Review

Physics of higher orbital bands in optical lattices: a review

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Abstract

The orbital degree of freedom plays a fundamental role in understanding the unconventional properties in solid state materials. Experimental progress in quantum atomic gases has demonstrated that high orbitals in optical lattices can be used to construct quantum emulators of exotic models beyond natural crystals, where novel many-body states such as complex Bose–Einstein condensates and topological semimetals emerge. A brief introduction of orbital degrees of freedom in optical lattices is given and a summary of exotic orbital models and resulting many-body phases is provided. Experimental consequences of the novel phases are also discussed.

Keywords: cold atoms, orbital, optical lattice

(Some figures may appear in colour only in the online journal)

1. Introduction

Optical lattices play a central role in studying strongly interacting many-body physics with ultracold atoms (Bloch \textit{et al} 2008, Lewenstein \textit{et al} 2012, Dutta \textit{et al} 2015a). Because of their unprecedented controllability, atomic gases confined in optical lattices enable quantum simulation of various lattice Hamiltonians, e.g. Bose and Fermi Hubbard models, where different aspects have been intensively investigated. With single-species of bosons, e.g. \textsuperscript{87}Rb, a quantum Mott-to-superfluid transition has been observed. Multi-component lattice models have been reached with atomic internal degrees of freedom. The SU(2) spinfull Fermi–Hubbard simulator has been carried out by using hyperfine states of \textsuperscript{6}Li or \textsuperscript{40}K. One theme along this direction is to emulate complex correlated phenomena of strongly interacting electrons. Such multi-component quantum simulators with atomic internal degrees of freedom have been very successful in simulating Hamiltonians with high symmetries.

For electrons, one important ingredient besides spin is the orbital degrees of freedom, which arises in a variety of condensed matter systems (Tokura and Nagaosa 2000). In solid state materials, orbitals originate from electron clouds surrounding the ions in the crystal. With tunnelings, these orbitals form Bloch bands. Orbitals are Wannier states corresponding to different bands. Degenerate orbitals (or bands) could emerge in the presence of point group symmetries, but the symmetry for orbitals is much lower than for spins. Understanding such orbitals degree of freedom is crucial to obtain a simple and yet powerful model that captures the essence of many complicated materials, such as transition metal oxides, pnictides, etc. A task of this kind however remains outstanding, much due to the complexity of multiple types of degrees of freedoms coupled together, including orbital, charge, spin, and crystal field. The intricate coupling makes it an expensive challenge, both analytically and numerically, to understand orbital physics alone first and to attempt to compare with any electronic solid state materials in experiments.
Given one important application of optical lattices is to simulate complex phenomena of electrons, it is rather essential to find ways to emulate electron orbitals with atoms. Actually with optical lattices, the ionic crystal trapping electrons is replaced by an artificial crystal of light, created by standing waves of laser beams. The Wannier orbitals in the lattice naturally mimic properties of that in ionic crystals. Due to the intrinsic spatial nature, orbital degree of freedom in both of these ionic and light crystals respect space point group symmetries rather than internal continuous group symmetries, which defines its uniqueness. Such symmetry properties of orbitals make them fundamentally difficult to be simulated with internal atomic degrees of freedom such as hyperfine spins. On this regard, the orbital states of an atom in an optical lattice provide a natural avenue to emulating the electronic orbital related physics.

Exploration of orbital physics in optical lattices is certainly not restricted to quantum simulations of electrons in solids. For example, orbital bosons are able to bring to the study of quantum matter some really novel concepts that have no prior analogue in systems of (fermionic) electrons. Moreover, bosons (e.g. \(^{87}\text{Rb}\) atoms) are more widely used in optical lattice experiments. In the first experimental demonstration of many-body orbital physics, bosons were loaded into the \(p\)-bands of an optical lattice, for which earlier theoretical studies had predicted interesting phenomena such as time-reversal symmetry breaking and spontaneous angular momentum order (Isacsson and Girvin 2005, Kuklov 2006, Liu and Wu 2006).

Strong interactions which are achievable in optical lattice experiments also lead to interesting orbital physics. Firstly, with strongly repulsive bosons loaded into higher orbital bands, they would form a Mott state with orbital degree of freedom. Orbital ordering in such a Mott state is drastically different from spin ordering in Mott states. For Mott states formed by spinor bosons (assuming no spin–orbital coupling), the super-exchange Hamiltonian typically has high symmetries. The orbital super-exchange Hamiltonian is generally more complicated and at the same time promises richer physics. Secondly, for strongly interacting atoms in a lattice (e.g. lattice bosons in the Mott regime, or a Feshbach resonant Fermi gas (Chin et al 2010) in a lattice), even without deliberately loading atoms into higher orbital bands, population of those bands is unavoidable due to interaction effects. This is because local interactions would mix all different orbitals. Recent works (Zhou et al 2011b, Soltan-Panahi et al 2012) have shown that the interaction-induced high-band population could give rise to significant physical effects, such as condensation of boson pairs, and exotic symmetry breaking orders. It is therefore essential rather than an option to account for orbital physics in modeling strong interaction effects in optical lattices.

Research of fermions in higher orbitals adds a remarkably distinct venue. Theoretical studies have also found quantum phases with angular momentum ordering that spontaneously break time-reversal symmetry. For fermions, this symmetry breaking leads to even more dramatic effects than the bosonic counterpart. Considering the angular momentum order and mixing of orbitals with opposite parities (like \(s\) and \(p\), or \(p\) and \(d\) orbitals), the fermionic atoms experience effective gauge fields, which then gives rise to topological phenomena, like quantum Hall, topological insulator, or certain topologically protected gapless phases. This route of engineering topological matter offers one way different from the Raman-induced synthetic gauge fields (Dalibard et al 2011) or the artificial spin–orbit couplings (Galitski and Spielman 2013, Zhai 2015). It has fundamentally distinct properties and is advantageous in certain aspects. For example, it does not involve complications of Raman couplings, and the resultant topological phases would have longer lifetime due to less heating effects. The finite temperature behaviors of the spontaneously generated gauge fields are also different from the the Raman-induced case.

In this review, we start by describing the basics of modeling orbitals in optical lattices. Then by using particular examples, we present a selection of many-body aspects of orbital physics that we find most interesting and novel, as sketched above. Along with developing theoretical concepts and models pedagogically, we review the recent experimental developments and the current status in this field, and outline several future directions.

2. High orbitals and band structures in optical lattices

Previous studies in optical lattices largely focused on atoms trapped in the lowest band and the resultant single-band Hubbard model, where correlated effects of bosons, e.g. the Mott-superfluid transition, have been intensively investigated (Bloch et al 2008, Lewenstein et al 2012, Dutta et al 2015a). In this section we present the procedure to construct tight binding models involving high orbital degrees of freedom, which is one essential step to study correlation effects in interacting atoms in lattices. To demonstrate the validity condition of tight binding models, we also show the exact results from plane-wave expansion for the tunneling amplitudes, band structures and Wannier functions of higher bands. A two dimensional square lattice is assumed in this section.

2.1. Harmonic approximation and tight binding models

In the tight binding regime, an optical lattice can be treated as individual harmonic oscillators, which are coupled by quantum tunnelings. On each harmonic oscillator centered at a lattice site labeled by its position \(\mathbf{R}\), we have discrete energy levels with orbital wavefunctions \(\phi_{\alpha}(\mathbf{x} - \mathbf{R})\). Associated with the localized orbital wavefunctions, we can define the lattice operators \(b_{\alpha}(\mathbf{R})\). To do this, it has to be enforced that the orbital wavefunctions are orthonormal. The simple eigen wavefunctions of harmonic oscillators do not satisfy orthonormal condition, for the reason that there are overlaps between orbital wavefunctions on neighboring sites.

The procedure to construct the orthogonal basis from the localized harmonic oscillator wavefunctions is the following. We start with the harmonic oscillator wavefunctions \(\phi_{\alpha}(\mathbf{x} - \mathbf{R})\)
localized on site \( \mathbf{R} \). These wavefunctions are already approximately orthogonal, i.e.

\[
\int \! d\mathbf{x} \phi^*_\alpha (\mathbf{x} - \mathbf{R}) \phi^*_{\alpha'} (\mathbf{x} - \mathbf{R}') = \delta_{\alpha\alpha'} \epsilon_{\alpha \mathbf{R}, \alpha' \mathbf{R}'} + \epsilon_{\alpha \mathbf{R}, \alpha' \mathbf{R}'} ,
\]

where \( \epsilon_{\alpha \mathbf{R}, \alpha' \mathbf{R}'} \) are small numbers. By definition we know that \( \epsilon \) is a traceless Hermitian matrix. Then we improve this basis by introducing

\[
\tilde{\phi}_\alpha (\mathbf{x}) = \phi_\alpha (\mathbf{x}) - \frac{1}{2} \sum_{\alpha' \mathbf{R}} \epsilon_{\alpha \mathbf{R}, \alpha' \mathbf{R}} \phi_{\alpha'} (\mathbf{x} - \mathbf{R}') .
\]

After that \( \tilde{\phi}_\alpha (\mathbf{x} - \mathbf{R}) \) is renormalized as

\[
\tilde{\phi}_\alpha (\mathbf{x}) \rightarrow \tilde{\phi}_\alpha (\mathbf{x}) / \sqrt{\int \! d\mathbf{x}' |\tilde{\phi}_\alpha (\mathbf{x}')|^2} .
\]

The improved wavefunctions satisfy a better approximate orthogonal condition

\[
\int \! d\mathbf{x} \tilde{\phi}^*_\alpha (\mathbf{x} - \mathbf{R}) \tilde{\phi}^*_{\alpha'} (\mathbf{x} - \mathbf{R}') = \delta_{\alpha\alpha'} \epsilon_{\alpha \mathbf{R}, \alpha' \mathbf{R}'} + O(\epsilon^2) .
\]

The above procedure can be iterated \( N \) times to get the orthonormal basis to the precision of \( O(\epsilon^N) \).

Once we have the orthonormal basis, the tunnelings between \( \mathbf{R} \) and \( \mathbf{R}' \) are calculated as

\[
t_{\alpha\alpha'} (\mathbf{R} - \mathbf{R}') = \int \! d\mathbf{x} \tilde{\phi}^*_\alpha (\mathbf{x} - \mathbf{R}) H (\mathbf{x}) \tilde{\phi}^*_{\alpha'} (\mathbf{x} - \mathbf{R}') ,
\]

where \( H (\mathbf{x}) \) is the Hamiltonian in the first quantization form \( H = -\frac{\hbar^2}{2m} \nabla^2 + V (\mathbf{x}) \). The lattice model Hamiltonian including tunnelings is given by

\[
\hat{H} = \sum_{\alpha\alpha'} \sum_{\mathbf{R}, \mathbf{R}'} t_{\alpha\alpha'} (\mathbf{R} - \mathbf{R}') \hat{b}^\dagger_{\alpha} (\mathbf{R}) \hat{b}^{}_{\alpha'} (\mathbf{R}') .
\]

Without truncating the basis, the Hamiltonian is exact, from which the band structure can be calculated. If we only keep the lowest harmonic wave functions, this lattice Hamiltonian gives qualitatively correct band structures for deep lattices.

The procedure described above to construct orthogonal orbital wave functions is one essential step if one uses harmonic approximation. In principle, the constructed wave functions are not the same as the maximally localized Wannier functions (Kivelson 1982, Marzari et al. 2012, Uehlinger et al. 2013, Gunzare et al. 2014). The procedure to calculate such-maximally localized Wannier functions is not as straightforward and is beyond the scope of this review.

2.1.1. Multi-band Hubbard model. Considering interacting bosonic atoms loaded on excited bands, the physics will be described by a multi-band Hubbard model

\[
H = \sum_{\alpha \mathbf{R}} \epsilon_{\alpha \mathbf{R}} \hat{b}^\dagger_{\alpha} (\mathbf{R}) \hat{b}^{}_{\alpha} (\mathbf{R}) + \sum_{\alpha \mathbf{R}, \alpha' \mathbf{R}'} t_{\alpha\alpha'} (\mathbf{R} - \mathbf{R}') \hat{b}^\dagger_{\alpha} (\mathbf{R}) \hat{b}^{}_{\alpha'} (\mathbf{R}') + \sum_{\alpha \mathbf{R}} U_{\alpha\alpha \mathbf{R}, \alpha \mathbf{R}'} \hat{b}^\dagger_{\alpha} (\mathbf{R}) \hat{b}^{}_{\alpha} (\mathbf{R}) \hat{b}^\dagger_{\alpha} (\mathbf{R}) \hat{b}^{}_{\alpha} (\mathbf{R}) .
\]

With weak interaction, the coupling constants \( U_{\alpha\alpha \mathbf{R}, \alpha \mathbf{R}'} \) can be estimated at tree-level as (Jaksch et al. 1998, Liu and Wu 2006, Zhou et al. 2011b, Li et al. 2016, Dutta et al. 2015a)

\[
U_{\alpha\alpha \mathbf{R}, \alpha \mathbf{R}'} = -\frac{4\pi a_s \hbar^2}{2m} \int \! d^3 \mathbf{x} \phi^*_{\alpha \mathbf{R}} (\mathbf{x}) \phi^*_{\alpha \mathbf{R}'} (\mathbf{x}) \phi^{}_{\alpha \mathbf{R}} (\mathbf{x}) \phi^{}_{\alpha \mathbf{R}'} (\mathbf{x})
\]

where \( a_s \) is the s-wave scattering length, tunable with Feshbach resonance techniques. With fermionic atoms, we have a similar Hubbard model with interactions between hyperfine states.

2.2. Band structures

In terms of field operators, the Hamiltonian of particles moving in optical lattices is

\[
\hat{H} = \int \! d^3 \mathbf{x} |\psi^\dagger (\mathbf{x}) - \frac{\hbar^2}{2m} \nabla^2 + V (\mathbf{x}) |\psi (\mathbf{x}) ,
\]

where \( |\psi (\mathbf{x}) \rangle \) is a field operator. It can be either bosonic or fermionic. Statistics is irrelevant here to determine single-particle band structures. We expand the operator \( |\psi (\mathbf{x}) \rangle \) in the momentum basis

\[
|\psi (\mathbf{x}) \rangle = \sum_{\mathbf{K}} \frac{1}{\sqrt{N_{\mathbf{K}}}} \sum_{\lambda} \hat{a}_{\mathbf{K}} (\mathbf{k}) e^{i(\mathbf{k} + \mathbf{K}) \cdot \mathbf{x}} .
\]

For example, the potential of a square lattice created by laser is

\[
V (\mathbf{x}) = -V_0 [\sin^2 (k_x) + \sin^2 (k_y)] = -V_0 \left[ \frac{1}{4} e^{i 2 k_x x} + e^{i 2 k_y y} + \text{c.c.} \right] + \text{const} .
\]

where \( k \) is the wavevector of the laser beams. The Hamiltonian in momentum space reads as

\[
\hat{H} = \sum_{\mathbf{K}} \sum_{\mathbf{k}} \hat{H}_{\mathbf{K}} (\mathbf{k}) \hat{a}^\dagger_{\mathbf{K}} (\mathbf{k}) \hat{a}^{\dagger}_{\mathbf{K}} (\mathbf{k}) ,
\]

with the matrix given by

\[
\hat{H}_{\mathbf{K}} (\mathbf{k}) = \frac{\hbar^2 (k_x + k_y)^2}{2m} \delta_{\mathbf{K}, \mathbf{k'}} + v (\mathbf{k} + \mathbf{K} - \mathbf{k}) .
\]

Diagonalizing this matrix, we get the band structure \( E_{\mathbf{k}} (\mathbf{k}) \) and the eigenvectors \( \lambda_{\mathbf{K}}^{(n)} (\mathbf{k}) \), with \( n \) the band index. The Hamiltonian in the eigen-basis reads

\[
\hat{H} = \sum_{\mathbf{k}} \sum_{n} E_n (\mathbf{k}) \hat{b}^\dagger_{\mathbf{k}} (\mathbf{k}) \hat{b}^{\dagger}_{\mathbf{k}} (\mathbf{k}) \hat{b}^{}_{\mathbf{k}} (\mathbf{k}) ,
\]

with \( \hat{b}_{\mathbf{k}} (\mathbf{k}) = \sum_{\mathbf{K}} \lambda_{\mathbf{K}}^{(n)} (\mathbf{k}) \hat{a}^{\dagger}_{\mathbf{K}} (\mathbf{k}) \).

The Wannier basis is given by

\[
\hat{b}_{\mathbf{k}} (\mathbf{R}) = \frac{1}{\sqrt{N_{\mathbf{K}}}} \sum_{\mathbf{k}} b_{\mathbf{k}} (\mathbf{k}) e^{i(\mathbf{k} + \mathbf{K}) \cdot \mathbf{R}} .
\]
Table 1. Tunneling amplitudes in a two-dimensional square lattice with potential $V(x) = -V_0[\sin^2(kx) + \sin^2(ky)]$.

| $V_0/E_R$ | $t_{nn}^R/E_R$ | $t_{nn}^L/E_R$ | $t_{nn}^R/E_R$ | $t_{nn}^L/E_R$ |
|-----------|----------------|----------------|----------------|----------------|
| 3         | -0.4441        | 0.0449         | 2.0074         | 0.3308         |
| 5         | -0.2631        | 0.0136         | 1.6912         | 0.2914         |
| 10        | -0.07673       | 9.1E-4         | 0.9741         | 0.1051         |
| 20        | -9.965E - 3    | 1.2E-5         | 0.2411         | 5.5E-3         |

Note: $E_R$ is the one photon recoil energy $\frac{k^2}{2m}$. $t_{nn}^R$ and $t_{nn}^L$ are nearest neighbor and next nearest neighbor tunnelings for the lowest $s$-band and the other two excited $d$-bands. $t_{nn}^R$ and $t_{nn}^L$ are nearest neighbor and next nearest neighbor tunnelings in the $x$ direction for the $p_y$ (first excited) band.

