Novel $\rho$-orbital physics in the honeycomb optical lattices

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Thank G. W. Chern (U Wisconsin), Y. P. Wang (IOP) for collaborations on various projects of orbital physics with cold atoms.

Thank I. Bloch, A. Hemmerich, T. L. Ho for helpful discussions.
• **Introduction: cold atoms in high orbital bands.**
  Why orbital physics with cold atoms is interesting?

• **Orbital fermions in the honeycomb lattice (fundamentally different from graphene)**

  Flat band physics: exact results of Wigner crystal (single component) and ferromagnetism (two-component).

  Exotic band insulator: topological quantum anomalous Hall insulator

Exotic Mott insulator: frustrated orbital exchange; **120 degree model → Kitaev model**

Unconventional f-wave Cooper pairing.
Research progress of cold atom physics

- Great successes of cold atom physics: BEC, BCS-BEC, etc...

- **Orbital** Physics: new physics of bosons and fermions in high-orbital bands in optical lattices.

Here orbital refers to the different energy levels (e.g. s, p) of each optical site.

Good timing: experiments on orbital-bosons.

Square lattice (Mainz); double well lattice (NIST, Hamburg); polariton lattice (Stanford).

Fundamental features of orbital physics

- Orbital: a degree of freedom independent of charge and spin.

- Orbital degeneracy.

\[ p\text{-orbitals: } p_x, p_y, p_z \]
\[ d\text{-orbitals: } d_{x^2-y^2}, d_{y^2-z^2}, d_{xy}, d_{yz}, d_{xz} \]

\[ t_{||} \gg t_{\perp} \]

- Spatial anisotropy.

\[ e_g \]

\[ t_{2g} \]

Crystal field splitting
Transition metal oxide orbital systems

- Orbitals play an important role in magnetism, superconductivity, and transport properties.

Manganite: $\text{La}_{1-x}\text{Sr}_{1+x}\text{MnO}_4$

Iron-pnictide: $\text{LaOFeAs}$
What is new? (I) Orbital bosons have no counterparts in solids

- Solid state orbital systems: orbital physics only of fermions.

- Cold atom orbital systems: both fermions and bosons.

The ordinary many-body ground states of bosons satisfy the “no-node” theorem, i.e., the wavefunction is positive-definite.

Orbital bosons: (meta-stable excited states of bosons).

New materials of bosons beyond the “no-node” theorem. Unconventional BECs with spontaneous time-reversal symmetry breaking.

(II) New materials of strongly correlated p-orbitals

• Solid state: strongly correlated orbital systems are usually $d$-orbital transition metal oxides and $f$-orbital rare-earth compounds.

• Most $p$-orbital solid state materials are weakly correlated (e.g. semiconductors).

• Not many $p$-orbital Mott-insulators. Exceptions: Cs3C60, …

• Cold atom orbital systems:

$p$-orbital has even stronger anisotropy than $d$ and $f$; Combination of strong anisotropy with strong correlation.
• **Introduction: cold atoms in high orbital bands.**
  
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**Flat band physics: exact results of Wigner crystal (single component)**

Exotic band insulator: topological quantum anomalous Hall insulator

Exotic Mott insulator: frustrated orbital exchange; 120 degree model $\rightarrow$ Kitaev model

Unconventional Cooper pairing: f-wave.
The p-orbital honeycomb lattice

- Three coherent laser beams polarizing in the z-direction.

also K. Sengstock’s recent work.
p-orbital fermions in the honeycomb lattice

Not our interest

\textit{cf.} graphene: $p_z$-orbital; Dirac cones.

Our interest!

$p_x, p_y$-orbitals: flat bands; interaction effects dominate $\rightarrow$ ferromagnetism.

$p_x, p_y$-physics: get rid of the hybridization with $s$

- $p_z$-orbital band is not a good system for orbital physics.

  isotropic within 2D; non-degenerate.

- Interesting orbital physics in the $p_x, p_y$-orbital bands.

- However, in graphene, $2p_x$ and $2p_y$ are close to $2s$, thus strong hybridization occurs.

