

# Orbital Phases of Cold Atoms – Unconventional BEC, ferromagnetism, and f-wave pairing states

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- Bosons: C. Wu, Mod. Phys. Lett. 23, 1(2009);  
C. Wu, W. V. Liu, J. Moore and S. Das Sarma, PRL 97, 190406 (2006).  
W. V. Liu and C. Wu, PRA 74, 13607 (2006).
- Fermions: S. Z. Zhang , H. H. Hung, and C. Wu, arXiv:0805.3031, to appear in PRA  
W. C. Lee, C. Wu, S. Das Sarma, arXiv:0905.1146, to appear in PRA.  
C. Wu, D. Bergman, L. Balents, and S. Das Sarma, PRL 99, 67004(2007).

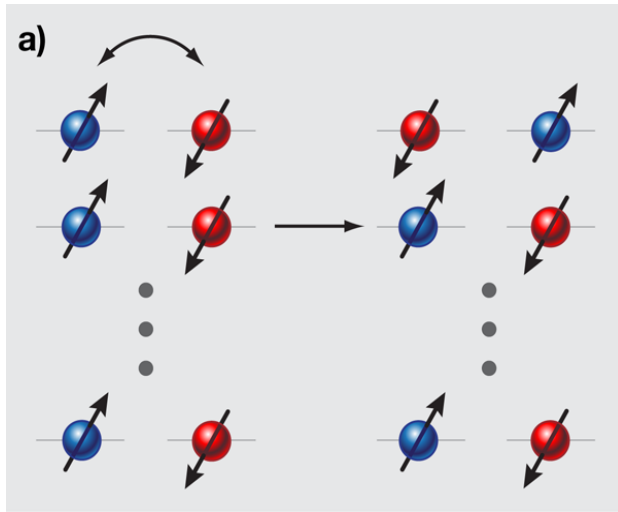
Other work: [http://www.physics.ucsd.edu/~wucj/Wu\\_Publication.html](http://www.physics.ucsd.edu/~wucj/Wu_Publication.html)

## Collaborators:

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W. V. Liu	(Pittsburgh)
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J. Moore	(Berkeley)
Shi-zhong Zhang	(UIUC/OSU)

Thank I. Bloch, L. M. Duan, T. L. Ho for helpful discussions.

# Large spin cold fermions: large S v.s. large N

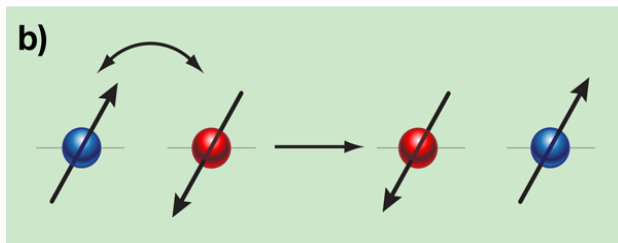


a) Large spin electron systems:  
weak quantum fluctuation.

$$\Delta S_z = \pm 1$$

b) Large spin cold atom systems:  
strong quantum fluctuation .

$$\Delta F_z = \pm 1, \pm 2, \dots \pm F$$



c) Spin-3/2 fermions: hidden **Sp(4)**  
**/SO(5)** symmetry without fine tuning.

Brief review: C. Wu, Mod Phys Lett B 20, 1707  
(2006)

Online talk: <http://online.itp.ucsb.edu/online/coldatoms07/wu2/>

Recent exp:  $^{87}\text{Sr}$  ( $I=9/2$ ) (T. Killian),  $^{173}\text{Yb}$  ( $I=5/2$ ) (Y. Takahashi)

Theory: large N, Hermele, Gurarie, Rey et al.

# Outline

- **Introduction: cold atoms in high orbital bands.**
  1. What is orbital physics in the condensed matter context?
  2. Why orbital physics with cold atoms is interesting? Some pioneering experiments.

- Orbital bosons: unconventional BEC beyond the “no-node” theorem.

- Orbital fermions:

Exotic band (quantum anomalous Hall) and Mott insulators (120 degree model): [http://online.itp.ucsb.edu/online/lowdim\\_c09/wu/](http://online.itp.ucsb.edu/online/lowdim_c09/wu/)

Itinerant ferromagnetism (FM): flat band FM.

Unconventional Cooper pairing: f-wave.

FFLO states of fermions in the p-bands: 1D Fermi surface+2D phase coherence.

# Research progress of cold atom physics

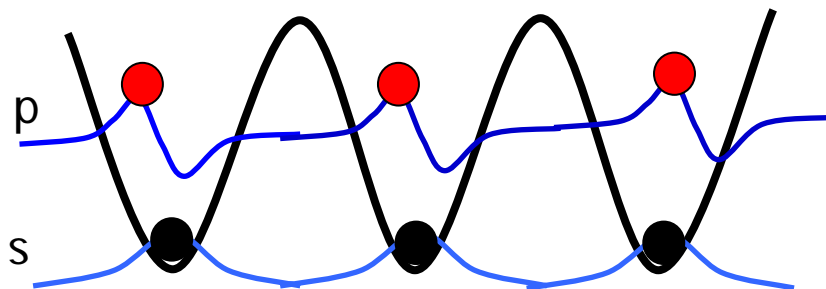
- Great success of cold atom physics in the past decade:  
BEC; superfluid-Mott insulator transition; multi-components bosons and fermions; BEC-BCS crossover ...

- **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: pioneering experiments on orbital-bosons.

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



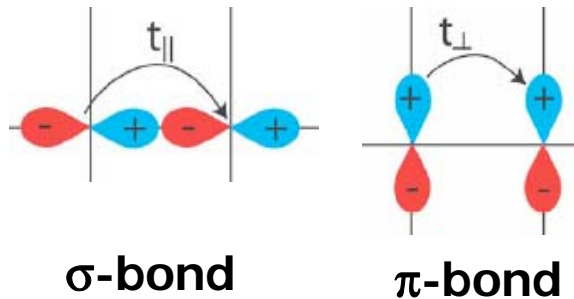
# Orbital physics

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

Tokura, et al., science 288, 462, (2000).

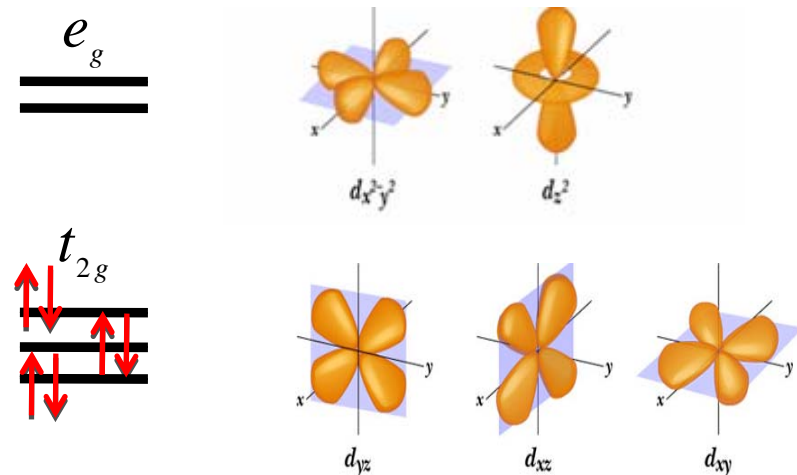
- Two fundamental features: orbital degeneracy and **spatial anisotropy**.

$p$ -orbitals:  $p_x, p_y, p_z$



$$t_{||} \gg t_{\perp}$$

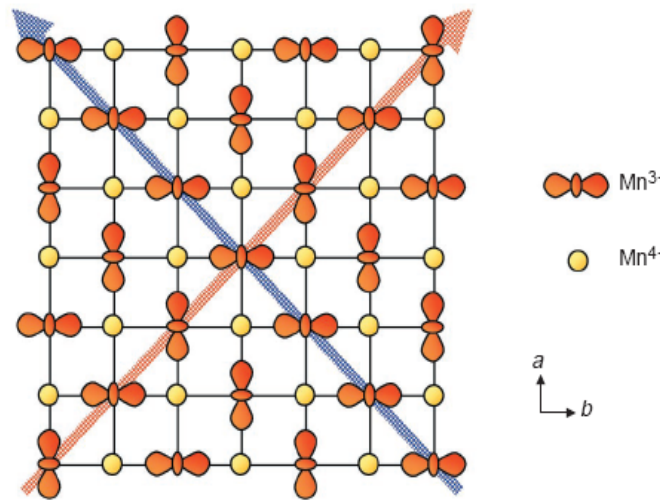
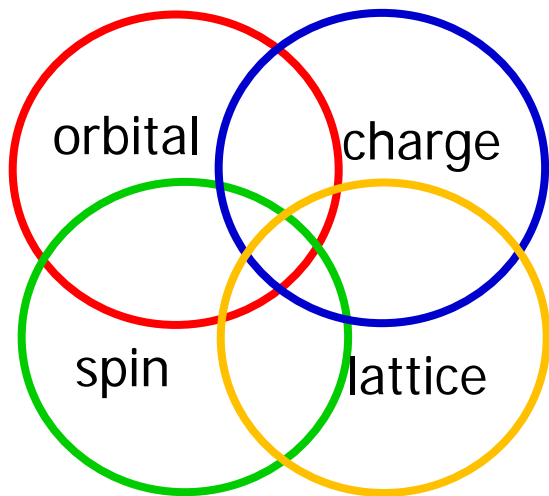
$d$ -orbitals:  $d_{x^2-y^2}, d_{r^2-3z^2}, d_{xy}, d_{yz}, d_{xz}$



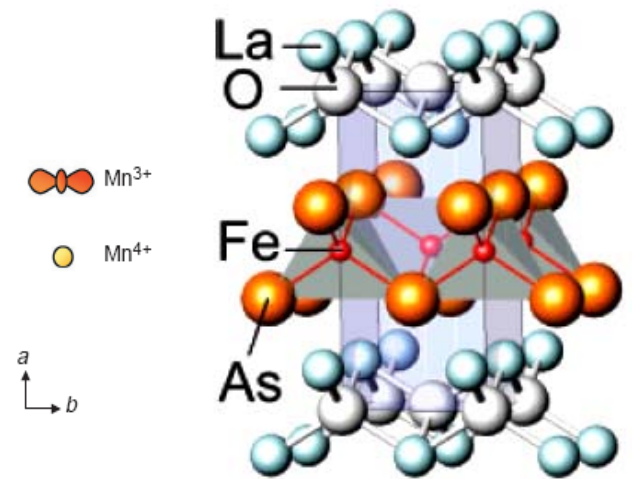
crystal field splitting

# Transition metal oxide orbital systems

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



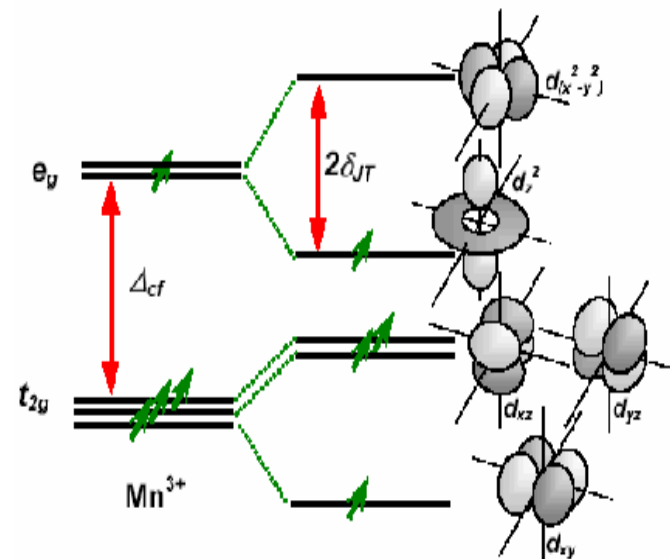
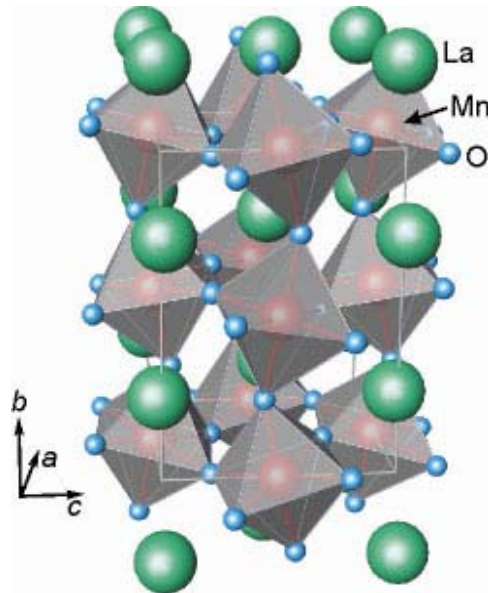
Manganite:  $\text{La}_{1-x}\text{Sr}_{1+x}\text{MnO}_4$



Iron-pnictide:  $\text{LaOFeAs}$

## Cold atom orbital systems (I): no Jahn-Teller distortion

- **Solid state orbital systems:** lattice is not rigid. Jahn-Teller distortion lifts the orbital degeneracy and **quenches** the orbital degree of freedom.



