Novel Orbital Phases of Fermions in *p*-band Optical Lattices

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W. C. Lee, C. Wu, S. Das Sarma, in preparation.
C. Wu, PRL 101, 168807 (2008).
C. Wu, PRL 100, 200406 (2008).
C. Wu, and S. Das Sarma, PRB 77, 235107 (2008).
S. Zhang , H. H. Hung, and C. Wu, arXiv:0805.3031.
C. Wu, D. Bergman, L. Balents, and S. Das Sarma, PRL 99, 67004(2007).

Collaborators: L. Balents, D. Bergman, S. Das Sarma, H. H. Hung, W. C. Lee, S. Zhang.

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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;

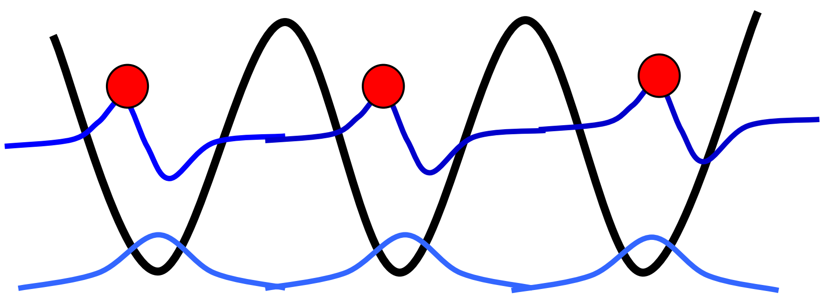
Multi-component bosons and fermions;

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 (NIST); polariton lattice (Stanford).

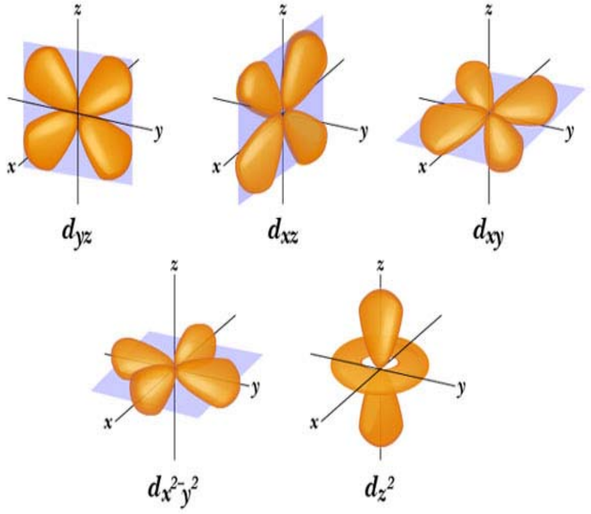


Orbital physics

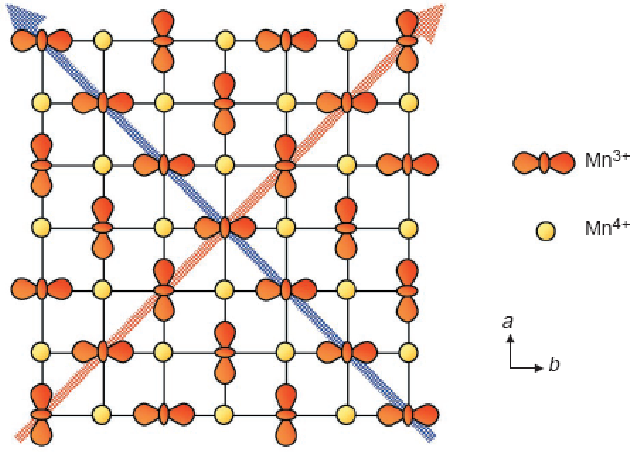
- Orbital: a degree of freedom independent of charge and spin.

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

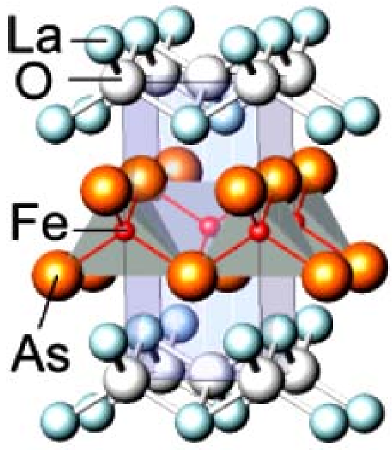
- Orbital band degeneracy and spatial anisotropy.



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



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



LaOFeAs

Advantages of optical lattice orbital systems

- Solid state orbital systems:

Jahn-Teller distortion quenches orbital degree of freedom;

only fermions;

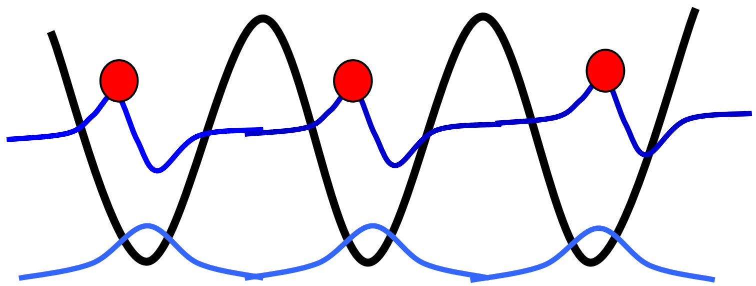
correlation effects in *p*-orbitals are weak.

- Optical lattices orbital systems:

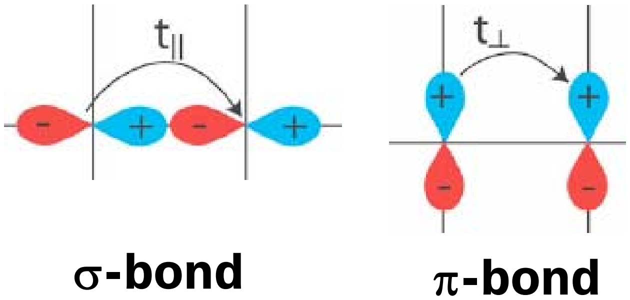
rigid lattice free of distortion;

both bosons (meta-stable excited states with long life time) and fermions;

strongly correlated $p_{x,y}$-orbitals: stronger anisotropy



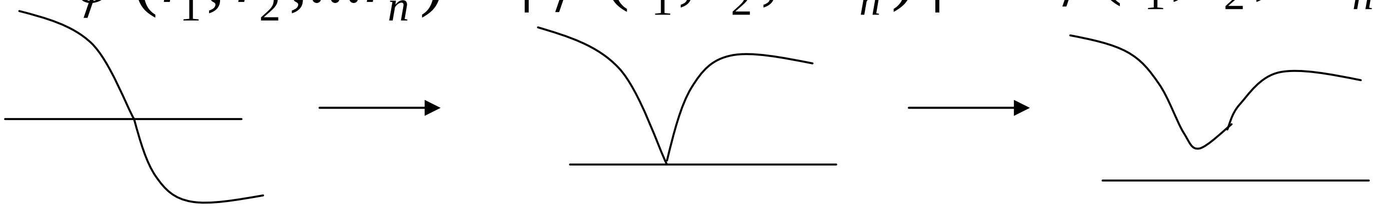
$$t_{//} >> t_{\perp}$$



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.

$$\psi(r_1, r_2, \ldots r_n) \qquad |\psi(r_1, r_2, \ldots r_n)| \qquad \phi(r_1, r_2, \ldots r_n) > 0$$



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

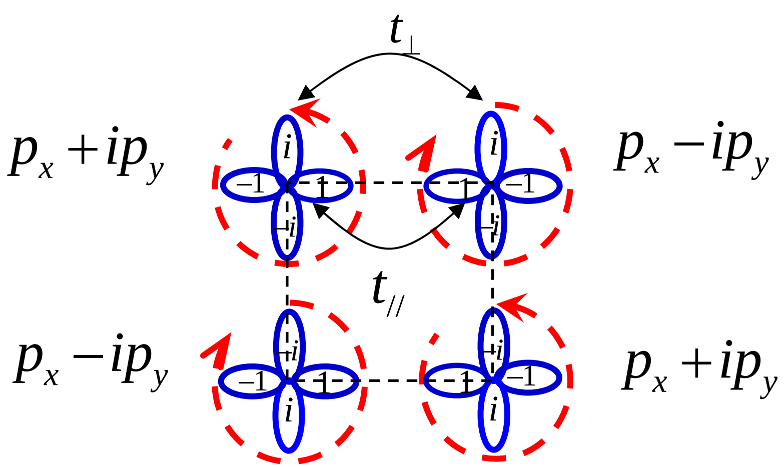
• Strong constraint: complex-valued WF → positive definite WF; time-reversal symmetry cannot be broken.

• Feynman's statement applies to all of superfluid, Mott-insulating, super-solid, density-wave ground states, etc.

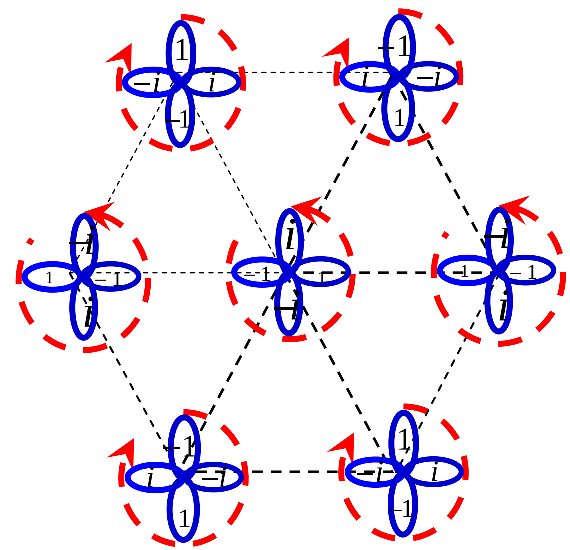
Orbital bosons: complex condensates beyond the no-node theorem

- Spontaneous time reversal symmetry breaking; orbital Hund's rule interaction.