- In optical lattices, $p_x$ and $p_y$-orbital bands are well separated from $s$. 

\[1/r\)-like potential\]
**p-orbital honeycomb optical lattice**

- Band Hamiltonian ($\sigma$-bonding) for spin-polarized fermions.

$$H_t = t_{//} \left\{ \sum_{\vec{r} \in A} [p_1^+(\vec{r})p_1(\vec{r} + \hat{e}_1) + h.c.] \right.$$ 

$$+ [p_2^+(\vec{r})p_1(\vec{r} + \hat{e}_2) + h.c]$$ 

$$+ [p_3^+(\vec{r})p_3(\vec{r} + \hat{e}_3) + h.c] \right\}$$

\[\begin{align*}
p_1 &= \frac{\sqrt{3}}{2} p_x + \frac{1}{2} p_y \\
p_2 &= -\frac{\sqrt{3}}{2} p_x + \frac{1}{2} p_y \\
p_3 &= -p_y
\end{align*}\]

\[p_1 + p_2 + p_3 = 0\]
Flat bands from **localized** eigenstates

- Flat band + Dirac cone.
- If $\pi$-bonding is included, the flat bands acquire small width at the order of $t_\perp$. Realistic band structures show $t_\perp / t_\parallel \rightarrow 1\%$
- localized eigenstates.

\[ t_\parallel \gg t_\perp \]

$\pi$-bond
Realistic Band structure with the sinusoidal optical potential

- Excellent band flatness.

\[ H = -\frac{\hbar^2 \nabla^2}{2m} + V \sum_{i=1}^{3} \cos(\vec{p}_i \cdot \vec{r}) \]
Exact solution for spinless fermions: Wigner crystallization

\[ \langle n \rangle = \frac{1}{6} \]

- Close-packed hexagons; avoiding repulsion.
- The crystalline ordered state is stable even with small \( t_\perp \).
- The result is also good for bosons.

\[ \langle n \rangle = 1/6 \]

Gapped state
Orbital ordering with strong repulsions

Various orbital ordering insulating states at commensurate fillings.

Dimerization at $\langle n \rangle = 1/2$! Each dimer is an entangled state of empty and occupied states.
Exotic quantum anomalous Hall insulators

The required experimental technique was **available** in Nate Gemelke and Steven Chu’s group at Stanford.


\[ \text{Ir}^{4+} \]

\[
\begin{align*}
\text{isospin up} & = \text{spin up, } l_z=0 + \text{spin down, } l_z=1
\end{align*}
\]
A brief review: quantum Hall effect (QHE)

- Landau levels quantization from external magnetic fields.

- Insulating bulk with **chiral gapless edge modes**. Quantized Hall conductance; dissipationless charge transport through edge states.

- Haldane: Landau level is not necessary for QHE. The key point is the non-trivial wavefunction topology ---- $1^{\text{st}}$ Chern number.
Quantum Anomalous Hall (QAHE)-- QHE without Landau levels

- Example: a two-band system. The pseudo-spin vector $\vec{d}$ exhibits a non-trivial configuration in the Brillouin zone.

$$H(k) = \vec{d}(k) \cdot \vec{\tau} = \left( \begin{array}{cc} d_3(\vec{k}) & d_1(\vec{k}) - id_2(\vec{k}) \\ d_1(\vec{k}) - id_2(\vec{k}) & -d_3(\vec{k}) \end{array} \right)$$

$$d_1(k) = t \sin k_x, \quad d_2(k) = t \sin k_y, \quad d_3(k) = m(2 - \cos k_x - \cos k_y) - \Delta$$

- Hall conductance is quantized to $n/2\pi$.

$$\sigma_{xy}^H = \frac{e^2}{\hbar} \frac{1}{8\pi^2} \int \int_{FBZ} d^2k \, \hat{d} \cdot (\partial_{k_x} \hat{d} \times \partial_{k_y} \hat{d})$$

$$= n \frac{e^2}{\hbar}$$

Haldane’s Quantum Anomalous Hall model

- Honeycomb lattice with complex-valued next-nearest neighbor hopping.

\[
H_{NN} = -t \sum_{\vec{r} \in A} \left\{ c^+ (\vec{r}_A) c(\vec{r}_B) + h.c. \right\}
\]

\[
H_{NNN} = -\sum_{\vec{r}} t' \left\{ e^{i\delta} c^+ (\vec{r}_A) c(\vec{r}_A') + e^{i\delta} c^+ (\vec{r}_B) c(\vec{r}_B') + h.c. \right\}
\]

- Topological insulator if \( \delta \neq 0, \pi \). Mass changes sign at \( K_{1,2} \).

