Novel *p*-orbital physics in the honeycomb optical lattices

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C. Wu, D. Bergman, L. Balents, S. Das Sarma, PRL 99, 70401 (2007);
C. Wu, S. Das Sarma, PRB 77, 235107(2008);
C. Wu, PRL 100, 200406 (2008);
C. Wu, PRL 101, 186807 (2008);
S. Zhang, H. Hung, and C. Wu, PRA, 053618 (2010);
W. C. Lee, C. Wu, and S. Das Sarama, PRA 82, 053611(2010);
M. C. Zhang, H. H. Hung, C. W. Zhang, and C. Wu, PRA 83, 023615 (2011).

Collaborators:

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Outline

• **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

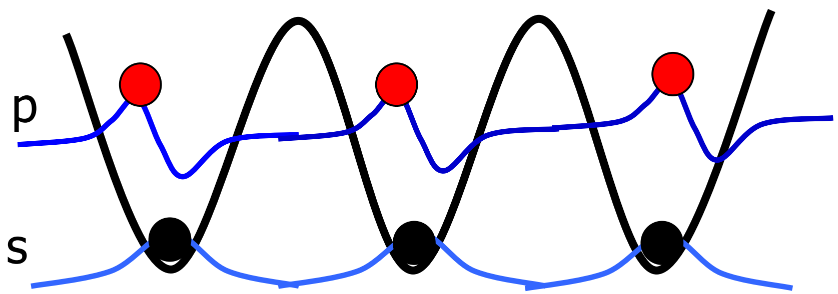
- Great successes of cold atom physics: BEC, BCS-BEC, etc…

- **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).



J. J. Sebby-Strabley, et al., PRA 73, 33605 (2006); T. Mueller et al., Phys. Rev. Lett. 99, 200405 (2007); C. W. Lai et al., Nature 450, 529 (2007).

Fundamental features of orbital physics

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

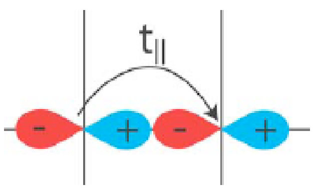
Tokura, et al., science 288, 462, (2000).

- **Orbital degeneracy.**

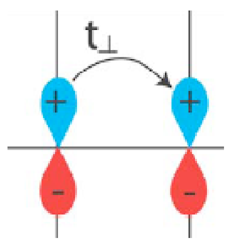
- **Spatial anisotropy.**

p-orbitals: p_x, p_y, p_z

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

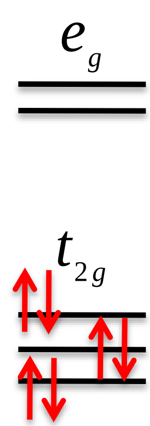


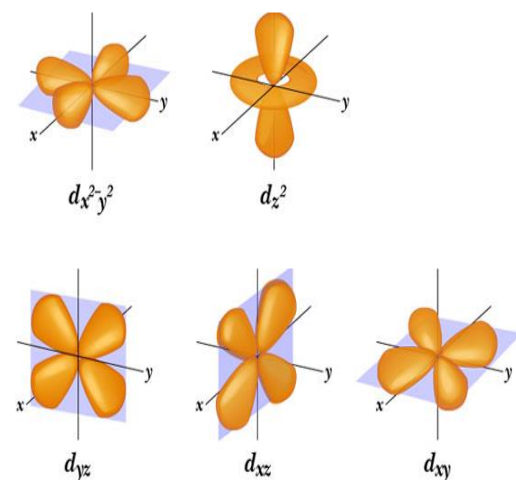
σ-bond



π-bond

$t_{//} >> t_{\perp}$

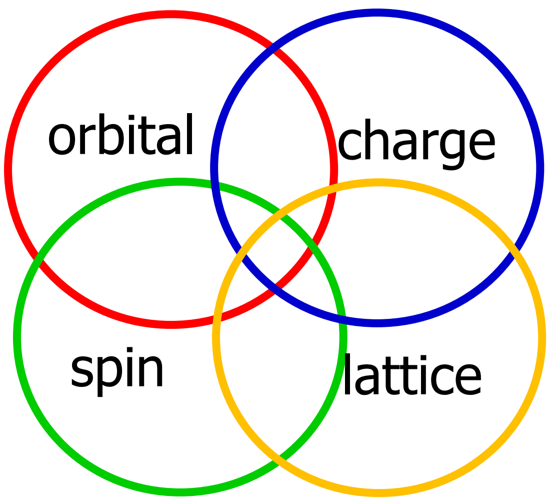


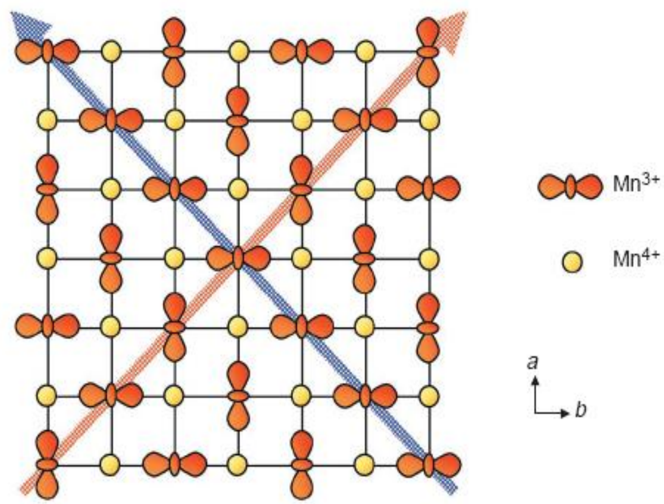


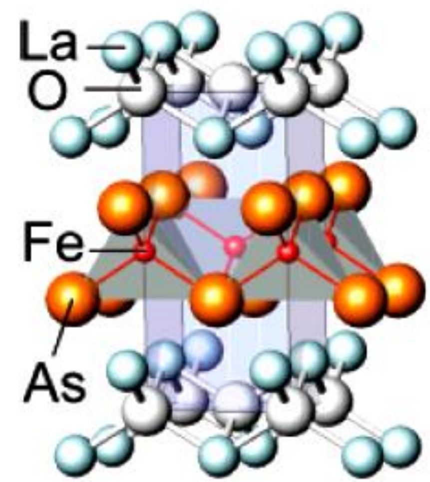
crystal field splitting

Transition metal oxide orbital systems

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







Manganite: $La_{1-x}Sr_{1+x}MnO_4$

Iron-pnictide: 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.

C. Wu, Mod. Phys. Lett. B 23, 1 (2009) —a short review.

(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.

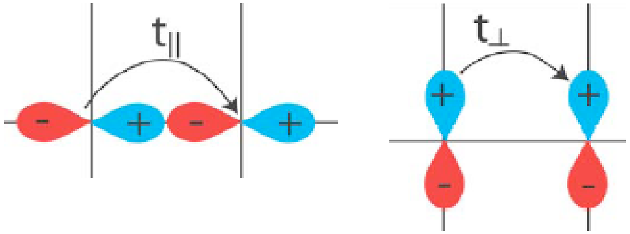
- Most *p*-orbital solid state materials are weakly correlated (e.g. semiconductors).

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

- Cold atom orbital systems:

$$t_{//} >> t_{\perp}$$

P-orbital has even **stronger anisotropy** than *d* and *f*;
Combination of strong anisotropy with strong **correlation.**



σ-bond π-bond

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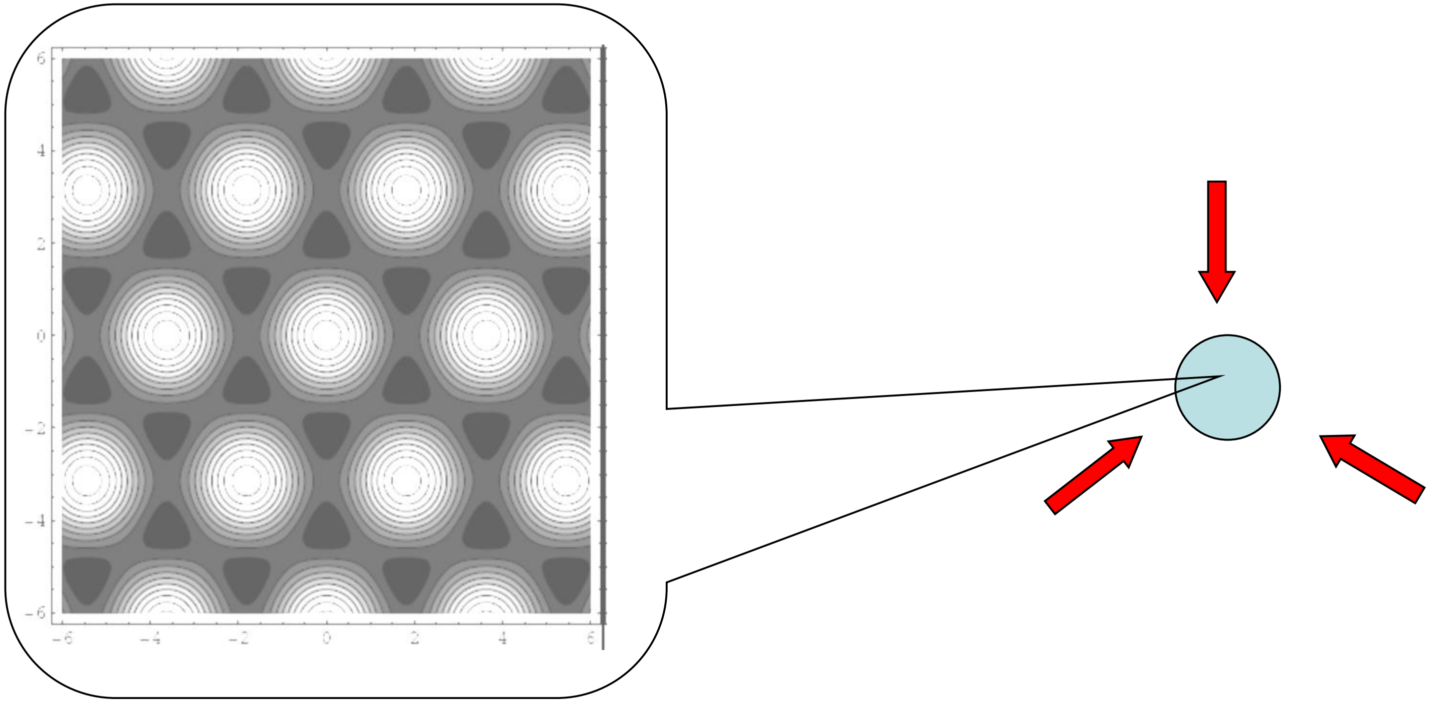
Unconventional Cooper pairing: f-wave.

The p-orbital honeycomb lattice

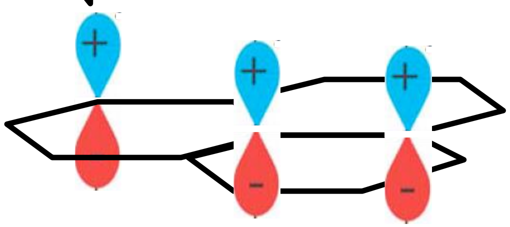


- Three coherent laser beams polarizing in the z-direction.

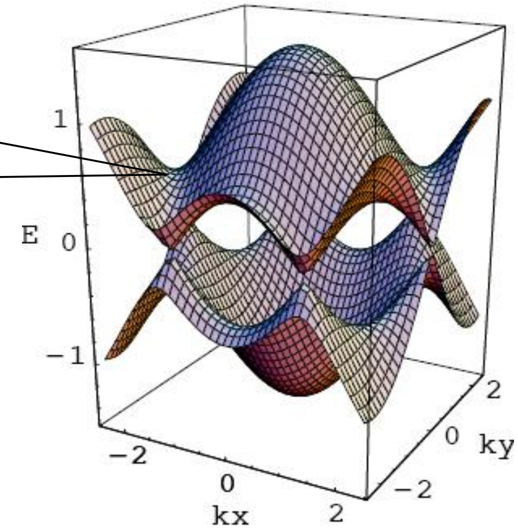
G. Grynberg et al., Phys. Rev. Lett. **70**, 2249 (1993).
also K. Sengstock's recent work.

p-orbital fermions in the honeycomb lattice

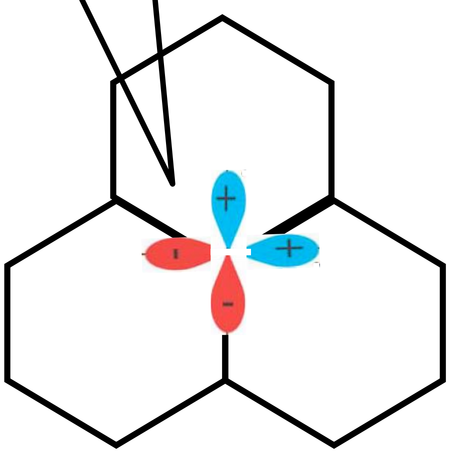
Not our interest



cf. graphene: p_z-orbital; Dirac cones.