- **Cold atom orbital systems:** atoms in external optical lattices.

Rigid lattice **free of distortion**; orbital degeneracy is robust.



## Cold atom orbital systems (II): orbital bosons

- 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** beyond the “**no-node**” theorem.

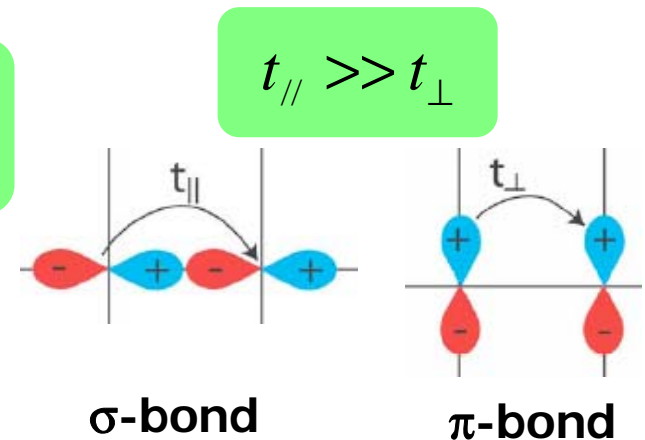
Unconventional BEC with spontaneous breaking of time-reversal symmetry.

## Cold atom orbital systems (III): 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.**
- Cold atom orbital systems:

**New materials:** strongly correlated  $p$ -orbital systems.

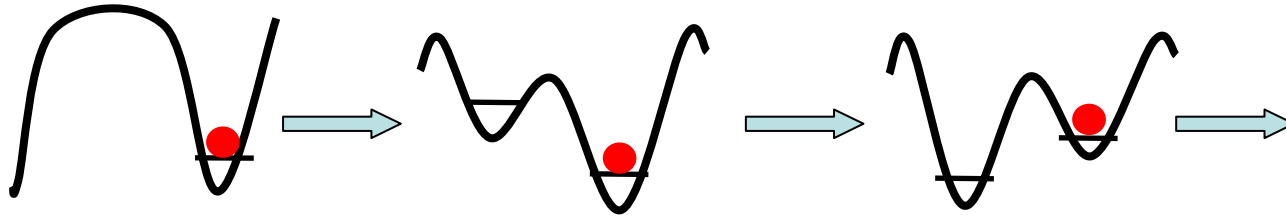
$p$ -orbital has even **stronger anisotropy** than  $d$  and  $f$ ; combined with strong **correlation**.



# Double-well lattice at NIST: transfer bosons to the excited band

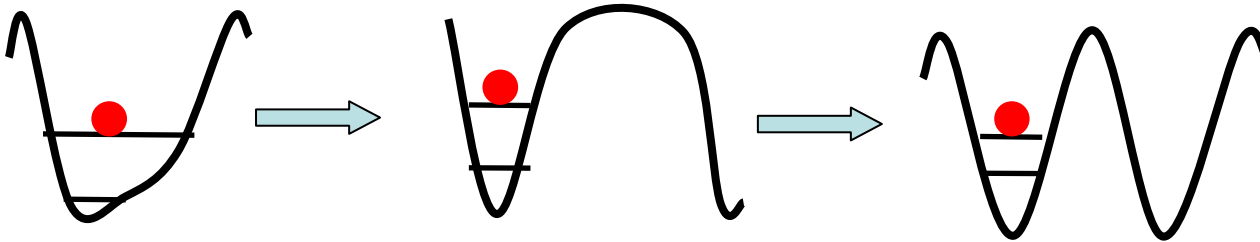
Grow the long period lattice

Avoid tunneling (diabatic)



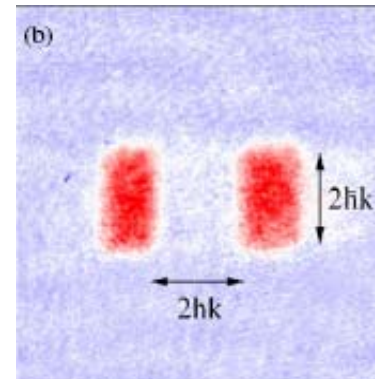
Create the excited state (adiabatic)

Create the short period lattice (diabatic)



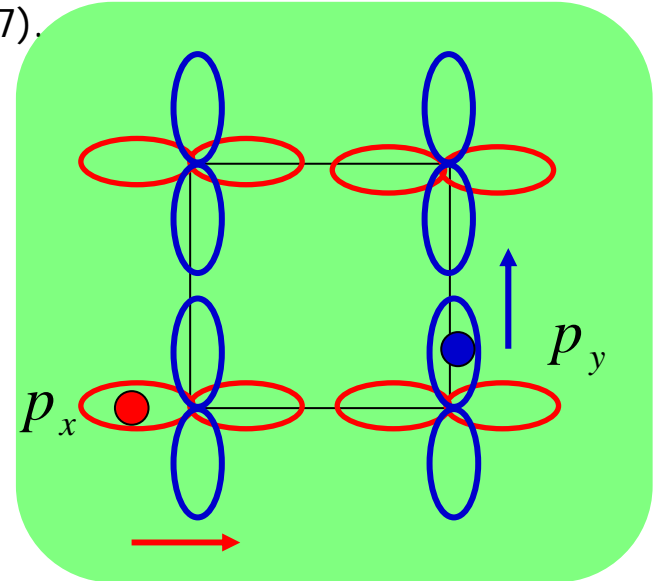
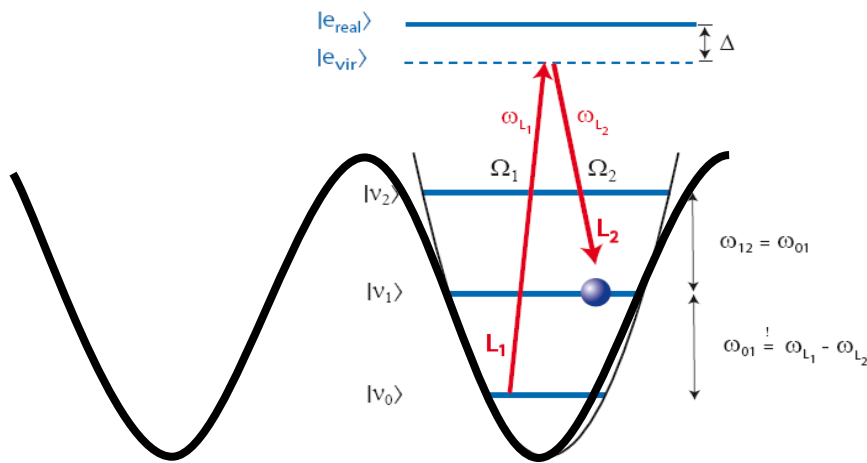
- Band mapping.
- Phase incoherence.

M. Anderlini, et al., J. Phys. B 39, S199 (2006).

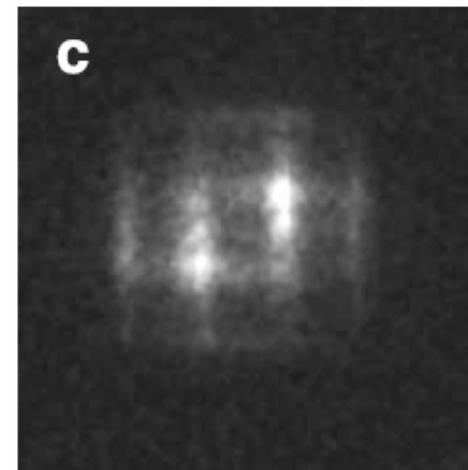


# Orbital bosons: pumping bosons by Raman transition

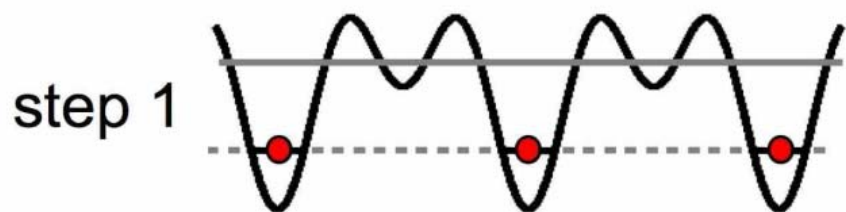
T. Mueller, I. Bloch et al., Phys. Rev. Lett. 99, 200405 (2007).



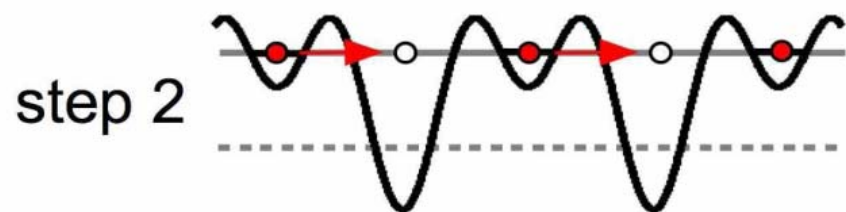
- Long life-time ( $\sim 100$  hopping time) to develop 1-d phase coherence.
- Quasi-1d band feature in the square lattice.



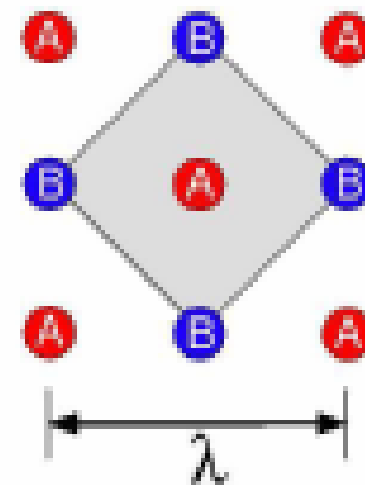
# P-orbital BEC with non-zero center of mass momentum