2.3. Heuristics to lifetime of high orbital atoms

Here the lifetime of $p$-orbital condensate in a one dimensional (1D) lattice is discussed based upon Fermi’s Golden rule calculation. The resulting time scale is expected to apply to two dimensional (2D) square and three dimensional (3D) cubic lattices as well (Isacsson and Girvin 2005). The $p$-orbital condensate wavefunction is given as

$$|\Psi\rangle = \frac{[b_{p}(Q = \pi)]^N}{\sqrt{N!}} \langle \text{vac} \rangle. \tag{15}$$

With interactions, two particles in the $p$-band can collide and one particle would decay to the lowest $s$-band and the other goes to the second excited $d$-band. This process is described by the following interaction term

$$H_{\text{int}}^{\text{quad}} = U/N|_{k_1+k_2+k_3=0} \times \{b_{p}^\dagger(k_1)b_{s}^\dagger(k_2)b_{p}(k_3)b_{s}(k_4) + \text{h.c.}\}. \tag{4}$$

The final state after the collision is

$$|\langle \Psi'; k_1, k_2 \rangle \rangle = b_{s}^\dagger(k_1)b_{s}^\dagger(k_2) \{b_{p}^\dagger(Q)\}^{N-2} \sqrt{(N-2)!} \langle \text{vac} \rangle. \tag{5}$$

The transition probability from second order perturbation theory is

$$P(k_1, k_2; t) \approx \frac{4 \sin^2(\Delta \varepsilon_{kk}/2)}{\Delta \varepsilon_{kk}^2} \langle \langle \Psi'; k_1, k_2 | H_{\text{int}}^{\text{quad}} | \Psi \rangle \rangle^2,$$

with $\Delta \varepsilon_{kk}$ being the difference of kinetic energy between $|\Psi\rangle$ and $|\Psi'; k_1, k_2 \rangle$. The loss rate from the $p$-band is obtained as

$$|w| = \sum_{k_2} \frac{1}{\bar{t}^2} P(k_1, k_2; t) \left|_{t \to \infty} \right. \approx \sum_{k_2} \frac{2\pi}{\hbar} \langle \langle \Psi'; k_2 | H_{\text{int}}^{\text{quad}} | \Psi \rangle \rangle^2 \delta(\Delta \varepsilon_{kk}) \approx \frac{4\pi U^2}{\hbar N} N(N-1) \left[ \frac{1}{\rho_{\varepsilon_{p}}(K)} + \frac{1}{\rho_{\varepsilon_{d}}(-K)} \right]^{-1}, \tag{16}$$

where $\rho_{\varepsilon}$ is the density of states and $K$ is determined by

$$\varepsilon_{p}(K) + \varepsilon_{d}(-K) = 2\varepsilon_{p}(Q), \tag{17}$$

which in general has two solutions when the band gap between $s$ and $p$ matches that between $p$ and $d$.

The loss rate per site is

$$w \approx \frac{4\pi(U^2)}{\hbar} \left[ \frac{1}{\rho_{\varepsilon_{p}}(K)} + \frac{1}{\rho_{\varepsilon_{d}}(-K)} \right]^{-1}, \tag{18}$$

with $\nu$ the filling factor. The lifetime $1/w$ is typically short for cubic or square lattices, where the condition of equation (17) may be satisfied. It was suggested that anharmonicity (Müller et al 2007) present in the actual optical lattice potential should help suppress the decay. Nonetheless, the lifetime can be significantly improved by using double-well lattice potentials to mismatch the band gaps as first discussed in Stojanović et al (2008) and further confirmed in the experiments (Wirth et al 2011).

3. Many-body phases and transitions

Orbital degrees of freedom play an important role in understanding many complex phases in solid state materials. For
example, high temperature superconductivity in the cuprates (Bednorz and Müller 1986) and pnictides (Kamihara et al. 2006), chiral $p$-wave superconductivity proposed in Sr$_2$RuO$_4$ (Luke et al. 1998), and Ferromagnetic superconductivities in oxide heterostructures such as LaAlO$_x$/SrTiO$_3$ (Ohtomo and Hwang 2004), are all nucelated by strong correlation effects in a multi-orbital setting (Tokura and Nagaosa 2000). In optical lattices, recent studies have shown that the interplay of high orbitals and interaction effects give rise to unconventional many-body phenomena (Lewenstein and Liu 2011).

For bosons loaded into high-orbital bands of an optical lattice, an analogue of Hund’s rule coupling leads to a complex Bose–Einstein condensate with spontaneous angular momentum order (Isacsson and Girvin 2005, Kuklov 2006, Liu and Wu 2006, Wu et al. 2006, Wu 2009). The bosonic analogue of Hund’s rule basically states that repulsive contact interactions favor maximization of the local angular momentum. Different aspects of the unconventional condensate have been theoretically investigated, e.g. rotation effects (Umucalilar and Oktel 2008), manifestations of lattice geometry and trapping potential (Lim et al. 2008, Cai et al. 2008, Zhai et al. 2008, Zhang et al. 2015), and novel quantum magnetism (Wang et al. 2013, Sowiński et al. 2012, Hett et al. 2011, Pinheiro et al. 2008, Cai et al. 2010, Zhang et al. 2008, Wu 2008b, Zhao and Liu 2008, Lu and Arrigoni 2009, Cai et al. 2012), unconventional Cooper pairings (Lee et al. 2012), unconventional orbital superconductivity (Liu and Wu 2006, Li et al. 2011b) and also by unbiased numerical methods (Li et al. 2012, Hébert et al. 2013, Sowiński et al. 2013). Even without deliberately loading atoms into the higher bands, it has been shown high-band population can be stabilized by interaction effects (Zhou et al. 2011b, Soltan-Panahi et al. 2012).

For fermions, it has been shown that interaction effects combined with the band topology of $p$-orbitals lead to various exotic quantum phases. With $p$-orbital fermions in two dimensions, interactions cause generic instabilities towards quantum density wave orders (modulations in spin, charge or orbital density) (Wu et al. 2006, 2012, Wu and Das Sarma 2008, Wu 2008b, Zhao and Liu 2008, Lu and Arrigoni 2009, Zhang et al. 2012), unconventional Cooper pairings (Lee et al. 2010, Zhang et al. 2010b, 2011, Cai et al. 2011, Hung et al. 2011, Liu et al. 2015), and novel quantum magnetism (Wang et al. 2008, Wu and Zhai 2008, Zhang et al. 2010a, Hauke et al. 2011, Zhou et al. 2015) at low temperature. From quantum engineering perspectives, the elongated spatial nature of $p$-orbitals makes them ideal building blocks for fascinating topological states, e.g. topological semi-metal (Sun et al. 2012b), quantum Hall phases (Wu 2008a, Wang and Gong 2010), topological insulators/superconductors (Liu et al. 2010, 2014, Liu et al. 2016, Li et al. 2013), and even fractional states (Sun et al. 2010).

In this section, we will review a selection of quantum many-body phases of $p$-orbital bosons and fermions.

**Figure 2.** Illustration of the tight binding model of $p$-orbital bosons on a square lattice (reproduced with permission from Liu and Wu 2006; copyright 2006 American Physical Society). The longitudinal tunneling amplitude $t_i$ is in general far greater than the transverse tunneling $t$. The ‘$\perp$’ symbols indicate the sign of two lobes of $p$-orbital wave functions.

### 3.1. Orbital $p + ip$ Bose–Einstein condensation

#### 3.1.1. Complex $p_x + ip_y$ Bose–Einstein condensation at finite momentum

For bosons loaded on $p$-orbitals of a 2D square lattice (Wirth et al. 2011) in the tight-binding regime, the tunneling Hamiltonian is

$$H_{\text{tun}} = \sum_r \left( t_0 [b_r^\dagger(\mathbf{r}, \mathbf{p}_x) + \mathbf{a}_x] + x \leftrightarrow y \right) - t_1 [b_r^\dagger(\mathbf{r}, \mathbf{p}_x) + \mathbf{a}_y] + \text{h.c.},$$  \hspace{1cm} (19)

where $b_x$ and $b_y$ are bosonic annihilation operators for $p_x$ and $p_y$ orbitals, respectively (figure 2). After a Fourier transformation, we get the energy spectra for the $p_x$ and $p_y$ bands. The dispersion for the $p_x$ band is

$$\epsilon_x(k) = 2t_1 \cos(k_x) - 2t_1 \cos(k_y).$$

The dispersion for the $p_y$ band is readily obtained with a lattice rotation ($C_4$). There are two degenerate minima—$Q_x = (\pi, 0)$ and $Q_y = (0, \pi)$ in the $p$-bands with the degeneracy protected by the $C_4$ symmetry. The ground state manifold of non-interacting $p$-orbital bosons is spanned by

$$|N_x, N_y\rangle = \frac{|b_r^\dagger(Q_x)|^N |b_r^\dagger(Q_y)|^N}{\sqrt{N_x! N_y!}} |\text{vac}\rangle,$$  \hspace{1cm} (20)

which has a large degeneracy that shall be lifted by interactions.

The interaction terms of repulsive $p$-orbital bosons read (Isacsson and Girvin 2005, Liu and Wu 2006, Li et al. 2011b)

$$H_{\text{int}} = \sum_r \left\{ \frac{1}{2} U_0 [n_r(\mathbf{r}) n_r(\mathbf{r}) + n_r(\mathbf{r}) n_r(\mathbf{r})] + 2U_0 n_r(\mathbf{r}) n_r(\mathbf{r}) \right. \right.$$

$$+ \left. \frac{1}{2} U_0 [b_r^\dagger(\mathbf{r}) b_r^\dagger(\mathbf{r}) b_r(\mathbf{r}) b_r(\mathbf{r}) + \text{h.c.}] \right\},$$  \hspace{1cm} (21)

where the density operators $n_r = b_r^\dagger b_r$. Approximating Wannier functions by localized harmonic wavefunctions, we have

$$U_1 = 3U_2 = 3U_3 \equiv U > 0,$$  \hspace{1cm} (22)

from which the interaction can be rewritten as

$$H_{\text{int}} = \frac{U}{2} \sum_{\mathbf{R}} \left[ n^2(\mathbf{R}) - \frac{1}{3} U^2(\mathbf{R}) \right],$$  \hspace{1cm} (23)
with $n = \sum b_i^\dagger b_i$ and $L_z = i b_1^\dagger b_y + \text{h.c.}$ We thus expect that the angular momentum order is ‘universally’ favorable in $p$-orbital Bose gases.

It is however worth emphasizing here that the angular momentum ordering does not rely on the strict equality in equation (22) or the interaction form in equation (23). This becomes more clear with Ginzburg–Landau or effective field theories analysis (Li et al 2012, 2016, Liu et al 2013). Detailed studies taking into account unharmonic corrections and trapping potentials also confirm that the angular momentum order indeed exists in the regimes accessible to optical lattice experiments (Collin et al 2010, Pinheiro et al 2012, Pietraszewicz et al 2013, Sowiński et al 2013).

To capture quantum/thermal fluctuations, two slowly varying bosonic fields are introduced as

$$\phi_\alpha(x) = \sum_k b_k(Q_\alpha + k)e^{ikx},$$

where $\Lambda$ is a momentum cut off. The effective field theory of $\phi_\alpha(x)$ is

$$H = \int d^3r \left[ K_0(\partial_x \phi_0^\dagger(\mathbf{r})\partial_x \phi_0(\mathbf{r}) + x \leftrightarrow y) + K_2(\partial_x \phi_0^\dagger(\mathbf{r})\partial_x \phi_0(\mathbf{r}) + x \leftrightarrow y) - \mu(\phi_0^\dagger \phi_0 + x \leftrightarrow y) + \frac{1}{2} g_0(\phi_0^\dagger \phi_0^\dagger \phi_0 + x \leftrightarrow y) + 2g_\varphi \phi_0^\dagger \phi_0^\dagger \phi_0^\dagger \phi_y + \frac{1}{2} g_\varphi \phi_0^\dagger \phi_0^\dagger \phi_0^\dagger \phi_y + h.c.) \right]. (24)$$

In a superfluid state, we have $\langle \phi_\alpha \rangle = \varphi_\alpha$. At mean field level, the energy of this state is

$$E = \frac{1}{2} g_0(|\varphi_\alpha|^4 + |\varphi_\alpha|^4) + 2g_\varphi |\varphi_\alpha|^2 |\varphi_\alpha|^2 + \frac{1}{2} g_\varphi (|\varphi_\alpha|^2 |\varphi_\alpha|^2 + c.c.).$$

From equation (22), we have $g_0 = 3g_\varphi = 3g_\varphi > 0$, and the relative phase between $p_1$ and $p_2$ is locked at $\pm\pi/2$, i.e. $\varphi_\alpha = \varphi e^{i\pi/2}$, where the ‘$\pm$’ sign is spontaneously chosen. The superfluid state has a staggered angular momentum order $(-1)^{R} \theta(L_z(R), R)$, which breaks time-reversal symmetry. Such a superfluid state is named transversely staggered orbital current (TSOC) superfluid. The phase configuration of this superfluid state and its momentum distribution are shown in figure 3.

An alternative way of looking at time-reversal symmetry breaking is to project interactions into the subspace spanned by $|NN\rangle$ in equation (20). In this subspace, the interaction reads

$$\langle NN'|NN||\text{Ham}|NN\rangle = \frac{U_1}{2N} \left[ (N'_z - N_z) \delta_{N'_z, N_z} + 2U_2 \sum_{N'_z} (N'_z + 1) \delta_{N'_z, N_z} + x \leftrightarrow y \right]$$

$$+ \frac{U_3}{2N} \left[ \sqrt{N'_z(N'_z - 1)} \sum_{N'_z} \delta_{N'_z, N_z} + x \leftrightarrow y \right]. (25)$$

For the two orbital components to be miscible, we need

$$2U_2 - |U_3| < U_1, \quad (26)$$

as analogous to spin miscible condition in spinor condensates (Pethick and Smith 2008).

The angular momentum correlation is given by

$$(-1)^{R} \theta(L_z(R), R) = \frac{1}{N} \sum_{N_z} \left[ \langle b_i^\dagger(Q_x) b_j(Q_y) \rangle^2 + h.c. \right]$$

$$- \langle n_z \rangle \langle n_z + 1 \rangle - \langle n_z \rangle \langle n_z + 1 \rangle, \quad (27)$$

with $\langle \ldots \rangle$ the ground state expectation value. With $U_3 > 0$, to minimize the energy in equation (25), $\langle b_i^\dagger(Q_x) b_j(Q_y) \rangle$ gets a negative value in the ground state and in the thermodynamical limit $\langle n_z \rangle \gg 1, \langle n_z \rangle \gg 1$, it approaches $-2\langle n_z \rangle \langle n_z \rangle$. The system thus has a long range correlation in angular momentum, i.e. $(-1)^{R} \theta(L_z(R), R) \bigg|_{R \to \infty}$ const. $\neq 0$. The corresponding Ising order parameter is a staggered angular momentum $L_z(R) \equiv (-1)^{R} \theta(L_z(R), R)$. When $U_3$ is negative, $\langle b_i^\dagger(Q_x) b_j(Q_y) \rangle$ becomes positive, and the angular momentum order $L_z$ vanishes and the system develops the other Ising orbital order $p_i \pm p_i$ with an order parameter $(-1)^{R} \theta(b_i^\dagger(R) b_i(R) + h.c.)$. From the above analysis, the transition at $U_3 = 0$ is predicted to be first order (figure 4), although fluctuations may stabilize some intermediate state and the first order transition could be replaced by a sequence of double second order transitions.

3.1.2. Symmetry based effective field theory description. The predicted TSOC superfluid state in the $p$-band tight binding model is also confirmed with effective field theory (EFT) treatment (Li et al 2016), which infers that the TSOC superfluid does not necessarily require a deep lattice. In the band structure calculation for the case of lattice rotation symmetry (Wirth et al 2011), dispersion of the relevant $p$-band $E_p(k)$ has two degenerate minima at $Q_x = (\pi, 0)$ and $Q_y = (0, \pi)$, around which low energy modes can be excited due to quantum or thermal fluctuations. This leads to a two-component EFT, where the fields are introduced as

$$\phi_\alpha(x) = \int d^3q \frac{b(Q_\alpha + q)e^{iqx}}{(2\pi)^2}, \quad (28)$$

![Figure 3. Transverse staggered orbital current superfluid state (Liu and Wu 2006, Li et al 2011b) (reproduced with permission from Liu and Wu 2006; copyright 2006 American Physical Society). (a) shows the phase configuration, from which one can infer the orbital current alternates from site to site. (b) shows the momentum distribution, which is confirmed in the experiments (Wirth et al 2011).](Image 520x777)
with a momentum cutoff and \(b(Q, \theta_q + q)\) annihilation operators for the Bloch modes near the band minima. The form of EFT is determined by considering lattice rotation and reflection symmetries, under which the fields \(\phi_0\) transform as

\[
\begin{bmatrix}
\phi_0(x, y) \\
\phi_0^*(x, y)
\end{bmatrix}
\rightarrow
\begin{bmatrix}
-\phi_0(-y, -x) \\
\phi_0(x, -y)
\end{bmatrix},
\]

respectively. The Hamiltonian density of the EFT consistent with these symmetries is

\[
\mathcal{H}_{\text{eff}} = \phi_0^*(x) \left( K_x \frac{\partial^2}{\partial x^2} + K_y \frac{\partial^2}{\partial y^2} - \mu \right) \phi_0(x) + x \rightarrow y
+ \sum_{\alpha \neq \alpha'} g_{\alpha \alpha'} |\phi_{\alpha'}|^2 |\phi_{\alpha'}|^2 + g_3 (|\phi_{\alpha'}|^2 |\phi_{\alpha'}|^2 + \text{h.c.}),
\]

with effective couplings \(K_x, K_y\) and \(g_3\). This form of EFT is solely symmetry based, i.e. independent of microscopic details. For weakly interacting bosons, the coupling constants in equation (31) can be calculated from microscopic models (see appendix).

In the vicinity of thermal phase transitions of the superfluid phases, classical phase fluctuations are expected to dominate the universal physics, which allows us to ignore the subdominant density fluctuations and to replace \(\phi_0\) by \(\sqrt{\rho} e^{i\theta_0}\) with \(\rho\) the total density. In terms of phases \(\theta_0\), the Hamiltonian density is rewritten as

\[
\mathcal{H}_{\text{eff}} = \left(-K_x \frac{\partial^2}{\partial x^2} - K_y \frac{\partial^2}{\partial y^2} + x \leftrightarrow y\right) + \frac{1}{2} g_3 \rho^2 \cos(2(\theta_0 - \theta_0)),
\]

Bearing in mind the periodic nature of the phases \(\theta_0\), a proper lattice regularization of this EFT leads to a coupled XY model,

\[
H_{\text{phase}}^{\text{eff}} = \sum_{\mathbf{r}} [2J_1 \cos(\Delta \theta_0(\mathbf{r})) - 2J_2 \cos(\Delta \theta_0(\mathbf{r}))]
+ \{x \leftrightarrow y\} - U \sum_{\mathbf{r}} \sin^2(\theta_0(\mathbf{r}) - \theta_0(\mathbf{r})),
\]

where \(\Delta \theta_0(\mathbf{r}) = \theta_0(\mathbf{r} + \mathbf{a}_x) - \theta_0(\mathbf{r})\) with \(j = x, y\). At zero temperature we have the TSOC superfluid where the phases are locked at \(\theta_0(\mathbf{r}) = \pi n\), \(\theta_0(\mathbf{r}) = \pi n + 2\pi s\), with \(s = \pm 1\) and \(\theta_0 \in [0, 2\pi)\) spontaneously chosen. At finite temperature, the coupled XY model supports two types of topological defects. The first is a vortex in the phase \(\theta_0\), which is a point defect with logarithmic energy cost. The second is a domain wall connecting two Ising domains with different \(s\). Upon heating the TSOC superfluid, vortex proliferation should drive a Kosterlitz–Thouless transition and the domain wall fluctuations should drive an Ising transition. Monte Carlo study finds that the Kosterlitz–Thouless transition temperature is lower than the Ising transition (Li et al 2016).

From the effective field theory analysis, the \(p\)-orbital angular momentum order, or equivalently the \(\pm \frac{1}{2}\) phase locking, does not rely on the precise form of the interaction (equation (23)). The requirements are \(g_3 > 0\) and two \(p\) orbitals being miscible.