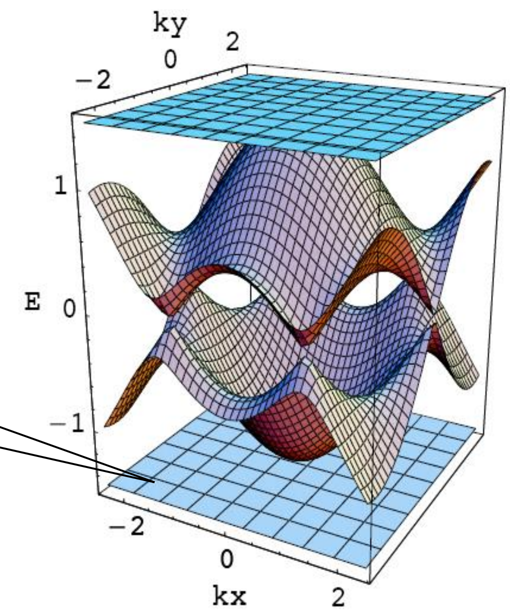


Our interest!



p_x;p_y-orbitals: flat bands; interaction effects dominate→ ferromagnetism.

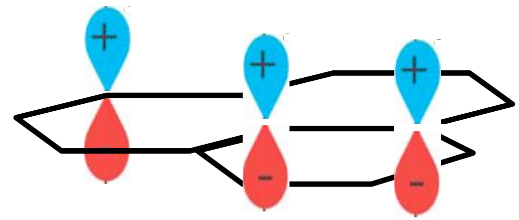
C. Wu, D. Bergman, L. Balents, and S. Das Sarma, PRL 99, 70401 (2007).



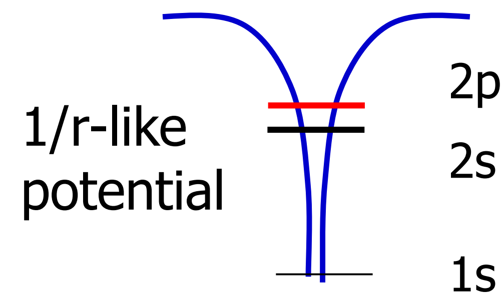
p_x, p_y-physics: get rid of the hybridization with s

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

isotropic within 2D; non-degenerate.

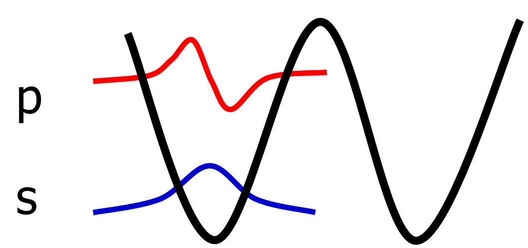


- Interesting orbital physics in the p_x, p_y-orbital bands.



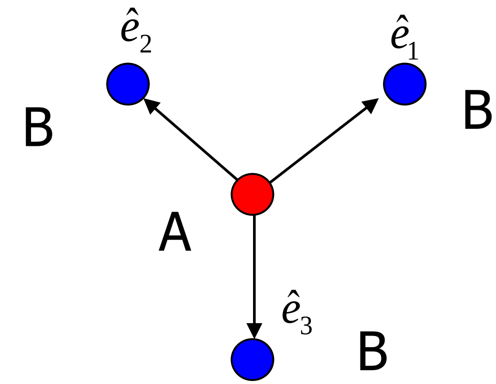
- However, in graphene, $2p_x$ and $2p_y$ are close to $2s$, thus strong hybridization occurs.

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

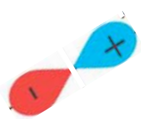


p-orbital honeycomb optical lattice

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



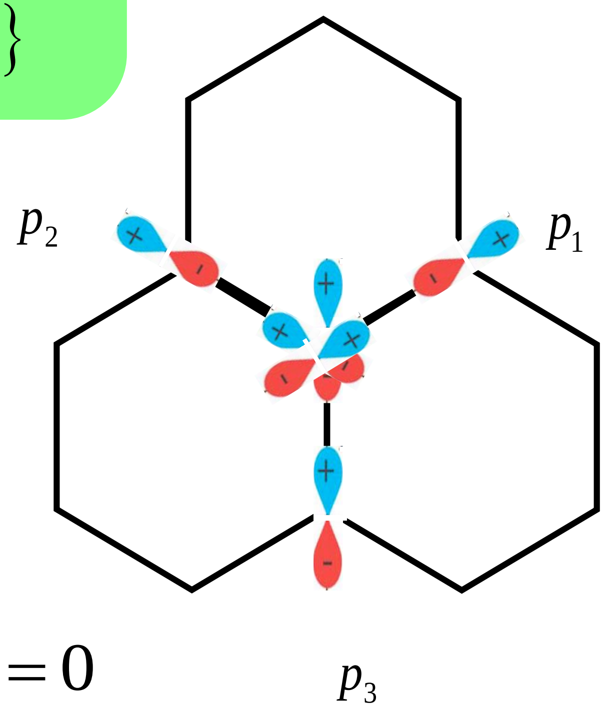
$$H_t = t_{//} \Big\{ \sum_{\vec{r}\in A} [p_1^+(\vec{r})p_1(\vec{r}+\hat{e}_1)+h.c.]$$
$$+[p_2^+(\vec{r})p_1(\vec{r}+\hat{e}_2)+h.c]$$
$$+[p_3^+(\vec{r})p_3(\vec{r}+\hat{e}_3)+h.c] \Big\}$$



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

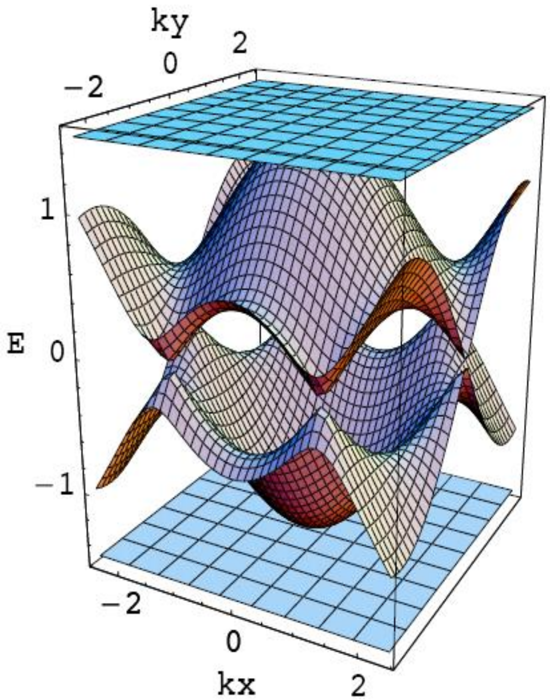
$$p_2 = -\frac{\sqrt{3}}{2} p_x + \frac{1}{2} p_y$$

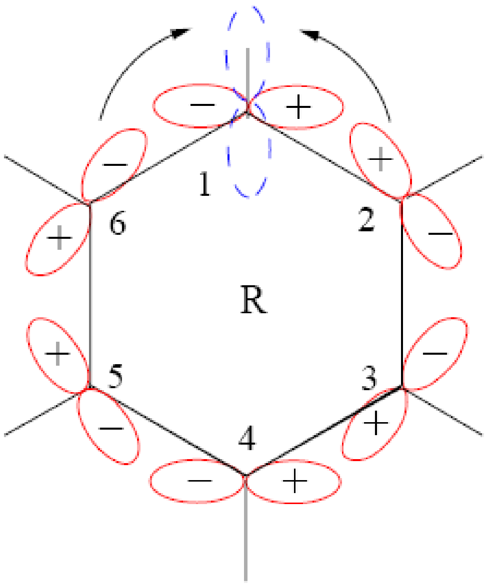
$$p_3 = -p_y$$



$$p_1 + p_2 + p_3 = 0$$

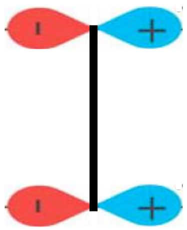
Flat bands from **localized** eigenstates





- Flat band + Dirac cone.
- localized eigenstates.

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



$t_{//} >> t_{\perp}$

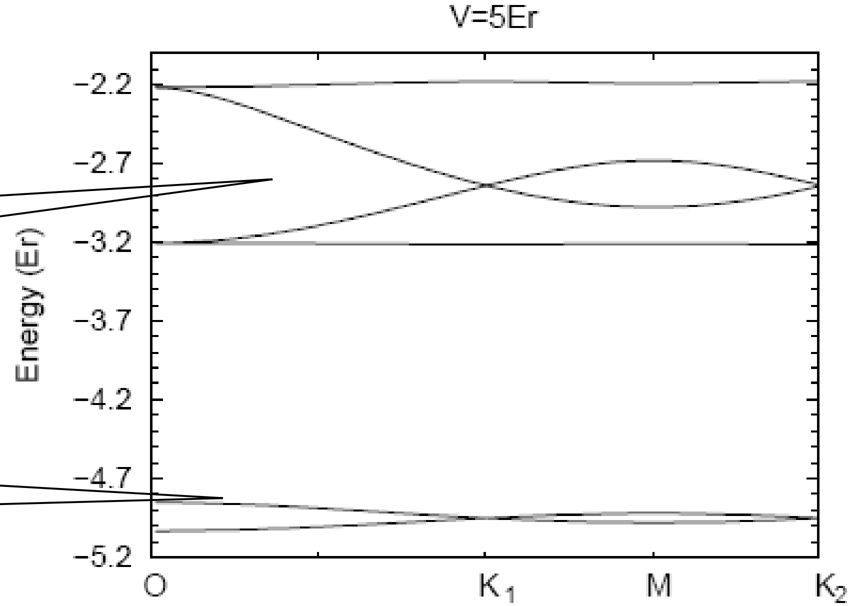
π-bond

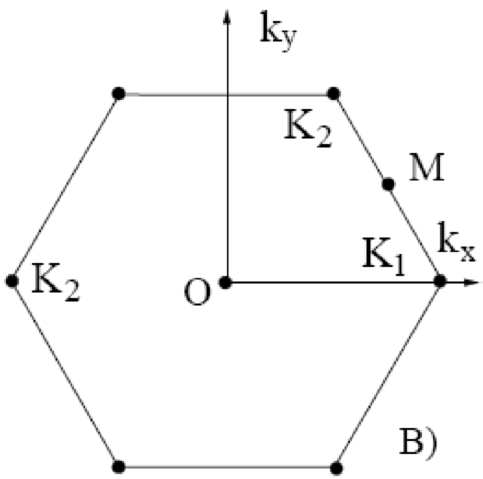
Realistic Band structure with the sinusoidal optical potential

- Excellent band flatness.

$p_{x,y}$-orbital bands

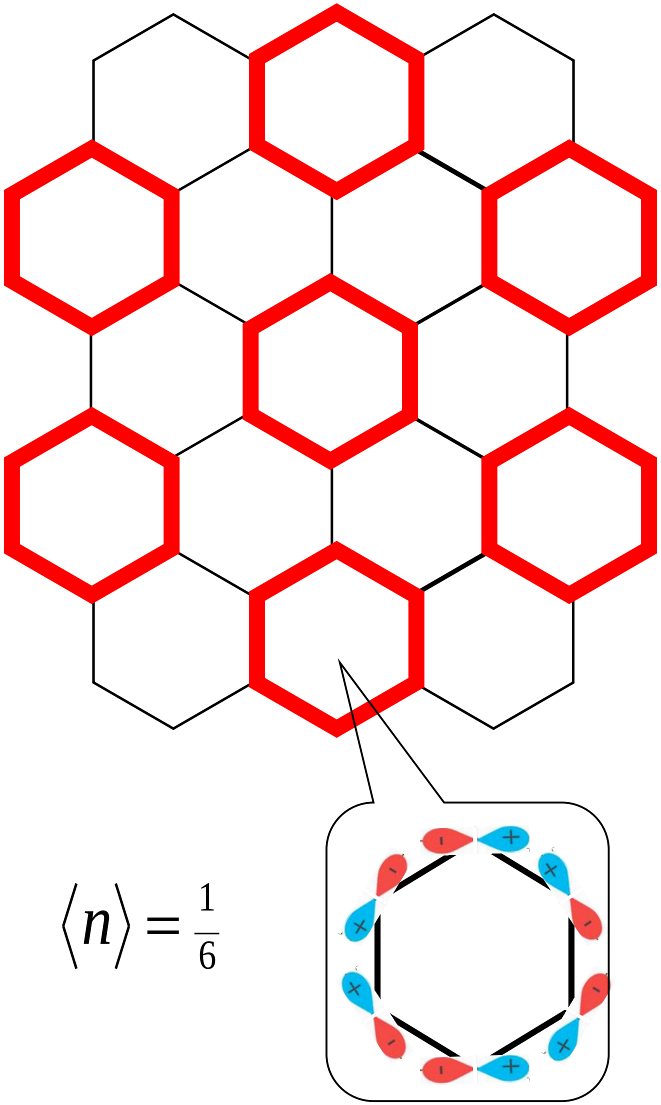
s-orbital bands



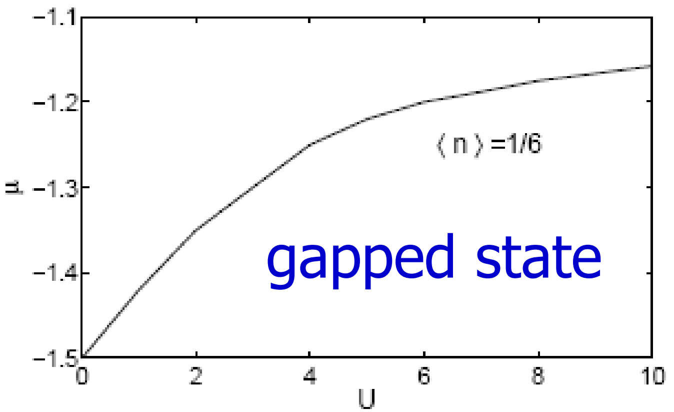


$$H = -\frac{\hbar^2\nabla^2}{2m} + V\sum_{i=1\sim 3}\cos(\vec{p}_i \cdot \vec{r})$$