W. V. Liu and C. Wu, PRA 74, 13607 (2006);
C. Wu, Mod. Phys. Lett. 23, 1 (2009).



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



Other group's related work: Ofir Alon et al, PRL 95 2005. V. W. Scarola et. al, PRL, 2005; A. Isacsson et. al., PRA 2005; A. B. Kuklov, PRL 97, 2006; C. Xu et al., cond-mat/0611620 .

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);
C. Wu et al, PRL 99, 67004(2007).
Shizhong Zhang and C. Wu, arXiv:0805.3031.

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

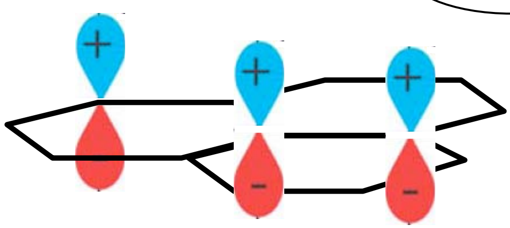
C. Wu et al, arxiv0701711v1; C. Wu, PRL 100, 200406 (2008).

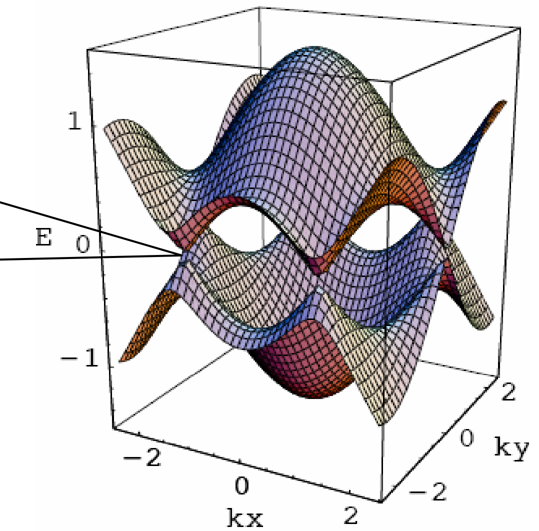
- Topological insulators in the p-band – orbital analogue of anomalous quantum Hall effect.

C. Wu, PRL 101, 186807 (2008).

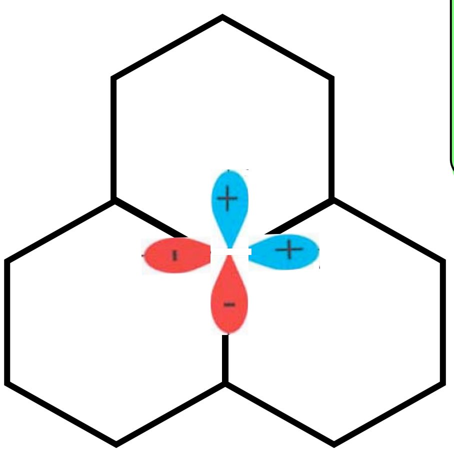
p-orbital fermions in honeycomb lattices

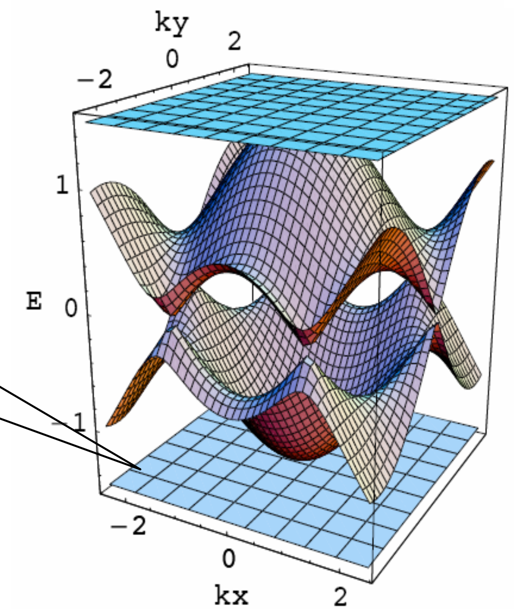
cf. graphene: a surge of research interest; p_z-orbital; Dirac cones.





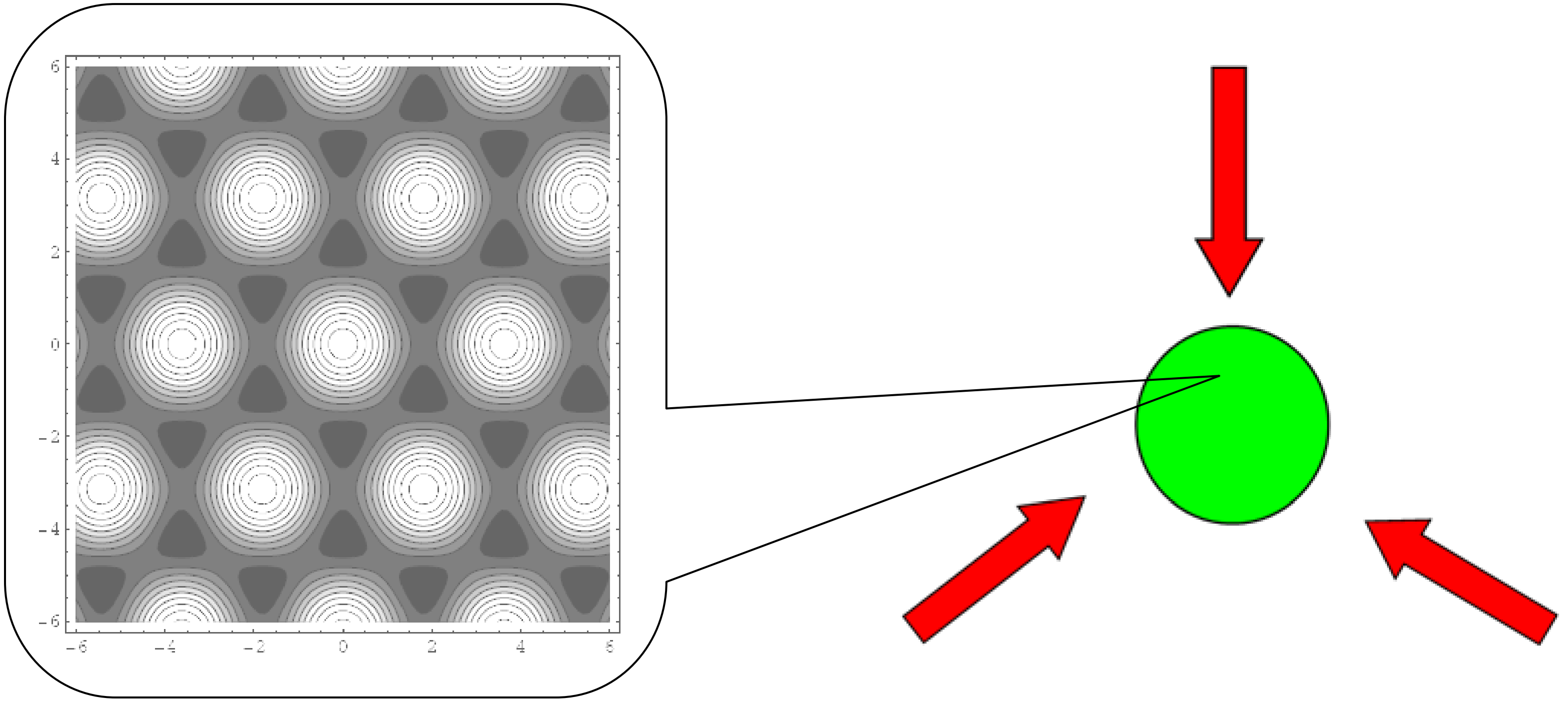
p_{xy}-orbital: flat bands; interaction effects dominate.





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

Honeycomb optical lattice with phase stability

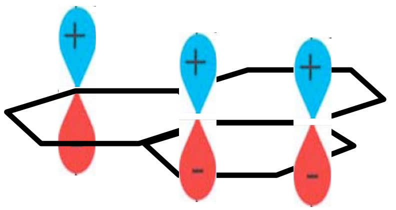


- Three coherent laser beams polarizing in the z-direction.
- Laser phase drift only results an overall lattice translation without distorting the internal lattice structure.

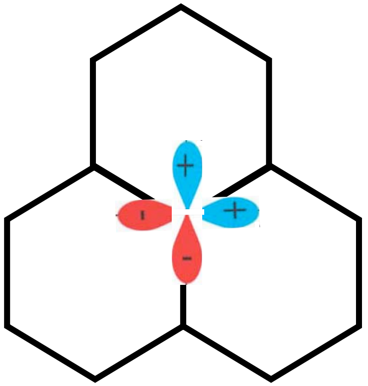
G. Grynberg et al., Phys. Rev. Lett. **70**, 2249 (1993).

What is the fundamental difference from graphene?