### 3.13. Population of higher bands by interaction

Here, we will focus on condensation of weakly interacting bosons in a lattice potential. With weak interaction, the condensate is well described by Gross–Pitaevskii approach where the condensate wavefunction \(\phi(\mathbf{x})\) is obtained by minimizing an energy functional

\[
E_{\text{GP}} = \int d^3x \phi^*(\mathbf{x}) \left( \frac{\nabla^2}{2m} + V(\mathbf{x}) - \mu \right) \phi(\mathbf{x}) + |g| |\phi(\mathbf{x})|^4.
\]

With infinitesimal interaction, the condensate wavefunction resembles the lowest band Bloch wavefunction with lattice momentum \(\mathbf{k} = 0\), i.e. \(\phi(\mathbf{x}) \propto \sum_{\mathbf{R}} w_\mathbf{R}(\mathbf{x} - \mathbf{R})\). This wavefunction preserves lattice translation and time-reversal symmetries meaning \(\phi(\mathbf{x}) = \phi(\mathbf{x} + \mathbf{a})\) and \(\phi = \phi^*\). From these preserved symmetries the generic form of the condensate wavefunction with weak interaction is

\[
\phi(\mathbf{x}) = \sum_{n} \lambda_n \sum_{\mathbf{R}} w_\mathbf{R}(\mathbf{x} - \mathbf{R}),
\]

provided that there are no first order transitions. The coefficients \(\lambda_n\) are real and the interaction induced high band condensate is at zero lattice momentum. In terms of \(\lambda_n\), the energy \(E_{\text{GP}}\) reads as

\[
E_{\text{GP}} = \sum_{n} (E_n(\mathbf{k} = 0) - \mu) \lambda_n^2 + U_{0000} \lambda_0^4
+ 4 \sum_{n=0} \lambda_{0000} \lambda_n^2 + 10 \sum_{n=0,m=0} U_{00mn} \lambda_0^2 \lambda_m \lambda_n + \mathcal{O}(\lambda_n^3),
\]

with the interactions \(U_{0000}, U_{0011}, \ldots\) introduced in equation (31). Minimizing this energy functional leads to

\[
\lambda_0^2 \approx \frac{\mu - E_0(0)}{2U_{0000}},
\]

\[
\lambda_{n>0} \approx - \frac{2U_{0000} \lambda_0^2}{E_0(0) - \mu}.
\]

The ratio \(\lambda_{n>0}/\lambda_0\) is readily given as

---

**Figure 4.** Staggered angular momentum order. For positive \(U_3\), the staggered angular momentum order is finite and the condensate has a staggered \(p_z \pm ip_y\) (TSOC) order; while for the negative case, the staggered angular momentum order vanishes and the condensate has a \(p_z \pm p_y\) order. In this plot, we assumed \(2U_2 < |U_3| < U_1\) such that the orbital mixed state has lower energy than \(p_z\) or \(p_y\) state.
Physically, the high band condensate is due to competition of interaction energy and lattice potential energy—the interaction favors an extended condensate; while the potential energy favors a condensate with high density at the lattice minima. The high band population due to interaction effects is found in various settings (van Oosten et al 2003, Alon et al 2005, Guo et al 2007, Kantian et al 2007, Larson et al 2009, Dutta et al 2011, Mering and Fleischhauer 2011, Sakmann et al 2011, Zhou et al 2011a, 2011b, Hofer et al 2012, Lühmann et al 2012,华北 (2013). In experiments, one can make a large fraction of high band condensate with double-well lattices, where the gap between lowest two bands is typically small and the fraction can be measured with band mapping techniques (Greiner et al 2002). Experimental evidence of this phenomenon has recently been achieved (Soltan-Panahi et al 2012). Furthermore, on general argument, the double-well lattices can have the energy gap between the ground s-band and the first excited p-bands significantly smaller than that between the first excited bands and higher bands (e.g. between p and d). This mechanism suppresses the decay by energy conservation law, making the first excited bands effectively metastable (Stojanović et al 2008). This will be further discussed in section 4.

For parity-symmetric lattices, the condensate wavefunction is parity even—\( \phi (x) = \phi (-x) \), which implies \( \tilde{\lambda}_{\text{odd}} = 0 \), \( n_{\text{odd}} \) referring to the parity odd bands with \( \tilde{w}_{\text{odd}}(x) = -\tilde{w}_{\text{odd}}(-x) \). At mean field level, parity odd bands do not contribute and \( \langle b_{n_{\text{odd}}} \rangle = 0 \). However, they can form pair condensate orderings—\( \langle b_n(\mathbf{r}) b_n(\mathbf{r}) \rangle \) due to Gaussian fluctuations (Zhou et al 2011a, 2011b). The mean field state is given by \( |M\rangle = \exp \left( \int d^3x \phi(x) \psi^\dagger(x) \right) |\text{vac}\rangle \). The effective Hamiltonian of high band modes at Gaussian level reads

\[
H_{\text{eff}} \approx \sum_{n, k} \left[ (E_n(k) - \mu) b_n^\dagger(k) b_n(k) \right] + \sum_{n, m, k, \ell} \left[ U_{nmmn} \lambda_n^2 b_n^\dagger(k) b_m^\dagger(-k) \right] \text{h.c.}. \tag{40}
\]

From standard perturbation theory, the correction on the mean field state from high band fluctuations is

\[
= \sum_{n, m, k} U_{nmmn} \lambda_n^2 b_n^\dagger(k) b_m^\dagger(-k) |M\rangle \text{h.c.}. \tag{41}
\]

which mediates pairings

\[
\langle b_n \dagger b_m \rangle = \frac{1}{N_k} \sum_k \langle b_n(k) b_m(-k) \rangle
\]

\[
= \int \frac{d^3k}{(2\pi)^3} U_{nmmn} \lambda_n^2 \left( E_n(k) + E_m(-k) - 2\mu \right). \tag{42}
\]

In parity odd bands, bosons form pair condensate with \( \langle b_{n_{\text{odd}}} \rangle = 0 \) and \( \langle b_{n_{\text{odd}}} b_{n_{\text{odd}}} \rangle = 0 \).

3.1.4. Three dimensional p-orbital BEC and frustrated orbital ordering. For bosons loaded on p-bands of a three dimensional cubic lattice, the tight binding Hamiltonian is (Liu and Wu 2006)

\[
H = \sum_{\mathbf{r}, \alpha, \beta, \gamma} \left[ t_{\alpha \beta \gamma} \hat{c}^\dagger \hat{c} \right] + \frac{U}{2} \sum_{\mathbf{r}} \left[ \hat{n}_n^2 - \frac{1}{3} \hat{L}_n^2 \right], \tag{43}
\]

where \( n \) and \( L \) are boson density and angular momentum operators \( n_\alpha = \sum \hat{b}_\alpha^\dagger b_\alpha \) and \( L_\alpha = -i \epsilon_{\alpha \beta \gamma} \hat{b}_\beta^\dagger b_\gamma \). Without interaction, there are three degenerate p-bands and the energy minima are at \( \mathbf{Q}_1 = (\pi, 0, 0), \mathbf{Q}_2 = (0, \pi, 0) \) and \( \mathbf{Q}_3 = (0, 0, \pi) \). The degenerate single-particle states are \( |\mathbf{Q}_n\rangle = b_\alpha^\dagger(\mathbf{Q}_n)|\text{vac}\rangle \). Thus any condensate wavefunction of a linear superposition of \( |\mathbf{Q}_n\rangle \) (Cai et al 2012b),

\[
|\hat{c}\rangle = \sum_{\alpha} c_\alpha |\mathbf{Q}_\alpha\rangle
\]

has the single-particle energy. Here \( \hat{c} = (c_x, c_y, c_z) \) is a complex vector normalized to 1, i.e. \( |\hat{c}| = 1 \). This complex vector could be parametrized as (Liu and Wu 2006)

\[
\begin{bmatrix}
  c_x \\
  c_y \\
  c_z
\end{bmatrix} = e^{i\epsilon_\chi - i\Theta_\chi} / \sqrt{2} \begin{bmatrix}
  \cos(\chi) \\
  i \sin(\chi) \\
  0
\end{bmatrix}, \tag{44}
\]

with \( \Theta_n = x, y, z \) the generators of SO(3) orbital rotation in the following matrix representation: \( [\Theta_n]_{\chi, \chi'} = -i \delta_{\chi, \chi'} \).

Although the SO(3) orbital rotation is not a symmetry of the total Hamiltonian, it keeps the interaction term invariant because \( n_\alpha \) and \( L_\alpha \) are both SO(3) scalars. With a condensate at the single-particle state \( |\hat{c}\rangle \), the mean field interaction energy is readily given as (Liu and Wu 2006)

\[
E_{\text{int}} = \frac{1}{2} U n_0^2 \left[ 1 - \frac{1}{3} \sin^2(2\chi) \right], \tag{45}
\]

with \( n_0 \) the boson occupation number per site. The interaction energy is minimized at \( \chi = \pm \frac{\pi}{2} \). Similar to the two dimensional case, the time-reversal symmetry is spontaneously broken in the p-band condensate. The ground state manifold is \( U(1) \times Z_2 \times SO(3) \) at mean field level. The \( Z_2 \times U(1) \) degeneracy remains due to the symmetries of the Hamiltonian, whereas the \( SO(3) \) degeneracy is an artifact of the mean field theory and such a degeneracy is lifted by fluctuations through an ‘order by disorder’ mechanism. Cai et al (2012b) carried out a variational comparison between the two superposition states

\[
|\text{planar}\rangle = \frac{1}{\sqrt{2}} (|\mathbf{Q}_1\rangle + i|\mathbf{Q}_2\rangle),
\]

and

\[
|\text{diag}\rangle = \frac{1}{\sqrt{3}} (|\mathbf{Q}_1\rangle + e^{i2\pi/3} |\mathbf{Q}_2\rangle + e^{-i2\pi/3} |\mathbf{Q}_3\rangle).
\]

It is found that the latter has lower energy under Bogoliubov approximation.

One interesting consequence is that the angular momentum (\( \hat{L} \)) order in the 3D p-orbital condensate state is noncollinear,
In other regions, one-loop corrections can be identified: (1) \(g g, r g, r g, r\) and (2) \(g g, r g, r, \omega\) and \(\phi_j(\omega, k)\). For general lattices lacking of \(C_4\) rotational symmetry, the energy potential parameters are not equal, \(r_i = r_j\). Performing a momentum shell renormalization group (RG) analysis, the fields are split into fast and slow parts, \(\phi^g_\alpha(\omega, k)|_{\omega \ll |k|}\) and \(\phi^\gamma_\alpha(\omega, k)|_{|k| < \Lambda}\). Following the standard Wilsonian RG procedure (integrating out fast modes and rescaling the effective action for the slow modes), the RG flow equations (or \(\beta\)-functions) for the potential parameters \(r_i\) to one-loop order are obtained to be

\[
\frac{d \tilde{r}_i}{d \tilde{l}} = 2 \tilde{r}_i + 4 \tilde{g}^g_1 \Theta(\tilde{r}_i - 1/2) + \tilde{g}_2 \Theta(\tilde{r}_i - 1/2), \\
\frac{d \tilde{r}_l}{d \tilde{l}} = 2 \tilde{r}_l + 4 \tilde{g}^g_1 \Theta(\tilde{r}_l - 1/2) + \tilde{g}_2 \Theta(\tilde{r}_l - 1/2). \tag{49}
\]

Here the dimensionless parameters are defined as \(\tilde{r} = r m \Lambda^2\) and \(\tilde{g} = g m(2 \pi)\) and \(\Theta(x)\) is the Heavyside step function. The RG flow equations for the quartic couplings are

\[
\frac{d \tilde{g}^g_1}{d \tilde{l}} = -2 \tilde{g}^g_1^2 - 2 \tilde{g}^g_2^2, \\
\frac{d \tilde{g}^g_2}{d \tilde{l}} = -2 \tilde{g}^g_1^2 - 2 \tilde{g}^g_2^2, \\
\frac{d \tilde{g}_2}{d \tilde{l}} = -\tilde{g}_2^2. \\
\frac{d \tilde{g}_3}{d \tilde{l}} = -2 \tilde{g}_3(\tilde{g}^g_1 + \tilde{g}^g_2). \tag{50}
\]

With bare repulsive interaction, these quartic couplings are all marginally irrelevant. However they could strongly modify the RG flow of \(r_i\) before they renormalize to zero.

In the region with \(\tilde{r}_i(0) \geq \frac{1}{2}\) and \(\tilde{r}_l(0) \geq \frac{1}{2}\) the solutions are

\[
\tilde{r}_i(I) = e^{2I} \left[ \tilde{r}_i(0) + \int_0^I dt e^{-2I(4 \tilde{g}^g_1(t) + \tilde{g}_2(t))} \right], \\
\tilde{r}_l(I) = e^{2I} \left[ \tilde{r}_l(0) + \int_0^I dt e^{-2I(4 \tilde{g}^g_1(t) + \tilde{g}_2(t))} \right]. \tag{51}
\]

In this region, \(\tilde{r}_i\) and \(\tilde{r}_l\) quickly run to positive infinity. In the region with \(\tilde{r}_i < \frac{1}{2}\) and \(\tilde{r}_l < \frac{1}{2}\), the solutions are

\[
\tilde{r}_i(l) = \tilde{r}_i(0) e^{2l}, \\
\tilde{r}_l(l) = \tilde{r}_l(0) e^{2l}, \tag{52}
\]

from which the behaviors of RG flow are also fully determined by initial values of \(\tilde{r}_i, \tilde{r}_l\). In other regions, one-loop corrections play more important roles in making the eventual values of \(\tilde{r}_i, \tilde{r}_l\) positive or negative. Numerical studies have found interesting regions in the phase diagram where \(\tilde{r}_i(0) < 0\) and \(\tilde{r}_l(0) > 0\) (or vice versa) flow to \(\tilde{r}_i \to +\infty\) and \(\tilde{r}_l \to +\infty\). Depending on the flow directions of \(\tilde{r}_i, \tilde{r}_l\), four states can be identified: (1) Complex BEC \((\tilde{r}_i \to +\infty, \tilde{r}_l \to +\infty)\); (2) \(p_r\) BEC \((\tilde{r}_i \to +\infty, \tilde{r}_l \to -\infty)\); (3) \(p_l\) BEC \((\tilde{r}_i \to -\infty, \tilde{r}_l \to +\infty)\); and (4) vacuum \((\tilde{r}_i \to -\infty, \tilde{r}_l \to -\infty)\).

The RG study sketched above does not really capture the TSOC state because \(g_3\) flows to 0, making an illusion that quantum
fluctuations wash away the phase locking between \( p_x \) and \( p_y \) components. However this is not physically correct. A more careful RG study requires introducing \( U(1) \) and \( Z_2 \) order parameters to characterize the fluctuation effects in the TSOC state.

### 3.2. Mott states, orbital exchange and frustration of bosons

In the strongly interacting regime, bosons localize and form Mott insulator phases. Unlike the ‘featureless’ \( s \)-band Mott insulators, the \( p \)-band Mott insulators have orbital degrees of freedom. Details of preparation of \( p \)-band Mott states including relaxation dynamics are studied in Challis et al (2009). The orbital ordering is governed by the orbital exchange interactions which result from virtual boson tunnelings. Here we will derive the orbital super-exchange interactions and discuss the orbital frustrations on certain lattice geometries.

#### 3.2.1. Mott states with filling factor larger than 1

The procedure to derive super-exchange interactions is to take the local terms as the leading part and the hopping terms as perturbation. Consider the two dimensional \( p \)-band Bose gas for example. The local interaction is given by

\[
H_U = \frac{U}{2} \left(n^2 - \frac{1}{3}L_z^2\right).
\]

(53)

It can be verified that the angular momentum operator \( L_z \) commutes with the local interaction, i.e.

\[
[L_z, H_U] = 0.
\]

Thus the eigenstates of the local interaction can be chosen as states with definite angular momentum. For filling factor \( \nu > 1 \), the degenerate eigenstates with lowest energy \( \frac{\nu^2}{4} U \) are

\[
|+\rangle = \frac{(b_+^\dagger)^{\nu}}{\sqrt{\nu!}} |\text{vac}\rangle,
\]

\[
|\rangle = \frac{(b_-^\dagger)^{\nu}}{\sqrt{\nu!}} |\text{vac}\rangle,
\]

(54)

where \( b_{\pm} = \frac{b_x \pm ib_y}{\sqrt{2}}. \) The states \(|+\rangle\) and \(|\rangle\) have angular momentum \( +\nu \) and \( -\nu \), respectively. On a square lattice, the tunneling Hamiltonian in the transformed basis reads

\[
H_t = \sum_{i, j, \pm x} T_{ij}(\vec{z}) b_{i, x}^\dagger b_{j, x} + \text{h.c.} + x \leftrightarrow y,
\]

(55)

with the matrices

\[
T(\vec{z}) = \begin{bmatrix}
\frac{\nu - t_x}{2} & \frac{\nu + t_x}{2} \\
\frac{\nu + t_y}{2} & \frac{\nu - t_y}{2}
\end{bmatrix},
\]

(56)

\[
T(\vec{y}) = \begin{bmatrix}
\frac{\nu - t_y}{2} & -\frac{\nu + t_y}{2} \\
\frac{\nu + t_x}{2} & \frac{\nu - t_x}{2}
\end{bmatrix}.
\]

The low energy sub-space is spanned by the product states

\[
|s(\vec{r})\rangle \equiv \otimes_{x} |s(x)\rangle,
\]

(57)

where \( s(\vec{r}) = \pm \) and \( \vec{r} \) runs over all lattice sites. All the states in this subspace have the same energy to leading order in \( U \) and there is thus a macroscopically huge degeneracy. The corrections due to the hopping term \( H_t \) lift the degeneracy. The first order corrections vanish because \( H_t \) does not connect any states in the low energy sub-space. The second order correction is calculated by the standard perturbation theory,

\[
\Delta E(|s(\vec{r})\rangle) = \sum_{m} \frac{|\langle m| H_t |s(\vec{r})\rangle|^2}{E_0^0(|s(\vec{r})\rangle) - E_0^0(|m\rangle)}.
\]

(58)

where \( \langle m| \) is a higher energy state orthogonal to the product states \( |s(\vec{r})\rangle \), and \( E_0^0 \) is the leading order energy.

Keeping only tunneling between nearest neighbors as in equation (54), \( \Delta E(|s(\vec{r})\rangle) \) simplifies to

\[
\Delta E(|s(\vec{r})\rangle) = \sum_{(r, r') \neq 0} \Delta E(|s(r)s(r')\rangle),
\]

(59)

Then the correction \( \Delta E(|s(\vec{r})\rangle) \) is given as

\[
\Delta E(|s(\vec{r})\rangle) = \sum_{(r, r')} \langle \nu, \nu' \rangle J_{\nu} \langle \nu, \nu' \rangle,
\]

(60)

with

\[
J_{\nu} = \frac{3\nu^2(\nu + 2) t_{\nu} t_{\nu'}}{2(\nu + 1)} > 0.
\]

Including this correction into the Hamiltonian, we get

\[
\hat{\Delta} H = \sum_{(r, r')} J_{\nu} \sigma_{\nu}(\vec{r}) \sigma_{\nu}(\vec{r'}),
\]

(61)

where \( \sigma_{\nu} \) is defined to be \( \sigma_{\nu} = \nu^{-1} P_{L_{\nu}} P \), with \( P \) a projection operator \( P = |+\rangle \langle +| + |+\rangle \langle -|-\rangle \langle -| \). The orbital super-exchange makes the staggered angular momentum ordering energetically favorable.