Exact solution for spinless fermions: Wigner crystallization



$$\langle n \rangle = \frac{1}{6}$$

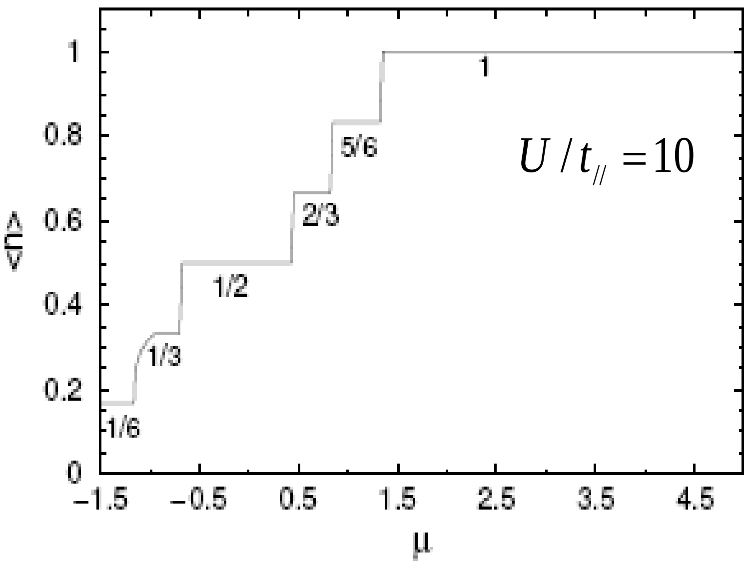


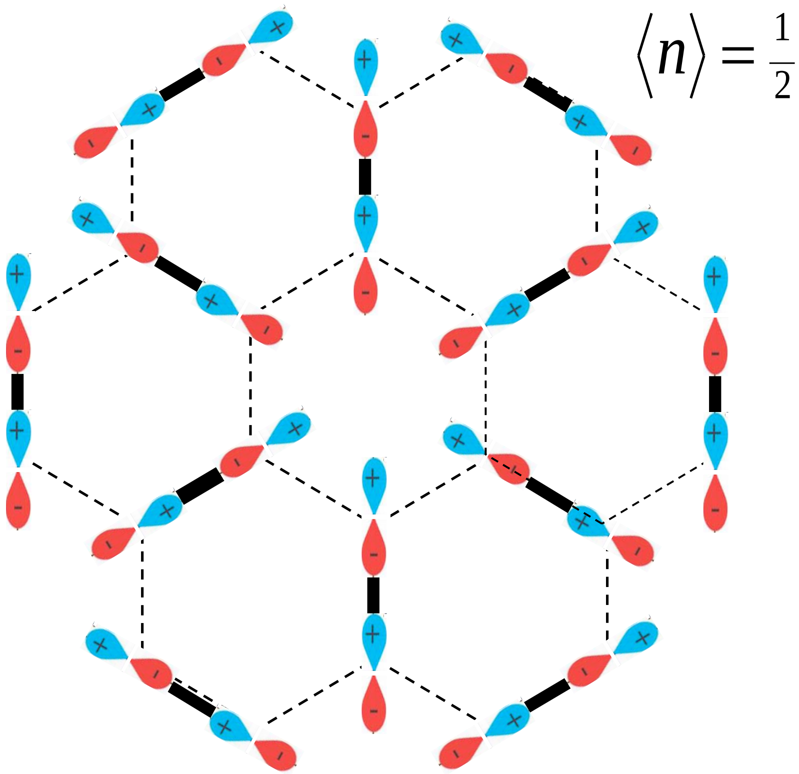
- Close-packed hexagons; avoiding repulsion.

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

- The result is also good for bosons.

Orbital ordering with strong repulsions

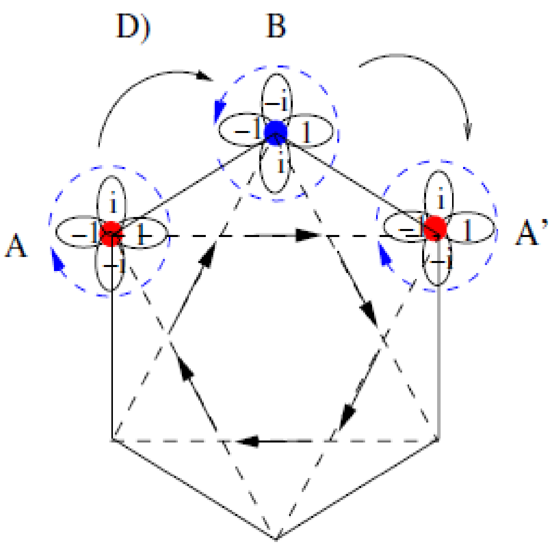




- Various orbital ordering insulating states at commensurate fillings.

- Dimerization at <n>=1/2! Each dimer is an entangled state of empty and occupied states.

Exotic quantum anomalous Hall insulators

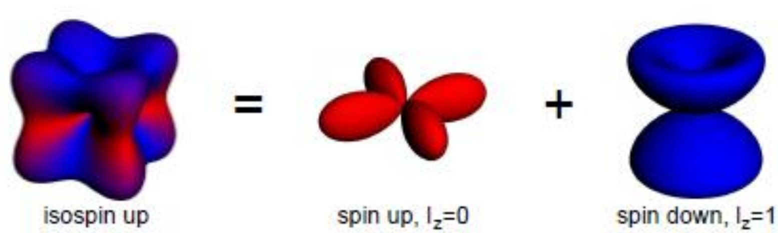


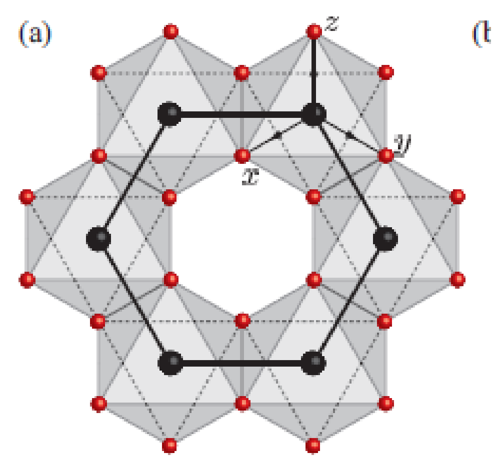
The required experimental technique was **available** in Nate Gemelke and Steven Chu's group at Stanford.

C. Wu, PRL 101, 186807 (2008).
Zhang, Hung, Zhang, Wu, PRA 83, 023615 (2011).

c.f. Condensed matter systems: Nagaosa et al, Na2IrO3, PRL 2009; Fang and Dai, science 2010.

Ir4+

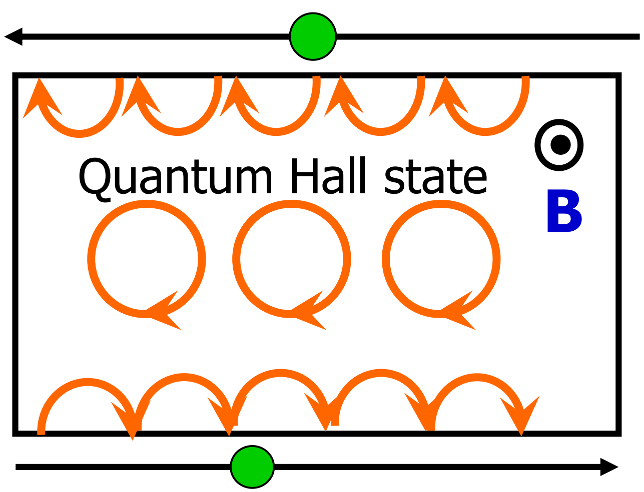


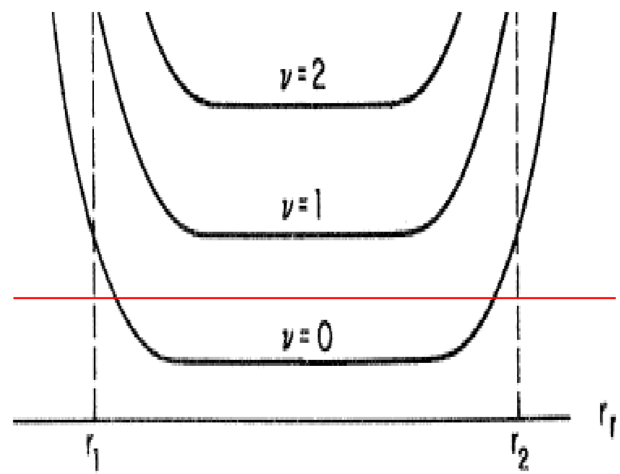


A brief review: quantum Hall effect (QHE)

- 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 ---- 1st Chern number.

Quantum Anomalous Hall (QAHE)– QHE without Landau levels

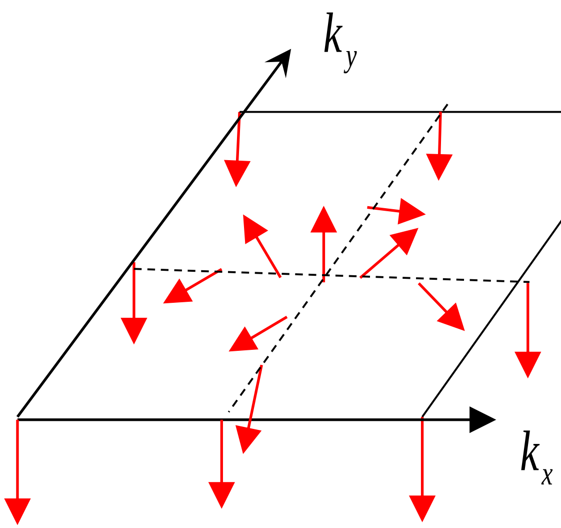
- Example: a two-band system. The pseudo-spin vector $\vec{d}$ exhibits a non-trivial configuration in the Brillouin zone.

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

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

- Hall conductance is quantized to n/2π.

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



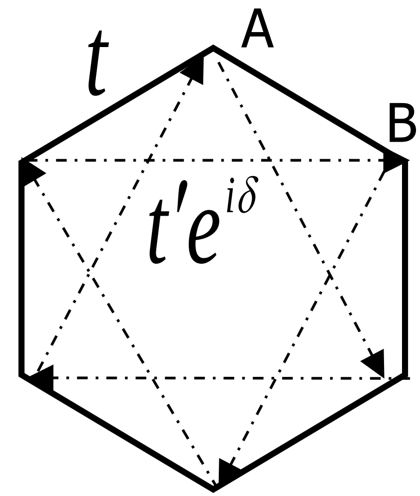
X. L Qi, et al, PRB 74,85308 (2006)

Haldane's Quantum Anomalous Hall model

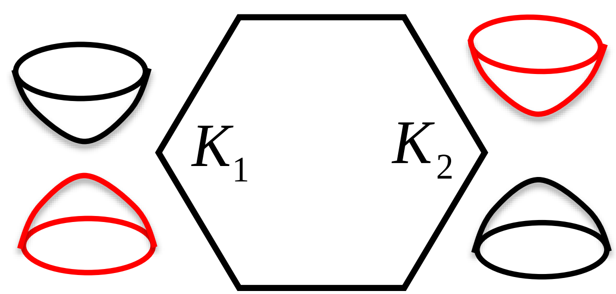
- Honeycomb lattice with complex-valued next-nearest neighbor hopping.