$$\theta < \frac{\pi}{2}$$

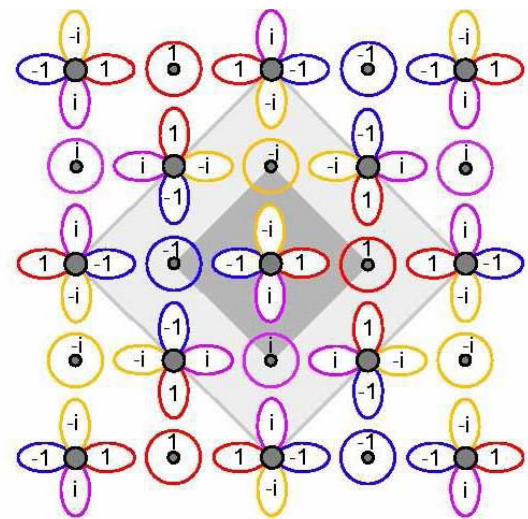
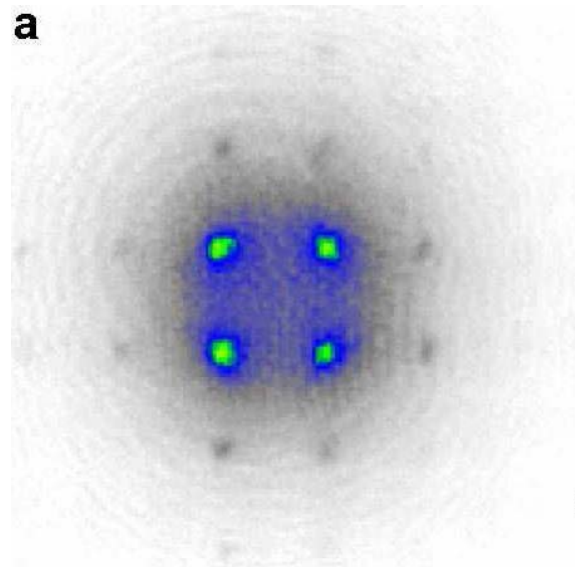
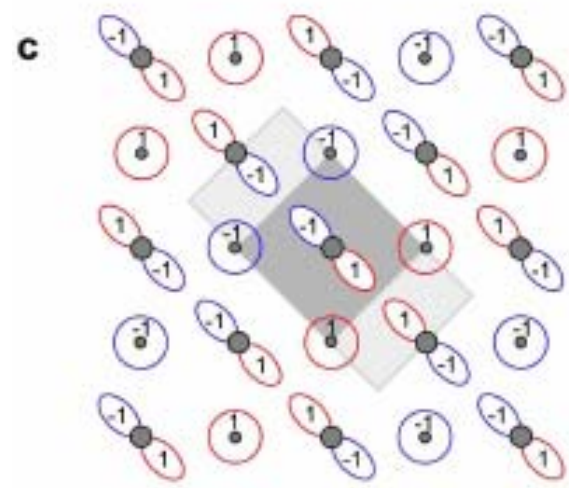
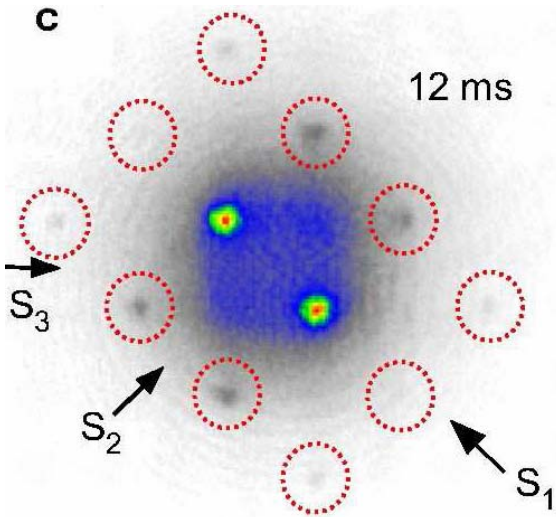


$$\theta > \frac{\pi}{2}$$



$$V(x, y) = -V_0 \left[ \sin^2(kx) + \sin^2(ky) + 2 \cos(\theta) \sin(kx) \sin(ky) \right]$$

# Asymmetric (real, nodal) to symmetric (complex) p-BEC



# Outline

- Introduction: orbital physics, a new research direction of cold atoms.
- Orbital bosons: unconventional BEC with spontaneous time reversal symmetry breaking.

C. Wu, Mod. Phys. Lett. 23, 1(2009) (brief review);

V. M. Stojanovic, C. Wu, W. V. Liu and S. Das Sarma, PRL 125301(2008);

C. Wu, W. V. Liu, J. Moore and S. Das Sarma, PRL 97, 190406 (2006);

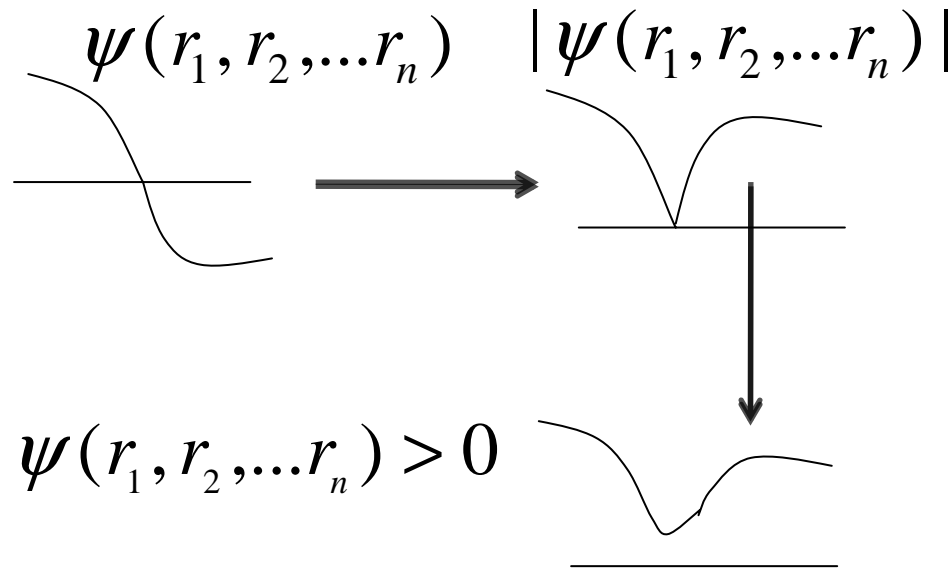
W. V. Liu and C. Wu, PRA 74, 13607 (2006).

Other group's related work: V. W. Scarola *et al.*, PRL, 2005; A. Isacson *et al.*, PRA 2005; A. B. Kuklov, PRL 97, 2006; C. Xu *et al.*, cond-mat/0611620 .....

- Orbital fermions in the hexagonal lattice.

# The "no-node" theorem (single component bosons)

- Many-body **ground state** wavefunctions of bosons in the coordinate-representation are positive-definite if without rotation.



R. P. Feynman

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



# Go beyond the “no-node” paradigm

- It applies to all of the ground states of bosons, (e.g. superfluid, Mott-insulating, super-solid, density-wave states).
- Strong constraint!

Complex-valued wavefunction reduces to positive-definite → quantum Monte-Carlo is free of the sign problem.

**Time-reversal (TR) symmetry cannot be spontaneously broken!**

- Our goal: unconventional BEC spontaneously breaking TR.

**Excited (meta-stable):** bosons in high orbital bands ----  
**orbital physics of bosons.**

**Spin-orbit** coupled BEC → spontaneous half-quantum vortex string.

# Ferro-orbital interaction for spinless p-orbital bosons

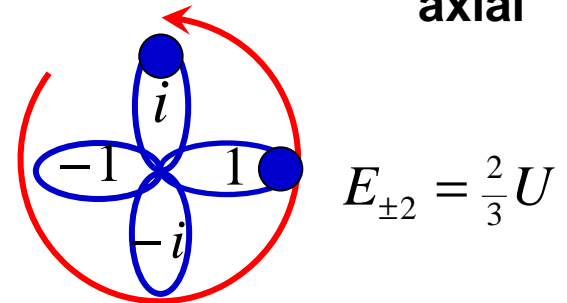
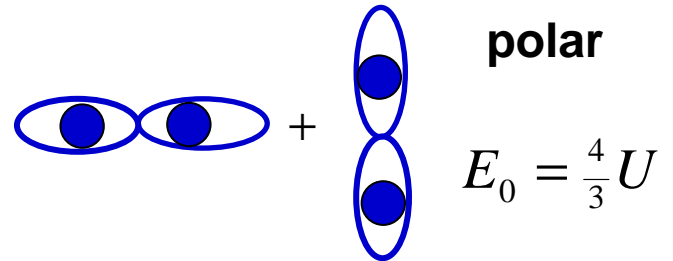
- **A single site** problem: two orbitals  $p_x$  and  $p_y$  with two spinless bosons.

$$V(r_1 - r_2) = g\delta(r_1 - r_2) \quad U = g \int dr |\phi_x(r)|^4 = g \int dr |\phi_y(r)|^4$$

$$x^2 + y^2 \quad L_z = 0: \frac{1}{\sqrt{2}} (p_x^+ p_x^+ + p_y^+ p_y^+) |0\rangle$$

$$(x \pm iy)^2 \quad L_z = \pm 2: \left\{ \frac{1}{\sqrt{2}} (p_x^+ \pm ip_y^+) \right\}^2 |0\rangle$$

$$= \left\{ \frac{1}{2} (p_x^+ p_x^+ - p_y^+ p_y^+) \pm \frac{i}{\sqrt{2}} p_x^+ p_y^+ \right\} |0\rangle$$



Axial states are spatially more extended!

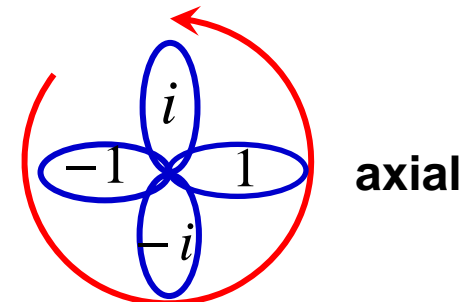
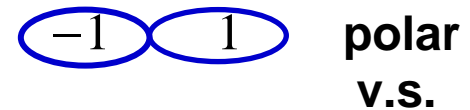
$$E_{\pm 2} < E_0$$

## Orbital Hund's rule for bosons

$$H_{\text{int}} = \frac{U}{2} \sum_r \left\{ n_r^2 - \frac{1}{3} (L_r^z)^2 \right\}$$

$$n = p_x^+ p_x + p_y^+ p_y, L_z = -i(p_x^+ p_y - p_y^+ p_x)$$

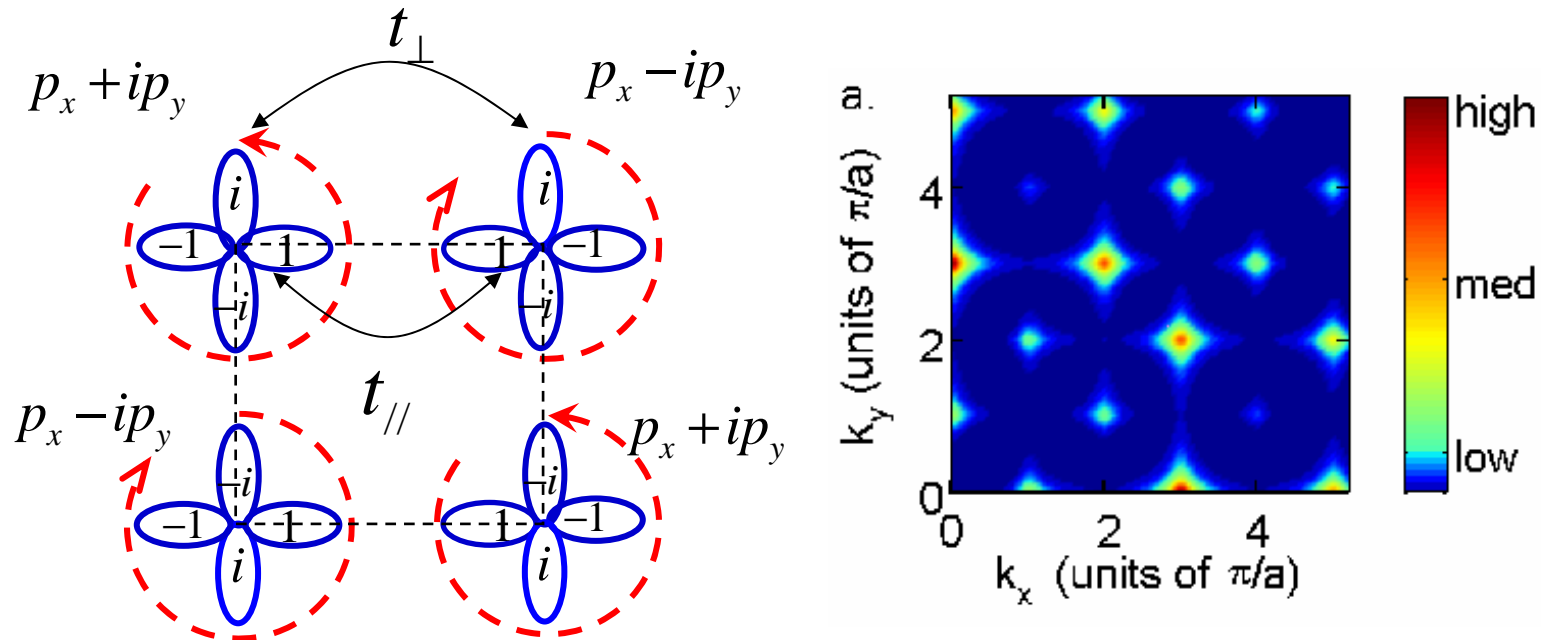
- If more than two bosons occupy in the same site, they aggregate into the same single-particle state.
- **Orbital angular momentum moments:** the same axial state (e.g.  $p+ip$ ) instead of the polar state (e.g.  $p_x$ ) to minimize repulsion.



- *cf.* Second Hund's rule for electrons.
- *c.f.*  $p+ip$  superconductors.

## Unconventional BEC with TR symmetry breaking: square lattice

- Inter-site tunneling orders the onsite orbital angular momentum (OAM) moments. Staggered OAM ordering.