It should be emphasized here that the energy corrections in equation (60) actually do not depend on the orientation of the link \( \vec{r} \rightarrow \vec{r'} \) and that the effective Hamiltonian in equation (61) is independent of lattice geometries. Considering \( p \)-band Mott insulators on a triangle lattice, the effective orbital model is geometrically frustrated making both of ferromagnetic and antiferromagnetic correlations suppressed.

The above analysis holds in the deep lattice regime. For a relatively shallow lattice, the degeneracy in local Hilbert space could be lifted up (Collin et al 2010). Treating such effects...
as perturbations, based on well established results in transverse field Ising models (Sachdev 2011) the staggered angular momentum order in the Mott state is expected to be stable when the perturbations are reasonably weak as compared to the super-exchange. But we would like to emphasize that the competition of charge (atom number for neutral atoms) and spin orders in the shallow lattice regime may alter the above speculation and lead to potentially rich physics.

### 3.2.2. Mott state with filling factor 1.

For Mott states with filling factor $\nu = 1$, the convenient basis to calculate the super-exchange interaction is the $p_x, p_y$ basis, rather than the $p_x \pm ip_y$ basis. The generic form of interaction in equation (21) is used here. Like deriving super-exchange for filling $\nu > 1$, we need to calculate the second order corrections of nearest neighbor product states $|1, 0; 0, 1\rangle, |0, 1; 0, 1\rangle, |0, 1; 1, 0\rangle$, and $|1, 0; 0, 1\rangle$, where a notation $H_\nu$ is adopted to save writing. The zeroth order energy corrections are given by

$$\Delta E(|1, 0; 1, 0\rangle) = -2\hbar \left\{ \frac{1}{U_1 + U_3} + \frac{1}{U_2 - U_3} \right\},$$

$$\Delta E(|0, 1; 0, 1\rangle) = 0,$$

$$\Delta E(|0, 1; 1, 0\rangle) = \Delta E(|1, 0; 1, 0\rangle) = -\frac{\hbar^2}{2U_2}. \tag{63}$$

(Note that the transverse tunneling is neglected here, for the reason that the longitudinal tunneling is enough to lift the degeneracy and is significantly stronger than the transverse one.) Mapping $p_x$ and $p_y$ orbitals to the pseudo-spin 1/2 states, $\sigma = \uparrow$ and $\downarrow$, respectively, the effective Hamiltonian on this link reads

$$H_\nu = J\sigma(s(r)\sigma(r + \hat{x}) + M_\nu [\sigma(r) + \sigma(r + \hat{y})], \tag{64}$$

with $J_1 = -\frac{\hbar^2}{2}[(U_1 + U_3)^{-1} - (U_1 - U_3)^{-1} - (2U_2)^{-1}]$, $M_\nu = -\frac{\hbar^2}{2}[(U_1 + U_3)^{-1} - (U_1 - U_3)^{-1}]$. Similarly, the effective Hamiltonian for the link $r' - r = \hat{y}$ is obtained as

$$H_\nu = J\sigma(s(r)\sigma(r + \hat{y}) - M_\nu [\sigma(r) + \sigma(r + \hat{y})]. \tag{65}$$

Then the total effective Hamiltonian for filling $\nu = 1$ on a square lattice is

$$\Delta H = \sum_r J_1 [\sigma(r)\sigma(r + \hat{x}) + \sigma(r)\sigma(r + \hat{y})]. \tag{66}$$

With $U_1 = 3U_2 = 3U_3$, the coupling $J_1$ is positive and the ground state has an antiferromagnetic ordering with alternating $p$-orbitals (see figure 6). For a one-dimensional lattice, $H_\nu$ makes $p_x$ orbitals favorable due to the effective Zeeman term $M_\nu$ (equation (64)). We mention here that including the transverse tunneling would give rise to even richer physics, e.g. an XYZ quantum Heisenberg model can emerge (Pinheiro et al 2013).

One key difference between filling $\nu = 1$ and higher fillings is that the super-exchange interaction depends on the orientation of the link $r' - r$, which makes the orbital frustration on triangle/Kagome lattices even more interesting.

### 3.2.3. Phase diagram of p-band Bose–Hubbard model.

The phase diagram of $p$-band Bose–Hubbard model in a two dimensional square lattice is studied by quantum (Hébert et al 2013) and classical (Li et al 2016) Monte-Carlo simulations. For filling of two particles per site or higher, a second order quantum phase transition from antiferromagnetic Mott state to the TSOC state is found at zero temperature in the quantum Monte-Carlo study as well as in Gutzwiller approach (Larson et al 2009, Collin et al 2010, Martikainen and Larson 2012). In the weakly interacting regime at finite temperature, the fluctuations are modeled by a phase-only model studied by the classical Monte-Carlo. It is found that the TSOC state develops a two-step phase transition to the normal state, a Kosterlitz–Thouless transition followed by a higher temperature Ising transition. Sandwiched between the two transitions is a time-reversal symmetry breaking non-superfluid intermediate state. By combining the numerical results from Monte Carlo in the weak coupling regime and the analytical exact result from mapping the Mott limit of the $p$-band model to the orbital equivalent of the Onsager Ising model (Onsager 1944), the phase diagram for $p$-band Bose–Hubbard model in two dimensions is proposed (figure 7). We would like to mention here that strong correlation effects may give rise to exotic intermediate phases between $p$-band Mott insulator and superfluid states (Xu and Fisher 2007).
The density is

\[ \Delta = \Delta_0 e^{i \mathbf{Q} \cdot \mathbf{r}} \]

and

\[ \Delta_\sigma = \Delta_{\sigma, x} = |\Delta| \cos(\mathbf{Q} \cdot \mathbf{r}) \]

The mean field phase diagram has been mapped out in Cai et al. (2011). The parameter regime supporting FFLO states is considerably large in spin imbalanced p-band fermions.

3.3.2. Nested Fermi surface—density stripes. Besides the superconducting stripes in FFLO states, p-orbital fermions also naturally support density stripe orders, again from Fermi superconducting stripes in FFLO states.

\[ H = \sum_{\mathbf{r} \alpha \beta} (\epsilon_{\alpha \beta} + \delta_{\alpha \beta} c_{\mathbf{r} \alpha \beta}^\dagger c_{\mathbf{r} \alpha \beta}) + \text{h.c.} - \mu \sum_{\mathbf{r} \alpha} n_\alpha(\mathbf{r}) - \frac{\hbar}{2}(n_1(\mathbf{r}) - n_1(\mathbf{r})) \]

with \( c_{\mathbf{r} \alpha \beta} \) the fermionic annihilation operators for \( p_\alpha(p_\beta) \) orbital with pseudo-spin \( \sigma = |1\rangle \) and \( n_\sigma = \sum_\alpha c_{\mathbf{r} \alpha \sigma}^\dagger c_{\mathbf{r} \alpha \sigma} \) the density operators for spin \( \sigma \). The transverse tunneling \( t_L (\ll \hbar) \) is neglected for simplicity and in presence of spin-imbalance, this leads to perfect nesting of p-orbital Fermi surfaces (see figure 8).

In atomic gases the pseudo-spin components are hyperfine states. The interactions between them maybe engineered by s-wave Feshbach Resonance. With the Feshbach Resonance, a matured technique in experiments, the induced interactions are given as (Zhang et al. 2010a)

\[ H_{\text{int}} = U \sum_{\mathbf{r}} [n_{x, \sigma} n_{y, \sigma} + n_{y, \sigma} n_{x, \sigma}] - \sum_{\mathbf{r}} J \left( \hat{s}_{x, \sigma} \cdot \hat{s}_{y, \sigma} - \frac{1}{4} n_{x, \sigma} n_{y, \sigma} \right) + \sum_{\mathbf{r}} V_{xy} \left| c_{x, x}^\dagger c_{y, y}^\dagger c_{y, x} c_{x, y} + \text{h.c.} \right| \]
The density fields are defined as

\[ \rho^{\pm}_{\alpha}(k) = \frac{1}{\sqrt{2N}} \int d\tau \psi^\dagger_{\alpha}(\mathbf{r}, \tau) \psi^{\pm}_{\alpha}(\mathbf{r}, \tau) e^{-i\mathbf{k} \cdot \mathbf{r}}. \]

The density correlations are given by

\[ \Pi_{\alpha\beta}(q) = N_0^2 \langle \rho^{+}_{\alpha}(q) \rho^{-}_{\beta}(-q) \rangle, \]

with \( q = (\mathbf{q}, \omega) \).

The action is parameterized by the field theory, where the Hamiltonian is approximated by

\[ H_{\text{MF}} = \sum_{\mathbf{r}, \alpha} t_{\alpha}(\epsilon^{\dagger}_{\alpha}(\mathbf{r}, \tau) + \text{h.c.}) - \mu \sum_{\mathbf{r}, \alpha} n_{\alpha \mathbf{r}} + g \sum_{\mathbf{r}} \langle n_{\mathbf{r}, \uparrow} M_{\mathbf{r}, \uparrow} + n_{\mathbf{r}, \downarrow} M_{\mathbf{r}, \downarrow} - M_{\mathbf{r}, \uparrow} M_{\mathbf{r}, \downarrow} \rangle, \]

with \( M_{\mathbf{r}, \alpha} = \langle n_{\alpha \mathbf{r}} \rangle \). Self-consistent mean field calculations confirm that repulsive and attractive interactions favor CDW.
and ODW, respectively. The density patterns of these density waves are shown in figure 9.

The order parameter for the charge density wave phase is introduced by

\[
\rho(r) = [\phi_1 e^{iQ_1 \cdot r} + \phi_2 e^{iQ_2 \cdot r} + \text{c.c.}] + \text{const.},
\]

where \(\phi_1\) and \(\phi_2\) are complex valued fields slowly varying in space. The phenomenological free energy reads

\[
F = \int d^2r \sum_{j=1,2} \left(K_j \nabla \phi_j^2 + \alpha_j |\phi_j|^2 + \beta_j |\phi_j|^4 + \nu |\phi_j|^2 |\phi_j|^2 \right).
\]

(76)

Here, incommensurate filling is assumed and the theory has an emergent \(U(1) \times U(1)\) symmetry; otherwise the terms such as \((\phi_j^2 + \text{c.c.})\) are allowed and the theory has lower symmetry.

The effective couplings, \(K, \alpha, \beta, \) and \(\nu\) in equation (76) have been connected to microscopic parameters by field theory calculations (Zhang et al. 2012). At low temperature, we have \((r < 0, u > 2v),\) and the system is in a striped CDW phase with the wavevector \(Q_1\) or \(Q_2\) spontaneously chosen. Assuming \(Q_1\) is spontaneously chosen then there is an algebraic long range order in \(\phi_r\), i.e. \(\langle \phi_r(r)\phi_r(r') \rangle \propto \frac{1}{|r-r'|} \). At higher temperature it is found that the striped CDW phase first melts to a nematic phase through an Ising transition and then to normal through a Kosterlitz–Thouless transition.

3.3.3. Strongly correlated orbital models. At half filling \(p\)-orbital fermions described by the Hamiltonian in equation (72) exhibits a Mott transition with strong repulsive interaction, which is studied in Wu (2008b) and Zhao and Liu (2008). In the fermionic Mott state, like in the bosonic case, fermions are localized on each lattice site. As a result, the low energy physics is described by an effective model of super-fermions.

Considering a link \((r, r')\) the super-exchange interactions are determined by energy corrections on the states \(|1, 0; 1, 0\rangle, \ |0, 1; 0, 1\rangle, \ |0, 1; 1, 0\rangle\) and \(|1, 0; 0, 1\rangle\), where a notation is taken from equation (62) with the bosonic operators \(b_\alpha\) replaced by fermionic ones \(c_\alpha\). Suppose this link is in the \(x\) direction, the tunneling is then \(H_{\text{eff}}^x = -t \sum_{r \rightarrow r'} c_\alpha^\dagger x_{r'} c_\alpha r + \text{h.c.}\), with the transverse tunneling neglected. From standard perturbation theory, the energy corrections due to virtual fermion fluctuations are

\[
\Delta E(|0, 1; 0, 1\rangle) = \Delta E(|1, 0; 1, 0\rangle) = 0,
\]

\[
\Delta E(|1, 0; 0, 1\rangle) = \Delta E(|0, 1; 1, 0\rangle) = 0
\]

(77)

(78)

Mapping \(p_x, p_y\) to pseudo-spin \(|\uparrow\rangle, |\downarrow\rangle\) states, the super-exchange interactions are given in a compact form as

\[
h_{\text{eff}}^x = J_s \sigma_x(r) \sigma_x(r') + \text{const.},
\]

(79)

\(J_s = \frac{t^2}{4U}\). Rotating \(p\)-orbitals by an angle \(\theta\), we have the following transformation

\[
\begin{pmatrix}
  c_x \\
  c_y
\end{pmatrix} \rightarrow \mathcal{U}(\theta) \begin{pmatrix}
  c_x \\
  c_y
\end{pmatrix},
\]

(80)

with

\[
\mathcal{U}(\theta) = \begin{pmatrix}
  \cos \theta & \sin \theta \\
  -\sin \theta & \cos \theta
\end{pmatrix}
\]

For a link oriented at an angle \(\theta\) with respect the \(x\) axis, the super-exchange interaction reads as

\[
h_{\text{eff}}^x = J_s \sigma_x(r) \sigma_x(r') + \text{const.}
\]

On a square lattice, the Hamiltonian describing the orbital order is

\[
H_{\text{eff}}^{\text{orb}} = J_s \sum_r \sigma_x(r) \sigma_x(r + \mathbf{a}_x) + \sigma_y(r) \sigma_y(r + \mathbf{a}_y),
\]

(82)

which has the same form as the \(p\)-band Mott insulator of bosons. This Hamiltonian supports an alternating \(p_x/p_y\) order as shown in figure 6. On a honeycomb lattice, the super-exchange Hamiltonian is

\[
H_{\text{eff}}^{\text{orb}} = J_s \sum_{r \rightarrow r'} T_j(r) T_j(r + \mathbf{e}_j),
\]

(83)

with

\[
T_1 = -\frac{\sqrt{3}}{2} \sigma_x + \frac{1}{2} \sigma_z,
\]

\[
T_2 = \frac{\sqrt{3}}{2} \sigma_x - \frac{1}{2} \sigma_z,
\]

\[
T_3 = -\sigma_z.
\]

(84)

Here the summation \(\sum_{r \rightarrow r'}\) includes one set of the ‘A’ sublattices (figure 10). This model, dubbed quantum 120° model (Wu et al. 2007, Zhao and Liu 2008, Wu 2008b), is geometrically frustrated. The complication of this model originates precisely from the spatial nature of orbitals, which makes orbital degrees of freedom drastically different from real spins.

In three dimensions on a diamond lattice, the \(p\)-orbital exchange interaction leads to an exact orbital Coulomb phase characterized by ice rules and emergent gauge structures (Chern and Wu 2011).

3.3.4. Anti-Ferromagnetic phases of spinor \(p\)-orbital fermions. As motivated by understanding the role of magnetism in high temperature superconductors, studies of antiferromagnetic transitions in \(s\)-band fermions attracted tremendous interest, but the transition temperature is still out of reach for current cooling techniques. One way to improve the transition temperature could be provided by considering \(p\)-band fermions. The antiferromagnetic transition of spin-1/2
fermions loaded in $p$-bands of a 3D cubic lattice are studied in Wu and Zhai (2008), where half filling (three fermions per lattice site) is assumed. The Hamiltonian describing such a system is $H = H_0 + H_{\text{int}}$, with

$$H_0 = \sum_{\alpha} (t_\alpha \Psi^\dagger_{\alpha \uparrow} \Psi_{\alpha \downarrow} + \text{h.c.}),$$

and

$$H_{\text{int}} = \sum_{\alpha} \left\{ \sum_{\alpha} n_{\alpha \uparrow} n_{\alpha \downarrow} + W \sum_{\alpha = \beta} (n_{\alpha \uparrow} n_{\beta \downarrow} + \text{h.c.}) \right\}.$$

With strong repulsion, we can project to the low-energy subspace determined by $H_{\text{int}}$; projecting out high energy subspace will contribute to super-exchange interactions. The low-energy states are the four degenerate components of total spin-$3/2$:

$$|\uparrow\uparrow\uparrow\rangle, \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle), \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle),$$

and $|\downarrow\downarrow\downarrow\rangle$, where a notation $|\downarrow\downarrow\uparrow\rangle = c_{\alpha \uparrow}^\dagger c_{\beta \downarrow}^\dagger c_{\gamma \downarrow}^\dagger |\text{vac}\rangle$ is used. This is manifestation of the Hund’s rule. It is quite involved to perform the quantum mechanical second order perturbation theory here. A more elegant way is to take the Brillouin–Wigner approximation where the super-exchange interaction is given by

$$H_j = -P_G H_0 P_G H_j P_G,$$  \hspace{1cm} (85)

Here $P_G$ and $P_G$ mean projections onto excited and low-energy subspaces, respectively.

The calculations are greatly simplified by two observations (Wu and Zhai 2008). Firstly, the hopping processes only take place within the same orbital. Secondly, all terms in $H_0$ acting on the low-energy subspace create eigenstates of $H_{\text{int}}$ with the same excitation energy $U + 2W$. Then the super-exchange Hamiltonian $H_j$ on a link $(r, r') = (r + \hat{x})$ is given by

$$\sum_{\alpha} \frac{2 |t_\alpha|^2}{U + 2W} P_G \left( \sum_{\alpha \alpha'} c_{\alpha \alpha', \sigma}^\dagger c_{\alpha \alpha', \sigma} P_G \right).$$

By symmetrizing $c_{\alpha \alpha', \sigma}^\dagger c_{\alpha \alpha', \sigma}$, one can show

$$P_G c_{\alpha \alpha', \sigma}^\dagger c_{\alpha \alpha', \sigma} P_G = \frac{1}{3} P_G \left( \frac{1}{3} c_{\alpha \alpha', \sigma}^\dagger c_{\alpha \alpha', \sigma} P_G \right).$$

Then the super-exchange Hamiltonian is obtained to be

$$H_j = J \sum_{(\alpha \beta)} \vec{S}_\alpha \cdot \vec{S}_\beta,$$  \hspace{1cm} (86)

with $\vec{S}_\alpha = \frac{1}{2} P_G \sum_{\alpha \alpha'} c_{\alpha \alpha', \sigma}^\dagger \sigma_{\alpha \alpha'} P_G$, and the effective coupling

$$J = 4(t_0^2 + 2t_1^2)/(9U + 18W) > 0.$$  \hspace{1cm} (87)

The effective description is an isotropic spin-3/2 Heisenberg model. We remind the reader that this is the model for half filling, with the full Hilbert space of each site being spanned by three $p$-orbitals and two spins. Hund’s rule reduces the low energy subspace to the total spin-3/2 space. The ground state of the system thus has an antiferromagnetic long range order.

This antiferromagnetic order is destroyed by thermal fluctuations when the temperature is above Néel temperature $\sim J$.

