Novel Orbital Phases of Fermions in $\rho$-band Optical Lattices

Congjun Wu

Department of Physics, UC San Diego

C. Wu, PRL 100, 200406 (2008).


Feb. 23, 2009, KITP
Outline

• Introduction to orbital physics.

New directions of cold atoms: orbital physics in high-orbital bands; pioneering experiments.

• Bosons: exotic condensate, complex-superfluidity breaking time-reversal symmetry.

• Fermions: $p_{x,y}$-orbital counterpart of graphene, flat bands and non-perturbative effects

• Orbital exchange, frustrations, order from disorder, orbital liquid.

• Topological insulators in the $p$-band – orbital analogue of anomalous quantum Hall effect.
Research focuses of cold atom physics

• Great success of cold atom physics in the past decade:
  
  BEC; superfluid-Mott insulator transition;
  
  Multi-component bosons and fermions;
  
  fermion superfluidity and BEC-BCS crossover; polar molecules ……

• **Oribtial** Physics: new physics of bosons and fermions in high-orbital bands.

Good timing: pioneering experiments on orbital-bosons.

Square lattice (Mainz); double well lattice (NI ST); polariton lattice (Stanford).
Orbital physics

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

• Orbital band degeneracy and spatial anisotropy.

• cf. transition metal oxides (d-orbital bands with electrons).

La$_{1-x}$Sr$_{1+x}$MnO$_4$

LaOFeAs
**Solid state orbital systems:**

- Jahn-Teller distortion quenches orbital degree of freedom;
- only fermions;
- correlation effects in $p$-orbitals are weak.

**Optical lattices orbital systems:**

- rigid lattice free of distortion;
- both bosons (meta-stable excited states with long life time) and fermions;
- strongly correlated $p_{xy}$-orbitals: stronger anisotropy
Bosons: Feynman’s no-node theorem

• The many-body ground state wavefunctions (WF) of bosons in the coordinate-representation are positive-definite in the absence of rotation.

\[
\psi(r_1, r_2, \ldots r_n) \quad |\psi(r_1, r_2, \ldots r_n)| \quad \phi(r_1, r_2, \ldots r_n) > 0
\]

\[
\langle H \rangle = \int dr_1 \ldots dr_n \frac{\hbar^2}{2m} \sum_{i=1}^{n} |\nabla_i \psi(r_1, \ldots r_n)|^2 + |\psi(r_1, \ldots r_n)|^2 \sum_{i=1}^{n} U_{ex}(r_i) + \\
|\psi(r_1, \ldots r_n)|^2 \sum_{i<j} V_{int}(r_i-r_j)
\]

• Strong constraint: complex-valued WF \(\rightarrow\) positive definite WF; time-reversal symmetry cannot be broken.

• Feynman’s statement applies to all of superfluid, Mott-insulating, super-solid, density-wave ground states, etc.
Orbital bosons: complex condensates beyond the no-node theorem

• Spontaneous time reversal symmetry breaking; orbital Hund’s rule interaction.

W. V. Liu and C. Wu, PRA 74, 13607 (2006);


Novel states of orbital fermions (honeycomb lattice)

• \( p_{x,y} \)-orbital counterpart of graphene,

  non-perturbative effects from band flatness

  (e.g. Wigner crystal, and flat band ferromagnetism.)

  C. Wu, and S. Das Sarma, PRB 77, 235107(2008);

• Orbital exchange; from Kitaev to quantum 120 degree model.

  C. Wu et al, arxiv0701711v1; C. Wu, PRL 100, 200406 (2008).

• Topological insulators in the p-band – orbital analogue of anomalous quantum Hall effect.

p-orbital fermions in honeycomb lattices

*cf.* graphene: a surge of research interest; $p_z$-orbital; Dirac cones.

$p_{xy}$-orbital: flat bands; interaction effects dominate.

Honeycomb optical lattice with phase stability

- Three coherent laser beams polarizing in the z-direction.
- Laser phase drift only results an overall lattice translation without distorting the internal lattice structure.

What is the fundamental difference from graphene?

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

• It is the other two $p_x$ and $p_y$ orbitals that exhibit anisotropy and degeneracy.

• 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 $s$. 
Artificial graphene in optical lattices

- Band Hamiltonian (σ-bonding) for spin-polarized fermions.

\[
H_t = t_{\parallel} \left\{ \sum_{\vec{r} \in A} \left[ p_1^+ (\vec{r}) p_1 (\vec{r} + \hat{e}_1) + h.c. \right] + \left[ p_2^+ (\vec{r}) p_1 (\vec{r} + \hat{e}_2) + h.c. \right] + \left[ p_3^+ (\vec{r}) p_3 (\vec{r} + \hat{e}_3) + h.c. \right] \right\}
\]

\[ p_1 = \frac{\sqrt{3}}{2} p_x + \frac{1}{2} p_y \]

\[ p_2 = -\frac{\sqrt{3}}{2} p_x + \frac{1}{2} p_y \]

\[ p_3 = -p_y \]
Flat bands in the entire Brillouin zone!