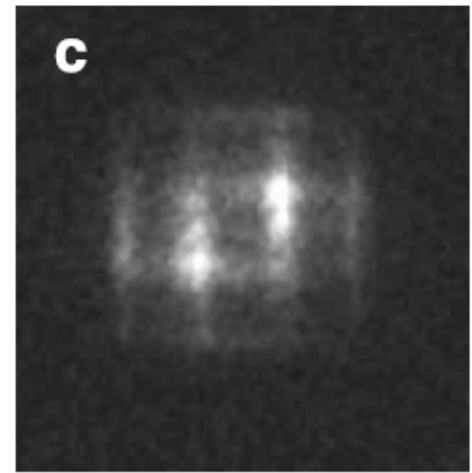
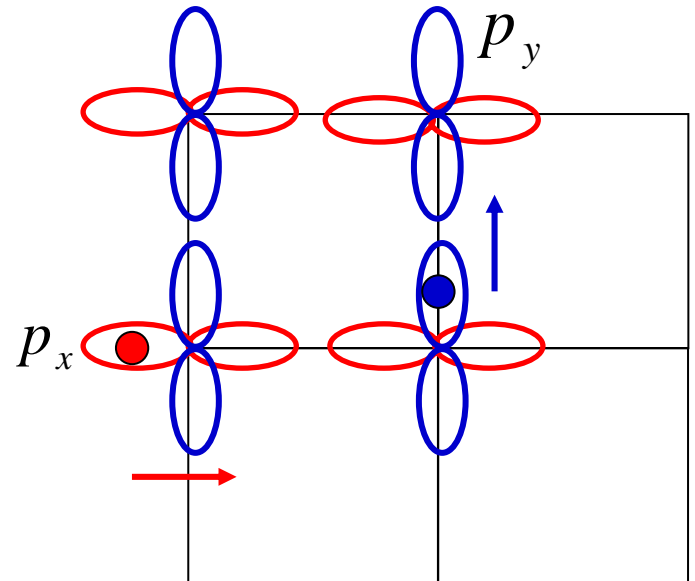
- Time of flight (zero temperature): Bragg peaks located at fractional values of reciprocal lattice vectors.

$$\left( \left(m + \frac{1}{2}\right) \frac{\pi}{a}, 0 \right) \quad \left( 0, \left(n + \frac{1}{2}\right) \frac{\pi}{a} \right)$$

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

# Quasi-1D behavior at finite temperatures

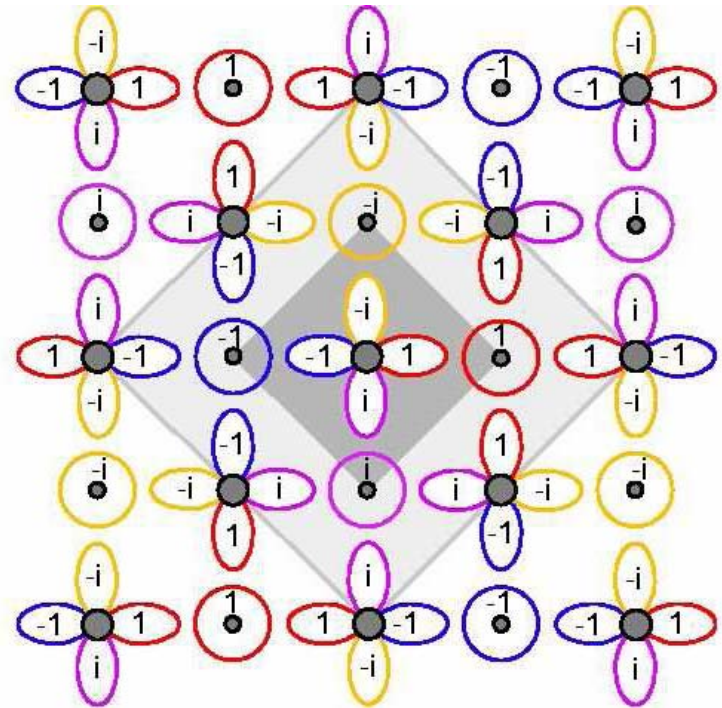
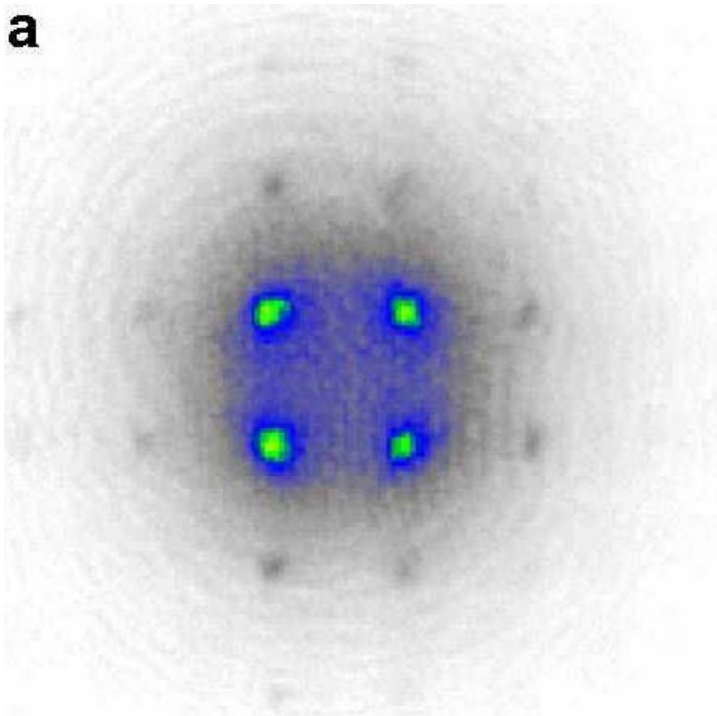
- Because  $t_{\perp} \ll t_{\parallel}$ ,  $p_x$ -particles can maintain phase coherence within the same row, but loose inter-row phase coherence at finite temperatures.
- Similar behavior also occurs for  $p_y$ -particles.
- The system effectively becomes 1D-like as shown in the time of flight experiment.



A. Isacsson et. al., PRA 72, 53604 (2005).

# Complex BEC beyond the “no-node” theorem

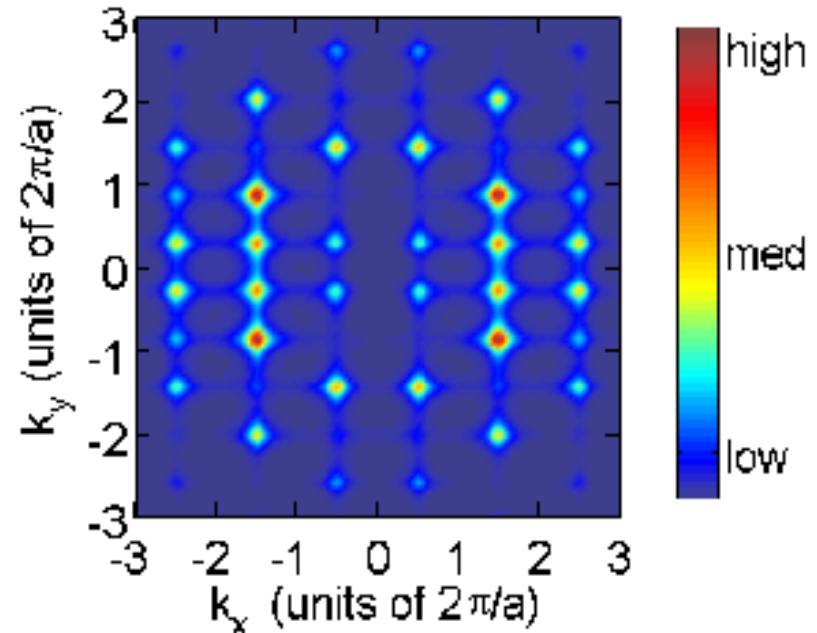
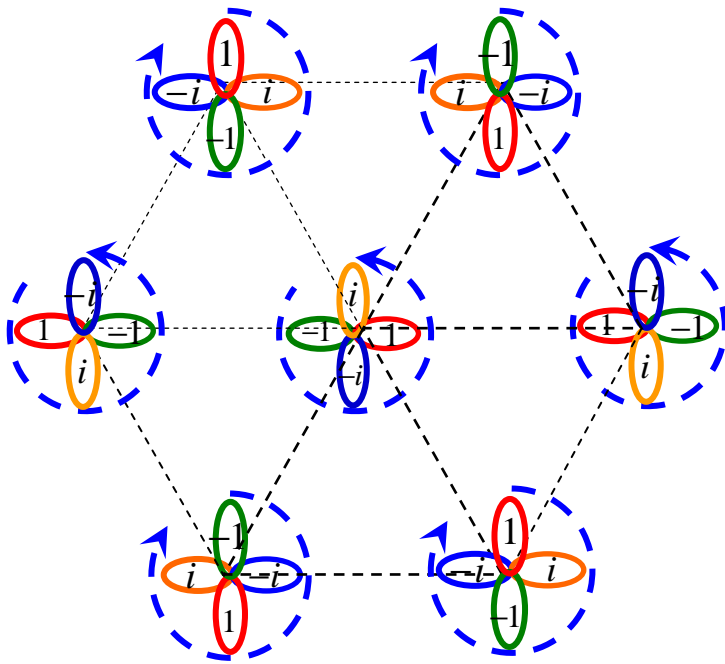
**a**



Wirth, Oelschlaeger, Hemmerich, arXiv:1006.0509.

# Unconventional BEC with TR symmetry breaking: triangular lattice

- Stripe ordering of orbital angular momentum moment in the triangular lattice.



- Each site behaves like a vortex with long range interaction in the superfluid state. Stripe ordering to minimize the global vorticity.

# Strong coupling analysis

- Ising variable for vortex vorticity:

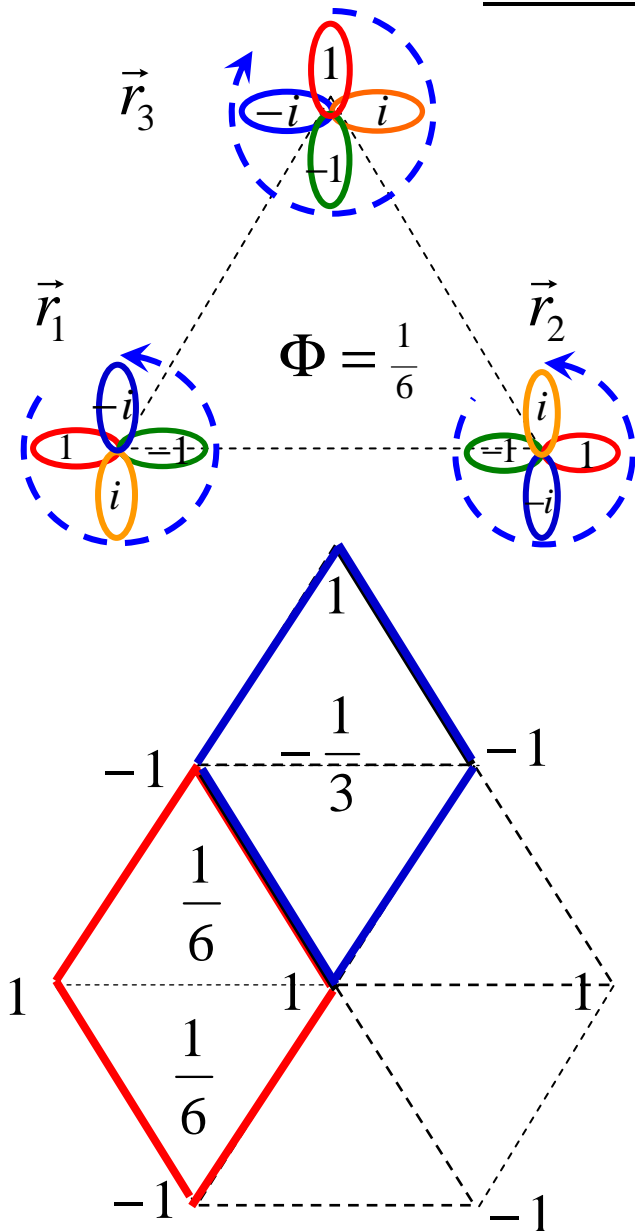
$$\sigma = \pm 1$$

- The minimum of the effective flux per plaquette is  $\pm 1/6$ .

$$\Phi_i = \frac{1}{2\pi} \sum_{\langle r, r' \rangle} A_{r, r'} = \frac{1}{6} (\sigma_{r1} + \sigma_{r2} + \sigma_{r3})$$

- The stripe pattern minimizes the ground state vorticity.