### 3.4. Topological bands and nontrivial orbital states

In optical lattice experiments considerable efforts have been made to create topological bands. Neutral atoms loaded in such bands would experience effective magnetic fields due to non-trivial Berry curvatures. These experimental developments are motivated by consideration of novel quantum many-body states such as quantum Hall states and topological insulators/superconductors. While previous experiments largely focused on manipulating different hyperfine states of atoms with synthetic gauge fields, recent theoretical studies (Liu et al 2010, 2014, Liu et al 2016, Sun et al 2011, 2012b, Li et al 2013, Dutta et al 2014a, 2014b, Yin et al 2015) point to alternate ways to achieve topological bands by considering high orbital states in the optical lattices of non-standard geometry.

#### 3.4.1. Topological sp-orbital ladder

A one dimensional ladder composed of two chains of $s$ and $p$-orbitals is shown in figure 11. The two orbitals are level in energy, and other lower orbitals are energetically separated with a large gap, and thus can be neglected when considering the $sp$ ladder. The Hamiltonian describing this orbital ladder system is given by

$$H_0 = \sum_j C_j^\dagger \left[ -t_{sp} P_G c_{\alpha \alpha', \sigma}^\dagger c_{\alpha \alpha', \sigma} P_G \right] C_j + \text{h.c.} - \sum \mu C_j^\dagger C_j,$$  \hspace{1cm} (88)

where $C_j^\dagger = [a_{s,j}(\alpha), a_{p,j}(\beta)]$, with $a_{s,j}(\alpha)$ and $a_{p,j}(\beta)$ being fermion creation operators for the $s$- and $p_{\alpha}$-orbitals on the A and B chain respectively. The relative sign of the hopping amplitudes is fixed by parity symmetry of the $s$ and $p_{\alpha}$ orbital wave functions. As depicted in figure 11, the hopping pattern plays a central role in producing a topological phase. With a proper global gauge choice, $t_s$, $t_p$, and $t_{sp}$ are all positive. Focusing on half filling with chemical potential $\mu = 0$, the Hamiltonian is particle-hole symmetric under transformation $C_j \rightarrow (-1)C_j^\dagger$. Heuristically, topologically non-trivial band structure of the $sp$-orbital ladder may be speculated by rewriting the staggered quantum tunneling as

$$t_{sp} \sum_j [C_j^\dagger (-i\sigma_y) C_j + \text{h.c.}]$$

resembling the spin–orbit interactions when the $s$ and $p$ orbitals are mapped to pseudo-spin ($1/2$) states. The physics of the $sp$ orbital ladder is also connected to the more familiar frustrated ladder with magnetic $\pi$-flux, but the $sp$-ladder appears much easier to realize in optical lattice experiments.

In the momentum space, the Hamiltonian takes a suggestive form

$$H(k) = h_0(k) 1 + \vec{h}(k) \cdot \vec{\sigma},$$  \hspace{1cm} (89)

where $h_0(k) = (t_s - t_p) \cos(k)$, $h_i = 0$, $h_{sp} = 2t_{sp} \sin(k)$ and $h_{p} = -(t_s + t_p) \cos(k)$. Here, $1$ is the unit matrix, and $\sigma_0, \sigma_i$ and $\sigma_z$ are Pauli matrices in the two-dimensional orbital space. The energy spectrum consists of two branches,
An interesting limit is that when $t_i = t_p = t_{pp}$ the two bands are both completely flat. As the momentum $k$ is varied from $-\pi$ to $+\pi$, crossing the entire Brillouin zone, the direction of the vector $\hat{h}(k)$ winds an angle of $2\pi$. In the notation of Wen (2012), the sp-orbital ladder belongs to the symmetry group $G_{\text{sp}} = U(T, C)$, as it has both particle-hole and time-reversal symmetries in addition to the usual charge $U(1)$ symmetry. At half filling, it is characterized by an integer topological invariant, in this case the winding number $1$.

A manifestation of the nontrivial band topology is existence of edge states. It is easiest to show the edge states in the flat band limit, $t_i = t_p = t_{pp} \equiv t$, by introducing auxiliary operators, $\phi_0(j) = [a_{p}^+(j) \pm a_s(j)]/\sqrt{2}$. Then the Hamiltonian only contains coupling between $\phi_0$ and $\phi_1$ of nearest neighbors,

$$H_0 \to 2t \sum_j \phi_0^+(j) \phi_1(j + 1) + \text{h.c.}$$

One sees immediately that the edge operators $\phi_0(1)$ and $\phi_1(N)$ are isolated from the bulk, i.e. decoupled from the rest of the system. These modes describe two edge states at zero energy. Away from the flat band limit, the wavefunctions of the edge states analytically constructed in Li et al (2013) are found not to confine strictly at the ends, but instead decay exponentially with a characteristic length scale

$$\xi = 2/\log\left((\sqrt{t_p} + t_p)/(\sqrt{t_p} - t_p)\right)$$

Here, recall that the implicit length unit is the lattice constant along the ladder direction. For $t_{pp} = \sqrt{t_p}$, which includes the flat band limit, the decay length $\xi$ vanishes and we have sharply confined edge states.

A topological phase transition to a trivial insulator state can be driven by inducing a coupling between $s$ and $p$ orbitals, $\Delta H = \Delta_0 \sum r C^\dagger_r p_r C_r$, which can be engineered by rotating the atoms locally on each site (Gemelke et al 2010). For the coupling strength $\Delta_0$ greater than some critical value $\Delta_0^c$, Berry phase vanishes and the system becomes a trivial band insulator, and the zero energy edge states disappear. Such a phase transition can be detected by measuring the density correlation between two ends in experiments.

Regarding practical experimental realizations, careful treatments of band structures and Wannier functions are required as the details of tight binding models could receive significant corrections beyond harmonic approximations (equation (2)) (Ganczarek et al 2014). One controllable way to couple $s$ and $p$ orbitals is to use a one dimensional shaking lattice (Sowiński 2012, Łącki and Zakrzewski 2013, Zhang and Zhou 2014, Dutta et al 2015a, Przysiężna et al 2015, Sträter and Eckardt 2015, Zhang et al 2015), which has recently been realized in experiments (Fort et al 2011, Parker et al 2013, Khamenehi et al 2016, Niu et al 2015, Weinberg et al 2015). The other way to systematically control the sp-orbital coupling is to consider a noncentrosymmetric lattice where the coupling can be turned on and off by manipulating inversion symmetries (Liu et al 2016).

### 3.4.2. Topological semimetal from mixing $p$ and $d$ orbitals.

We now turn to two dimensions and study how degeneracy of higher orbital bands may give rise to topological phases (Liu et al 2010, Sun et al 2012b). Consider a double-well optical lattice of the configuration shown in figure 12 (Sun et al 2012b). By the space group symmetry $(D_4)$ of the lattice, the two $p$-orbital states ($p_s$ and $p_p$) are degenerate with the lowest $d$-orbital (i.e. $d_{x^2-y^2}$) at high symmetry points in the momentum space. The lattice configuration is found to exhibit degenerate $p$ and $d$ orbitals. Considering a square lattice with three orbitals on each site ($p_s$, $p_p$, and $d_{x^2-y^2}$), the Hamiltonian of the tight binding model takes the following form (Sun et al 2012b)

$$H_0 = \delta \sum_r d_r^\dagger d_r - t_{dd} \sum_r (a_{rs}^\dagger a_{rs} + a_{rp}^\dagger a_{rp}) + \text{h.c.}$$

$$- t_{pp} \sum_r (a_{ps}^\dagger a_{ps} + a_{pp}^\dagger a_{pp} + \text{h.c.})$$

$$+ \sum_r (p_{sx}^\dagger p_{sx} + p_{px}^\dagger p_{px} + \text{h.c.})$$

$$+ \sum_r (p_{sy}^\dagger p_{sy} + p_{py}^\dagger p_{py} - p_{dx}^\dagger p_{dx} + p_{dy}^\dagger p_{dy} + \text{h.c.})$$

(90)

where $a_r$ ($a_r^\dagger$) is the lattice vector in $(x,y)$ direction, and $p_{sx}$, $p_{sy}$, $p_{px}$, $p_{py}$ are fermionic annihilation operators for $p_s$, $p_p$, and $d_{x^2-y^2}$ orbitals at site $r$. The amplitudes of tunneling between these orbitals at nearby sites are $t_{dd}$, $t_{pp}$, and $t_{pp}$. With a proper gauge choice, these tunneling amplitudes are all positive. Here a point group $D_4$ and time-reversal symmetries have been assumed. This tight binding Hamiltonian can be realized by a double-well optical lattice potential

$$V(x, y) = -V_1[\cos(kx) + \cos(ky)] + V_2[\cos(kx + ky) + \cos(kx - ky)]$$

(91)

A typical configuration and the experimental protocol to realize it are shown in figure 12 (Sun et al 2012b). By the point group symmetry $(D_4)$ of the lattice, the two $p$-orbital states ($p_s$ and $p_p$) are degenerate at high symmetry points in the momentum space. By dialing the relative strength of $V_1$ and $V_2$, the two $p$-orbitals may be tuned to degeneracy with the lowest $d$-orbital (i.e. $d_{x^2-y^2}$). That corresponds to the control
The Berry flux orbitals are weakly hybridized, with orbital band is + − z, and δt is the eigenstate of the given by c. c.

\[ \mathcal{H}(k) = \sum_k (d^+_{k,p} p^+_x, p_y^+ k) \mathcal{H}(k) \left( \begin{array}{ccc} d_x^k & p_x^k & p_y^k \\ \end{array} \right) \]

with \( \mathcal{H}(k) \) given by

\[
\begin{pmatrix}
-2t_{2d}(\cos k_x + \cos k_y) + \delta & 2it_{pd} \sin k_x & 2it_{pd} \sin k_y \\
-2it_{pd} \sin k_x & 2t_x \cos k_x - 2t_y \cos k_y & 0 \\
-2it_{pd} \sin k_y & 0 & 2t_y \cos k_y - 2t_x \cos k_x 
\end{pmatrix}
\]

Depending on the value of the energy difference \( \delta \), there are two types of band structures for this model. For \( \delta > 4t_{2d} + 2t_y - 2t_x \), d-orbitals are weakly hybridized with p-orbitals; for \( 0 < \delta < 4t_{2d} + 2t_y - 2t_x \), the orbitals are strongly hybridized. For the latter case, a band touching point between the top and middle bands shows up at \( k_x = 0, k_y = 0 \) (\( \Gamma \) point) This band touching point has non-trivial topological property, which is characterized by the Berry flux defined as the contour integral of the Berry connection in the momentum space,

\[ \gamma_n = \oint_C dk \cdot A_n(k), \]

with \( n \) the band index, \( C \) a close contour enclosing the band-touching point, and the Berry connection \( A_n(k) = i \langle \psi_k | \hat{\partial}_k | \psi_k \rangle \), where \( | \psi_k \rangle \) is the eigenstate of the Hamiltonian \( \mathcal{H}(k) \). The Berry flux \( \gamma_n \) is quantized to an integer multiplied by \( 2\pi \), and only two cases \( \gamma_n = 0 \) or \( \pi \) are distinguishable without any symmetry requirement due to the gauge choice in \( | \psi_k \rangle \). However, with space-inversion symmetry, we can restrict \( | \psi_k \rangle = | \psi_k(-k) \rangle \), with \( I \) the space-inversion operator. The Berry flux then becomes well defined up to mod \( 4\pi \) (Sun et al. 2012b). For the band touching point considered here, \( \gamma_n = 2\pi \), and this band touching is topologically protected (in presence of symmetry). Filling fermions up to such a touching point gives rise to a topological semimetal.

A more illuminating way to show the topological protection is to construct an effective two band Hamiltonian in the vicinity of \( \Gamma \) point. Near this point, the d−→−− orbital band is far below in energy and can thus be eliminated. With standard perturbation theory, the effective Hamiltonian is given to second order as (Sun et al. 2012b)

\[
\mathcal{H}_{\text{eff}} = \left( \frac{\mathcal{H}_2}{\mathcal{H}_3} \right) - \frac{1}{\mathcal{H}_1 - \mu} \left( \frac{\mathcal{H}_3}{\mathcal{H}_2} \right),
\]

with \( \mu \) the chemical potential of the topological semimetal. Further expanding momentum around 0, the effective Hamiltonian takes the following form

\[
\mathcal{H}_{\text{eff}} = \frac{t_1 + t_2}{2}(k^2_x + k^2_y) + 2t_3 k_x \sigma_x + \frac{t_1 - t_2}{2}(k^2_x - k^2_y) \sigma_z,
\]

where \( t_1 = t_\uparrow + \frac{4t_{2d}}{2t_y - 2t_x + 4t_d} \), \( t_2 = -t_y \), \( t_3 = \frac{-2t_{2d}}{2t_y - 2t_x + 4t_d} \). The absence of \( \sigma_z \) component is protected by time-reversal and space-inversion symmetries. The energy gap near \( \Gamma \) point is \( 2|\hbar| \), \( \hbar \) a planar vector \( \mathcal{H}(k) = (2t_3 k_x k_y, \frac{-2\hbar}{2}(k^2_x - k^2_y)) \). The vector \( \hbar \) forms a vortex configuration with winding number 2 in the momentum space. At the vortex core (the \( \Gamma \) point \( k = (0, 0) \)), it is guaranteed that \( \hbar = 0 \), which means the degeneracy (or band touching) point is topologically protected.

A question naturally arising is whether the required time-reversal and space inversion symmetries can spontaneously break at low temperature. Renormalization group analysis (Sun et al. 2009, 2012b) points to the spontaneous symmetry breaking of time-reversal, and a state with angular momentum order \( \langle p_x p_y \rangle \) is stabilized at low temperature, if the interaction is repulsive. Taking this into the effective Hamiltonian, a gap opens at \( \Gamma \) point. As a result, the topological semimetal gives way to an insulator state at low temperature. This insulator is topologically non-trivial with finite Chern number. If the bare interaction is attractive, the renormalization equation shows that it flows to the fixed point of zero (usually called a marginally irrelevant term). In other words, the topological semimetal phase is stable against any attractive interaction in the perturbative renormalization group sense.

3.4.3. Nearly flatbands with nontrivial topology. In the system described by equation (92) at low temperature, the developed angular momentum order generates an additional coupling between two p orbitals,

\[ \Delta H = \sum_k i\Delta p^+_{x,k} p_{y,k} + \text{h.c.}, \]
which breaks time-reversal symmetry and thus allows the Chern number to be non-trivial. With the parameter choice $\delta = -4t_{dd} + 2t_{g} + \Delta - 2t_{g}\Delta/(4t_{g} + \Delta)$, the energies of the top band at $K$ and $M$ points are equal (Sun et al 2011). Varying $\Delta$ with $t_{dd} = t_{pd} = t = t_{f}$ fixed, they found that the ratio of the bandwidth/band gap is minimized ($\approx 1/20$) at $\Delta/t = 2.8$ for the top band. The top and bottom bands carry $q_{\perp}$ into condensate and fluctuation parts, i.e.,

$$q_{\perp} = -\frac{\Delta}{2(4t_{g} + \Delta)}.$$ Note that the vector $\mathbf{q}$ is the lattice momentum after doubling periods to make $\mathbf{q}$ a good quantum number, and that $u_{q}$ and $v_{q}$ are periodic—$u_{q}(x + 2a_{i}) = u_{q}(x)$, $v_{q}(x + 2a_{i}) = v_{q}(x + 2a_{i}) = v_{q}(x)$. The eigenvalues of $\sigma_{\mathbf{q}}\mathcal{K}_{\mathbf{q}}$ determine the Bogoliubov spectra, which are studied for square and checkerboard lattices. The fluctuations would grow in time if the eigenvalues are imaginary, leading to dynamical instability. This instability is cross checked by simulating real time dynamics in the continuous space where the optical lattice is treated exactly by a periodic potential (Xu et al 2013), beyond the standard tight-binding model approximation.

For a square lattice, the TSOC superfluid state is found to be dynamically unstable unless the interaction strength is extremely weak. In presence of dynamical instability, the lifetime of the TSOC superfluid state in a simple square lattice could be tens of milliseconds, rendering that such a state is experimentally unreachable for the simple square lattice. This conclusion is fully consistent with the experimental finding of a relatively fast decay of the $p$-orbital atoms in a quasi-1D lattice system (Müller et al 2007). In contrast, for the checkerboard lattice as used in experiments (Ölschläger et al 2011, Wirth et al 2011), when the lattice is not too shallow and the interaction is not too strong, the TSOC superfluid state is shown numerically to be dynamically stable. This is consistent with the long lifetime as observed in experiments. Similar improvement with superlattices is also found in one dimension (Martikainen 2011). When the interaction is stronger than some critical value, the TSOC superfluid is no longer dynamically stable even for the checkerboard lattice. Based on the dynamical stability, a phase diagram is predicted in Xu et al (2013), which is consistent with experimental observations.

Another way to understand the dynamical instability is to look at the energy cost for fluctuations $u_{q}$, $v_{q}$, which takes the following form Wu and Niu (2001),

$$\delta E_{q} = \int d^{2}x(v_{q}^{*}(x)v_{q}(x))^{2}.$$ Note that the vector $\mathbf{q}$ is the lattice momentum after doubling periods to make $\mathbf{q}$ a good quantum number, and that $u_{q}$ and $v_{q}$ are periodic—$u_{q}(x + 2a_{i}) = u_{q}(x)$, $v_{q}(x + 2a_{i}) = v_{q}(x + 2a_{i}) = v_{q}(x)$. The eigenvalues of $\sigma_{\mathbf{q}}\mathcal{K}_{\mathbf{q}}$ determine the Bogoliubov spectra, which are studied for square and checkerboard lattices. The fluctuations would grow in time if the eigenvalues are imaginary, leading to dynamical instability. This instability is cross checked by simulating real time dynamics in the continuous space where the optical lattice is treated exactly by a periodic potential (Xu et al 2013), beyond the standard tight-binding model approximation.

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4. Experimental probes and novel lattices

The theoretical discovery of richness of many-body physics with $p$-orbital atoms has motivated considerable experimental efforts in recent years. So far the experiments have been done only for bosonic atoms. It has been demonstrated in a checkerboard optical lattice that the chiral $p + ip$ Bose–Einstein condensate gives rise to nontrivial quantum interference. In this section, we will review the experimental challenges to detect the chiral order, the recent proposals in theory and attempts in experiment, and the current status.

4.1. Early experimental observations of higher bands in a cubic lattice

Coherent bosonic cold atoms were observed in the higher bands of an optical lattice in the pioneering experiments of accelerating lattices (Browaeys et al 2005) and of cross-band Raman transitions (Müller et al 2007).

In the experiment of Müller et al (2007), the sample is prepared by first loading a Bose–Einstein condensate of $^{87}$Rb atoms into a deep symmetrically simple cubic 3D optical lattice formed by three far detuned laser standing waves. For this deep lattice, it can be treated as an array of 3D harmonic oscillators with discrete vibrational levels, which can be labeled as $|m_x, m_y, m_z\rangle$ with $m_j$ the vibrational quantum number along the $j$ axis. Population transfer in these orbital levels can be controlled using a stimulated two-photon Raman process with propagating laser beams along the $x$ axis (see figure 13), which provides an inter-orbital coupling

$$\Omega_{\text{eff}}|m_x', m_y, m_z\rangle\langle m_x, m_y, m_z|,$$

with $\Omega_{\text{eff}}$ the effective Rabi frequency. The experiment restricts the Raman coupling to the lowest Bloch bands and demonstrates orbital transition from the $|000\rangle$ state (s-orbital) to $|100\rangle$ ($p_x$-orbital). Rabi oscillations between the two orbitals have been observed. A maximal transfer efficiency of nearly 80% is achieved.