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

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



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

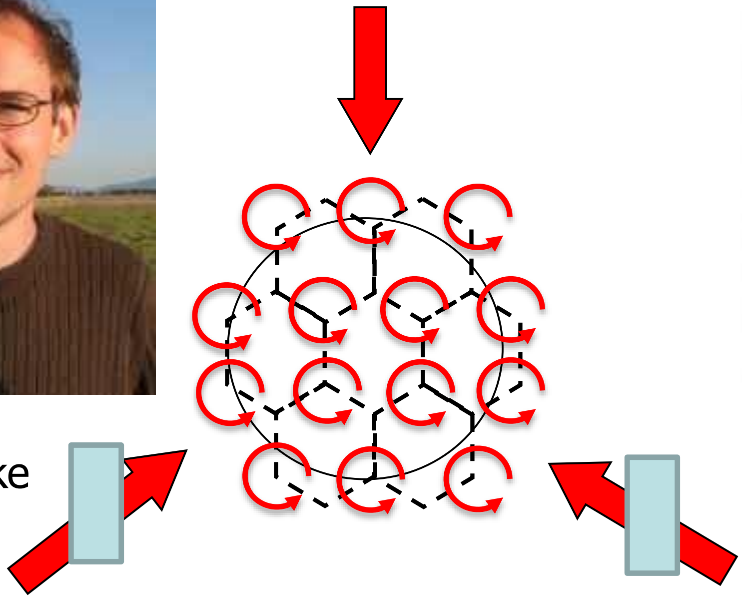


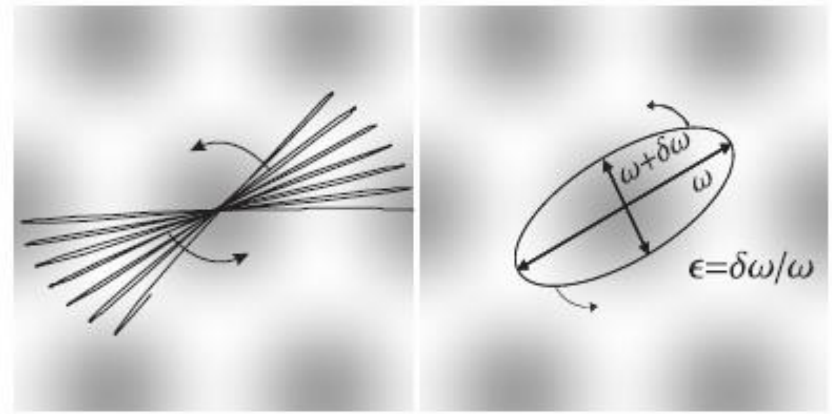
- **QAHE has not been experimentally realized yet in both CM and AMO systems.**

F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988)

Rotate each site around its own center

N. Gemelke





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

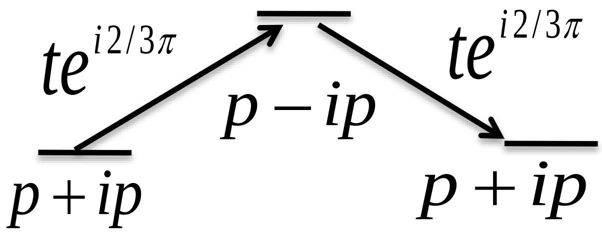
- Orbital Zeeman term.

$$H_{zmn} = -\Omega \sum_{r \in A} L_z(\vec{r})$$
$$= i\Omega \sum_{\vec{r} \in A} \{ p_x^+(\vec{r}) p_y(\vec{r}) - p_y^+(\vec{r}) p_x(\vec{r}) \}$$

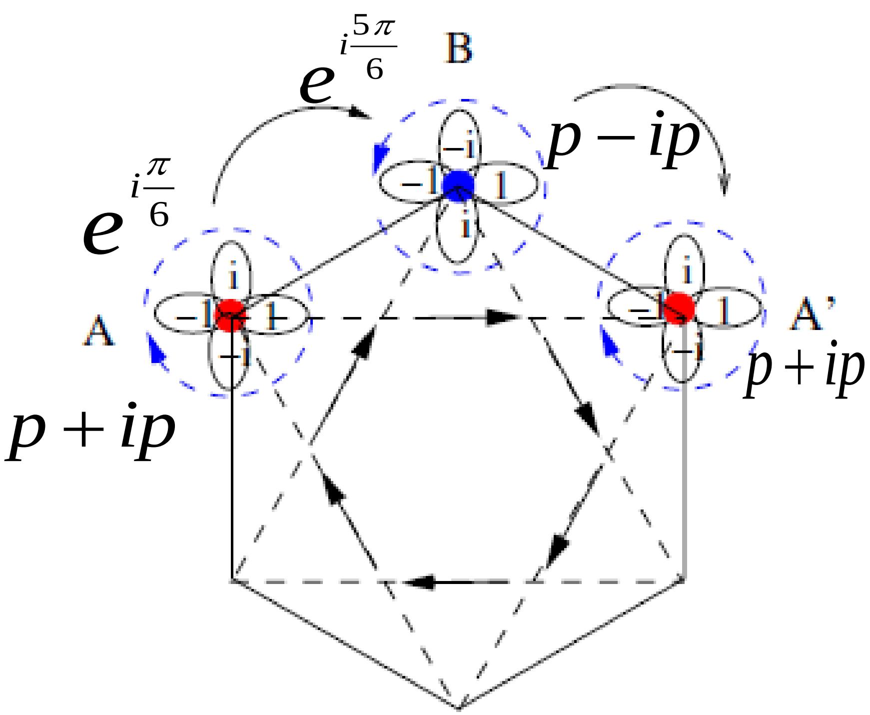
- The oscillation axis slowly precesses at the angular frequency of Ω .

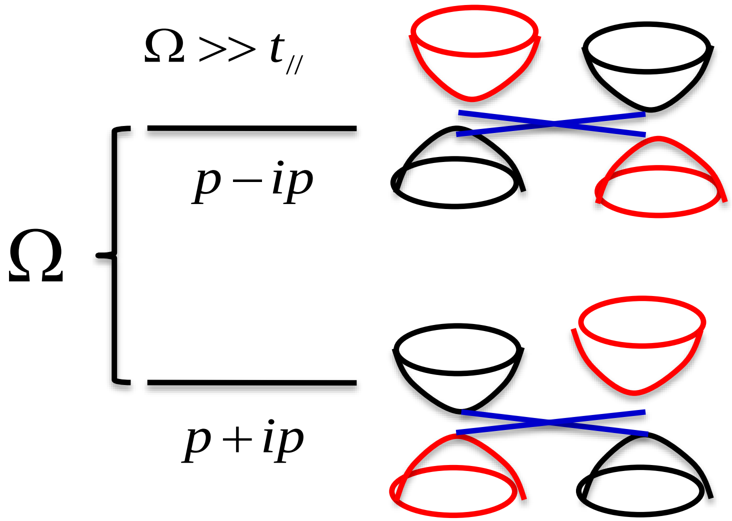
Large rotation angular velocity $\Omega >> t_{//}$

- The second order perturbation generates the NNN complex hopping.