- cf. The same analysis also applies to p+ip Josephson junction array.





# 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 honeycomb lattice. **P-orbital Fermions are stable due to Pauli’s exclusion principle!**

**Ferromagnetism** from band flatness.

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

C. Wu et al, PRL 99, 67004(2007).

Shi-zhong zhang, Hsiang-hsuan Hung, and C. Wu, arXiv:0805.3031, to appear in PRA.

A new mechanism for the **unconventional pairing: the f-wave.**

# The early age of ferromagnetism



World's first compass  
(司南 South-pointer)

↑  
south

Thales says that a stone (lodestone) has a soul because it causes movement to iron.

----*De Anima*, Aristotle (384-322 BC)

The magnetic stone attracts iron.

慈 (ci) 石(shi) 召(zhao) 铁(tie)

---- *Guiguzi* (鬼谷子), (4<sup>th</sup> century BC)

慈 (loving, kind): the original Chinese character for magnetism

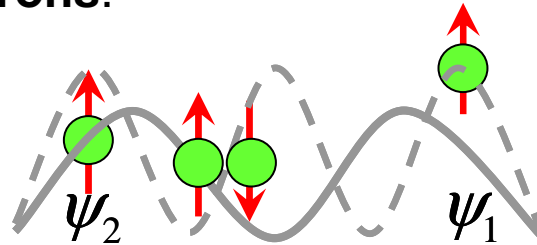
磁: magnetism, magnetic

# Itinerant ferromagnetism (FM): one of the central problems in condensed matter physics



E. C. Stoner

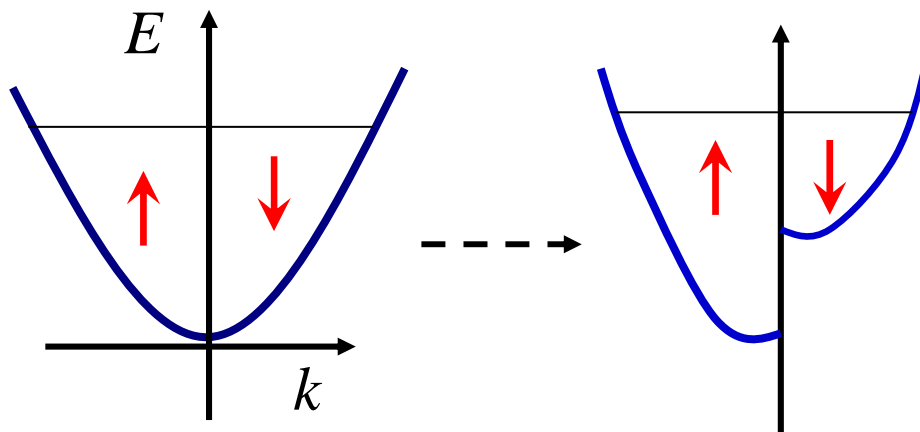
- Driving force: direct **exchange interaction among electrons.**



$$E_{\uparrow\uparrow} < E_{\uparrow\downarrow}$$

- Stoner criterion:

$$UN_0 > 1$$



$U$  – average interaction strength;  $N_0$  – density of states at the Fermi level

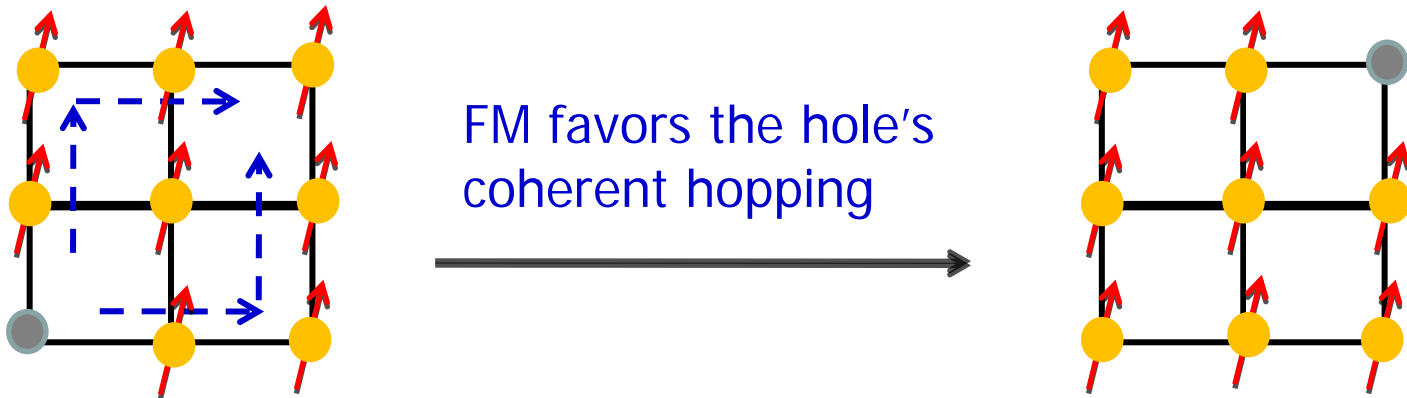
Fe	Co	Ni
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# A major challenge of condensed matter physics

- FM is essentially strong coupling physics. **NO** reliable weak coupling picture. In comparison, for superconductivity, we still have weak coupling BCS theory.

## Few Exact results:

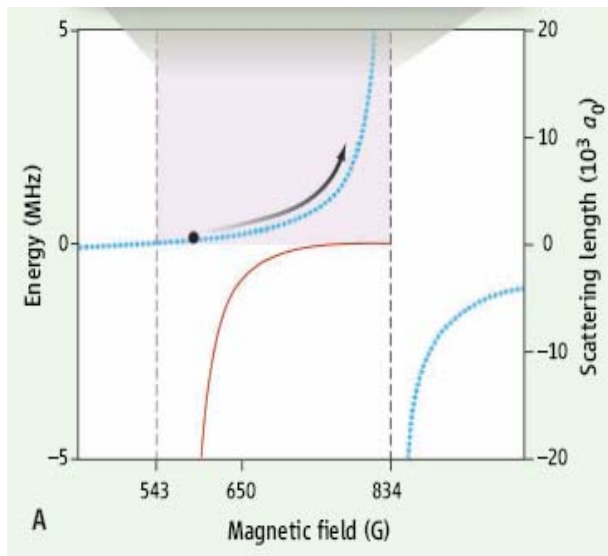
1. Nagaoka FM in Hubbard models ( $D \geq 2$ ) with a single hole and  $U \rightarrow +\infty$



2. Flat band FM: divergence of density of states stabilize ferromagnetism.

# Evidence of FM with cold atoms?

- Two-component fermions through Feshbach resonances from the side of **positive** scattering lengths.



When  $k_f a_s > 1.9$ , the increase of kinetic energy and the decrease of three-body loss are observed.

G. B. Jo, et al., Science 325, 1521(2009).

- Criticism: Magnetic domains are not observed.

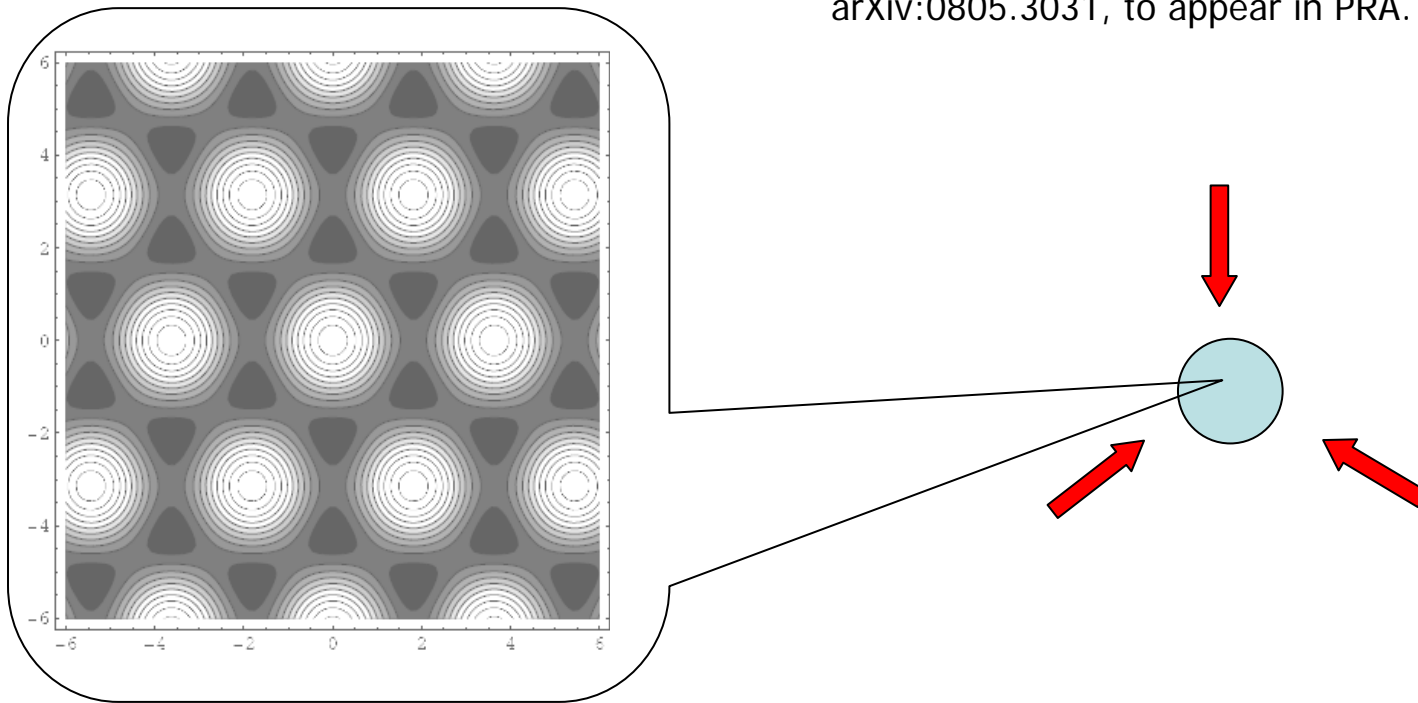
Hui Zhai, arxiv:0909.4917.

- Drawback: unstable to the dimer formation. To avoid this, fast ramping is needed, thus adiabaticity is not be ensured.

# The p-orbital honeycomb lattice

- Our approach: flat band FM to avoid the stability issue.

S. Z. Zhang, H. H. Hung, and C. Wu,  
arXiv:0805.3031, to appear in PRA.

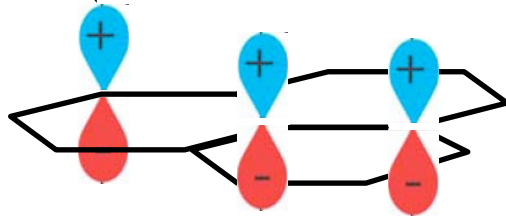


- Three coherent laser beams polarizing in the z-direction.

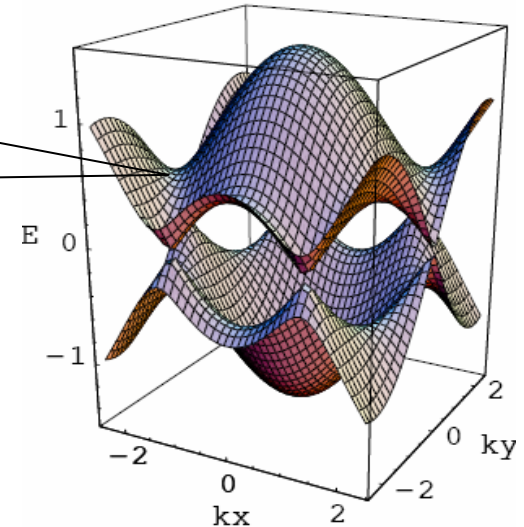
G. Grynberg et al., Phys. Rev. Lett. **70**, 2249 (1993).  
also K. Sengstock's recent work.