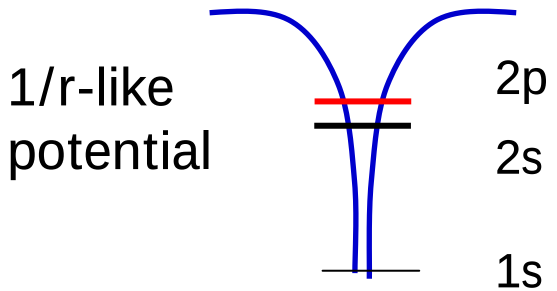
- p_z-orbital band is not a good system for orbital physics.



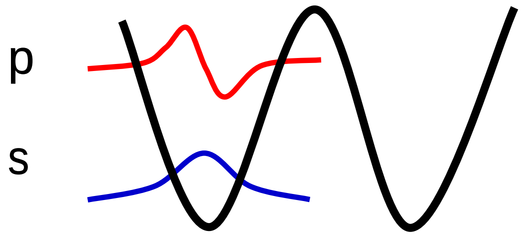
- It is the other two p_x and p_y orbitals that exhibit anisotropy and degeneracy.



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

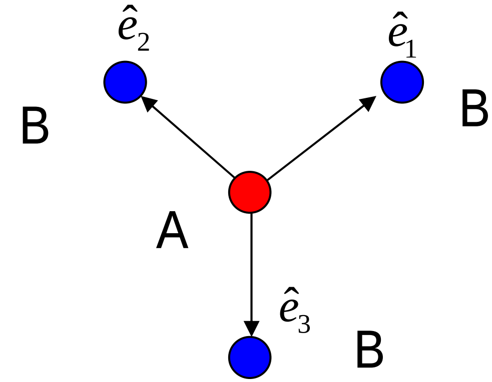


- In optical lattices, p_x and p_y-orbital bands are well separated from s.

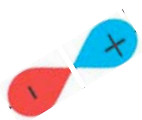


Artificial graphene in optical lattices

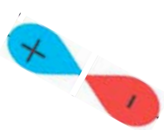
- Band Hamiltonian (σ-bonding) for spin-polarized fermions.



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

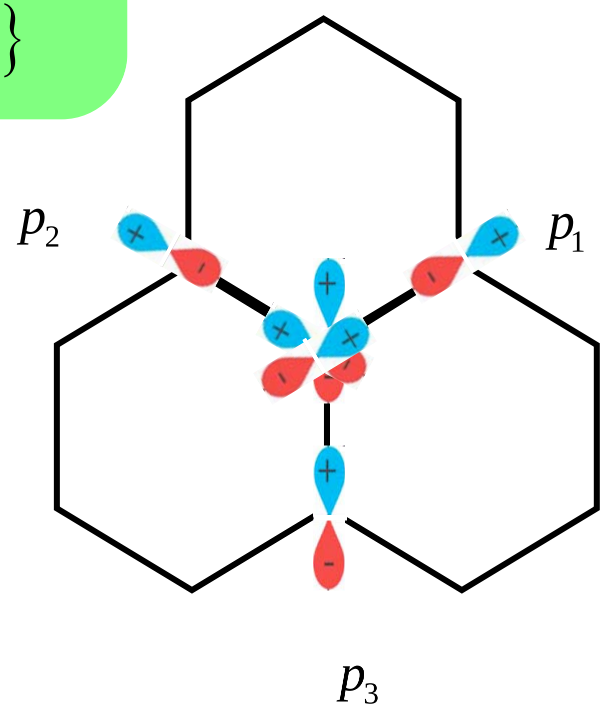


$$p_1 = \tfrac{\sqrt{3}}{2} p_x + \tfrac{1}{2} p_y$$

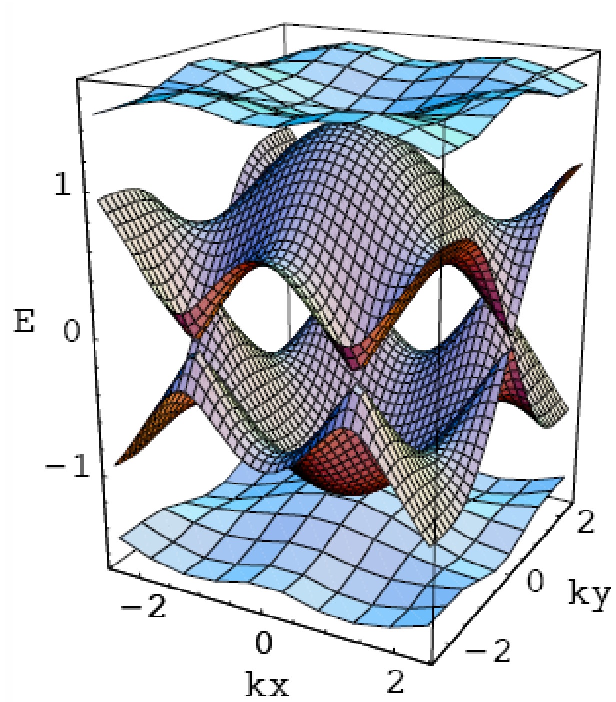


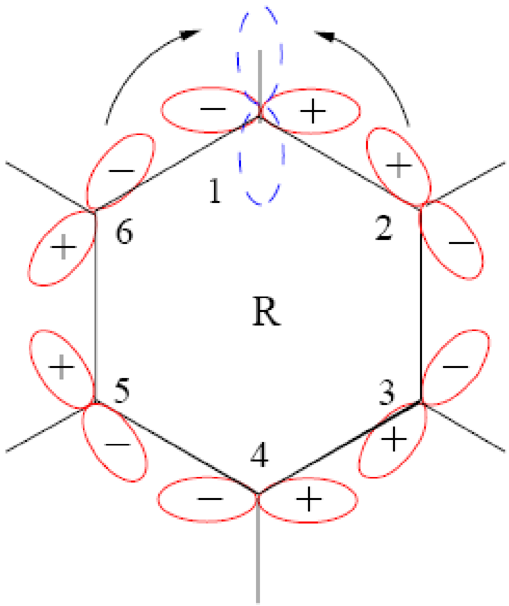
$$p_2 = -\tfrac{\sqrt{3}}{2} p_x + \tfrac{1}{2} p_y$$

$$p_3 = -p_y$$



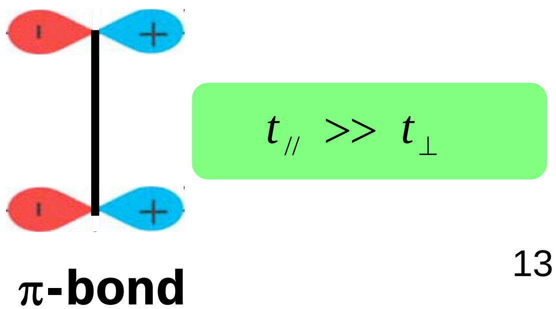
Flat bands in the entire Brillouin zone!





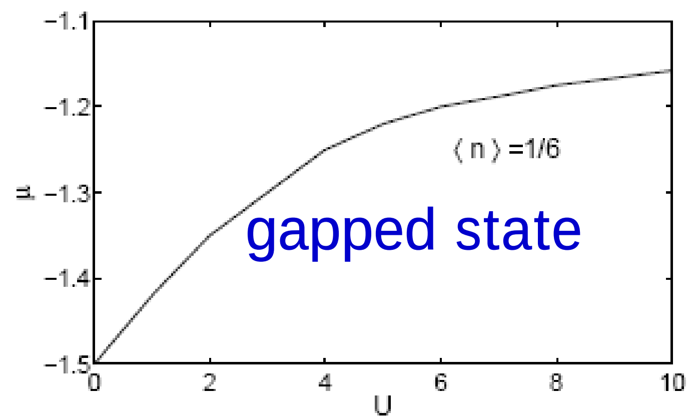
- Flat band + Dirac cone.
- localized eigenstates.

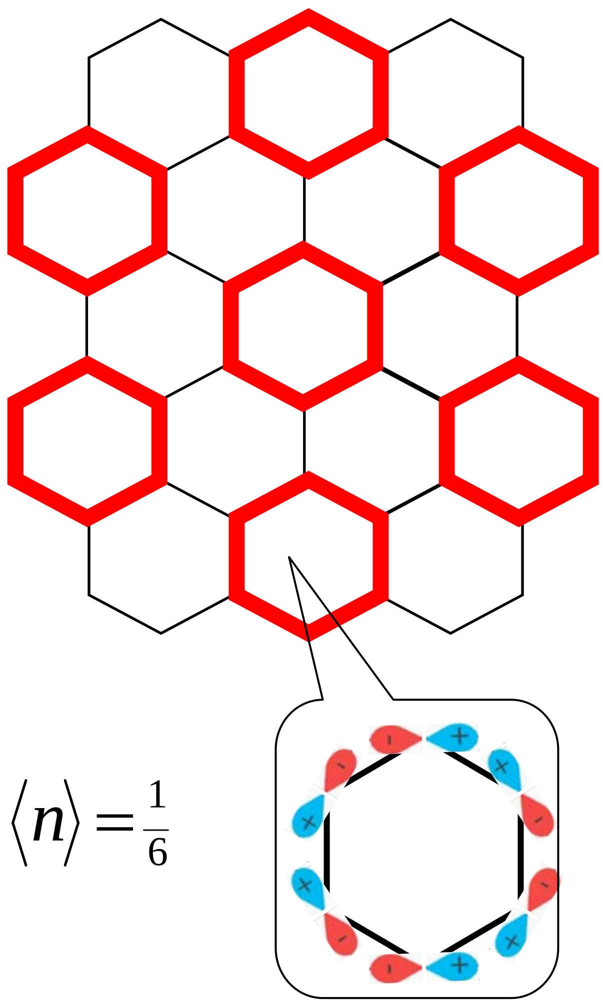
- If π-bonding is included, the flat bands acquire small width at the order of $t_\perp$. Realistic band structures show $t_\perp / t_{//} \to 1\%$