- QAHE has not been experimentally realized yet in both CM and AMO systems.

Rotate each site around its own center

- Phase modulation on laser beams: a fast overall oscillation of the lattice. Atoms cannot follow and feel a slightly distorted averaged potential.

- Orbital Zeeman term.

\[
H_{znm} = -\Omega \sum_{r \in A} L_z (\vec{r})
\]

\[
= i\Omega \sum_{\vec{r} \in A} \left\{ p^+_x (\vec{r}) p_y (\vec{r}) - p^+_y (\vec{r}) p_x (\vec{r}) \right\}
\]

- The oscillation axis slowly precesses at the angular frequency of \( \Omega \).
Large rotation angular velocity $\Omega >> t_{\parallel}$

- The second order perturbation generates the NNN complex hopping.

$$t' = -\left(te^{i2/3\pi}\right)^2 / 2\Omega$$
Small rotation angular velocity

\[ \Omega = 0 \]

\[ \Omega = 0.3t_{//} \]

Berry curvature and Chern numbers

\[ C = 0 \]

\[ C = -1 \]

\[ C = 1 \]
Large rotation angular velocity

\[ \Omega = \frac{3}{2} t_{//} \quad \Omega = 3 t_{//} \]

Berry curvature.

\[ C = -1 \]

\[ C = 1 \]
Soft confining potential: exact diagonalization for the non-interacting system

- Density plateaus in the insulating regimes.
- Metallic region between density plateaus.

Density profile: local density approx. works well.

\[ V_t(r) = \frac{1}{2} m \omega_0^2 r^2 \]

\[ \mu(r) = \mu - V_{tr}(r) \]
Equilibrium Anomalous Hall currents in the trap
Quantized and non-quantized Hall conductance

- Normalized conductance is quantized in the plateaus.

\[ \sigma_H = j_\theta / \partial V_r / \partial r = \frac{m}{2\pi h} \sum_n \int dk \ B_n (k_x, k_y) \]


\[ j_H = \sigma_H (F_{\text{drift}} + F_{\text{diff}}) \]
\[ F = \partial_r [(\mu(r) - E_b) n(r)] / n(r) \]
\[ = \partial_r \mu(r) + (\mu(r) - E_b) \partial_r \ln \mu(r) \]
• Orbital exchange in the Mott-insulating state; orbital frustration: quantum 120 degree model; solvable quantum orbital ice.

\[ (\vec{\tau} \cdot \hat{e}_2)(\vec{\tau} \cdot \hat{e}_2) \]

\[ (\vec{\tau} \cdot \hat{e}_1)(\vec{\tau} \cdot \hat{e}_1) \]

\[ (\vec{\tau} \cdot \hat{e}_3)(\vec{\tau} \cdot \hat{e}_3) \]

C. Wu, PRL 100, 200406 (2008); G-W Chern, C. Wu, arxiv1104.1614

c.f. Khaliullin et al, PRL 2009
Mott insulator of SPINLESS fermions: orbital exchange

\[ H_{\text{int}} = U \sum_{\vec{r}} n_{p_x}(\vec{r}) n_{p_y}(\vec{r}) \]

- Pseudo-spin representation.

\[ \tau_1 = \frac{1}{2} (p_x^+ p_x - p_y^+ p_y) \quad \tau_2 = \frac{1}{2} (p_x^+ p_y + p_y^+ p_x) \quad \tau_3 = \frac{i}{2} (p_x^+ p_y - p_y^+ p_x) \]

- Orbital exchange: no orbital flipping process.

\[ H_{\text{ex}} = J \tau_1(r) \tau_1(r + \hat{x}) \]

\[ J = 0 \quad \text{for} \quad J = 2t^2 / U \]

\[ J = 2t^2 / U \]
**Hexagon lattice: quantum 120° model**

- Non-triviality: Ising quantization axis depends on bond orientation. For a bond along the general direction $\hat{e}_\phi$, $p_x', p_y'$: eigen-states of $\vec{\tau} \cdot \hat{e}_{2\phi} = \cos 2\phi \tau_x + \sin 2\phi \tau_y$

$$H_{ex} = J(\vec{\tau}(r) \cdot \hat{e}_{2\phi})(\vec{\tau}(r + \hat{e}_\phi) \cdot \hat{e}_{2\phi})$$