# p-orbital fermions in the honeycomb lattice

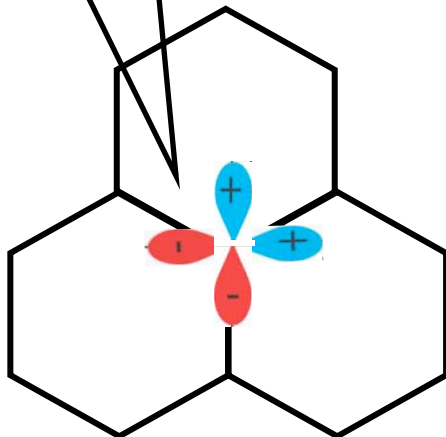
Not our interest



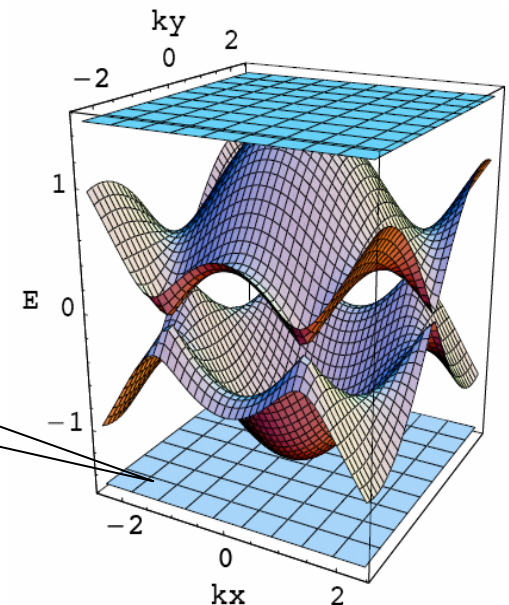
*cf.* graphene:  $p_z$ -orbital;  
Dirac cones.



Our interest



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

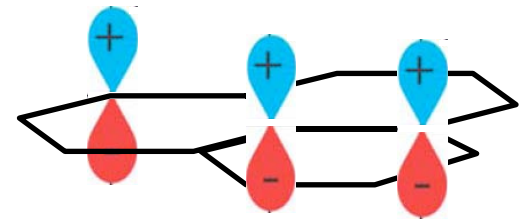


C. Wu, D. Bergman, L. Balents,  
and S. Das Sarma, PRL 99,  
70401 (2007).

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

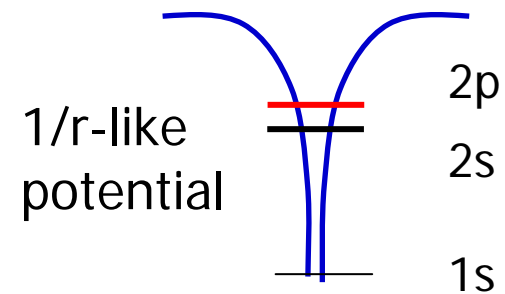
- $p_z$ -orbital band is not a good system for orbital physics.

isotropic within 2D; non-degenerate.

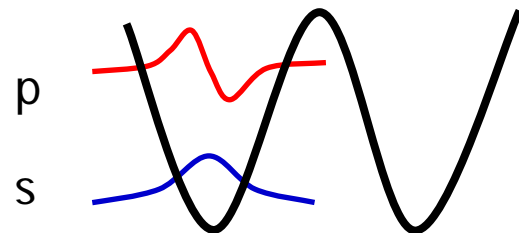


- Interesting orbital physics in the  $p_x, p_y$ -orbital bands.

- 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  $s$ .

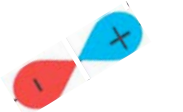
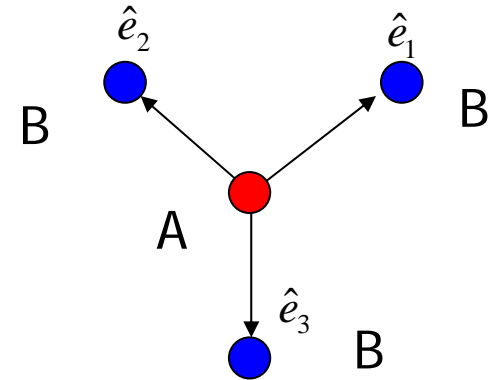




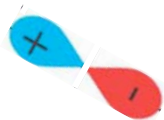
# p-orbital honeycomb optical lattice

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

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



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

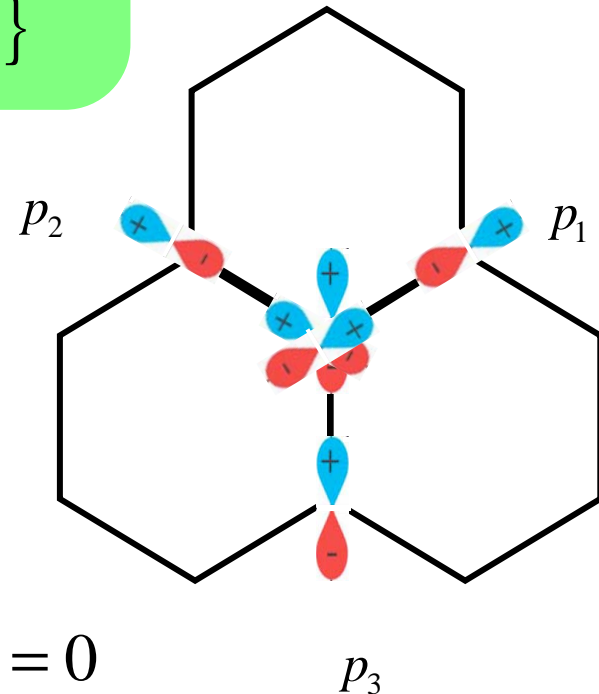


$$p_2 = -\frac{\sqrt{3}}{2} p_x + \frac{1}{2} p_y$$

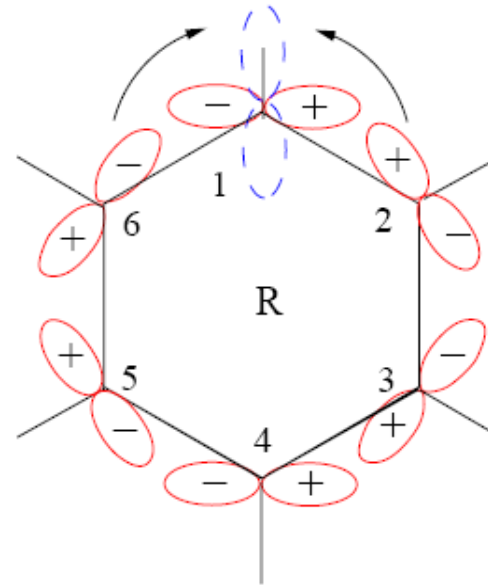
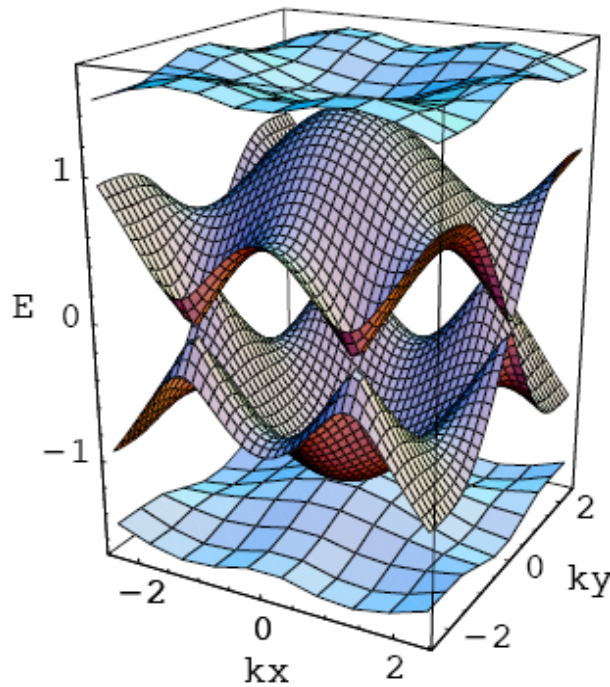


$$p_3 = -p_y$$

$$p_1 + p_2 + p_3 = 0$$



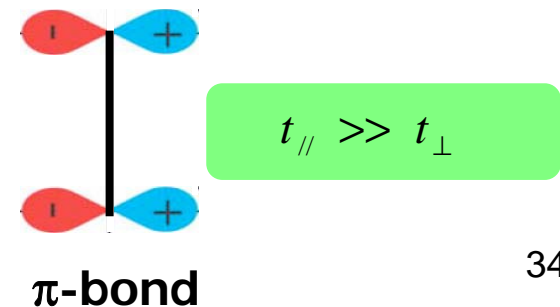
# Flat bands from **localized** eigenstates



- Flat band + Dirac cone.

- localized eigenstates.

- If  $\pi$ -bonding is included, the flat bands acquire small width at the order of  $t_{\perp}$ . Realistic band structures show  $t_{\perp} / t_{\parallel} \rightarrow 1\%$

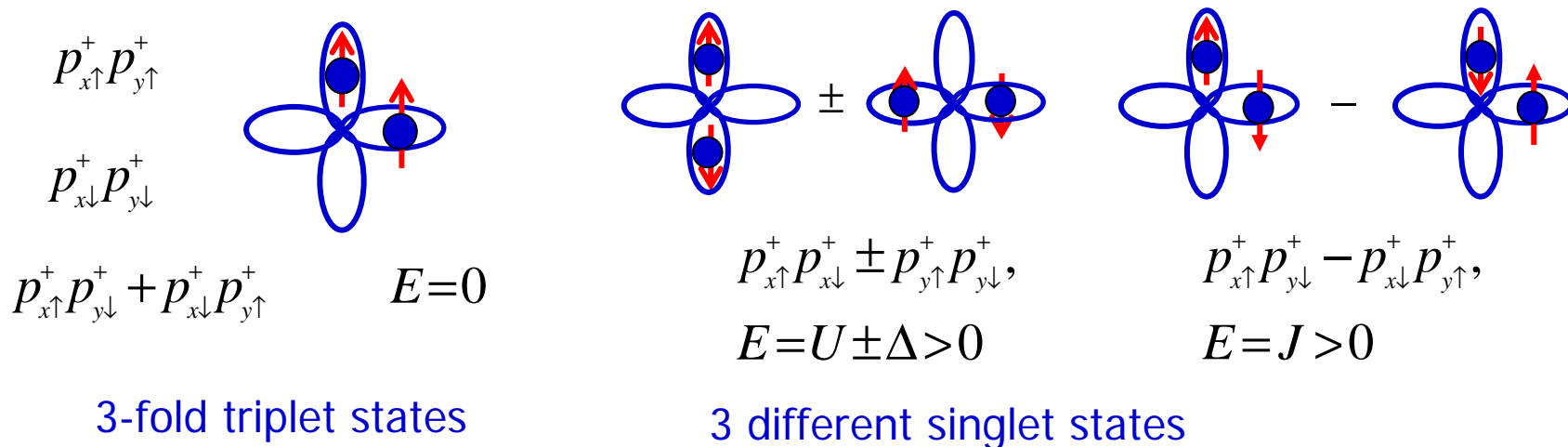


# Two-component fermions: six two-particle onsite states

- Multi-orbital Hubbard model:  $U$ , Hund's rule  $J$ , pair hopping  $\Delta$ .

$$H_{\text{int}} = U \sum_{\vec{r}} [n_{p_{x,\uparrow}}(\vec{r}) n_{p_{x,\downarrow}}(\vec{r}) + n_{p_{y,\uparrow}}(\vec{r}) n_{p_{y,\downarrow}}(\vec{r})] - J \sum_{\vec{r}} [\vec{S}_{p_x}(\vec{r}) \cdot \vec{S}_{p_y}(\vec{r}) - \frac{1}{4} n_{p_x}(\vec{r}) n_{p_y}(\vec{r})] + \Delta \sum_{\vec{r}} [p_{x,\uparrow}^+(\vec{r}) p_{x,\downarrow}^+(\vec{r}) p_{y,\downarrow}(\vec{r}) p_{y,\downarrow}(\vec{r}) + h.c.]$$

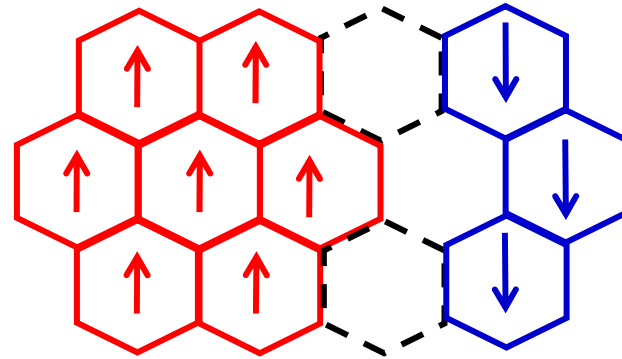
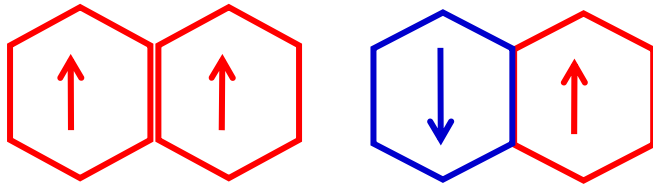
- A single site problem: the onsite triplet states do not cost energy within the s-wave scattering approximation.