The decay of atoms into the lowest orbital due to collisional events has also been measured. The lifetime was found to be 10–100 times longer than the tunneling scale. Emergence of coherence compatible with a Bose–Einstein condensation to a nonzero momentum state has been seen; yet the experimental system was anisotropic and the predicted $p_x + ip_y$-wave condensate was not studied for the absence of $p_x$ and $p_y$ orbital symmetry.

4.2. Observation of high-band condensation in a checkerboard lattice

After the early observation of higher band population (Müller et al 2007, Johnson et al 2009), long-lived Bose–Einstein condensate in the high-bands was not achieved until the groundbreaking experiment (Wirth et al 2011). In this experiment, a square optical lattice, composed of two classes (A and B) of (tube-shaped) lattice sites is used (see figure 14). Formed by two standing waves oriented along the $x$ and $y$ axes with polarization along the $z$ axis, the lattice potential is

$$V(x, y) = -\frac{\hbar}{4} \left[ \eta \left( \epsilon \cos(\alpha) + \gamma \sin(\alpha) \right) e^{ikx} + \epsilon^* e^{-ikx} \right] + e^{i\theta} \left( \epsilon e^{iky} + \epsilon^* e^{-iky} \right)^2,$$

where $\eta \approx 0.95$ accounts for a small difference in the powers directed to interferometer branches, $\epsilon \approx 0.81$ accounts for the imperfect retro-reflections, and the angle $\alpha$ permits tunability of anisotropy in the $x$-$y$ plane. An isotropic $p$-band with degenerate band minima arises when $\cos(\alpha) \approx \epsilon$ (or $\alpha = \alpha_{iso} \approx \pi/5$). The controllability of the phase difference $\theta$ allows to adjust the relative depth of potentials at A and B sites, which is crucial in this experiment to populate higher bands. For $\theta < \pi/2$ the A sites are shallower than the B sites and vice versa.

Initially a Bose–Einstein condensate of rubidium ($^{87}$Rb) atoms is prepared and the lattice potential is adiabatically turned on with $\theta = 0.38\pi$ such that B-sites are much lower than A. A lowest band lattice Bose–Einstein condensate is thus created with most of atoms confined in B sites. Then $\theta$ is rapidly increased to a final value $\theta_f > \pi/2$ such that the $s$-orbitals in the B sites are level with the $p$-band of the lattice in energy. In doing so, atoms are efficiently transferred to the $p$-band. Since this preparation procedure is abrupt, the prepared state is not immediately a condensate state but rather an incoherent state, in which the atomic distribution in the Brillouin zone is fairly uniform. Surprisingly, after some holding time around 10 ms, sharp peaks arise at $p$-band minima and the $p$-band Bose–Einstein condensate spontaneously emerges. In theory the emergence of phase coherence is beyond the scope of Gross–Pitaevskii
approach, and can be studied by constructing a quantum rotor model (Sau et al. 2012), where the dynamics is well captured by the truncated Wigner approximation (Polkovnikov et al. 2002).

The p-band condensate is not a ground state of the system but a metastable state; decaying into the lowest band is unavoidable. In this checkerboard lattice, the band gap between p-band and the lowest band is largely mismatched with the gap between p-band and the higher band, and Fermi’s golden rule calculation (see section 2.3) predicts a significant improvement of stability. In the experiment, the lifetime of the p-band condensate could reach 100 ms or longer.

From the measurements of momentum distribution, the experimental evidence of p-band condensate is conclusive. However, there is no direct evidence for the orbital ordering in the TSOC state as predicted in theory. As a step further, a phase diagram is mapped out with varying α (controlling the anisotropy) and the phase diagram is quantitatively consistent with theoretical predictions (Ölschläger et al. 2013). The remarkable consistency of experimental observations with theories strongly suggests the p-band condensate be a TSOC state. Yet, direct evidence of the orbital order requires further experimental investigation.

Population of even higher bands, say f-bands, is also achieved in this checkerboard lattice (Ölschläger et al. 2011) thanks to the tunability of relative depth between two sublattices. Similar procedure was implemented as in preparing the p-band condensate. The resulting f-band condensate also has a complex nature. The condensate wavefunction locally resembles the superposition \( \psi_{13,0} \pm i\psi_{03,0} \) of eigenfunctions \( \psi_{n,m} \) of a 2D harmonic oscillator with \( n \) and \( m \) oscillator quanta in \( x \) and \( y \) directions, which has a spatial \( (2x^2 - 3x) \pm i(2y^3 - 3y) \) dependence locally. The complex f-band condensate emerges from the same mechanism as the TSOC state of the p-band, namely maximizing the local angular momentum.

Besides the way of loading atoms into the excited bands demonstrated in the checkerboard lattice, there are other possibilities, for example by Bloch oscillation techniques (Larson and Martikainen 2011, Tarruell et al. 2012) or by vibrating lattices (Sowiński 2012, łącki and Zakrzewski 2013).

### 4.3. Early experimental realization of double-well lattices

Observations of higher bands in optical lattices are achieved in the early experiments manipulating double-well lattices, which were largely motivated by implementing coherent control of quantum degrees of freedom (Sebby-Strabley et al. 2006, Anderlini et al. 2007, Cheinet et al. 2008, Lundblad et al. 2008, Trotzky et al. 2008).

Here we use the experiment (Sebby-Strabley et al. 2006) to demonstrate how the higher bands are populated in double-well lattices and what consequent observables are achieved. This double-well lattice is a two dimensional lattice formed by superimposing two lattices with orthogonal polarizations. Having a laser setup as shown in figure 15(a), the electric field generated by the four laser beams is \( \text{Re}(\hat{E}(x,y))e^{i\lambda x} \), with

\[
\hat{E}(x,y) = E(e^{ikx} + e^{i(2\theta + 2\phi - 2\pi) - 2\pi}e^i)\hat{e}_1 + E(e^{i(\theta + 4\pi)} + e^{i(\theta + 2\pi + k\phi)})\hat{e}_2,
\]

where \( k = 2\pi/\lambda \) (\( \lambda \) is the wavelength of the laser light), \( \theta = kdx + \delta\theta \), and \( \phi = kdy + \delta\phi \) (the extra phase shifts \( \delta\theta \) and \( \delta\phi \) are polarization dependent and can be controlled in experiments). We have neglected several imperfections such as imperfect alignment and reflections for simplicity here. In experiments these imperfections could cause technical challenges. For light polarizations being all in plane such that \( \hat{e}_1 = \hat{\theta} = \hat{\phi} = \hat{x} \), we have a laser intensity field

\[
I(x,y)I_{\theta\phi,0} = 2\cos(2kx - 2\delta\theta_0 - 2\delta\phi_0) + 2\cos(2ky + 2\delta\phi_0) + 4,
\]

(101)

with subscripts in \( \theta \) and \( \phi \) specifying the polarization dependence. For the out-of-plane case, \( \hat{e}_2 = \hat{\tilde{e}}_2 = \hat{\tilde{z}} \), the laser intensity field is

\[
I(x,y)I_{\theta\phi,0} = 16 \left[ \cos \left( \frac{k}{2}(x + y) - \frac{\theta_0}{2} \right) - \cos \left( \frac{k}{2}(x - y) - \frac{\theta_0}{2} - \phi_0 \right) \right]^2.
\]

(102)

The laser field creates an optical potential \( V(x,y) \propto (I_{\theta\phi}(x,y) + I(x,y)) \). With in-plane and out-plane polarized laser beams combined, a double-well lattice can be created (figure 15(b)).

![Figure 14. Population of excited bands (figure courtesy of A. Hemmerich). (a), the checkerboard lattice with two sublattices A and B. (b), the experimental sequence to populate excited bands versus the final value of \( \theta \) (see equation (99)) in step 2 in (b). (c), the populations of higher bands with varying \( \theta \). The upper panel illustrates momentum distributions in different Brillouin zones (top row), and their dependence on \( \theta \). (d) shows the condensation in the \( X \) point and the band relaxation to the first BZ after long times. (e) three momentum spectra are shown, with the middle one corresponding to the interesting case of equal populations in \( X \) and \( Y \). Original results in a different form were published in Wirth et al. (2011).](image-url)
Ground state can be achieved by adiabatically loading atoms into the lattice. For the double-well lattice, different from simple Bravais lattices, the band gap could be very small compared with the energy scale $hT_{\text{load}}^{-1}$ with $T_{\text{load}}$ the loading time. Then the Landau–Zener transitions across the lowest and first excited bands can be significant. The population of the first excited band causes the oscillations in the momentum distribution measured in time-of-flight, which are observed in experiments.

The relation between the observed oscillations in the momentum distribution and the population of the excited band can be quantified by constructing a two-band model,

$$H = \sum_{\mathbf{r}, \mathbf{r}'} \phi^\dagger_{\mathbf{r}} T_{\mathbf{r}\mathbf{r}'} \phi_{\mathbf{r}'}.$$

with $\phi_\mathbf{r} = [\phi_\mathbf{r}^A, \phi_\mathbf{r}^B]^T$ where $\phi_\mathbf{r}^A$ and $\phi_\mathbf{r}^B$ are annihilation operators for the localized orbitals, $\omega_0(\mathbf{x} - \mathbf{r})$ and $\omega_0(\mathbf{x} - \mathbf{r})$, in the two sub-wells at site $\mathbf{r}$ in the double-well lattice. In momentum space, the Hamiltonian then reads $H = \sum_\mathbf{k} \phi^\dagger_\mathbf{k} H(\mathbf{k}) \phi_\mathbf{k}$, with $\phi_\mathbf{k}$ Fourier transform of $\phi_\mathbf{r}$. After loading bosonic atoms into the lattice, the condensate is a superposition of the ground state and excited state at lattice momentum $\mathbf{k} = 0$,

$$|\psi\rangle = \psi_0 |g\rangle + \psi_1 |e\rangle.$$

Writing $\mathcal{H}(0)$ as

$$\mathcal{H}(0) = h_0 |1\rangle + h_\alpha |\alpha\rangle,$$

the dynamics of the state $|\psi\rangle$ is given as $|\psi(t)\rangle = \psi_0 e^{i\Delta t/2} |g\rangle + \psi_0 e^{-i\Delta t/2} |e\rangle$, with $\Delta = 2\sqrt{h_0^2 + h_\alpha^2}$. In terms of $\phi_\mathbf{k}$ basis, we have

$$|\psi(t)\rangle = \left[ |\psi_0 e^{-i\Delta t/2} \cos(\gamma/2) - \psi_0 e^{i\Delta t/2} \sin(\gamma/2)\rangle \phi_\mathbf{k}^A(0) \right] + \left[ |\psi_0 e^{-i\Delta t/2} \sin(\gamma/2) + \psi_0 e^{i\Delta t/2} \cos(\gamma/2)\rangle |\phi_\mathbf{k}^B(0)\rangle \right]|0\rangle,$$

with $\gamma$ the polar angle of the vector $(h_\gamma, h_\alpha)$. The momentum distribution is then given as

$$\rho_\mathbf{k}(\theta) = \text{const.} + 2\text{Re} \left[ \psi_0^* \psi_0 e^{i\Delta t/2} (\tilde{\omega}_\mathbf{k}(\theta/2) + \tilde{\omega}_\mathbf{k}(\theta/2)) \times (\tilde{\omega}_\mathbf{k}(\theta/2) + \tilde{\omega}_\mathbf{k}(\theta/2)) \right]$$

where $\tilde{\omega}_\mathbf{k}(\theta)$ is the Fourier transform of $\sum_\mathbf{r} \omega_\mathbf{r}(\mathbf{x} - \mathbf{r})$. The population fraction of the excited band could thus be extracted from the dynamical evolution of momentum distribution.

Although the above discussions were restricted to the setup in the experiment (Sebby-Strabley et al 2006), the coherent oscillation in time-of-flight is a generic phenomenon when a superposed state of ground and excited bands is prepared. And indeed similar oscillations are observed in other double-well lattices as well (Anderlini et al 2007, Müller et al 2007, Trotzky et al 2008).

4.4. Theoretical understanding of experiments

Early theoretical studies of $p$-band condensates focus on the case with the point group $D_4$ symmetry. For the lattice potential realized in the experiment of Hamburg (equation (99)), the point group symmetry is maintained only for the ideal case $\epsilon = 1$ and $\alpha = 0$, where the potential reduces to $V = -V_0(\eta^2 \cos^2 kx + \cos^2 ky + \eta \cos \theta \cos kx \cos ky)$. For the realistic situation with $\epsilon < 1$, the $D_4$ symmetry is thus broken and only reflection symmetry with respect to the $x$-axis is preserved. The asymmetry can be partially compensated by setting $\alpha = \alpha_{\text{iso}}$ for which the potential reads $V = -V_0[(\eta^2 \cos^2 kx + \cos^2 ky) - \eta \cos \theta \cos kx \cos ky + \epsilon^2 \cos(\eta \cos(\theta + \epsilon)) \cos ky - \theta \cos ky)]$. The consequences of asymmetry are studied in detail in Cai and Wu (2011) and Shchesnovich (2012).

The band structure is calculated by plane-wave expansion (Cai and Wu 2011). The reciprocal lattice vectors are defined as $G_{m,n} = mb_1 + nb_2$, with $b_{1,2} = (\pm \pi/a, \pi/a)$ ($a$ the lattice constant). Taking the single-particle Hamiltonian $H_0 = -\hbar^2 \nabla^2 / (2M) + V(\mathbf{x})$, the diagonal matrix elements are $\left( \mathbf{k} + G_{m,n} \right)|H_0| \mathbf{k} + G_{m,n} = E_1|ak_x/\pi + (m-n)|^2 + |ak_y/\pi + (m+n)|^2$, with $E_1$ the single-photon recoil energy, and the off-diagonal matrix elements are

$$\langle \mathbf{k}|H_0| \mathbf{k} + G_{1,0}\rangle = \frac{V_0}{4} \eta^2 \cos \alpha, \langle \mathbf{k}|H_0| \mathbf{k} + G_{0,1}\rangle = \frac{V_0}{4} \eta e^{i\pi} \cos \alpha,$$

$$\langle \mathbf{k}|H_0| \mathbf{k} + G_{1,1}\rangle = \frac{V_0}{4} \eta e^{i\pi} \cos \alpha,$$

$$\langle \mathbf{k}|H_0| \mathbf{k} + G_{0,0}\rangle = \frac{V_0}{4} \eta e^{i\pi} \cos \alpha.$$

There are four time-reversal invariant points in the Brillouin zone, $O = (0,0)$, $X_\alpha = (\pm \pi/2a, \pm \pi/2a)$, and $M = (\pi/a, \pi/a)$, at which the Bloch functions are real valued. The band spectra are symmetric at these points, and consequently $\partial_\mathbf{k} \epsilon(0) = 0$, which means that they are saddle points in the band structure. For the choice $\alpha = \alpha_{\text{iso}}$, the second band has double degenerate minima at $X$ and $X_\alpha$. For $\alpha < \alpha_{\text{iso}} (\alpha > \alpha_{\text{iso}})$, $X_\alpha$ ($X_\alpha$) becomes the unique band minimum.

To investigate the interaction effects, the Gross–Pitaevskii equation

![Figure 15. Laser beams to generate a double-well lattice (redrawn from Sebby-Strabley et al 2006; copyright 2006 American Physical Society). (a) shows the laser setup. The incoming beam with wave vector $\mathbf{k}_1$ is reflected by mirrors M1 and M2 and after traveling distance $d_1$ returns to the cloud with a wave vector $\mathbf{k}_1$. The beam is then retro-reflected by M3 and returns with a wave vector $\mathbf{k}_3$, having traveled with an additional distance $2d_2$. (b) shows the generated double-well lattice with $h_{s1,0}=0.4$, $\phi_{s1} - \phi_{s2} = \pi/2$ and $\theta_{s1} - \theta_{s2} = -\pi/2$ (see text). The darker (lighter) regions represent areas where the potential is low (high).]
\[
\left\{-\frac{\hbar^2\nabla^2}{2M} + V_{\text{eff}}(\mathbf{x})\right\}\Psi(\mathbf{x}) = E\Psi(\mathbf{x}),
\]  

(106)

with \( V_{\text{eff}}(\mathbf{x}) = V(\mathbf{x}) + g_0|\Psi(\mathbf{x})|^2 \), is solved self-consistently by assuming the condensate wavefunction is a superposition of Bloch functions at \( X_{+} \).

\[ \Psi(\mathbf{x}) = \cos(\delta)\psi_{X_{+}}(\mathbf{x}) + \sin(\delta)e^{i\phi}\psi_{X_{-}}(\mathbf{x}). \]  

(107)

The Bloch functions \( \psi_{X_{\pm}} \) have nodal lines in space, while the variational condensate wavefunction could avoid nodal lines by having complex values (with \( \delta = 0 \) or \( \pi/2 \), and \( \phi = 0 \)). The complex solution is spatially more uniform and thus more favorable by interactions, but at the same time costs more kinetic energy when \( \alpha = \alpha_{\text{iso}} \).

The competition between interactions and anisotropy leads to an interesting phase diagram containing two real and one complex states of Bose–Einstein condensation. The Gross–Pitaevskii approach finds second order transitions at zero temperature (Cai and Wu 2011). The phase transitions can be understood within a Ginzburg–Landau theory,

\[ F = -r_1|\psi_{X_{+}}|^2 - r_2|\psi_{X_{-}}|^2 + g_1|\psi_{X_{+}}|^4 + g_2|\psi_{X_{-}}|^4 + g_3(\psi_{X_{+}}^*\psi_{X_{-}}^2 - c.c.) \]

(108)

with \( \psi_{X_{\pm}} \) describes the condensate component at \( X_\pm \). The Umklapp term \( g_3 > 0 \) favors the complex state. Assuming \( r_1, r_2 \), and \( g_3 - 2g_4 > 0 \), the complex state occurs in the regime

\[ \frac{g_3 - 2g_4}{2g_2} < \frac{r_1}{r_2} < \frac{2g_4}{g_3 - 2g_4}. \]  

(109)

The predicted phase diagram is confirmed in the experiment (Ölschläger et al 2013).