- After a suitable transformation, the Ising quantization axes can be chosen just as the three bond orientations.

$$H_{ex} = -\sum_{r, r'} J(\vec{\tau}(r_i) \cdot \hat{e}_{ij})(\vec{\tau}(r'_j) \cdot \hat{e}_{ij})$$

From the Kitaev model to 120 degree model


\[ H_{kitaev} = -J \sum_{r \in A} (\sigma_x(r)\sigma_x(r+e_1) + \sigma_y(r)\sigma_y(r+e_2) + \sigma_z(r)\sigma_z(r+e_3)) \]
Large S picture: heavy-degeneracy (frustration) of classic ground states

- Ground state constraint: the two $\tau$-vectors have the same projection along the bond orientation.

$$H_{ex} = \sum_{r,r'} J\{[(\bar{\tau}(r) - \bar{\tau}(r')) \cdot \hat{e}_{rr'}]\}^2 + J\sum_r \tau_z^2(r)$$

- Ferro-orbital configurations.
- Loop config: $\tau$-vectors along the tangential directions.
Heavy-degeneracy of the classic ground states

- General loop configurations
Global rotation degree of freedom

• Each loop config remains in the ground state manifold by a suitable arrangement of clockwise/anticlockwise rotation patterns.
“Order from disorder”: 1/S orbital-wave correction
Zero energy flat band orbital fluctuations

- Each un-oriented loop has a local zero energy model up to the quadratic level.

\[ \Delta E = 6JS^2(\Delta \theta)^4 \]

- The above config. contains the maximal number of loops, thus is selected by quantum fluctuations at the 1/S level.

- Project under investigation: the quantum limit (s=1/2)? A very promising system to arrive at orbital liquid state? What is the physics after doping? Add rotation → Topo Mott Insulator.
Outline

• Introduction: orbital physics is an interesting research direction of cold atoms.

• Orbital bosons: unconventional BEC beyond the "no-node" theorem.

• Orbital fermions in the hexagonal lattice.

  Ferromagnetism from band flatness.

  **The unconventional f-wave Cooper pairing of the spinless fermions.**

Conventional v.s. unconventional Cooper pairings

- **Conventional superconductivity:**
  
s-wave: pairing amplitude does not change over the Fermi surface.

- **d-wave (high T_c cuprates).** Pairing amplitude changes sign on the Fermi surface.
Unconventional Cooper pairing

• Most of unconventional pairing states arise from strong correlation effects. Predictions and analysis are difficult.

  p-wave: superfluid $^3$He-A and B; Sr$_2$RuO$_4$;
  d-wave: high $T_c$ cuprates;
  Extended s-wave: iron-pnictide superconductors (?);

• Can we arrive at unconventional pairing in a simpler way, say, from nontrivial band structures but with conventional interactions?


• No strong correlation effects. Analysis is controllable.

• **f-wave** pairing with spinless fermions in the p-orbital hexagonal optical lattice.
Nontrivial orbital configurations between time reversal (TR) partners

- Along the three middle lines of Brillouin zone, eigen-orbitals are real.
- At K and K', eigen-orbitals are complex and orthogonal.
The f-wave structure because of the symmetry reason

• Along middle lines, TR pairs cannot be paired → nodal lines.
• The TR pair at K and K’ has the largest pairing.
• Odd parity.

• The mean-field gap value can reach 10nK; and the 2D Kosterlitz-Thouless temperature can reach 1nK.
Phase sensitive detection: zero energy Andreev bound states

With zero energy Andreev Bound States

No Andreev Bound States
Summary: $p$-orbital fermions in the honeycomb lattice – Novel physics beyond graphene

- Strong correlation effect from band flatness: Exact results of Wigner crystal and ferromagnetism.

- Mott-insulator: a new type of frustrated magnet-like model.

- Band insulator (topological): quantum anomalous Hall effect.

- Novel mechanism for the f-wave Cooper pairing.