- 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.

\[ t_\parallel >> t_\perp \]
Hubbard model for spinless fermions:

Exact solution: Wigner crystallization

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

- Close-packed hexagons; avoiding repulsion.

- The crystalline ordered state is stable even with small \( t_\perp \).

- Particle statistics is **irrelevant**. The result is also good for bosons.
Exact solution: Wigner crystallization at 1/6-filling

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

- Spinless fermions with onsite repulsion: close-packed hexagons; avoiding repulsion.
- Gapped state which is stable even with small \( t_\perp \).
- The result is also valid for bosons.

• Dimerization at \( \langle n \rangle = 1/2! \) (Mean-field result). Each dimer is an entangled state of empty and occupied states.
Flat-band itinerant ferromagnetism (FM)

• FM requires strong enough repulsion and thus FM has no well-defined weak coupling picture.

• It is commonly accepted that Hubbard-type models cannot give FM unless with flat band structure.


• In spite of its importance, **FM has not been paid much attention in cold atom community** because strong repulsive interaction renders system unstable to dimer-molecule formation.

• Flat-band ferromagnetism in the p-orbital honeycomb lattices.

• Interaction amplified by the divergence of DOS. **Realization of FM with weak repulsive interactions in cold atom systems.**

Novel states of orbital fermions (honeycomb lattice)

• $p_{x,y}$-orbital counterpart of graphene,
  non-perturbative effects from band flatness
  (e.g. Wigner crystal, and flat band ferromagnetism.)

  C. Wu, and S. Das Sarma, PRB 77, 235107(2008);

• Orbital exchange; from Kitaev to quantum 120 degree model.

  C. Wu, PRL 100, 200406 (2008);  C. Wu et al, arxiv0701711v1;

• Topological insulators in the $p$-band – orbital analogue of anomalous quantum Hall effect.

Mott-insulators with orbital degrees of freedom: orbital exchange of spinless fermion

• Pseudo-spin representation.

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

• No orbital-flip process. Antiferro-orbital Ising exchange.

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

\[
J = 0
\]

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

• For a bond along the general direction $\hat{e}_\varphi$.

$p'_x, p'_y$ : eigen-states of $\bar{\tau} \cdot \hat{e}_{2\varphi} = \cos 2\varphi \tau_x + \sin 2\varphi \tau_y$

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

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

$$H_{ex} = -\sum_{r,r'} J(\bar{\tau}(r) \cdot \hat{e}_{ij})(\bar{\tau}(r') \cdot \hat{e}_{ij})$$
From the Kitaev model to 120 degree model


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

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

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

- Ferro-orbital configurations.

- Oriented loop config: $\tau$-vectors along the tangential directions.
Heavy-degeneracy of 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.

• Starting from an oriented loop config with fixed loop locations but an arbitrary chirality distribution, we arrive at the same unoriented loop config by performing rotations with angles of $\pm 30^\circ, \pm 90^\circ, \pm 150^\circ$. 
“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?
Novel states of orbital fermions (honeycomb lattice)

- $p_{x,y}$-orbital counterpart of graphene,

  non-perturbative effects from band flatness

  (e.g. Wigner crystal, and flat band ferromagnetism.)

  C. Wu, and S. Das Sarma, PRB 77, 235107(2008);

- Orbital exchange; from Kitaev to quantum 120 degree model.

  C. Wu, PRL 100, 200406 (2008);  C. Wu et al, arxiv0701711v1;

- Topological insulators in the $p$-band - orbital analogue of anomalous quantum Hall effect.

Topological insulators: Haldane’s QHE Model without Landau level

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

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

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

+ h.c.} \]

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

\[ H(\vec{k}) = a(\vec{k}) \tau_1 + b(\vec{k}) \tau_3 + m(\vec{k}) \tau_2 \]

\[ + c(\vec{k}) I \]
Phase modulation on laser beams: a fast overall oscillation of the lattice. Atoms cannot follow and feel a slightly distorted averaged potential.

The oscillation axis slowly precesses at the angular frequency of $\Omega$.

$H_{zmnn} = -\Omega \sum_{\vec{r} \in A} L_z(\vec{r})$

$= i\Omega \sum_{\vec{r} \in A} \left\{ p_x(\vec{r}) p_y(\vec{r}) - p_y(\vec{r}) p_x(\vec{r}) \right\}$
Large rotation angular velocity

- Second order perturbation generates the NNN complex hopping.

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

\[ \Omega = 0 \]

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

Berry curvature.

\[ C = 0 \]

\[ C = -1 \]

\[ C = 1 \]
Large rotation angular velocity

\[ \Omega = \frac{3}{2} t_{\parallel} \]

\[ \Omega = 3 t_{\parallel} \]

Berry curvature.

\[ C = -1 \]

\[ C = 1 \]
Summary

\(\rho_{x,y}\)-orbital counterpart of graphene: strong correlation from band flatness.

orbital exchange: frustration, quantum 120 degree model

Topological insulator: quantum anomalous Hall effect.