4.5. Measurement of orbital orders by quench dynamics

Direct measurement of orbital ordering, namely the staggered angular momentum, was thought to be an experimental challenge, which motivates a theoretical proposal of using quench dynamics (Li et al 2016). The key idea could be understood by drawing an analogy between the two orbital states at each site \( (p_x, p_y) \), and a pseudospin-1/2 degrees of freedom \( (\uparrow, \downarrow) \). In this analogy, the \( p_x \pm ip_y \) state corresponds to a pseudospin pointing along the \( y \) direction in space. Applying a ‘magnetic field’ along the \( x \) direction to this pseudospin should then induce Larmor precession, leading to periodic oscillations of the \( z \)-magnetization, corresponding to the population imbalance between two \( p \)-orbitals, \( \Delta N = N(p_x) - N(p_y) \). Here we consider a square lattice. We can take a certain initial state and then quickly turn on a strong ‘magnetic field’

\[ H_{\text{mag}} = \sum_{\mathbf{r}} (-1)^{r_y+r_x}\lambda(\mathbf{r})[\hat{b}_\uparrow(\mathbf{r})\hat{b}_\downarrow(\mathbf{r}) + \text{h.c.}] \]

(110)

at time \( \tau = 0 \). For simplicity, the ‘magnetic field’ is assumed to be strong enough to completely dominate the short-time dynamics. If initially a staggered superposition \( p_x \pm e^{i\phi}p_y \) is prepared, all local Larmor precessions add up to produce a macroscopic oscillation in the orbital imbalance \( \Delta N \). This imbalance evolves within a Heisenberg picture as

\[ \frac{d\Delta N(\mathbf{r}, \tau)}{d\tau} = -i[\Delta N(\mathbf{r}, \tau), H_{\text{mag}}] = -2\lambda(\mathbf{r})\lambda_{\text{mag}}(\mathbf{r}, \tau), \]  

(111)

with \( \lambda_{\text{mag}} \) the staggered angular momentum operator, whose time evolution is described by

\[ \frac{d\lambda_{\text{mag}}(\mathbf{r}, \tau)}{d\tau} = 2\lambda(\mathbf{r})\Delta N(\mathbf{r}, \tau). \]  

(112)

This leads to oscillations in \( \langle \Delta N(\mathbf{r}, \tau) \rangle \),

\[ \langle \Delta N(\mathbf{r}, \tau) \rangle = \langle \Delta N(\mathbf{r}, 0) \rangle \cos(2\lambda(\mathbf{r})\tau) - \langle L_{\text{mag}}(\mathbf{r}, 0) \rangle \sin(2\lambda(\mathbf{r})\tau) \]

\[ \equiv A(\mathbf{r})\cos(2\lambda(\mathbf{r})\tau) + \phi(\mathbf{r}), \]

(113)

where \( \langle \Delta N(\mathbf{r}, 0) \rangle \) and \( \langle L_{\text{mag}}(\mathbf{r}, 0) \rangle \) denote the orbital imbalance and staggered angular momentum for the initial state. The trigonometric form of this time-dependent equation thus defines the quantities \( A(\mathbf{r}) \) and \( \phi(\mathbf{r}) \), ready to compare with the experimental measurement of \( \Delta N \).

Neglecting spatial inhomogeneity in \( \lambda(\mathbf{r}) \) and \( \phi(\mathbf{r}) \), we can set \( \lambda(\mathbf{r}) = \lambda \) and \( \phi(\mathbf{r}) = \phi \), and extract the initial angular momentum order from the amplitude \( A \) and the phase shift \( \phi \) in the dynamics of the spatially averaged orbital imbalance \( \langle \Delta N(\tau) \rangle = 1/N\sum_\mathbf{r}\Delta N(\mathbf{r}, \tau) \). The coefficient \( \lambda \) can be read off from the oscillation period \( \tau_0 \equiv \pi/\lambda \). The orbital population imbalance can be measured directly in time-of-flight experiments.

For a \( C_4 \) symmetric initial state with non-zero staggered angular momentum, but no orbital imbalance, \( \langle \Delta N(\tau) \rangle \) is expected to oscillate with a non-zero amplitude and phase shift \( \phi \equiv \pm \pi/2 \) whose sign will fluctuate from realization to realization. By contrast, for a state with angular momentum order, the spontaneous time-reversal symmetry breaking yields a finite phase shift \( \phi \neq 0 \), which would vanish in a singular fashion as we tune from the angular momentum ordered to disordered regime through a second order phase transition.

The required coupling \( H_{\text{mag}} \) can be engineered by adding a quench potential \( V_{\text{mag}}(\mathbf{x}) \) modulated in the \( (1,1) \) direction with respect to the original lattice potential. The add-on potential generates a coupling between \( p_x \) and \( p_y \) orbitals

\[ \epsilon(\mathbf{r}) \approx \frac{\hbar}{4m_\omega_0} \partial^2 V_{\text{mag}}(\mathbf{r}) + \frac{1}{\hbar^2} \left( \frac{\mathbf{a} + \mathbf{b}}{\sqrt{2}} \right)_r \]

(114)

where \( \omega_0 \) is the harmonic oscillator frequency of the lattice wells hosting the \( p \)-orbitals and \( a = |\mathbf{a}| = |\mathbf{b}| \) is the lattice.
constant. The above estimate for the coupling strength is valid in the tight binding regime when the quench potential is weak as compared with the original optical lattice. Without loss of generality, one may consider an add-on optical potential of the form

$$V_{\text{add}}(x) = -\Gamma \cos^2 \left( \frac{2\nu + 1}{4} (K_x + K_y) \cdot x \right),$$

(115)

with some integer \( \nu \geq 0 \), a positive amplitude \( \Gamma \), and \((K_x, K_y)\) denoting the primitive vectors of the reciprocal lattice. This potential leads to a \( p_x/p_y \) coupling

$$\epsilon(r) = \frac{E_r}{\hbar \omega_0} \left( 2\nu + 1 \right)^2 (-1)^{x+y},$$

(116)

with \( E_r \) the photon recoil energy with wave number \( 1/2 |K_x + K_y| \). The staggering factor in the engineered coupling is crucial to probe the staggered angular momentum order.

This quench proposal brings other interesting possibilities in addition to providing a method to probe orbital order. For instance, one can simulate spin dynamics in solid state materials by studying orbital dynamics of \( p \)-band bosons. One advantage about orbital dynamics is that engineering artificial effective magnetic fields is intrinsically easier due to the spatial nature of orbital degrees of freedom than engineering real staggered magnetic fields.

### 4.6. Measurement of the complex phase by Raman transitions

There is another proposed scheme to measure the inter-orbital phase coherence in \( p_x \pm ip_y \) superfluid by Raman transition (Cai et al. 2012a). In the \( p_x \pm ip_y \) superfluid, condensation takes place at \( X_+ \) and \( X_- \) and the condensate state is \( |\Psi_0 \rangle \propto (b_{X_+}^\dagger + e^{i\phi} b_{X_-}^\dagger) |0 \rangle \) in general. The idea is to transform the phase coherence to number difference in momentum space. With a Raman operation, bosons in the original condensate can be transformed to a state with

\[
\begin{align*}
\tilde{b}_{X_+} &= \frac{1}{\sqrt{2}} (b_{X_+} - ie^{i\phi} b_{X_-}), \\
\tilde{b}_{X_-} &= \frac{1}{\sqrt{2}} (b_{X_-} - e^{-i\phi} b_{X_+}).
\end{align*}
\]

(117)

With \( \phi = 0 \), the phase coherence in the \( p_x \pm ip_y \) state is then transformed as

\[
(i\tilde{b}_{X_+}^\dagger b_{X_-} + \text{h.c.}) = (b_{X_+}^\dagger b_{X_-}^\dagger - b_{X_+}^\dagger b_{X_-}^\dagger) \equiv \delta n',
\]

(118)

which can be extracted in time-of-flight experiment.

The required Raman transition can be implemented by two traveling-wave laser beams along different directions with corresponding wave vector \( k_{1,2} \) and frequency \( \omega_{1,2} \) (Duan 2006). These laser beams induce an effective Raman Rabi frequency with a spatially varying phase \( \Omega(x,t) = \Omega_0 e^{i(k_x x - k_y y + \phi)} \), where \( \delta k = k_1 - k_2 \), \( \delta \omega = \omega_1 - \omega_2 \), and \( \phi \) is the relative phase between the two laser beams (see figure 16(a)). The effective Hamiltonian for the Raman process is described by

\[
H_R = \int dx \Omega(x,t) \phi^\dagger(x) \phi(x) + \text{h.c.},
\]

(119)

where \( \phi(x) \) is the boson annihilation operator in continuous space. The generated spatially dependent potential couples the two condensate components at the two momentum points (in the Hamburgh experiment (Wirth et al. 2011) \( X_+ = (\pm \pi/2, \pi/2) \), requiring \( \delta k = X_+ - X_- = (\pi, 0) \)).

To avoid complications of interband transitions (with band gap \( \Delta \)) and dynamics caused by tunnelings \( t \), an optimal choice for the Raman coupling strength is \( t \ll \hbar \Omega_0 \ll \Delta \). For the experimental situation, the Raman coupling strength should be chosen to be \( \Omega_0 \approx 2\pi \times 0.5 \text{ kHz} \). Thus the required duration of the Raman pulse is around 1 ms. To get efficient Raman operation, the frequency \( \delta \omega \) should match the energy difference between the initial and final states which is around a few Hz. Therefore the phase accumulation \( \delta \omega t \) within the duration of Raman pulse is negligible. With this approximation the Raman coupling is simplified to be

\[
H_R \approx \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \lambda(\mathbf{k}) b_{k_1}^\dagger b_{k_2} + \text{h.c.}
\]

(120)

Here \( \lambda(\mathbf{k}) \) is the \( \mathbf{k} \) dependent effective coupling, which can be calculated from the Bloch functions. For the Hamburgh experiment, it is estimated that \( \lambda(\mathbf{k}) \approx 0.98 \Omega_0 \propto \lambda \). Choosing the duration of the Raman pulse to be \( \lambda \delta t = \pi/4 \), the required state transfer in equation (117) is achieved. The resultant density difference is

\[
\delta n' = (ie^{i\phi} b_{X_+}^\dagger b_{X_-} + \text{h.c.}).
\]

(121)
The density difference would be superfluid. In this experiment, two independent superfluid. (c), 4 superfluid (reproduced with permission from Kock et al 2015; copyright 2015 American Physical Society). (a) shows the experimental protocol to prepare two copies of lattice condensates (red and blue). (b) shows the momentum distribution for the $p_x + ip_y$ superfluid. (c) shows the atomic spatial distribution after ballistic expansion of the two condensates. The four Bragg peaks are labeled by 1–4. (d) shows the experimental observation of the interference pattern of the four Bragg peaks. The interference structure is along the $z$ direction.

For the $p_x \pm ip_y$ superfluid, the density difference would be $bn^2 \propto \cos(\phi)$. With $\phi = 0$, $bn^2 = (\hbar b_x b_{X'} + \text{h.c.})$ represents the order parameter of the complex orbital ordering (figure 16).

4.7. Interference measurement of the complex phase

In a recent experiment (Kock et al 2015), that generalizes the idea of Young’s double slits, an interference measurement has been implemented to detect the inter-orbital phase coherence in the $p_x + ip_y$ superfluid. In this experiment, two independent copies of the lattice condensates are prepared with the experimental setup as illustrated in figure 17. The condensates are simultaneously prepared in the second band in two spatially separated regions of the lattice. After the state preparation, all potentials are switched off. The zeroth-order Bragg peaks observed in the $xy$-plane carry interference patterns in the $z$ direction due to overlapping contributions from the condensates originally separate in space. In the simplified picture approximating the two condensates by two point sources, the wave length of the density grating in the interference is $\lambda_c = \frac{2\pi bn z}{\sin(\theta)}$, with $t_{TO}$ the time of ballistic expansion, $d_z$ the spatial separation of the two condensates. This estimate is quantitatively consistent with experimental results.

In the ballistic expansion, the Bragg peaks (labeled by 1, 2, 3 and 4 in figure 17) yield the Fourier components of the condensate wavefunction, and we can associate a phase for each component, $\theta_{1,2,3,4}$. Since the spatially separate condensates are decoupled, they carry different phases, $\theta_i$ and $\theta'_i$. From the relative phase $\Delta \theta_i = \theta_i - \theta'_i$, we can introduce $\Delta \theta_{ij} = \Delta \theta_i - \Delta \theta_j$, which directly determines the correlation among the interference patterns in the Bragg peaks. If $\Delta \theta_{ij} = 0$ ($\pi$), the density patterns of the $i$th and $j$th peak are positively (negatively) correlated.

5. Discussion and outlook

5.1. Orbital physics in electronic materials

The crystal structure of the atomic ions in solids provide confining potential for electrons due to strong Coulomb force. Electrons in solids are usually nearly localized on atomic ions and the resulting orbital wavefunctions (or the shape of the electron cloud) are determined by the strong confining potential. This orbital degree of freedom is of great importance in correlated materials such as transition metal oxides (Tokura and Nagaosa 2000). Many intriguing phenomena such as metal-insulator transitions and colossal magnetoresistance can be attributed (or partially attributed) to the interplay of $d$-orbitals with charge and spin degrees of freedom.

Considering a transition-metal oxide material with perovskite crystal structure, $d$-orbital electrons localized on the transition-metal atom are surrounded by six oxygen ions $O^{2-}$, which give rise to crystal field and consequent energy splitting of the $d$-orbitals. Orbital wavefunctions pointing towards the negative-charged oxygen ions (the $e_g$ orbitals, $d_{x^2−y^2}$ and $d_{3z^2−r^2}$) have higher energy compared with those pointing in other orientations (the $t_{2g}$ orbitals, $d_{xy}$, $d_{yz}$ and $d_{xz}$) due to Coulomb repulsion (see figure 18). The spatial nature of orbital makes it intrinsically attached to the crystal fields, even in the absence of the relativistic spin–orbit interaction, and this intrinsic coupling of orbital degree of freedom to crystal fields

![Figure 17. Interference measurement of inter-orbital coherence in the $p_x + ip_y$ superfluid (reproduced with permission from Kock et al 2015; copyright 2015 American Physical Society). (a) shows the experimental protocol to prepare two copies of lattice condensates (red and blue). (b) shows the momentum distribution for the $p_x + ip_y$ superfluid. (c) shows the atomic spatial distribution after ballistic expansion of the two condensates. The four Bragg peaks are labeled by 1–4. (d) shows the experimental observation of the interference pattern of the four Bragg peaks. The interference structure is along the $z$ direction.](image1)

![Figure 18. Five $d$-orbitals. In the presence of crystal field, the orbital degeneracy splits into two groups, $e_g$ and $t_{2g}$.](image2)
and the resultant crystal symmetry make it distinct from real spins. When orbitals are modeled as pseudo-spins, the model Hamiltonian is in general lack of SU(2) symmetry. Consider a typical Mott insulator LaMnO$_3$ as an example. A neutral Mn atom has an electron configuration 3d$^5$4s$^2$. Losing three electrons, Mn$^{3+}$ in this material has four electrons in those five $d$-orbitals. From Hund’s rule, the spins are aligned ferromagnetically, and there are thus two possibilities for $e_x$ orbitals with either $d_{z^2}$ or $d_{x^2}$ being occupied. This represents the orbital degree of freedom in this Mott insulator, which can be modeled as pseudo-spins $T_{x,y,z}$. The model Hamiltonian is

$$H = \sum_{r,r'} J_{uu}(r)T_{i}(r)T_{i}(r'),$$

which is typically not SU(2) symmetric. With a long range orbital order, spin magnetism would be strongly affected by so called Jahn-Teller effect (Jahn and Teller 1937).

Most $p$-orbital solid state materials, for example the semiconducting silicon and graphene, are actually weakly correlated. However, recent studies in one oxide heterostructure LAO/STO have found that correlated physics such as ferromagnetism emerges from the effective $p$-orbitals, where $p_x$ and $p_y$ are mimicked by $d_{z^2}$ and $d_{x^2}$ orbitals (the degeneracy with $d_{xy}$ orbital is broken due to lack of out-of-plane inversion symmetry at the interface). In $d$-orbital systems, correlated effects usually emerge due to large Hubbard $U$ interaction because of the tight confinement of these orbitals. The emergence of correlated physics in $p$-orbital systems on the other hand could be attributed to a different origin, which is the quasi-one dimensionality (Chen and Balents 2013, Li et al 2014). In one dimension at low filling, the magnetic susceptibility diverges as $\chi_{pd} \sim 1/\rho^2$, where $\rho$ is the occupation number per site. Even for infinitesimal interaction $U$, there is a strong interaction effect: the ratio of the interacting to free fermion susceptibility diverges, $\chi_{pd} / \chi_{ff} \to \infty$ for $\rho \to 0$. A general result for the free energy (per site) versus magnetization at low density is obtained to be

$$F = 2\rho J_{dd}F_{dd}\left(M, k_{B}T / J_{dd}\right) - J_{dd}M^2,$$

(122)

where $M$ is the magnetization (per site), $J_{dd}$ is the Hund’s rule coupling, $J_{dd}$ is the effective antiferromagnetic coupling, and $F_{dd}(m,t)$ is the free energy per site of the one-dimensional antiferromagnetic chain, with reduced magnetization $m$ and temperature $t$ (this is known from thermodynamic Bethe ansatz). The effective coupling $J_{dd}$ is reasonably conjectured to scale as $J_{dd} \propto \rho^3$ (Chen and Balents 2013). From the free energy, the Hund’s energy is dominant and favors a ferromagnetic state with sufficiently low density for arbitrarily weak Hund’s coupling $J_{dd}$. A rigorous work (Li et al 2014) studies the higher filling regime (but assumes no double occupancy), where a ferromagnetic ground state for $p$-orbital fermions is proved based on transitivity and non-positivity of the many-body Hamiltonian. Further studies are required to find out the boundary of the ferromagnetism in $p$-orbital fermions.

5.2. Synthetic orbital matter and material design

In material science, design of materials for applications is an important subject. Recent developments involve engineering heterostructures with hybrid materials. For example oxide heterostructures such as LaAlO$_3$/SrTiO$_3$ and GdTiO$_3$/SrTiO$_3$ have been created and extensively studied. While the properties of many materials can be calculated within the density functional theory (DFT), this approach fails for ones of strong correlation for which $d$-orbital electrons typically play an important role. At the same time, these strongly correlated materials could have fascinating properties including important applications. High $T_c$ superconductivity belongs to this class. Lots of efforts have been made in searching for materials with higher $T_c$, but there is no real improvement in the last two decades. Lack of reliable tools in predicting $T_c$ leaves the design of high $T_c$ superconductivity essentially to empirical trials, which are costly in both time and materials. Developing new tools to simulate strongly correlated materials by incorporating correlation effects in DFT has triggered tremendous interest but appears to be very challenging.

To address the challenge of simulating correlated $d$-orbital electrons in classical computers, one alternative way is to create synthetic orbital matter with optical lattices and take it as a quantum orbital simulator. With this optical-lattice-based quantum orbital simulator, the ultimate procedure for material design would be—(1) conceive a particular design of materials; (2) determine the orbital configuration of the imagined material by quantum chemistry; and (3) apply cold atoms in optical lattices to simulate the properties. In such a way, we could explore the imagined quantum materials for desired properties, bypassing the often tedious chemical process of really fabricating them from electronic compounds. This would significantly speed up the material design and should help improve key quantities of great interest, for instance, the value of critical temperature $T_c$ of superconductivity in future. Although the optical lattice experiment is still at a very early stage, with future developments, synthetic orbital matter in optical lattices could be extremely helpful to the design of real materials.