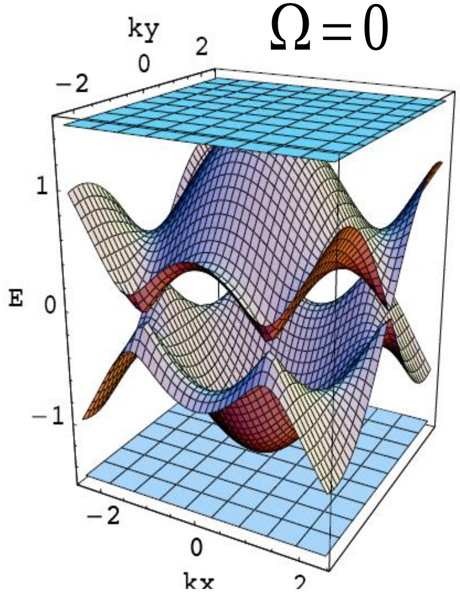
$$t' = -(te^{i2/3\pi})^2 / 2\Omega$$



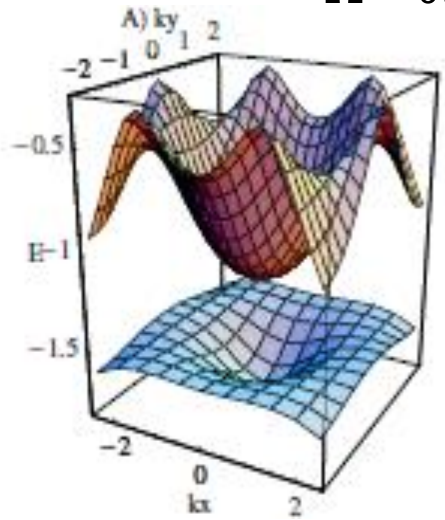


Small rotation angular velocity

$\Omega = 0$

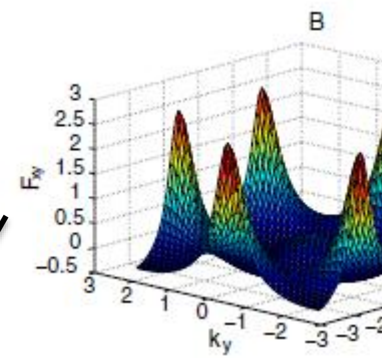


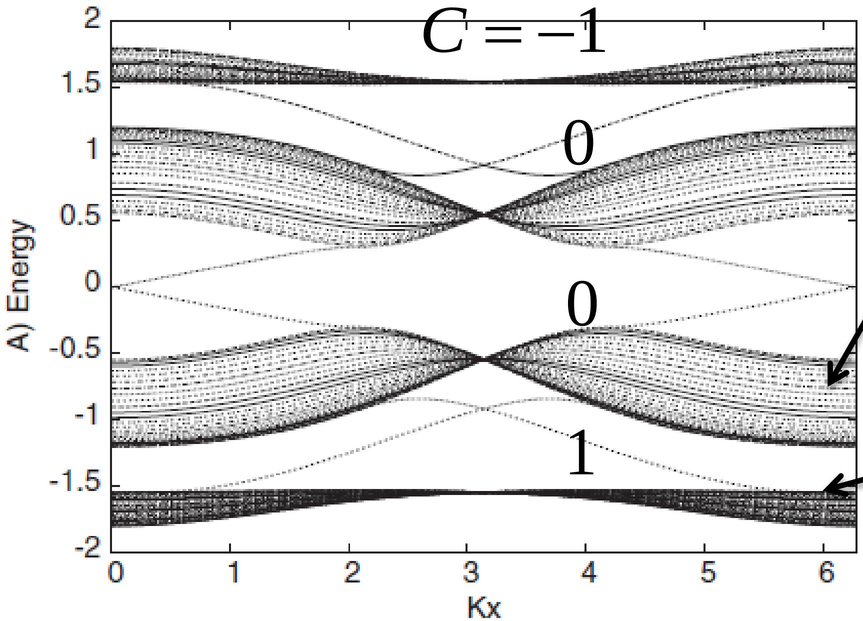
$\Omega = 0.3t_{//}$



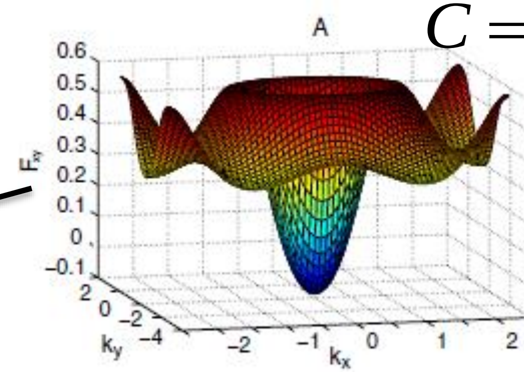
Berry curvature and Chern numbers

$C = 0$



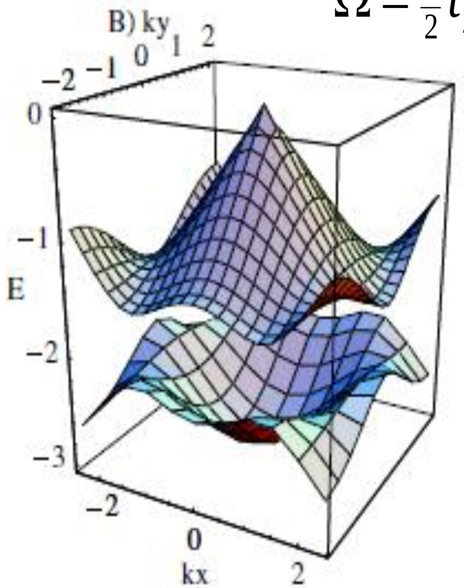


$C = 1$

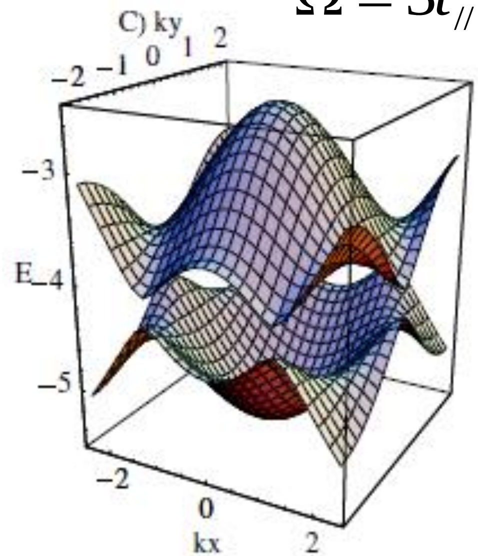


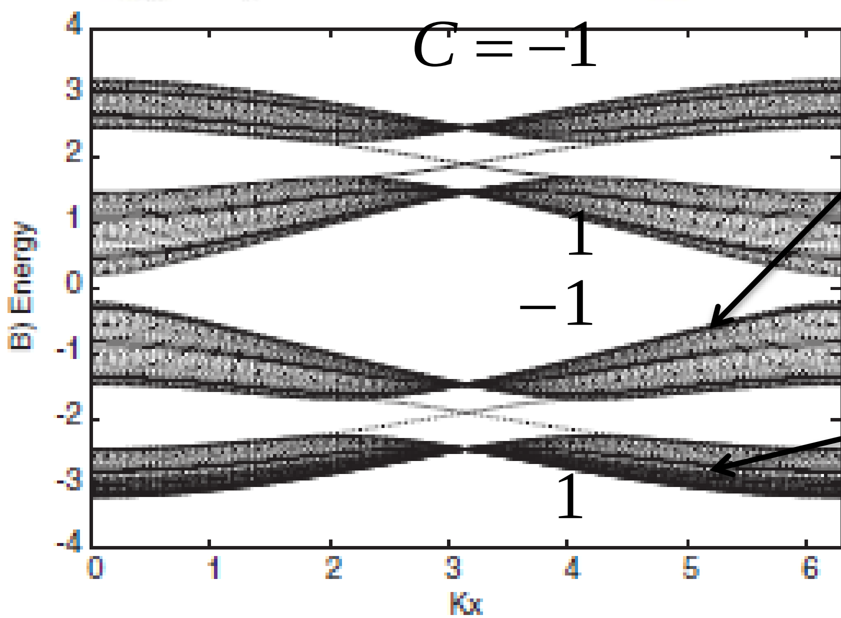
Large rotation angular velocity

$\Omega = \frac{3}{2} t_{//}$



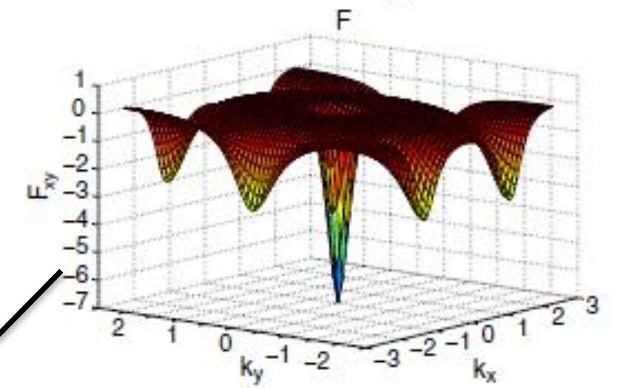
$\Omega = 3 t_{//}$



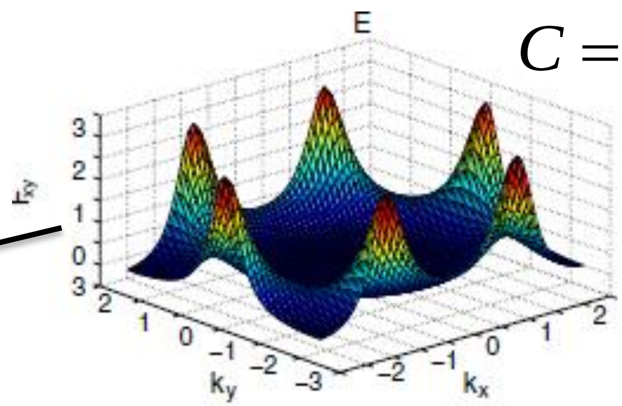


Berry curvature.

$C = -1$

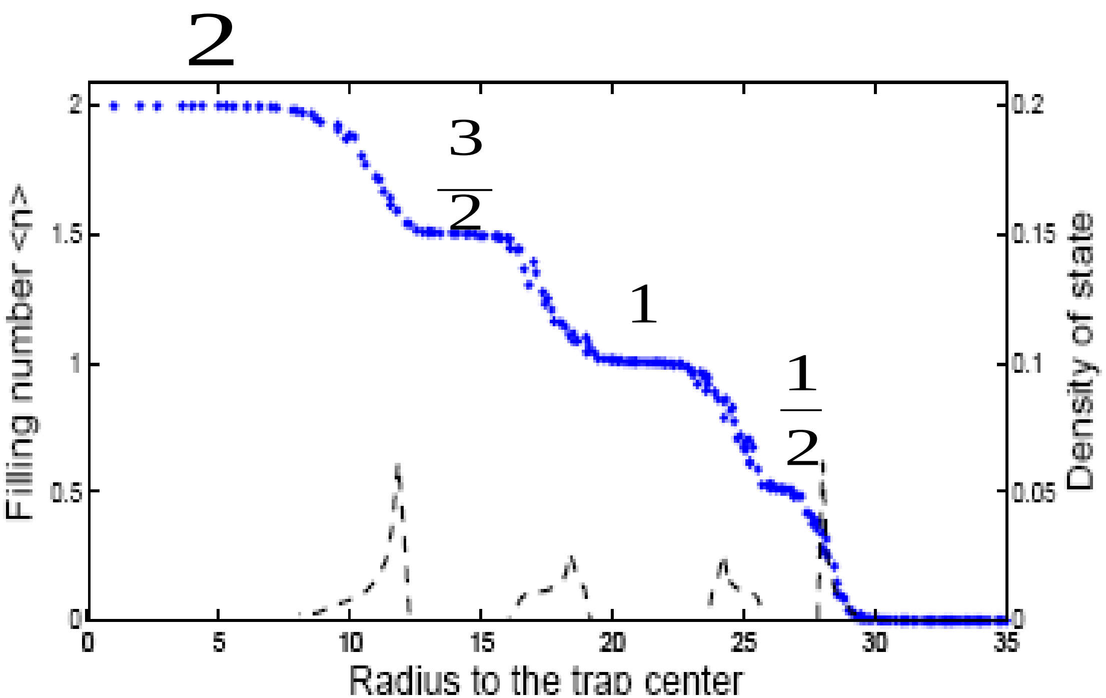


$C = 1$



Soft confining potential: exact diagonalization for the non-interacting system

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



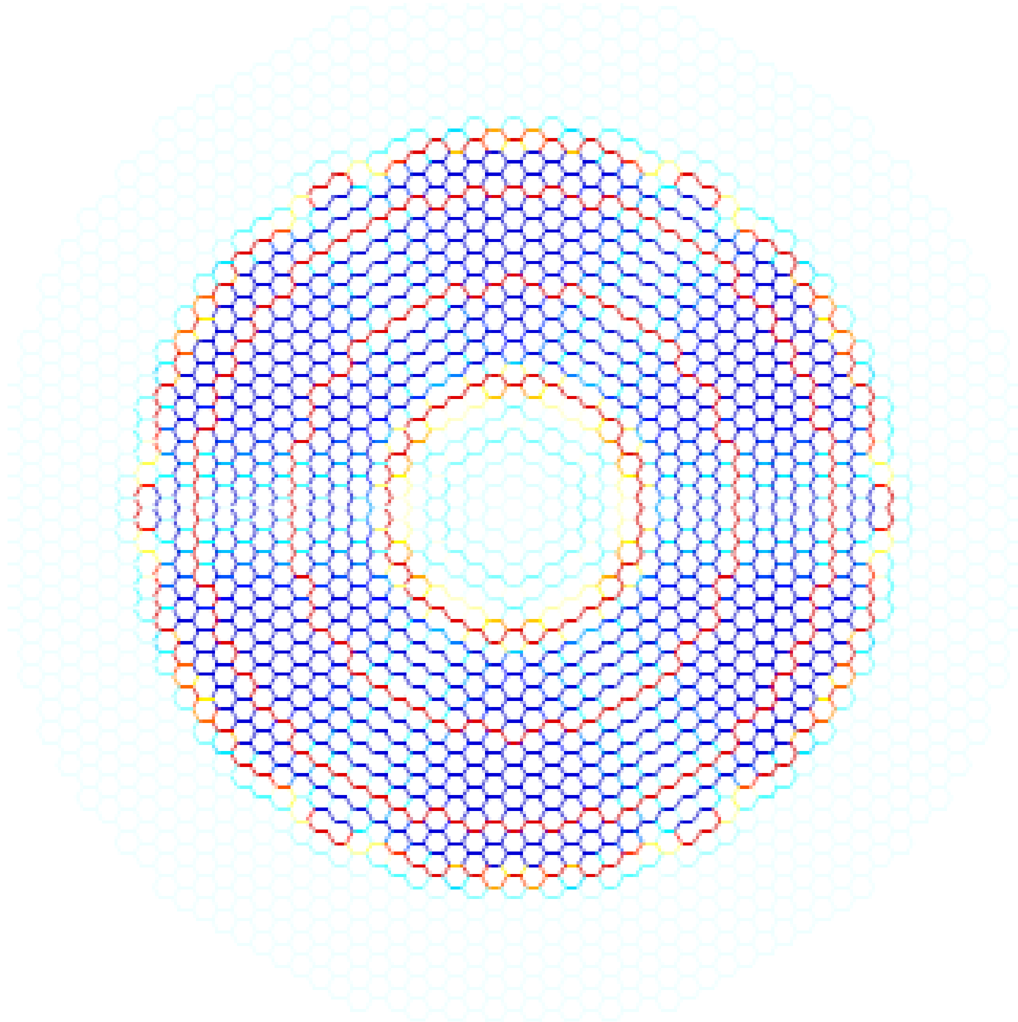
$(a)\Omega/t_{||} = \frac{1}{2}$

density profile: local density approx. works well.

$$V_t(r) = \tfrac{1}{2} m\omega_0^2 r^2$$

$$\mu(r) = \mu - V_{tr}(r)$$

Equilibrium Anomalous Hall currents in the trap

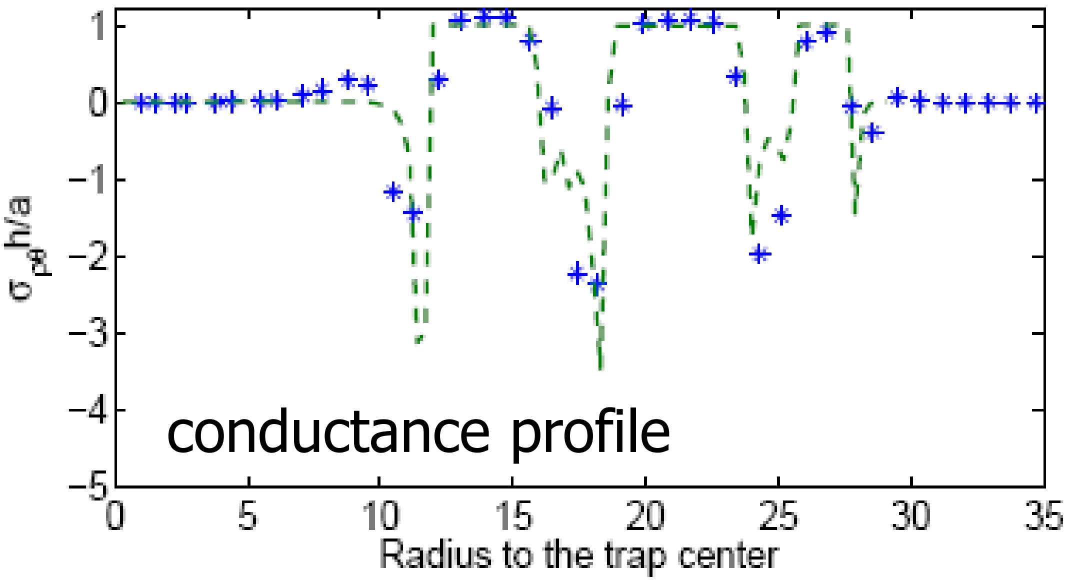


Quantized and non-quantized Hall conductance

- Normalized conductance is quantized in the plateaus.

$$\sigma_H = j_\theta / \tfrac{\partial V_{tr}(r)}{\partial r} = \frac{m}{2\pi h} \sum_n \int dk\, B_n(k_x, k_y)$$

- Metallic regime: reversed Hall current. Extra contribution from Hall diffusion current.