Hubbard model for spinless fermions: Exact solution: Wigner crystallization

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



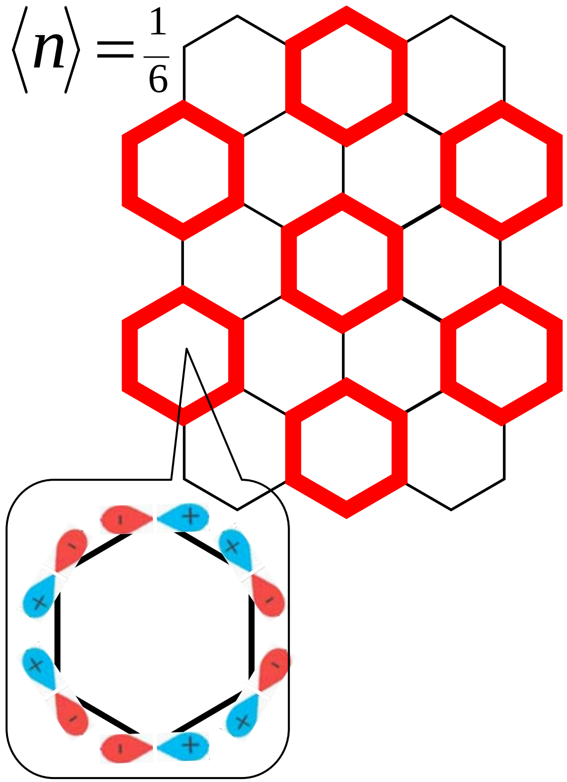


$$\langle n \rangle = \frac{1}{6}$$

- 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

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

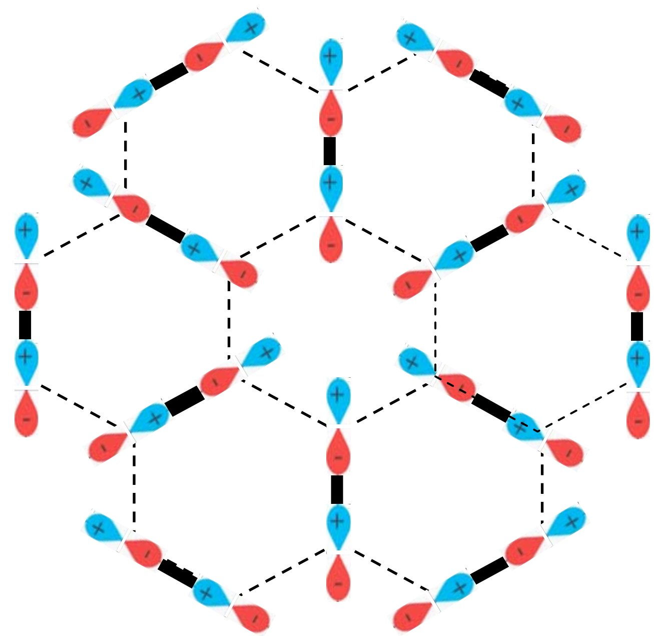


• Spinless fermions with onsite replusion: close-packed hexagons; avoiding repulsion.

• Gapped state which is stable even with small $t_\perp$.

• The result is also valid for bosons.

• Dimerization at <n>=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.

A. Mielke and H. Tasaki, Comm. Math. Phys 158, 341 (1993).

• 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**.

Shizhong Zhang and C. Wu, arXiv:0805.3031.

Novel states of orbital fermions (honeycomb lattice)

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

  non-perturbative effects from band flatnes

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

  C. Wu, and S. Das Sarma, PRB 77, 235107(2008);
  C. Wu et al, PRL 99, 67004(2007).
  Shizhong zhang and C. Wu, arXiv:0805.3031.

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

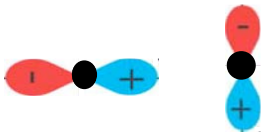
  C. Wu, PRL 100, 200406 (2008);   C. Wu et al, arxiv0701711v1;
  E. Zhao, and W. V. Liu, Phys. Rev. Lett. 100, 160403 (2008).

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

  C. Wu, PRL 101, 186807 (2008).

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

- Pseudo-spin representation.

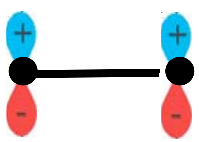


$$\tau_1 = \tfrac{1}{2}(p_x^+ p_x - p_y^+ p_y) \quad \tau_2 = \tfrac{1}{2}(p_x^+ p_y + p_y^+ p_x) \quad \tau_3 = \tfrac{i}{2}(p_x^+ p_y - p_y^+ p_x)$$

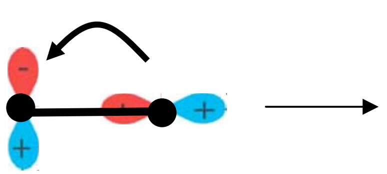
- No orbital-flip process. Antiferro-orbital Ising exchange.

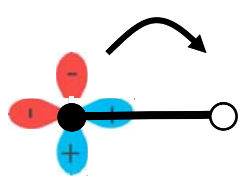
$J = 0$

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

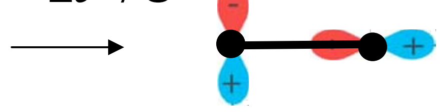


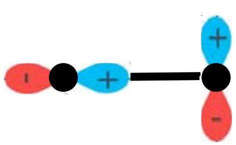
$J = 0$





$J = 2t^2/U$





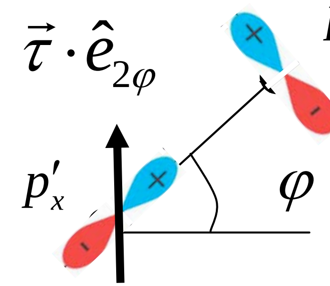
$J = 2t^2/U$

Hexagon lattice: quantum 120° model

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

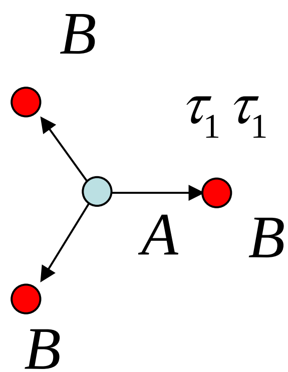
p'_x, p'_y : eigen-states of $\vec{\tau}\cdot\hat{e}_{2\varphi} = \cos 2\varphi\,\tau_x + \sin 2\varphi\,\tau_y$

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



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

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



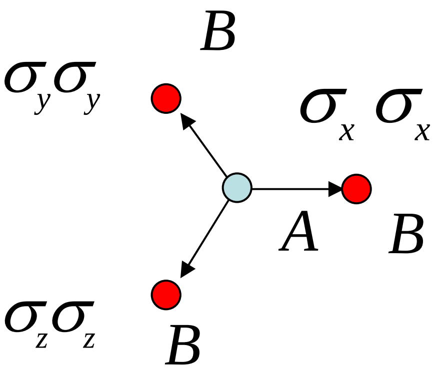
$$(-\tfrac{1}{2}\tau_1-\tfrac{\sqrt{3}}{2}\tau_2)(-\tfrac{1}{2}\tau_1-\tfrac{\sqrt{3}}{2}\tau_2)$$

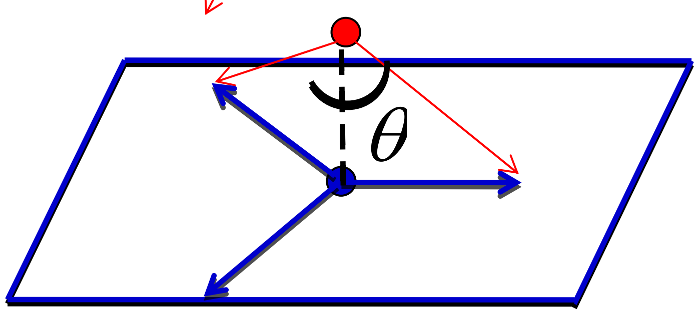
$$H_{ex} = -\sum_{r,r'} J(\vec{\tau}(r_i)\cdot\hat{e}_{ij})\,(\vec{\tau}(r'_j)\cdot\hat{e}_{ij})$$

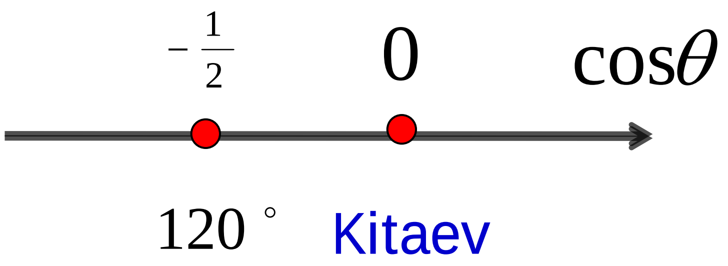
From the Kitaev model to 120 degree model