Finally, we would like to point out that orbital degrees of freedom are found to play an important role for a vast majority of intriguing electronic quantum materials that condensed matter physicists have found since 1970s. Magnetic materials of spin only are an important class of systems that have been studied with great progress and remain to pose new challenges, such as frustrated magnets possibly showing spin liquid phases. In fact, the spin-only systems represent a small fraction of the world of real materials. Furthermore, past theoretical studies predicted exotic phenomena for model systems that have no spin but only orbital degrees of freedom. Such hypothetical models, which previously might have seemed too special and excessive, now become readily realizable with optical lattices. On this regard, using higher orbital bands of the optical lattice appears to open up a new front to explore orbital physics, both for understanding the electronic systems and for exploring artificial quantum orbital-only models that have no prior analogue in solids.
5.3. Many-body dynamics of high orbital atoms

Coherent dynamics across different bands has been observed in many experiments (Jona-Lasinio et al. 2003, Sebbey-Strabley et al. 2006, Anderlini et al. 2007, Cheinet et al. 2008, Trotzky et al. 2008, Zhai et al. 2013, Hu et al. 2015). In particular the recent experiments (Zhai et al. 2013, Hu et al. 2015) have demonstrated fast coherent controllability of orbital degrees of freedom. These experimental developments open up possibilities of studying many-body dynamics of high orbital, where the observed Rabi-like oscillations between different bands can be affected by interaction. One particular example would be orbital Josephson effect, which has been studied for double-well potentials (Garcia-March et al. 2011, Garcia-March et al. 2012, Gillet et al. 2014, Garcia-March and Carr 2015). This effect has also been seen in numerical simulations of a dynamical procedure, proposed to detect the $p + ip$ BEC (Cai et al. 2012a, Li et al. 2016).

The orbital Josephson effect is expected to be generic for various experimental setups for high orbital atoms. Here we consider the specific setup proposed to probe the complex order parameter (see section 4.5). Assuming all atoms condense, the dynamics is then approximately captured by a two-mode Hamiltonian,

$$H = \lambda b^{\dagger}_{k_1}b_{k_2} + \text{h.c.} + g(b^{\dagger}_{k_1}b_{k_1}b^{\dagger}_{k_2}b_{k_2} + K_1 \rightarrow K_2) + g_3(b^{\dagger}_{k_1}b_{k_1}b^{\dagger}_{k_2}b_{k_2} + b^{\dagger}_{k_1}b_{k_1}b^{\dagger}_{k_2}b_{k_2} + \text{h.c.}),$$

(123)

where $b_{k_1, 2}$ are the two condensed modes and the last term $g_3$ is a Umklapp process. Following the treatment of Josephson effect developed for double-well Bose-Einstein condensates (Smerzi et al. 1997, Zapata et al. 1998), the dynamical state could be approximated by

$$|\Psi(t)\rangle = \frac{1}{\sqrt{N}}(\psi_1(t)b^{\dagger}_{k_1} + \psi_2(t)b^{\dagger}_{k_2})^N|0\rangle.$$

(124)

The corresponding time-dependent Gross–Pitaevskii equation is (Cai et al. 2012a)

$$i\partial_t\psi_1(t) = \lambda\psi_1(t) + (2g_1|\psi_1|^2 + g_2|\psi_2|^2)\psi_1 + 2g_3\psi_1^\dagger\psi_2^\dagger, \quad i\partial_t\psi_2(t) = \lambda\psi_2(t) + (2g_1|\psi_1|^2 + g_2|\psi_2|^2)\psi_2 + 2g_3\psi_2^\dagger\psi_1^\dagger,$$

(125)

To make the dynamics more physical, one can rewrite the wavefunctions $\psi_i(t)$ in terms of densities and phases as

$$\psi_1 \rightarrow \sqrt{\rho_1} e^{i\phi_1}, \quad \psi_2 \rightarrow \sqrt{\rho_2} e^{i\phi_2}.$$

The equation of motion is most easily derived by constructing the Lagrangian, which takes the form,

$$L = -\rho_1\partial_\phi \theta_1 - \rho_2\partial_\phi \theta_2 - \{2\lambda\sqrt{\rho_1\rho_2} \cos(\theta_2 - \theta_1) + 2g_3\rho_1\rho_2\cos(2(\theta_2 - \theta_1)) + 2g_1\rho_1 + g_2\rho_2 + g_3\rho_1\rho_2 \}.$$

(126)

From Euler–Lagrangian equations,

$$\partial_\rho_1 = -\frac{\partial L}{\partial \rho_1}, \quad \partial_\phi \rho_1 = 0,$$

(127)

one gets

$$\partial_\phi \rho_1 = -\frac{\partial_\phi L}{\partial \rho_1} = -\partial_\phi \left\{2\lambda\sqrt{\rho_1\rho_2} \cos(\theta_2 - \theta_1) + 2g_3\rho_1\rho_2\cos(2(\theta_2 - \theta_1)) + 2g_1\rho_1 + g_2\rho_2 + g_3\rho_1\rho_2 \right\},$$

$$\partial_\phi \rho_2 = -\frac{\partial_\phi L}{\partial \rho_2} = -\partial_\phi \left\{2\lambda\sqrt{\rho_1\rho_2} \cos(\theta_2 - \theta_1) + 2g_3\rho_1\rho_2\cos(2(\theta_2 - \theta_1)) + 2g_1\rho_1 + g_2\rho_2 + g_3\rho_1\rho_2 \right\},$$

$$\partial_\phi \theta_1 = -\frac{\partial_\phi L}{\partial \phi_1} = -\partial_\phi \left\{2\lambda\sqrt{\rho_1\rho_2} \cos(\theta_2 - \theta_1) + 2g_3\rho_1\rho_2\cos(2(\theta_2 - \theta_1)) + 2g_1\rho_1 + g_2\rho_2 + g_3\rho_1\rho_2 \right\},$$

$$\partial_\phi \theta_2 = -\frac{\partial_\phi L}{\partial \phi_2} = -\partial_\phi \left\{2\lambda\sqrt{\rho_1\rho_2} \cos(\theta_2 - \theta_1) + 2g_3\rho_1\rho_2\cos(2(\theta_2 - \theta_1)) + 2g_1\rho_1 + g_2\rho_2 + g_3\rho_1\rho_2 \right\}.$$

To make a direct connection to Josephson effects, the number imbalance and phase difference are defined to be $z = \rho_1 - \rho_2$ and $\phi = \theta_1 - \theta_2$, whose dynamical evolution is governed by

$$\partial_t z = 2\left(\lambda\sqrt{1 - z^2}\sin(\phi) + g_3(1 - z^2)\sin(2\phi)\right),$$

$$\partial_t \phi = (2g_1 - g_2)z - \frac{2\lambda z}{1 - z^2}\cos(\phi) - 2g_3z\cos(2\phi).$$

(128)

Compared with Josephson effects in double-well Bose–Einstein condensates (Smerzi et al. 1997, Zapata et al. 1998), the key difference is that here we have $\sin(2\phi)$ and $\cos(2\phi)$ terms which are generated by the Umklapp process $g_3$. In the ground state, these terms give rise to the spontaneous time-reversal symmetry breaking.

In the noninteracting limit, $g_{1,2,3} \rightarrow 0$, the Rabi-like oscillation with frequency $2\lambda$ is easily recovered. In the linear regime, $|z| \ll 1$, the dynamics in $z$ and $\phi$ is simplified to

$$\partial_t z \approx (2\lambda + 4g_3)\delta\phi, \quad \partial_t \delta\phi \approx (2g_1 - g_2 - 2\lambda - 2g_3)z,$$

assuming $\phi \ll 2\pi$. This gives rise to oscillatory dynamics with a frequency

$$\omega_{\text{real}} = \sqrt{(2\lambda + 4g_3)(2\lambda - 2g_1 + g_2 + 2g_3)},$$

(129)

which is the Josephson frequency for a real superposition state $p_1 + p_2$. For the complex superposition $p_1 \pm ip_2$, expressing $\phi$ in terms of fluctuation field $\delta\phi$, $\phi \rightarrow \phi + \delta\phi$ ($\delta\phi \ll 2\pi$), the linear dynamics is

$$\partial_t z \approx -2g_3\left(\delta\phi - \frac{\lambda}{g_3}\right), \quad \partial_t \delta\phi \approx (2g_1 - g_2 + 2g_3)z,$$

which predicts a Josephson frequency

$$\omega_{\text{complex}} = \sqrt{2g_3(2g_1 - g_2 + 2g_3)},$$

(130)

with $\lambda/g_3$ assumed to be small. In the Josephson effects, the frequency is different from that in non-interacting Rabi oscillations. This frequency difference is also seen in the numerical simulations based on Gross–Pitaevskii equations (Cai et al. 2012a) and Gutzwiller methods (Li et al. 2016).

The nonlinear effects of dynamics in equation (128) are expected to be more interesting, because of the $\sin(2\phi)$ term, than the usual Josephson physics of double-wells. For example the analogy of self-trapping effect in double-wells would certainly exist in this orbital setting, and very likely would lead to new possibilities beyond the standard double-well Josephson effect. Details of such orbital Josephson effects call for further theoretical and experimental investigations.
5.4. Relation to spin–orbit coupled quantum gases

Orbital degree of freedom can certainly be mapped to pseudospins. In doing so, spin–orbit couplings of certain types usually arise naturally due to the spatial nature of orbitals (Liu et al 2010, 2014, Sun et al 2012a, 2012b, Li et al 2013, Belenky et al 2014, Zhou et al 2015). The tunneling Hamiltonian of orbital models mixes different orbitals. In particular mixing of different parities could lead to non-trivial effective spin orbit couplings and consequent topological properties. Mixing of \( s \) and \( p \)-orbitals in a ladder system (Li et al 2013) closely mimics the one dimensional spin orbital coupling recently engineered in cold gases by Raman transitions (Lin et al 2011, Galitski and Spielman 2013). Such \( sp \) orbital mixing is recently achieved in a shaken lattice experiment of \(^{133}\text{Cs}\) Bose–Einstein condensates (Parker et al 2013) and a similar band structure with double minima like the spin–orbit coupled case is indeed obtained. Mixing of \( p \) and \( d \)-orbitals gives rise to the phases of topological semimetal and topological insulator (Sun et al 2012b). One recent work shows that mixing of \( p \)-orbitals in spin imbalanced fermions leads to topological superconductivity with novel features (Liu et al 2014). We note however that some of these novel predictions are made for fermionic species of atoms, whereas the high band experiments have been explored only for bosons so far as to this time. Further experimental developments are expected.

With strong repulsion, particles could form Mott states with the charge degrees of freedom frozen. The orbital ordering in Mott states is then described by super-exchange interactions of orbitals, which typically depend on the orientation of links. This orientation dependent orbital super-exchange gives rise to novel pseudo-spin models such as quantum 120° model (Zhao and Liu 2008, Wu 2008b) (see equation (83)).

With spin–orbit couplings, many interesting quantum phases such as skyrmions and topological states have been investigated. The connection of orbital physics to spin–orbit coupling suggests possibilities of novel orbital states. One reason to study spin–orbit coupled physics in orbital systems (with atoms loaded into higher bands) is that there appears no additional heating in this system, in contrast with the heating challenge faced by engineered spin–orbital couplings by the advanced Raman laser technique. In this regard, orbital physics provides an alternative platform to investigate spin–orbit coupled phenomena, which is a direction worth future exploration.

5.5. Periodic driving induced orbital couplings

In recent optical lattice experiments (Aidelsburger et al 2013, Miyake et al 2013, Parker et al 2013, Struck et al 2013, Jotzu et al 2014, Niu et al 2015, Weinberg et al 2015), periodically driven systems have been developed with a motivation to create exotic atomic phases. In such systems time reversal symmetry is explicitly broken. With the driving frequency matching band gaps, energetically separated orbital bands can be efficiently coupled.

Here we use one example to demonstrate the key idea of using lattice shaking to induce/control orbital couplings. Consider a one dimensional shaking lattice as implemented in experiments (Parker et al 2013). The time-dependent optical potential of this lattice reads

\[
V(x, t) = V_0 \cos[k(x - x_0(t))],
\]

with \( x_0(t) \) a periodic function, \( x_0(t) = X_0 \sin(2\pi t/T) \). Taking \( X_0 = 0 \), we have static lattice potential where \( s \) and \( p \)-orbital bands are decoupled and well separated by an energy gap. With weak driving, we have \( V(x, t) \approx V_0 [\cos(kx) + kx_0(t) \sin(kx)] \). The time-dependent term introduces an effective coupling between \( s \) and \( p \) orbitals, approximately given by

\[
\lambda_{sp} = kV_0 x_0(t) \int dx \sin(kx) w_p^*(x) w_p(x),
\]

with \( w_p(x) \) the orbital wavefunction. With frequency \( 2\pi/T \) matching the band gap, the system is approximately described by a static two-band model with \( s \) and \( p \) orbitals coupled, under a rotating wave approximation.

It appears natural to engineer orbital couplings by lattice modulation/shaking techniques. But the problem is that heating effects are fundamentally unavoidable in periodically driven quantum systems. Since periodic driving breaks time translational symmetry, energy is no longer a conserved quantity. It follows that driven systems (assumed ergodicity) at long time would necessarily be described by infinite temperature ensemble. Nonetheless, there could be long lifetime transient states that manifest interesting topological features. This requires more careful treatment of quantum dynamics than just solving for the ground states of effective static Hamiltonians. One way out is to combine with dissipation. Driven-dissipative orbital models may exhibit steady quantum many-body states with interesting topological properties. This is worth future exploration.

5.6. Open questions

For bosons, firstly, it remains open how to experimentally reach the Mott insulator phases of the \( p \)-band and study the \( p \)-band superfluid-Mott insulator transition. The current experiments at Hamburg are performed with a two-dimensional checkerboard lattice and a relatively shallow harmonic trap in the third dimension. Introducing an additional optical lattice potential in the third dimension is required to access the Mott regime. Unfortunately that would also increase the on-site interaction between \( p \)-orbital bosons, which leads to faster decay (Hemmerich 2014).

Secondly, it is intriguing to find out what type of new topological defects, other than vortices, may possibly occur in the staggered \( p_x \pm ip_y \)-orbital Bose–Einstein condensate. The state breaks not only \( U(1) \) but also other interesting symmetries that are usually not broken in other conventional Bose condensates, including for example, time-reversal, lattice translational and rotational symmetries. On the general ground of broken symmetries, new classification of topological defects is expected but remains unknown.

For fermions, the stability of the \( p \) and higher orbital bands is protected by Fermi statistics, if the experimental system is prepared with the lowest ground band being completely filled, as opposed to the method of band population inversion (Müller et al 2007, Wirth et al 2011, Ölschläger et al 2012, Ölschläger et al 2013, Kock et al 2015). Nevertheless, this approach would require a higher density of fermions, which in turn requires a higher efficiency of cooling fermions down to degeneracy. The recent breakthrough in the Rice experiment
of fermions on lattice (Hart et al 2015) is promising for studying the higher orbital bands.

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\[
\begin{align*}
V_{\text{int}} &= \frac{2\pi a_s \hbar^2}{m} \int d^3x \left[ \prod_{j=1}^4 \frac{d^3q_j}{(2\pi)^3} \right] e^{-iq_1 \cdot q_2 - q_3 \cdot q_4} \\
&\times \left\{ b_{Q_1}^\dagger q_1 b_{Q_2} q_2 b_{Q_3}^\dagger q_3 b_{Q_4}^\dagger q_4 + b_{Q_1} q_1 b_{Q_2}^\dagger q_2 b_{Q_3} q_3 b_{Q_4}^\dagger q_4 \\
&+ 4 \times b_{Q_1}^\dagger q_1 b_{Q_2} q_2 b_{Q_3}^\dagger q_3 b_{Q_4} q_4 + b_{Q_1} q_1 b_{Q_2} q_2 b_{Q_3}^\dagger q_3 b_{Q_4}^\dagger q_4 + b_{Q_1}^\dagger q_1 b_{Q_2} q_2 b_{Q_3}^\dagger q_3 b_{Q_4} q_4 \right\} \to \psi(x)
\end{align*}
\]

where \( \psi(x) \) is the bosonic field operator, \( m \) is the mass of atoms and \( a_s \) is the 3D scattering length. With bosons loaded into the \( p \)-band of a 2D lattice that has band minima at \( Q_\pi = (\pi, 0) \) and \( Q_x = (0, \pi) \), the field operator is expanded by the low energy modes as (Li et al 2016)

\[
\psi(x) = \int d^3q \left\{ e^{iQ \cdot x} b_{Q_1} + e^{iQ \cdot x} b_{Q_2} + e^{iQ \cdot x} b_{Q_3} + e^{iQ \cdot x} b_{Q_4} \right\},
\]

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**Appendix. Tree level estimate of couplings in effective field theory for \( p \)-orbital bosons**

In this appendix, the coupling constants in the effective field theory (equation (31)) are related to a microscopic model. We start with the contact interaction for a 3D Bose gas, which reads

\[
\begin{align*}
g_{\alpha_1 q_1 q_2 q_3} &= \frac{2\pi a_s \hbar^2}{ma^2} \int d^3x u_{Q_1} q_1(x') u_{Q_2} q_2(x') u_{Q_3} q_3(x') u_{Q_4} q_4(x'), \\
g_{\alpha_2 q_1 q_2 q_3} &= \frac{2\pi a_s \hbar^2}{ma^2} \int d^3x u_{Q_1} q_1(x') u_{Q_2} q_2(x') u_{Q_3} q_3(x') u_{Q_4} q_4(x'), \\
g_{\alpha_3 q_1 q_2 q_3} &= \frac{2\pi a_s \hbar^2}{ma^2} \int d^3x u_{Q_1} q_1(x') u_{Q_2} q_2(x') u_{Q_3} q_3(x') u_{Q_4} q_4(x'), \\
g_{\alpha_4 q_1 q_2 q_3} &= \frac{2\pi a_s \hbar^2}{ma^2} \int d^3x u_{Q_1} q_1(x') u_{Q_2} q_2(x') u_{Q_3} q_3(x') u_{Q_4} q_4(x'), \\
g_{\beta q_1 q_2 q_3} &= \frac{4\pi a_s \hbar^2}{ma^2} \int d^3x u_{Q_1} q_1(x') u_{Q_2} q_2(x') u_{Q_3} q_3(x') u_{Q_4} q_4(x'), \\
g_{\gamma q_1 q_2 q_3} &= \frac{4\pi a_s \hbar^2}{ma^2} \int d^3x u_{Q_1} q_1(x') u_{Q_2} q_2(x') u_{Q_3} q_3(x') u_{Q_4} q_4(x').
\end{align*}
\]
Neglecting the momentum dependence of $g_{a2}$ and $g_3$, the derived couplings simplify to
\[g_{xx} = g_{yy} = \frac{2\pi a_0^2 \hbar^2}{ma^2} \int d^d \mathbf{X} |u_{Q_0}(\mathbf{X})|^4,\]
\[g_{xy} = g_{yx} = \frac{4\pi a_0^2 \hbar^2}{ma^2} \int d^d \mathbf{X} |u_{Q_0}(\mathbf{X})|^2 |u_{Q_0}(\mathbf{X})|^2,\]
\[g_3 = \frac{2\pi a_0^2 \hbar^2}{ma^2} \int d^d \mathbf{X} u_{Q_0}(\mathbf{X})^2 u_{Q_0}(\mathbf{X})^2,\]

The calculation of $K_0$ and $K_1$ is straightforward at tree level, and they are estimated to be $K_0 = -\frac{1}{2 \omega^2} E_p(k)_{\mathbf{k} \rightarrow \mathbf{Q}}$, and $K_1 = -\frac{1}{2 \omega^2} E_p(k)_{\mathbf{k} \rightarrow \mathbf{Q}}$, with $E_p(k)$ the dispersion of the $p$-band.

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