$(a)\Omega/t_\parallel = \frac{1}{2}$

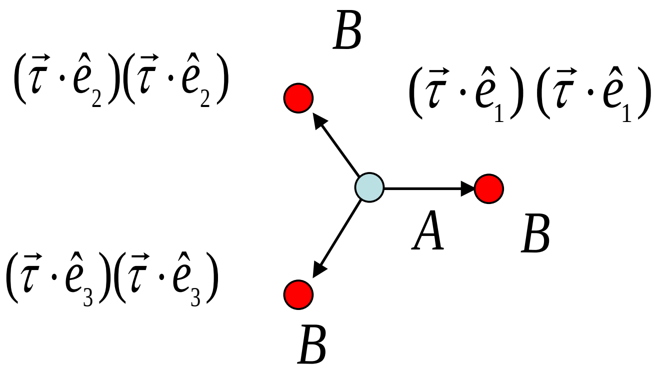
$$j_H = \sigma_H (F_{drift} + F_{diff})$$

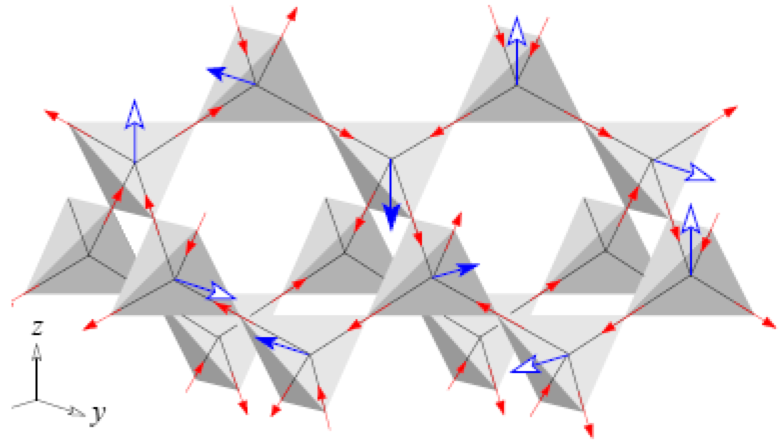
$$F = \partial_r [(\mu(r) - E_b) n(r)] / n(r)$$

$$= \partial_r \mu(r) + (\mu(r) - E_b) \partial_r \ln \mu(r)$$

Outline

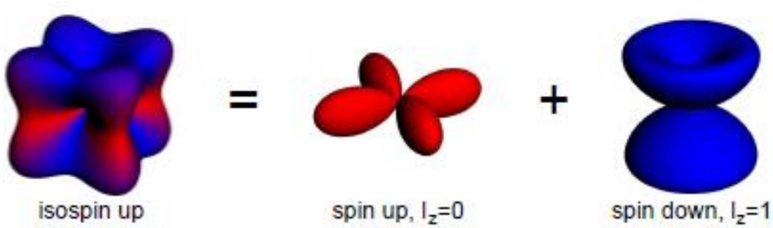
- Orbital exchange in the Mott-insulating state; orbital frustration: quantum 120 degree model; solvable quantum orbital ice.

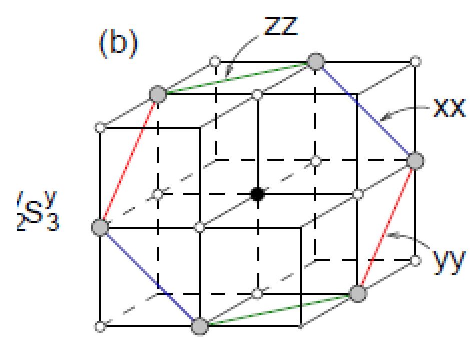




C. Wu, PRL 100, 200406 (2008).; G-W Chern, C. Wu, arix1104.1614

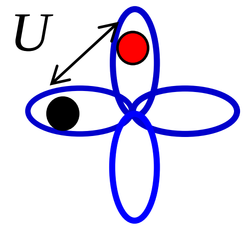
c.f. Khaliullin et al, PRL 2009



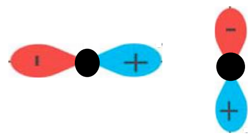


Mott insulator of SPINLESS fermions: orbital exchange

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

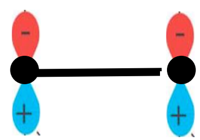


- Pseudo-spin representation.



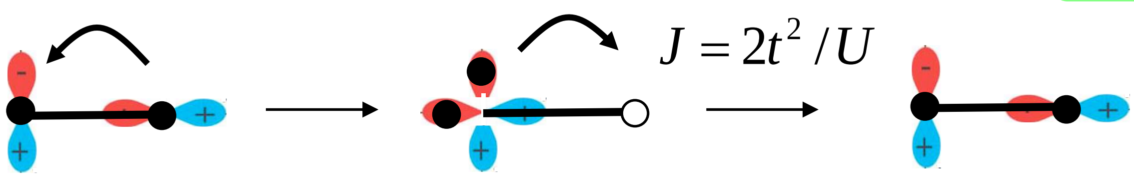
$$\tau_1 = \tfrac{1}{2}(p_x^+ p_x - p_y^+ p_y) \quad \tau_2 = \tfrac{1}{2}(p_x^+ p_y + p_y^+ p_x) \quad \tau_3 = \tfrac{i}{2}(p_x^+ p_y - p_y^+ p_x)$$

- Orbital exchange: no orbital flipping process.

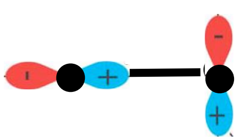


$J = 0$

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



$J = 2t^2 / U$

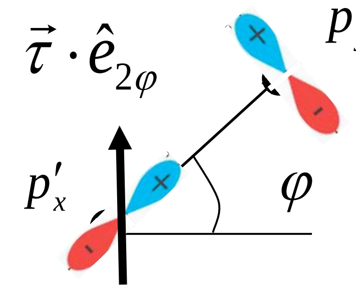


$J = 2t^2 / U$

Hexagon lattice: quantum 120° model

- Non-triviality: Ising quantization axis depends on bond orientation. For a bond along the general direction $\hat{e}_\varphi$,

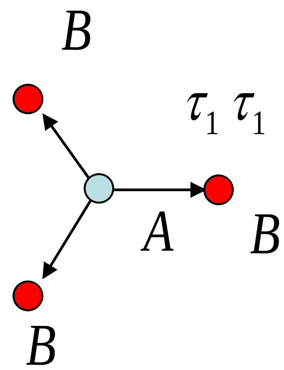
p'_x, p'_y : eigen-states of $\vec{\tau}\cdot\hat{e}_{2\varphi} = \cos 2\varphi\, \tau_x + \sin 2\varphi\, \tau_y$



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

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

$$(-\tfrac{1}{2}\tau_1 + \tfrac{\sqrt{3}}{2}\tau_2)(-\tfrac{1}{2}\tau_1 + \tfrac{\sqrt{3}}{2}\tau_2)$$



$$(-\tfrac{1}{2}\tau_1 - \tfrac{\sqrt{3}}{2}\tau_2)(-\tfrac{1}{2}\tau_1 - \tfrac{\sqrt{3}}{2}\tau_2)$$

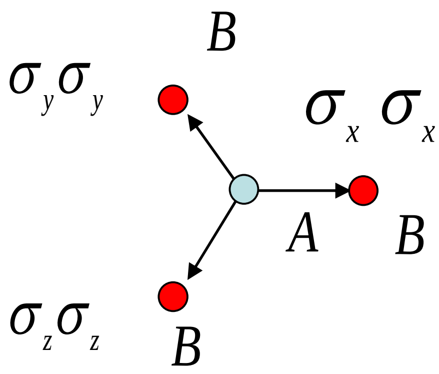
$$H_{ex} = -\sum_{r,r'} J(\vec{\tau}(r_i)\cdot\hat{e}_{ij})\,(\vec{\tau}(r'_j)\cdot\hat{e}_{ij})$$

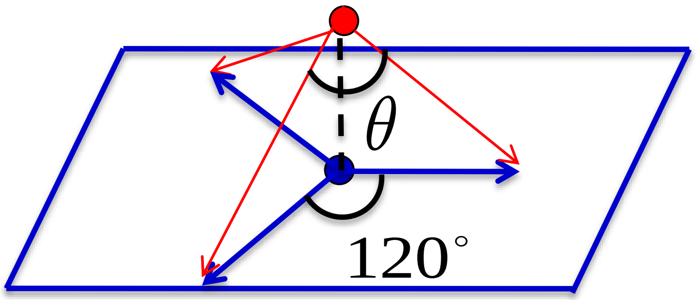
C. Wu et al, arxiv0701711v1; C. Wu, PRL 100, 200406 (2008). E. Zhao, and W. V. Liu, Phys. Rev. Lett. 100, 160403 (2008)

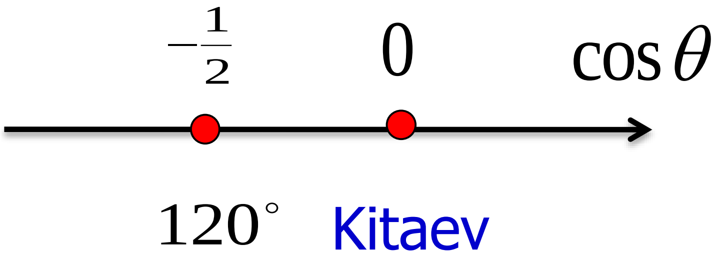
From the Kitaev model to 120 degree model

- cf. Kitaev model: Ising quantization axes form an orthogonal triad.

$$H_{kitaev} = -J \sum_{r \in A} (\sigma_x(r)\sigma_x(r+e_1) + \sigma_y(r)\sigma_y(r+e_2)$$
$$+\sigma_z(r)\sigma_z(r+e_3))$$



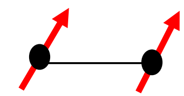




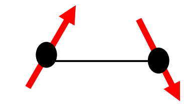
Large S picture: heavy-degeneracy (frustration) of classic ground states

- Ground state constraint: the two τ-vectors have the same projection along the bond orientation.

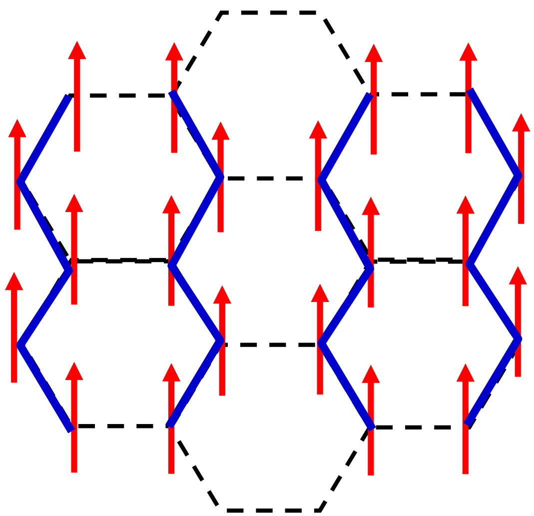
$$H_{ex} = \sum_{r,r'} J\{[(\vec{\tau}(r) - \vec{\tau}(r')] \cdot \hat{e}_{rr'}\}^2 + J\sum_{r} \tau_z^2(r)$$



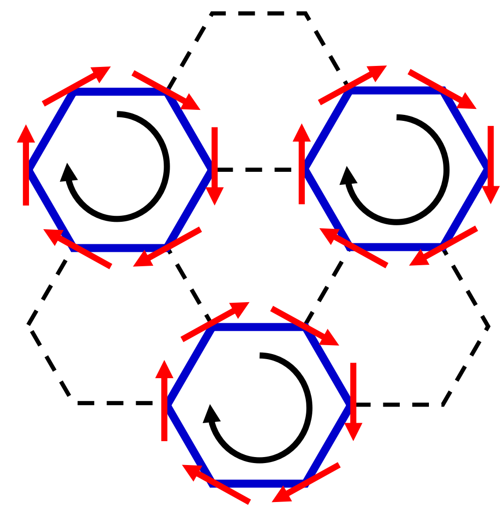
or



- Ferro-orbital configurations.