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

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



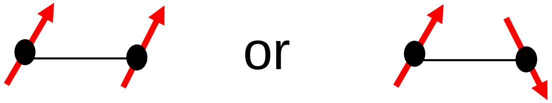




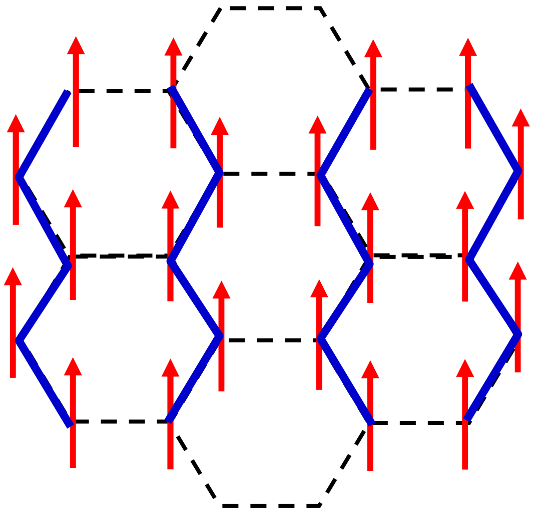
Large S picture: heavy-degeneracy of classic ground states

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

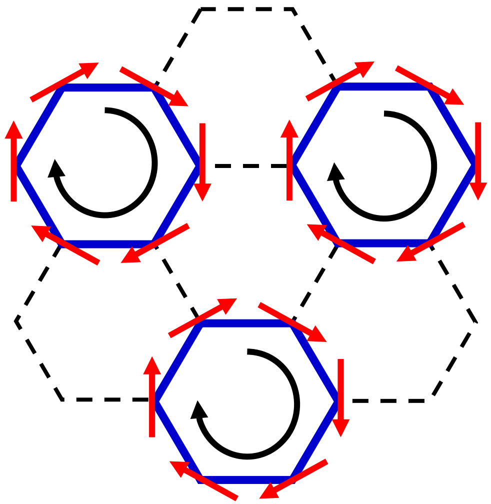
$$H_{ex} = \sum_{r,r'} J\{[(\vec{\tau}(r) - \vec{\tau}(r')] \cdot \hat{e}_{rr'}\}^2 + J\sum_{r} \tau_z^2(r)$$



- Ferro-orbital configurations.

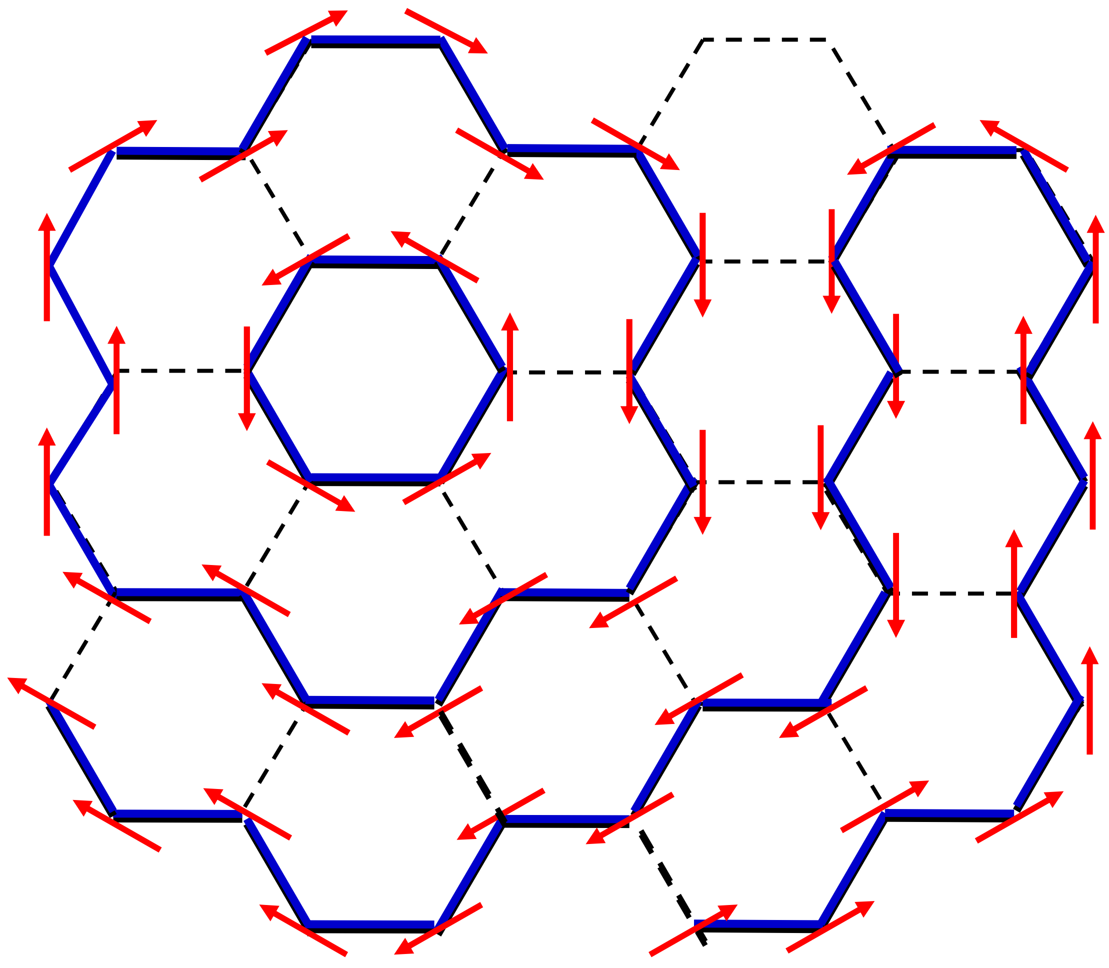


- Oriented loop config: τ-vectors along the tangential directions.



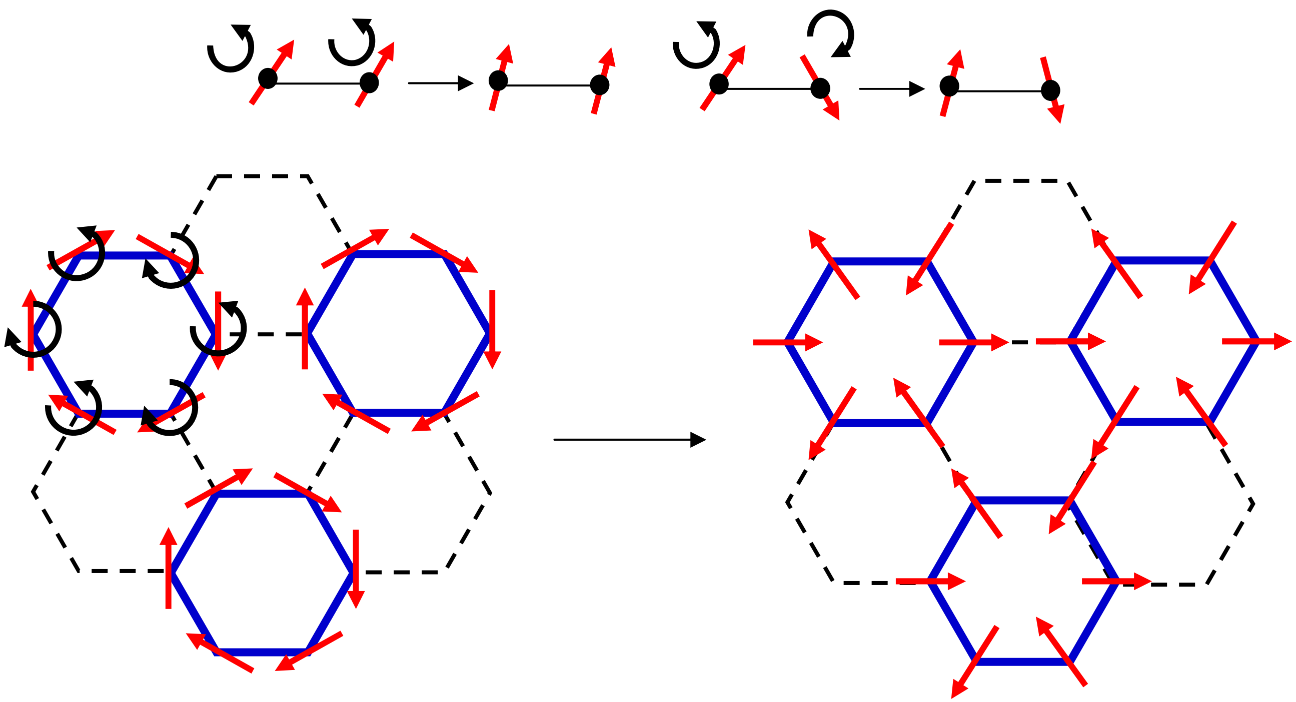
Heavy-degeneracy of classic ground states