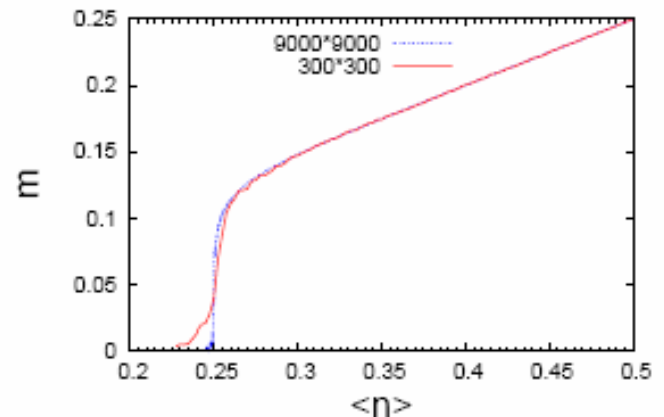
# Two-component fermion: interaction and percolation

- When localized eigenstates touch, their spins are aligned by the direct exchanges  $\rightarrow$  formation of FM clusters.
- Spins in disconnected clusters are uncorrelated.

No cost  $\Delta E \approx U / 36$



- **Exact** result in homogenous systems: FM appears above the percolation threshold while filling remains in the flat band:  $0.25 < n < 0.5$



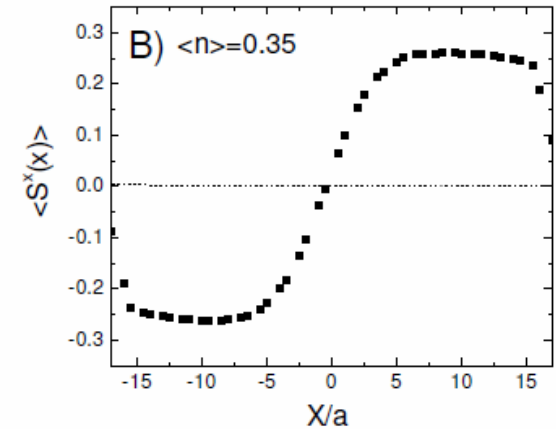
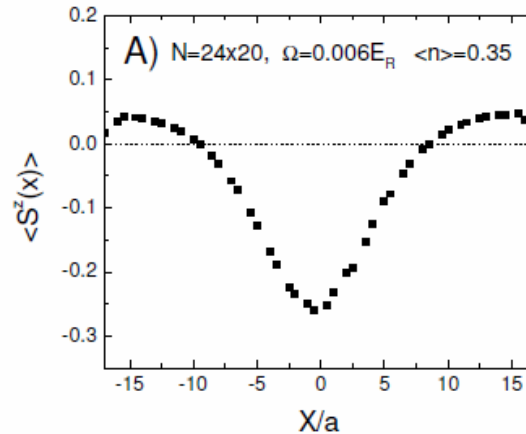
# Flat-band ferromagnetism in the p-orbitals

- Realistic system with a soft harmonic trap. Particle numbers of spin up and down are separately conserved.

$$\Omega = 0.005E_R, l = 4.5a,$$

$$N_{\uparrow} = N_{\downarrow} = 255,$$

$$t_{//} = U = 0.24E_R$$



- Self-consistent B-de G calculation. Skyrmion spin texture. It is reliable for soft inhomogeneity because of its exact starting point.

• Advantage: FM stabilized by weak or intermediate repulsions. The instability towards to the dimer molecule states is avoided.

• Entropy is large!

# 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.**

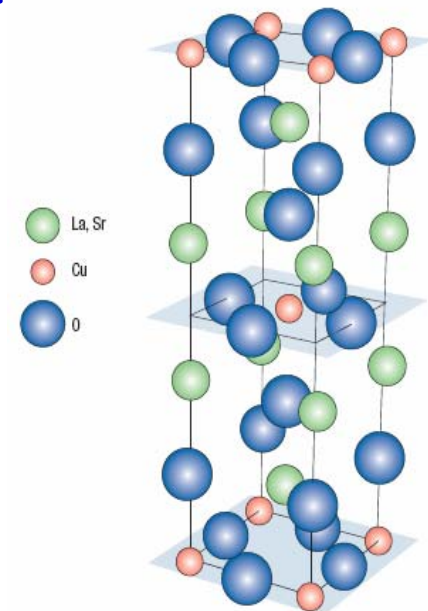
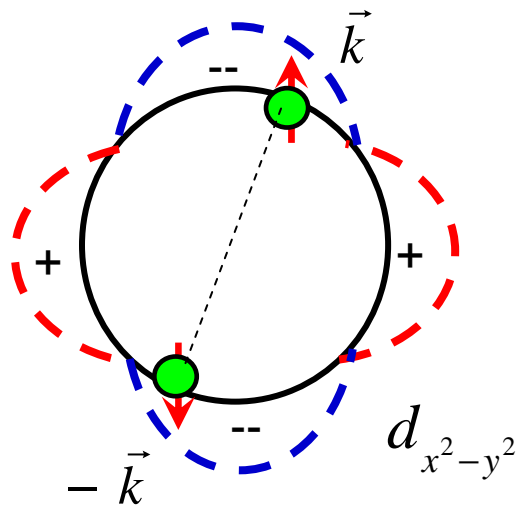
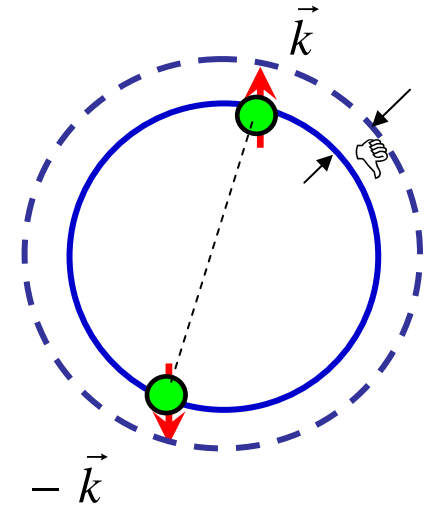
W. C. Lee, C. Wu, S. Das Sarma, arXiv:0905.1146, to appear in PRA.

# 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  $^3\text{He}$ -A and B;  $\text{Sr}_2\text{RuO}_4$ ;

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?

C. W. Zhang et al., Phys. Rev. Lett. 101, 160401 (2008).

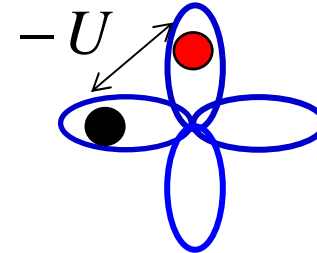
- No strong correlation effects. Analysis is controllable.
- **f-wave** pairing with spinless fermions in the p-orbital hexagonal optical lattice.



# Onsite attraction for **SPINLESS** $p$ -orbital fermions

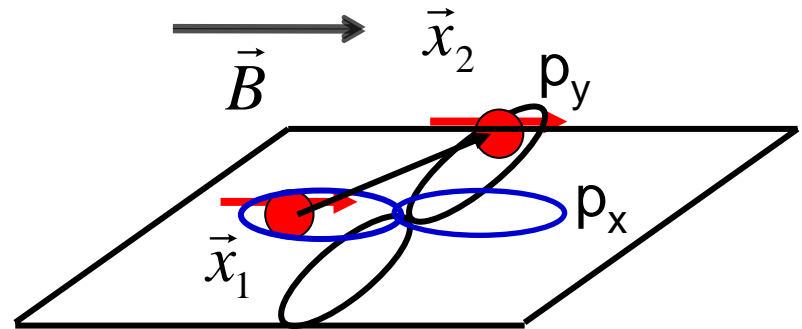
$$H_{\text{int}} = -U \sum_{\vec{r}} n_{p_x}(\vec{r}) n_{p_y}(\vec{r})$$

$$= -U \sum_{\vec{r}} n_{p_x + ip_y}(\vec{r}) n_{p_x - ip_y}(\vec{r})$$

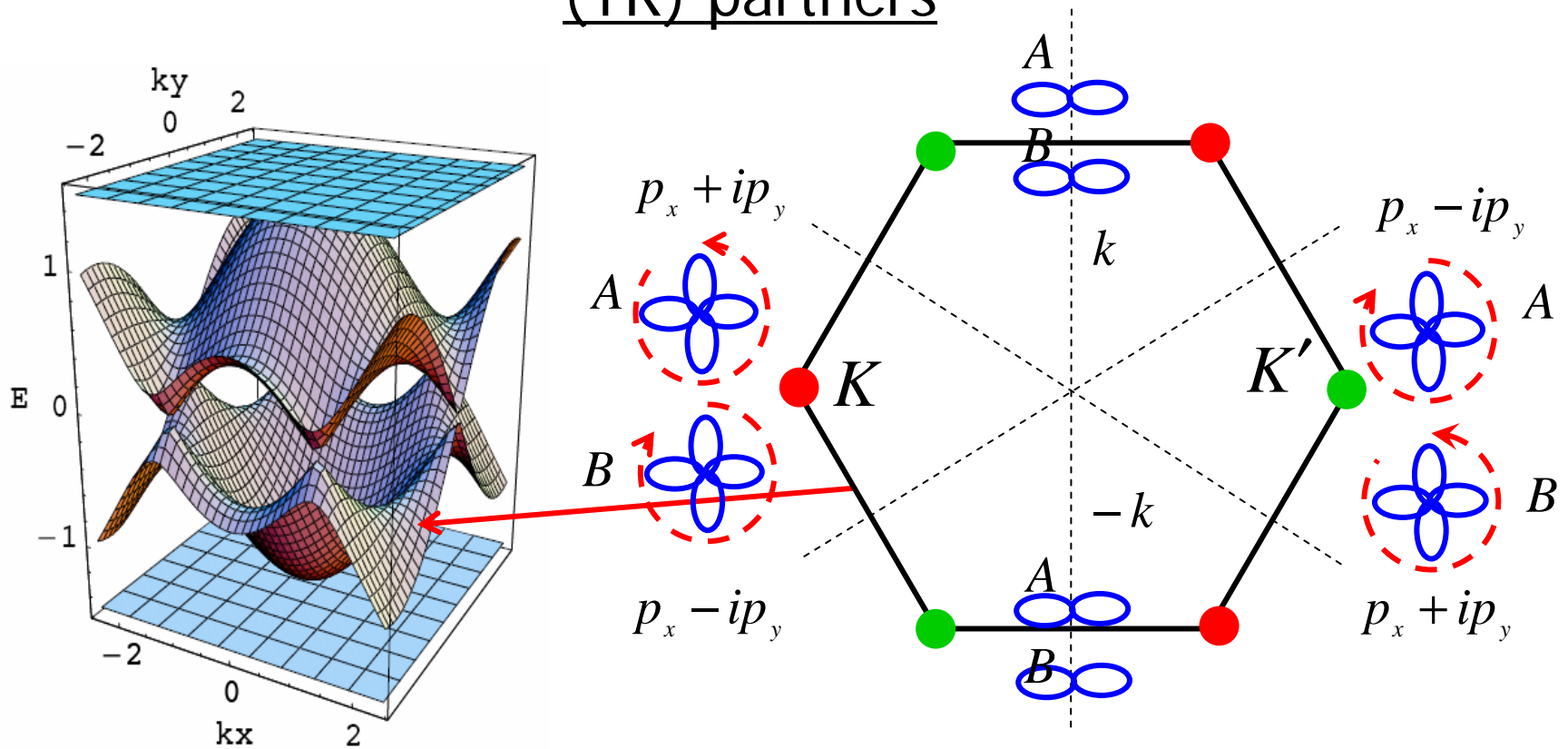


- Problem: contact interaction vanishes for spinless fermions.
- Use fermions with large magnetic moments whose laser cooling has been performed.
- Under strong 2D confinement,  $U$  is attractive and can reach the order of 100nK.