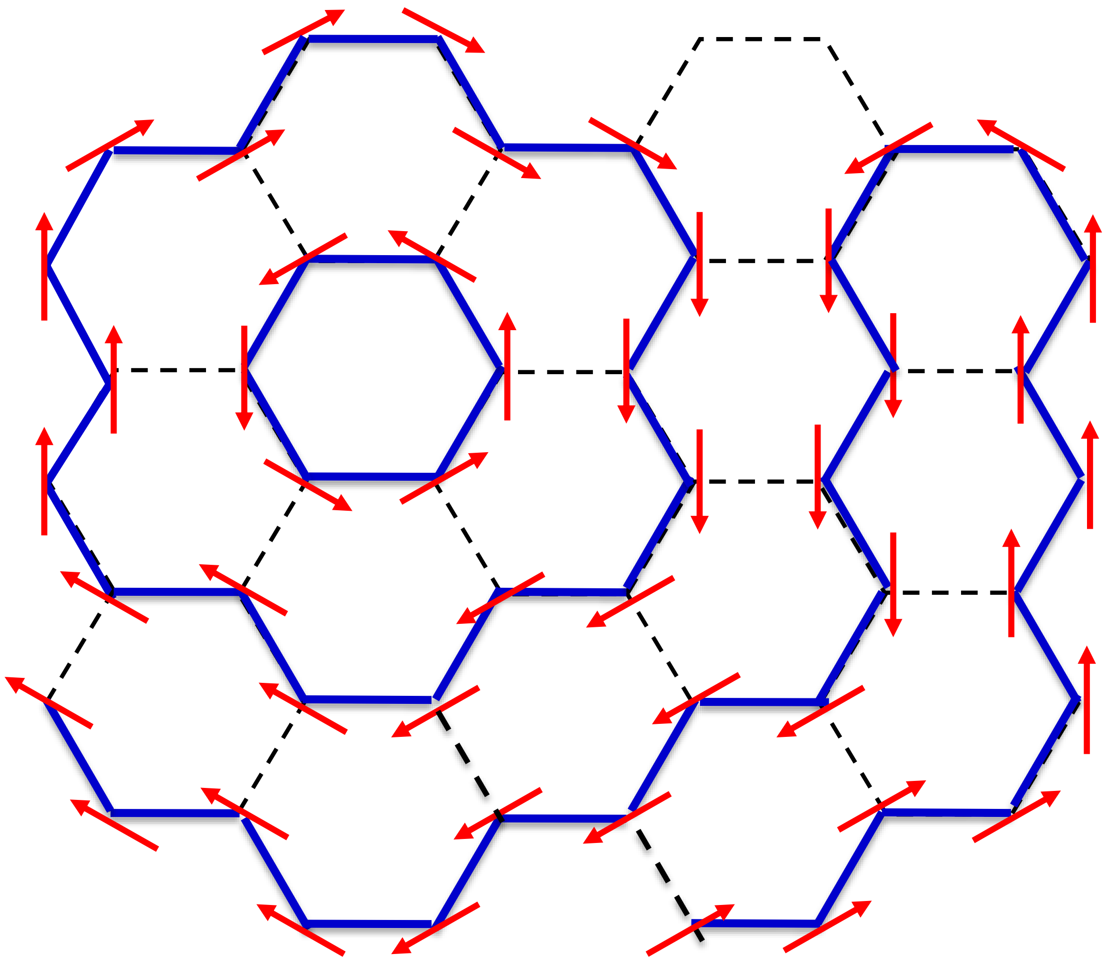


- Loop config: τ-vectors along the tangential directions.



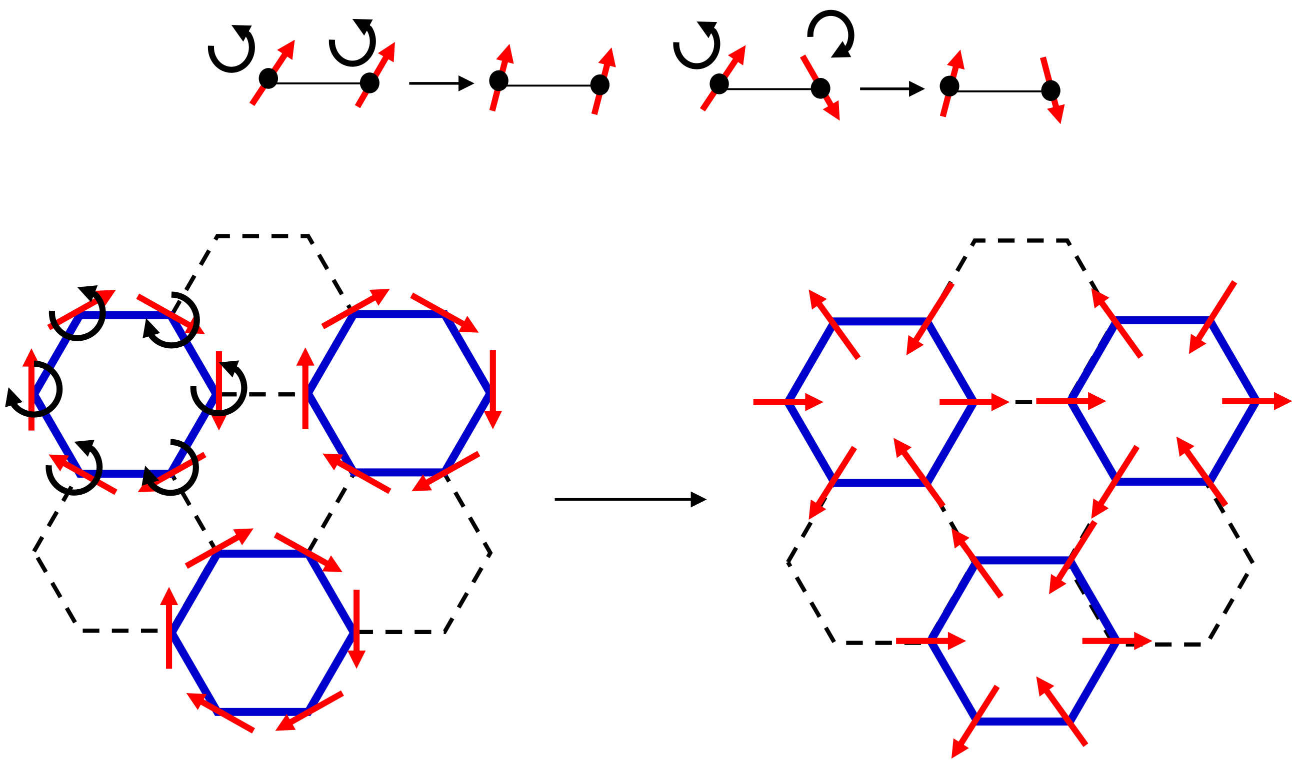
Heavy-degeneracy of the classic ground states

- General loop configurations

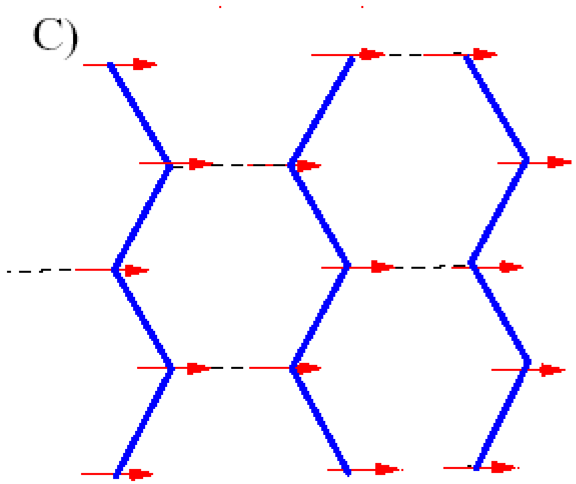


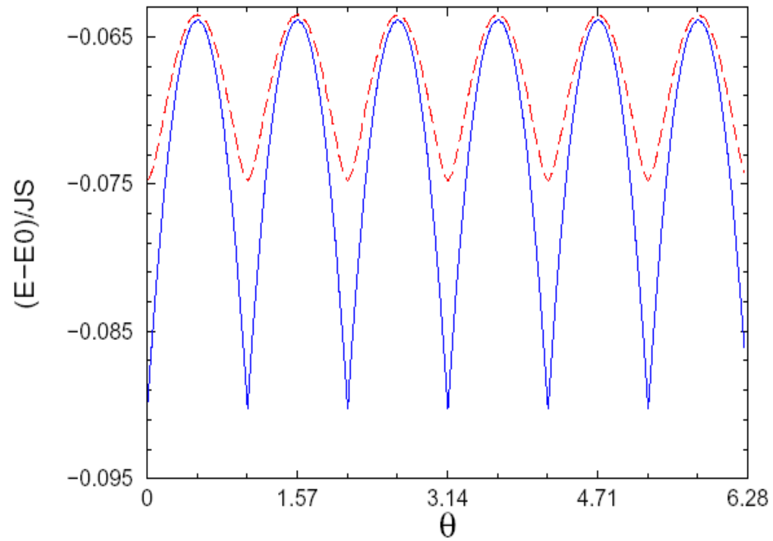
Global rotation degree of freedom

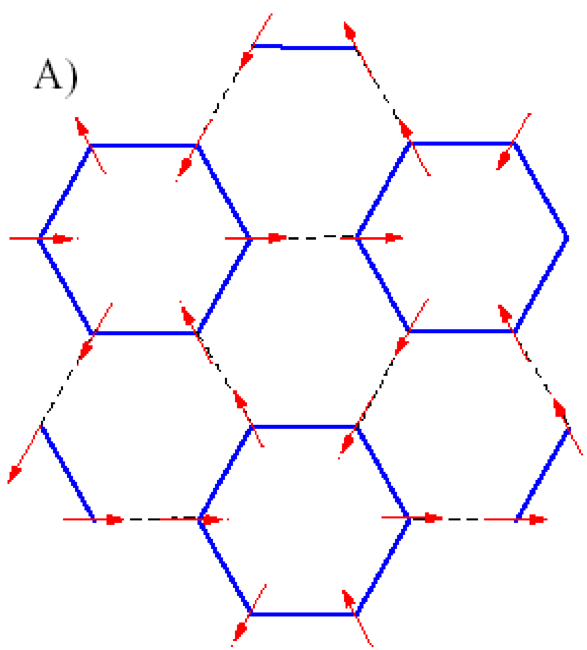
- Each loop config remains in the ground state manifold by a suitable arrangement of clockwise/anticlockwise rotation patterns.

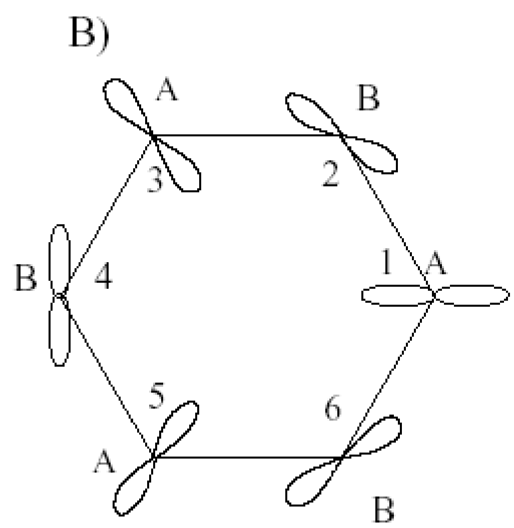


“Order from disorder”: 1/S orbital-wave correction



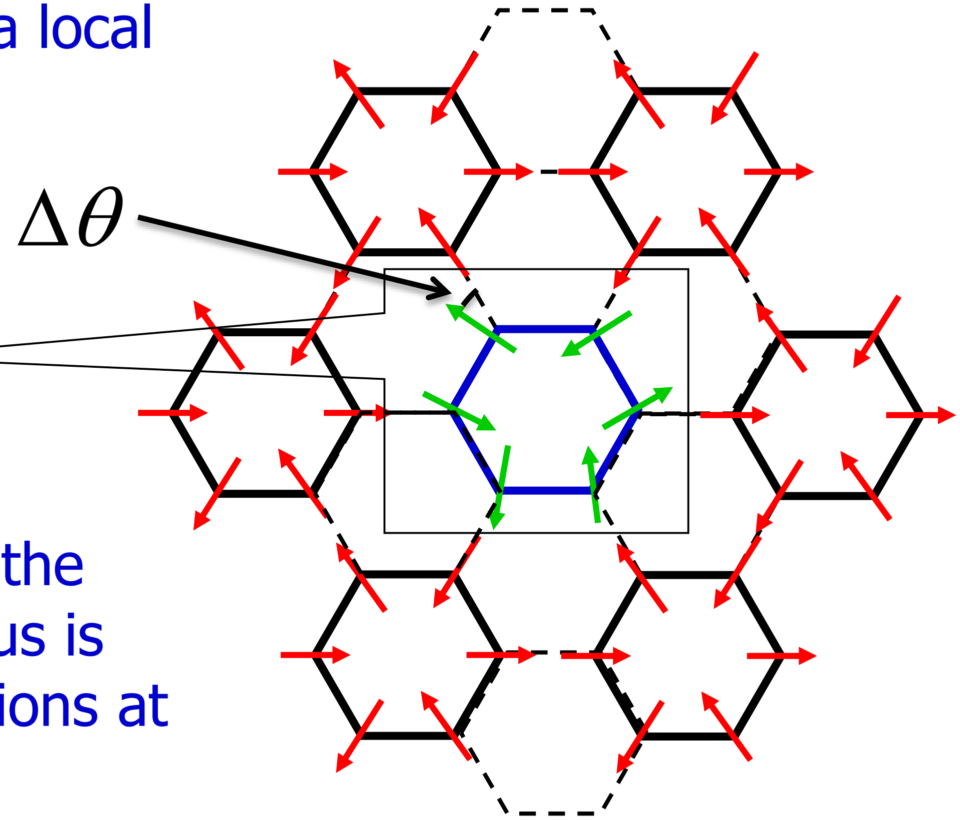






Zero energy flat band orbital fluctuations

- 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.