- General loop configurations



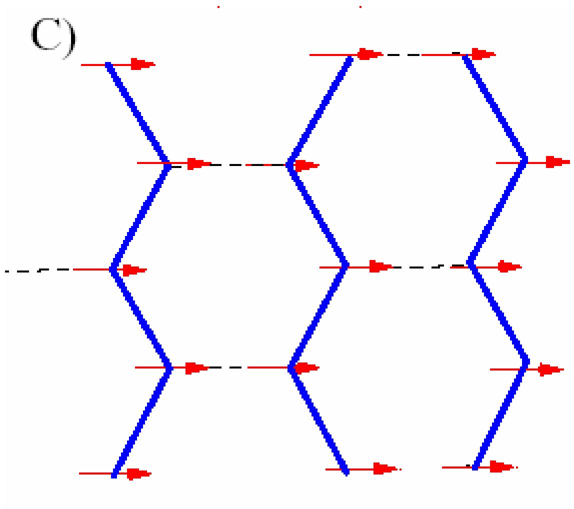
Global rotation degree of freedom

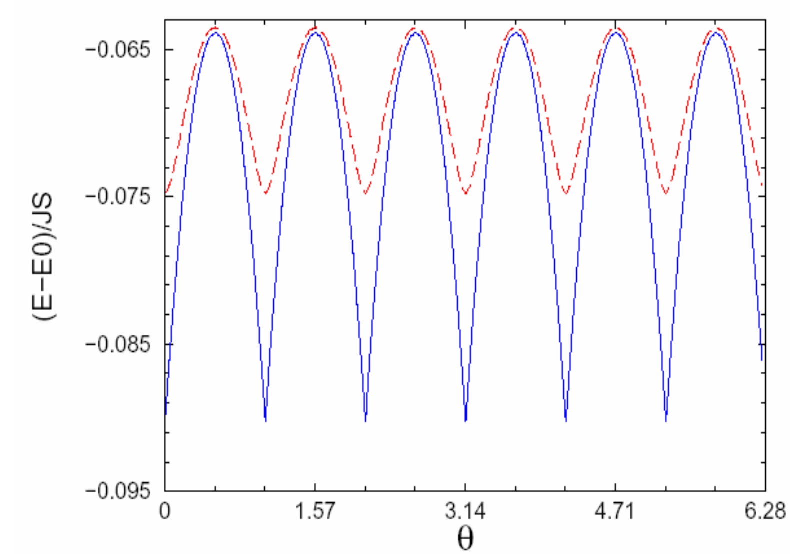
- Each loop config remains in the ground state manifold by a suitable arrangement of clockwise/anticlockwise rotation patterns.

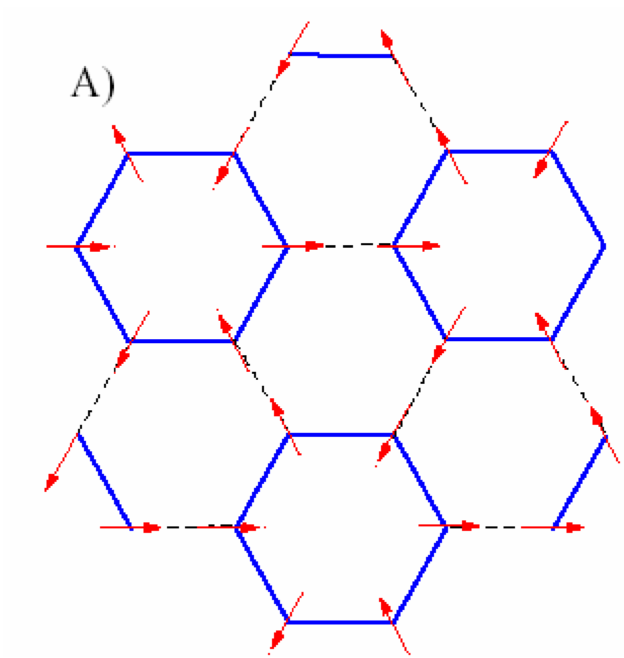


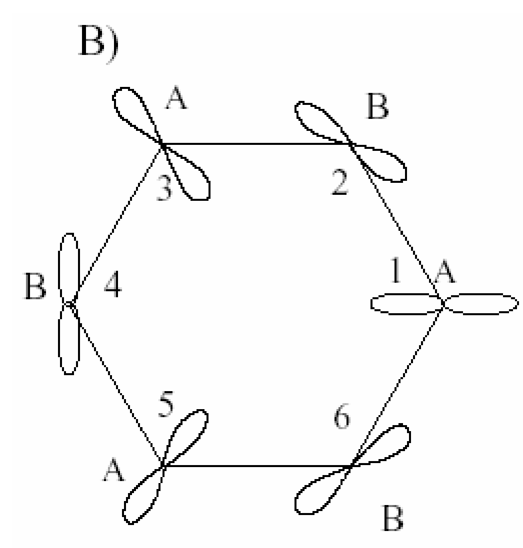
- Starting from an oriented loop config with fixed loop locations but an arbitrary chirality distribution, we arrive at the same unoriented loop config by performing rotations with angles of $\pm 30^{\circ}, \pm 90^{\circ}, \pm 150^{\circ}$.

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



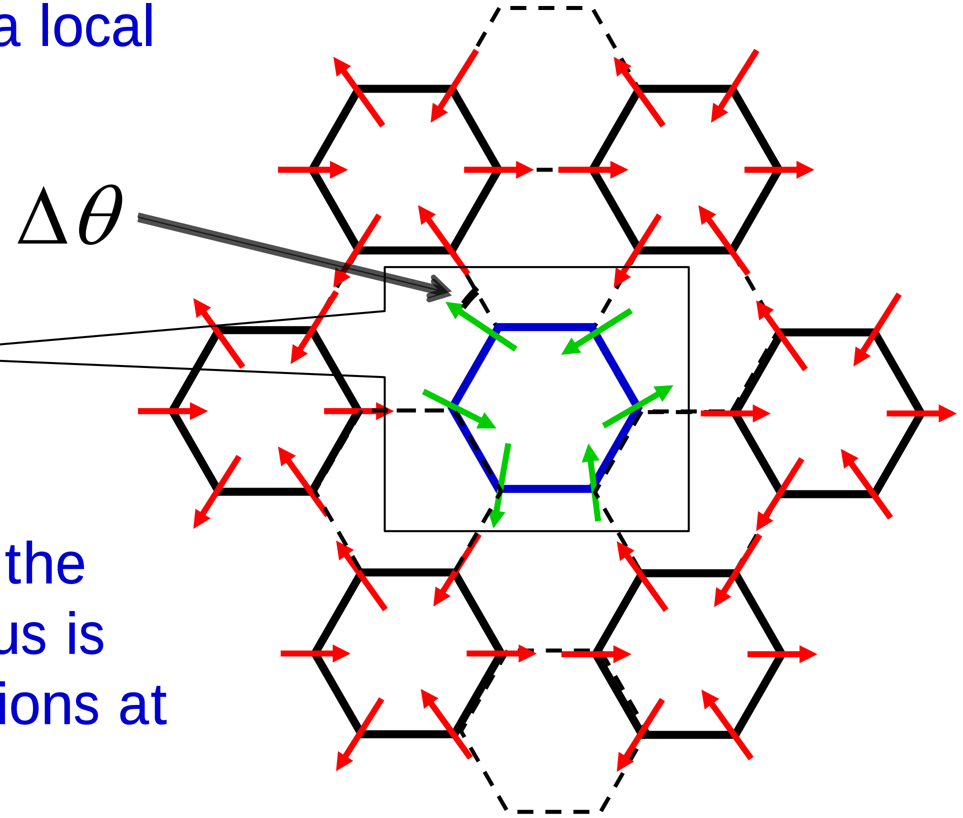






Zero energy flat band orbital fluctuations

- 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 flatnes

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

  C. Wu, and S. Das Sarma, PRB 77, 235107(2008);
  C. Wu et al, PRL 99, 67004(2007).
  Shizhong zhang and C. Wu, arXiv:0805.3031.

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

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

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

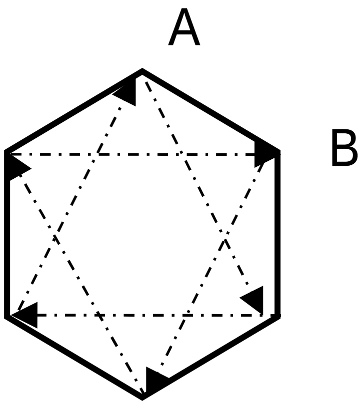
  C. Wu, PRL 101, 186807 (2008).