$^{167}\text{Er} (7\mu_B)$



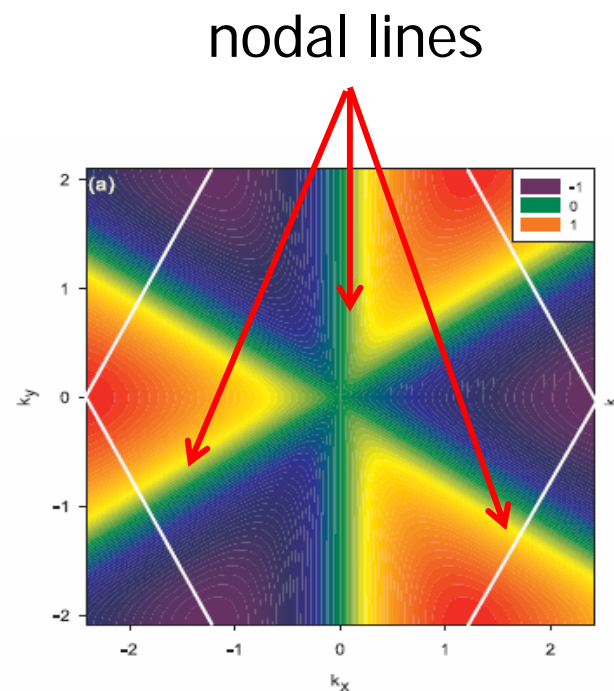
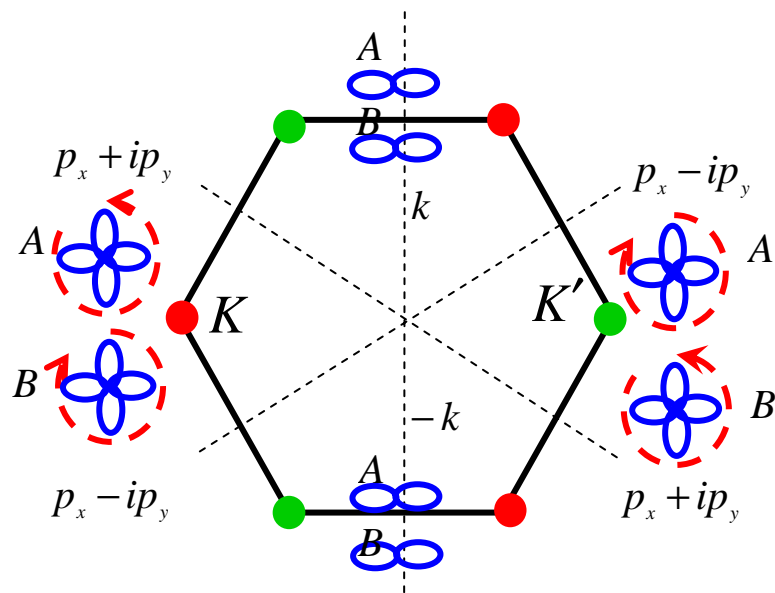
# Nontrivial orbital configurations between time reversal (TR) partners



- 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

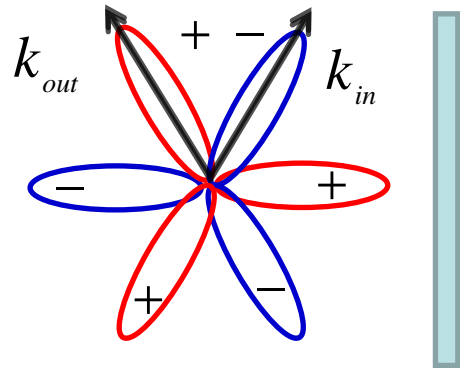
- Along middle lines, TR pairs cannot be paired  $\rightarrow$  nodal lines.
- The TR pair at K and K' has the largest pairing.
- Odd parity.



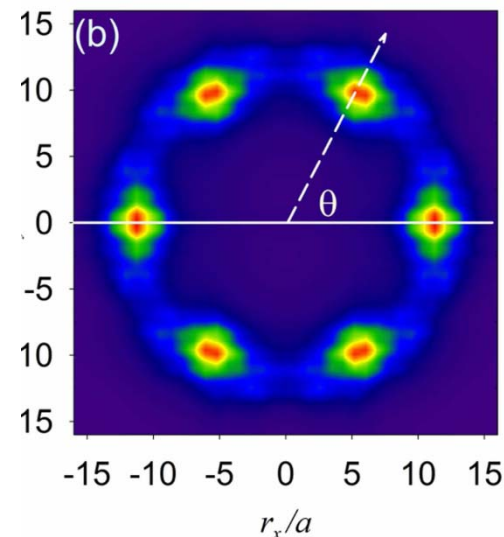
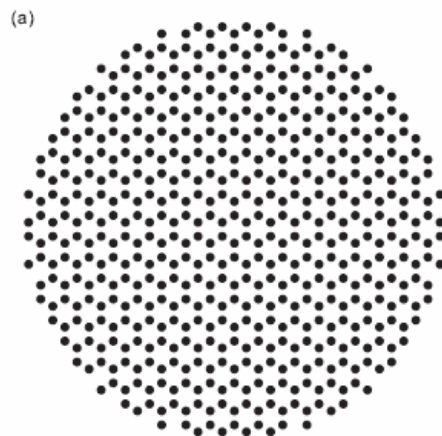
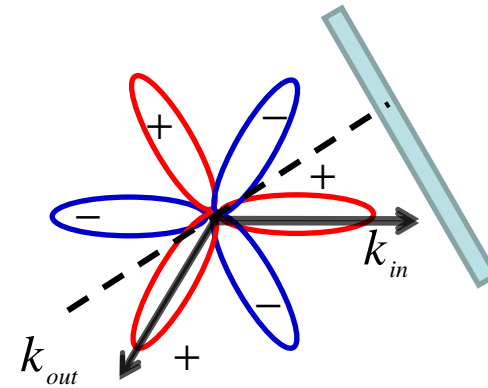
- The mean-field gap value can reach 10nK; and the 2D Kosterlitz-Thouless temperature can reach 1nK.

# Phase sensitive detection: zero energy Andreev bound states

**With zero energy Andreev Bound States**

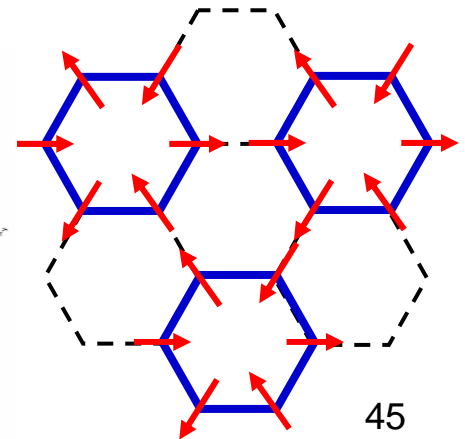
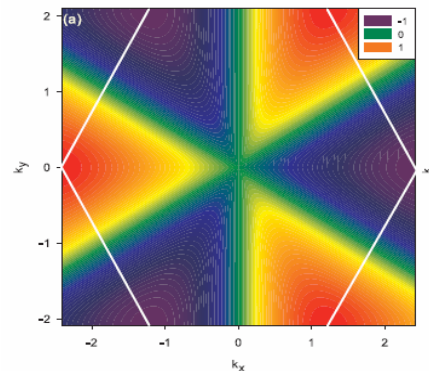
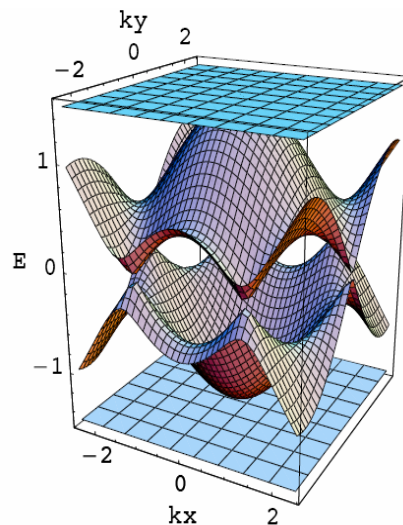
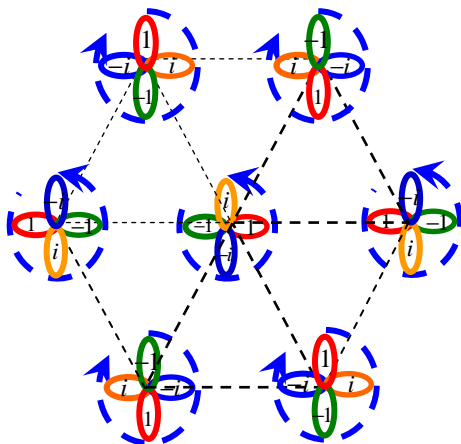


**No Andreev Bound States**



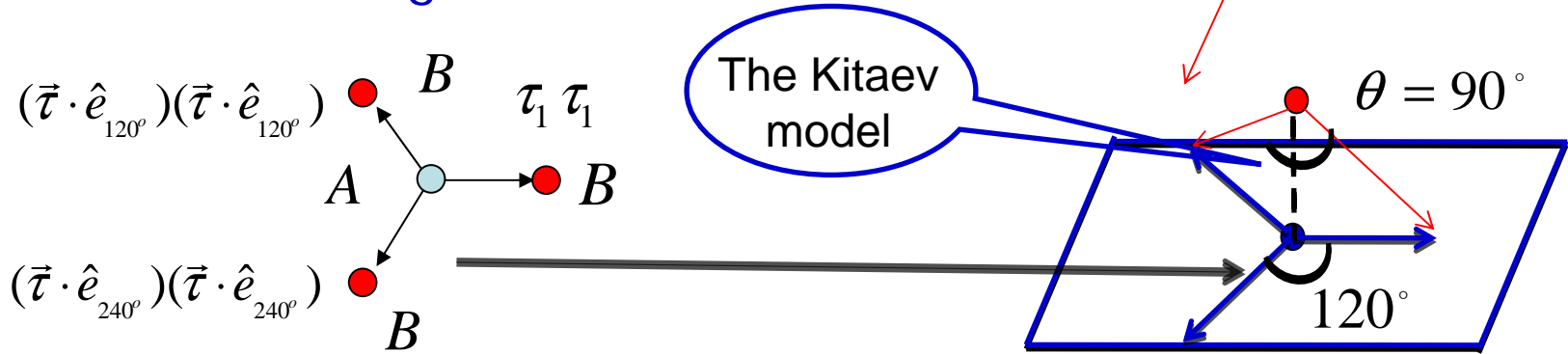
# Summary: orbital physics with cold atoms

- Unconventional BEC beyond the “no-node” theorem.
- Exact flat-band ferromagnetism.
- Novel mechanism for f-wave Cooper pairing;
- Mott-insulator: a new type of frustrated magnet-like model.
- Band insulator (topological): quantum anomalous Hall effect.



# Other selected work

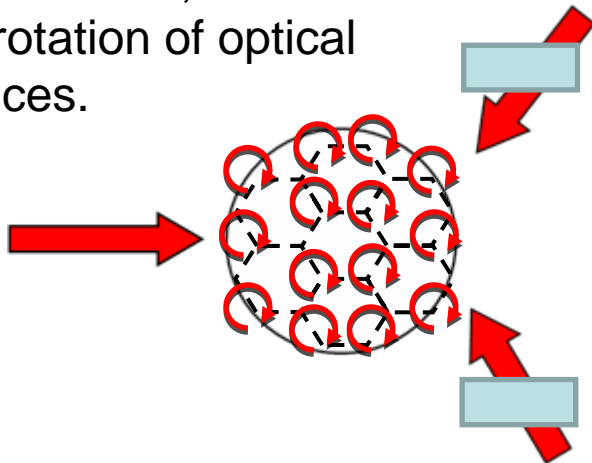
- Mott-insulator: quantum  $120^\circ$  model in the honeycomb lattice. A new frustrated magnet-like model.



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

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

N. Gemelke, S. Chu et al. rotation of optical lattices.



C. Wu, PRL 101, 168807 (2008).