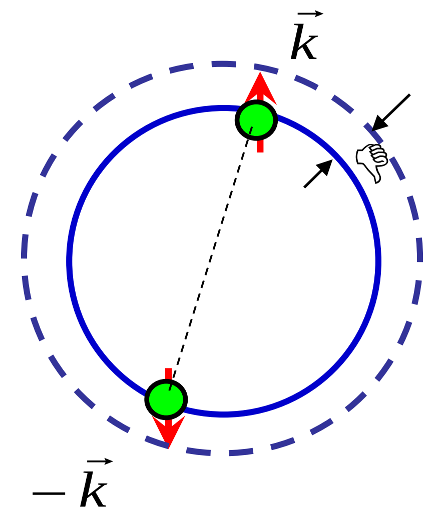
- Orbital fermions in the hexagonal lattice.

Ferromagnetism from band flatness.

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

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

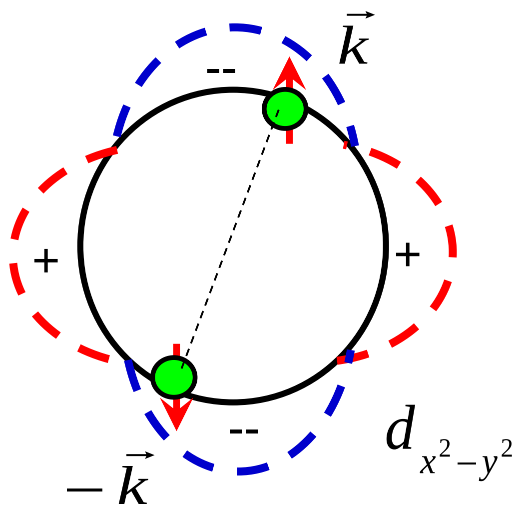
Conventional v.s. unconventional Cooper pairings

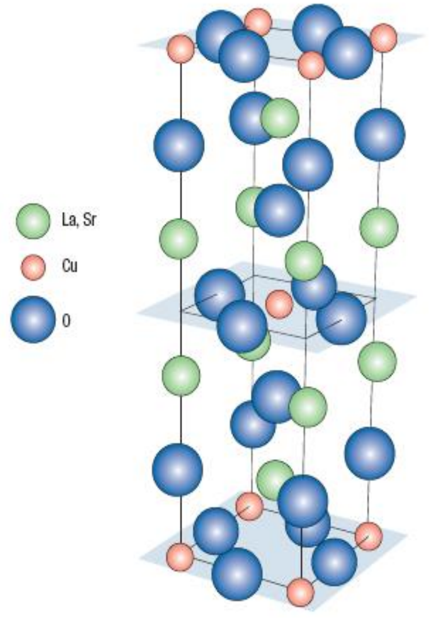


- Conventional superconductivity:

  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}He-A and B; Sr_2RuO_4;

d-wave: high T_c cuprates;

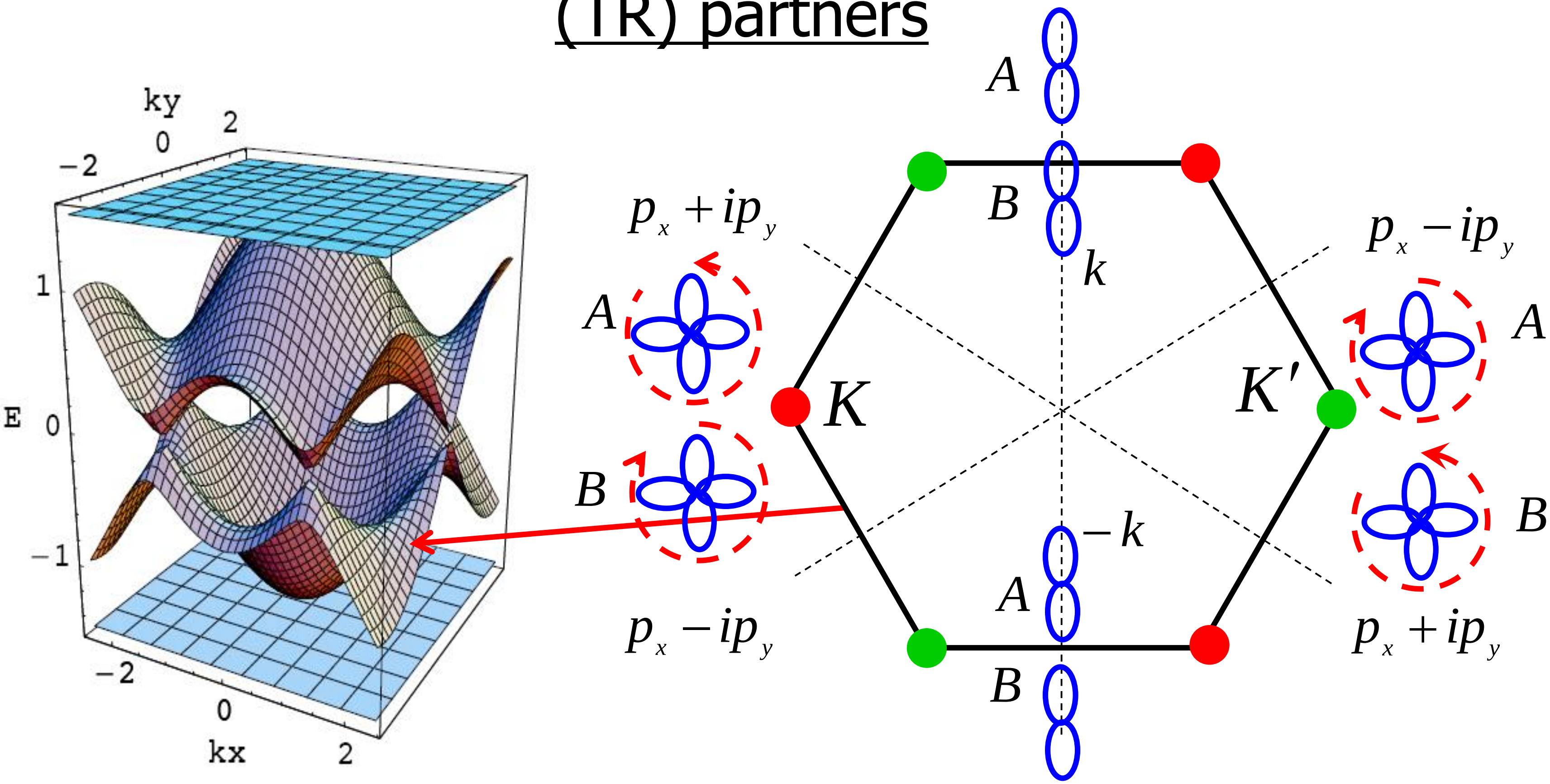
Extended s-wave: iron-pnictide superconductors (?);

- 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.

Nontrivial orbital configurations between time reversal (TR) partners

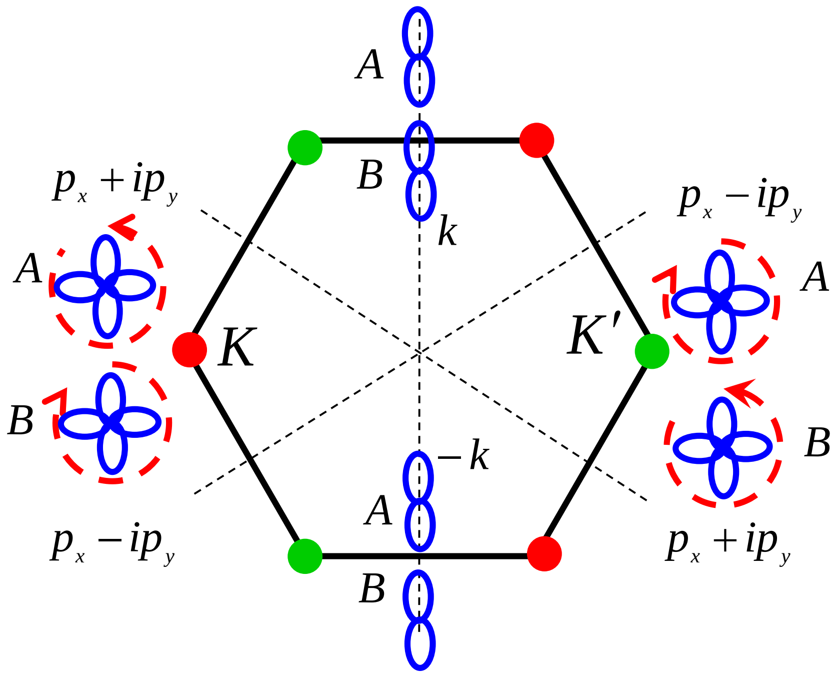


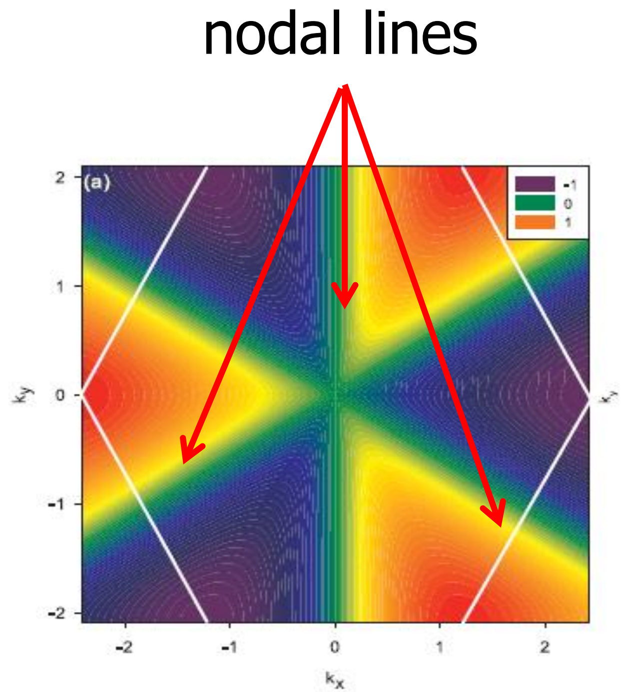
- Along the three middle lines of Brillouin zone, eigen-orbitals are real.

- At K and K′, eigen-orbitals are complex and orthognoal.

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.

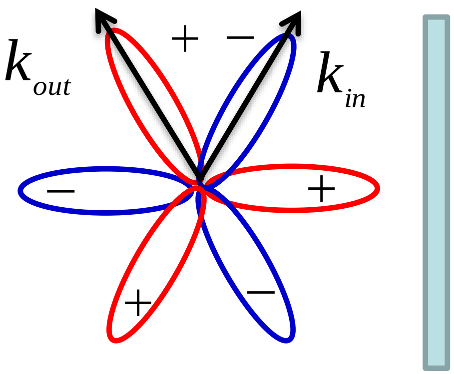


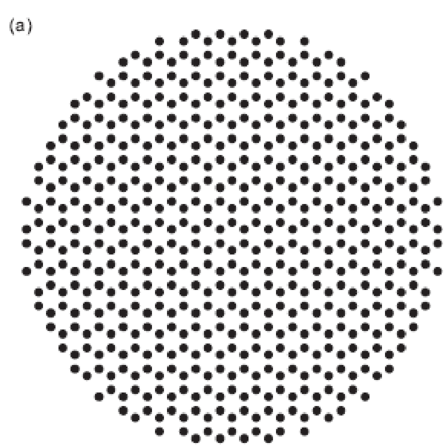


- The mean-field gap value can reach 10nK; and the 2D Kosterlitz-Thouless temperature can reach 1nK.

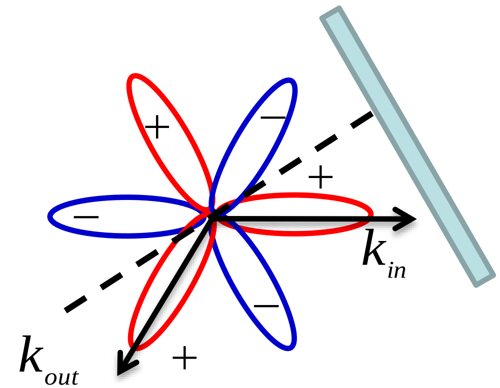
Phase sensitive detection: zero energy Andreev bound states

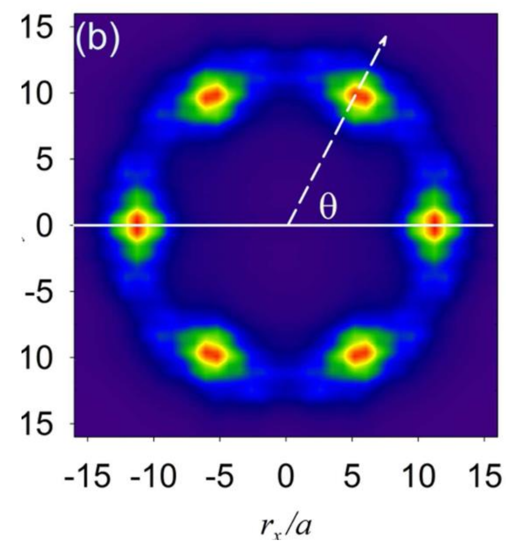
With zero energy Andreev Bound States





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.