Topological insulators: Haldane's QHE Model without Landau level

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

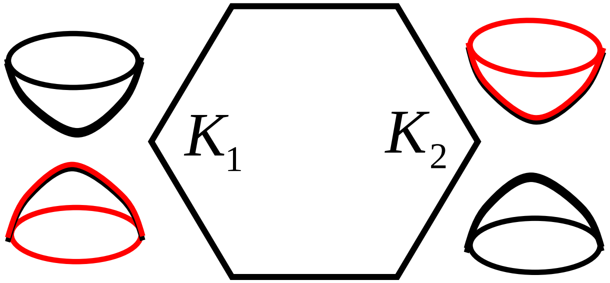
$$H_{NN} = -t \sum_{\vec{r} \in A} \{ c^{+}(\vec{r}_A) c(\vec{r}_B) + h.c. \}$$

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



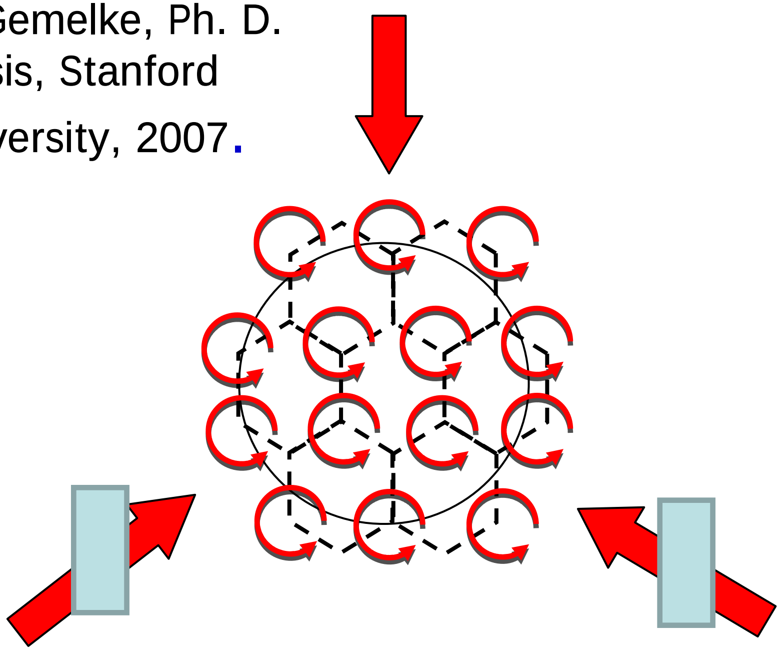
- Topological insulator at $\delta \neq 0, \pi$. Mass changes sign at $K_{1,2}$.

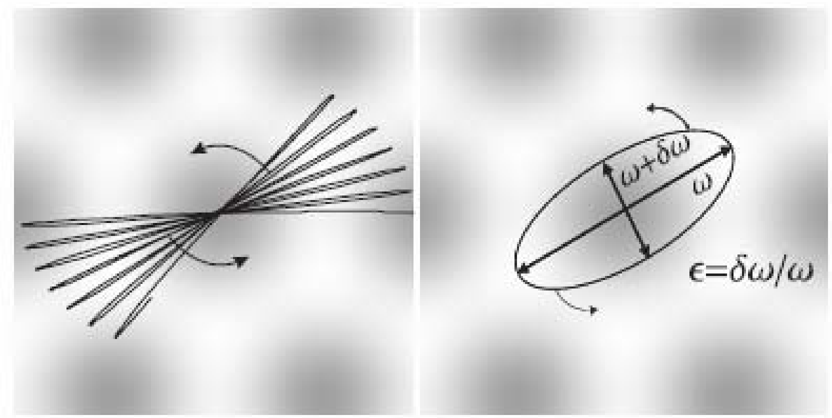
$$H(\vec{k}) = a(\vec{k})\tau_1 + b(\vec{k})\tau_3 + m(\vec{k})\tau_2 + c(\vec{k}) I$$



Rotate each site around its own center

N. Gemelke, Ph. D. thesis, Stanford University, 2007.





- 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.

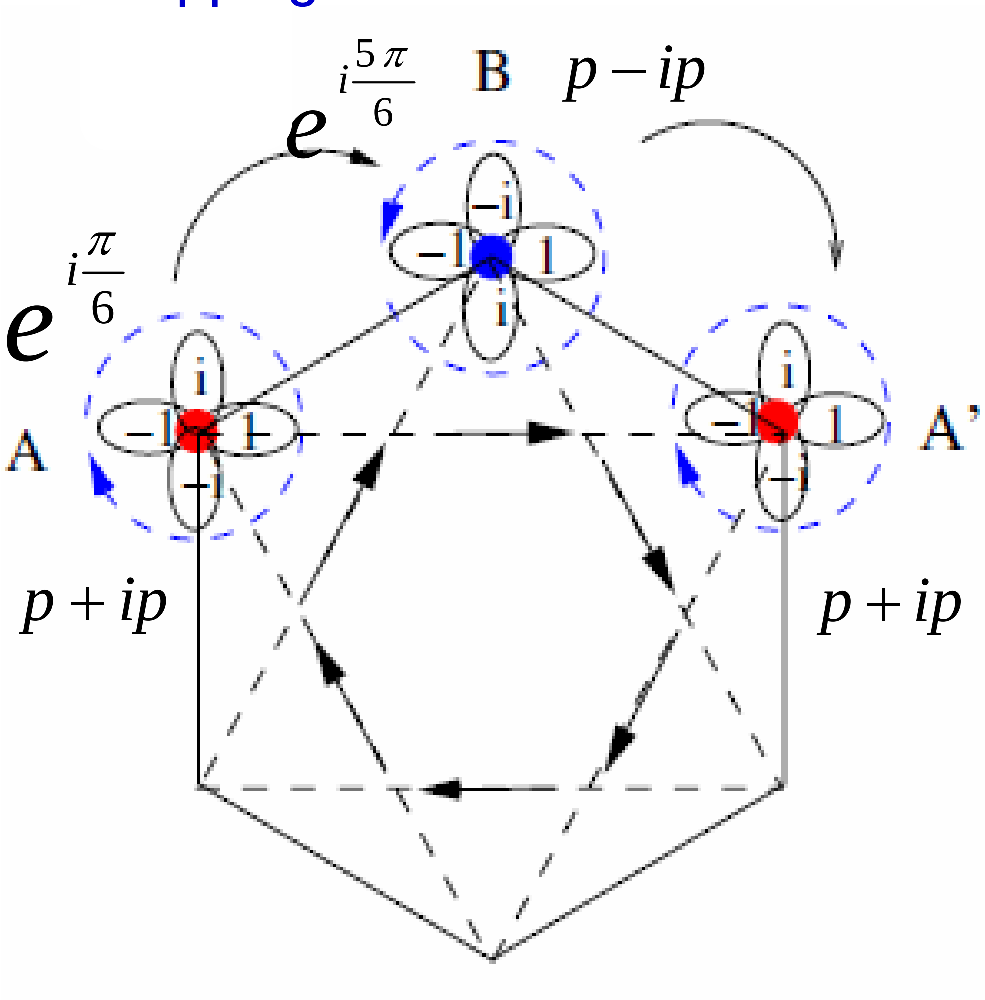
$$H_{zmn} = -\Omega \sum_{r \in A} L_z(\vec{r})$$
$$= i\Omega \sum_{\vec{r} \in A} \{ p_x^+(\vec{r}) p_y(\vec{r}) - p_y^+(\vec{r}) p_x(\vec{r}) \}$$

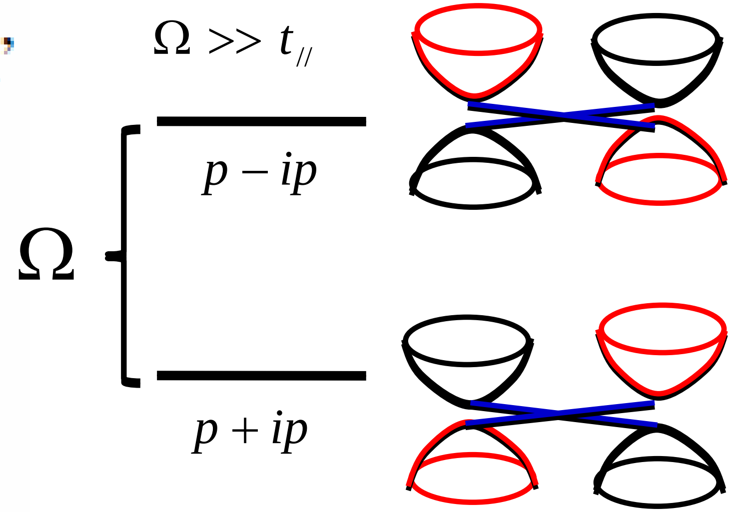
- The oscillation axis slowly precesses at the angular frequency of Ω .

Large rotation angular velocity

- Second order perturbation generates the NNN complex hopping.

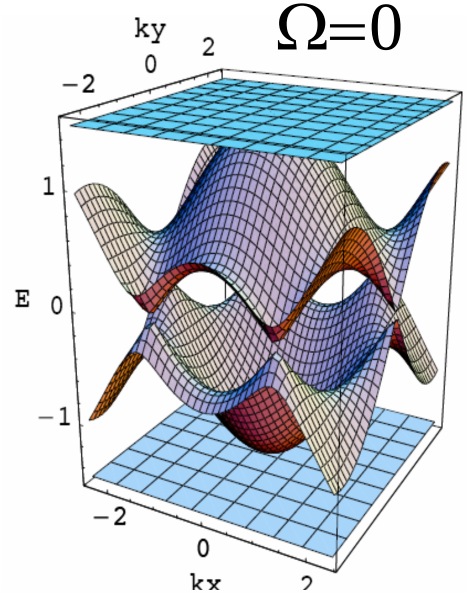
$$t' = -(t e^{i2/3\pi})^2 / 2\Omega$$



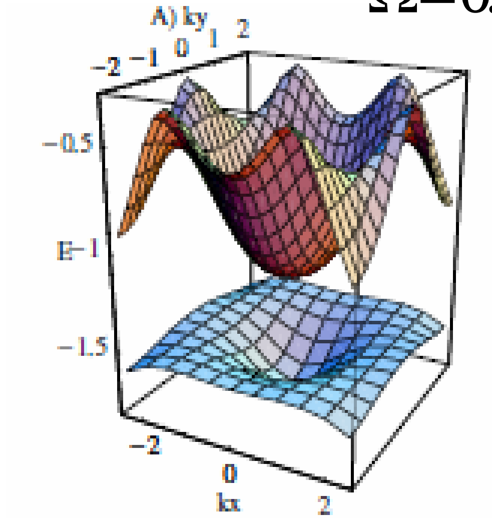


Small rotation angular velocity

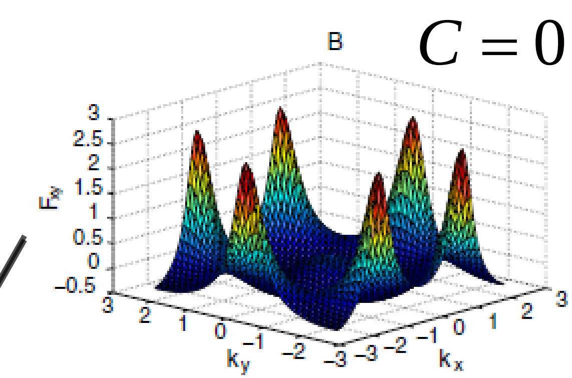
$\Omega=0$

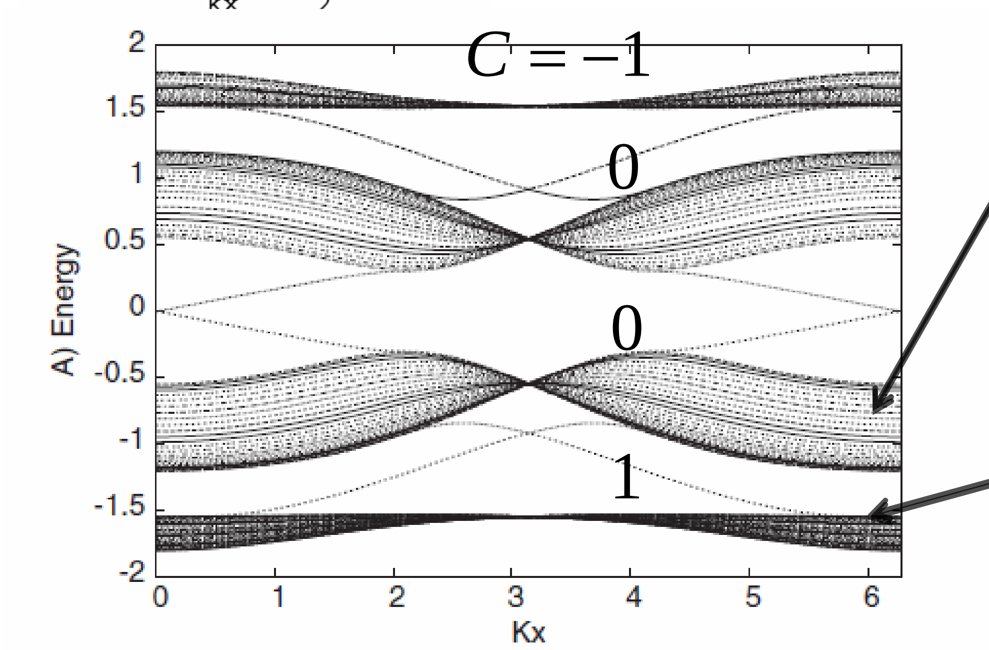


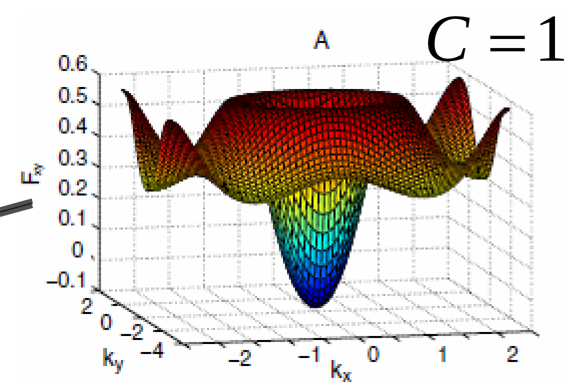
$\Omega=0.3t_{//}$



Berry curvature.

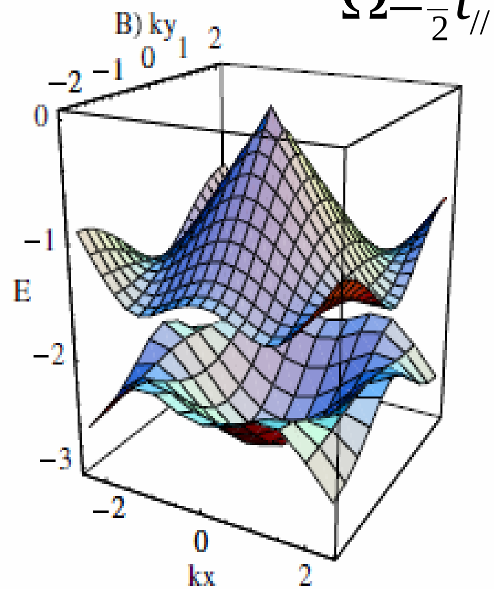




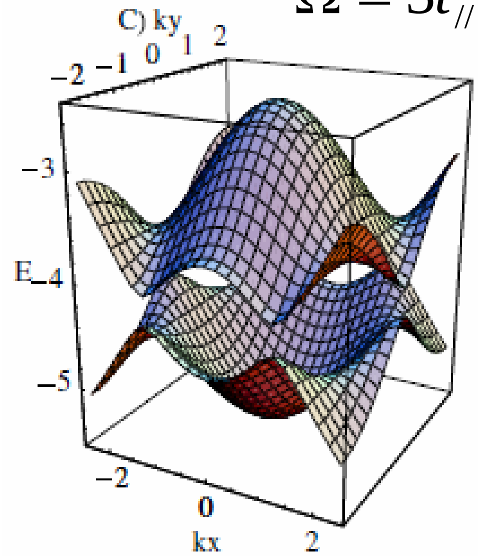


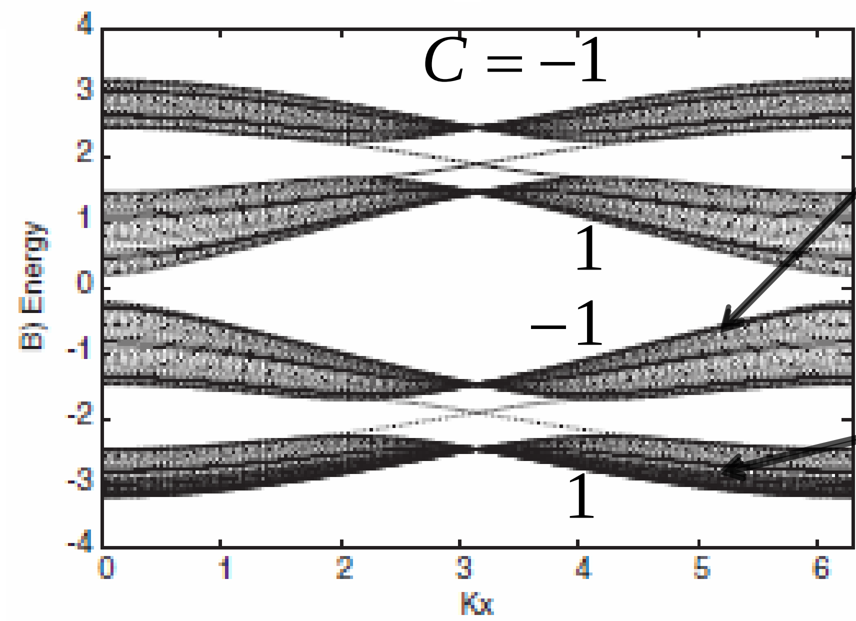
Large rotation angular velocity

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



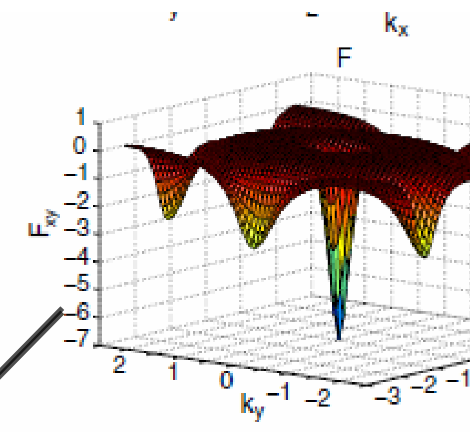
$\Omega = 3 t_{//}$



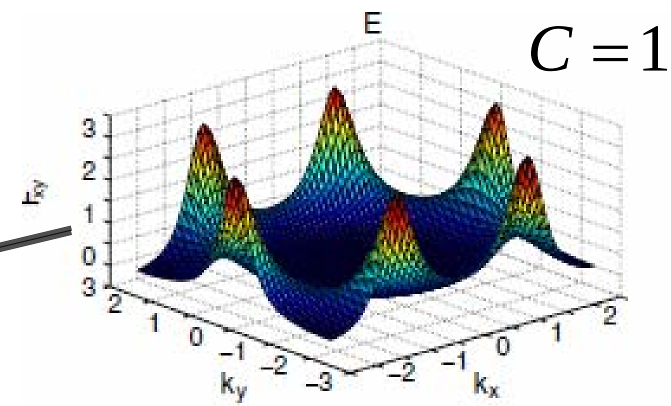


Berry curvature.

$C = -1$



$C = 1$



Summary

$p_{x,y}$-orbital counterpart of graphene: strong correlation from band flatness.

orbital exchange: frustration, quantum 120 degree model

Topological insulator: quantum anomalous Hall effect.