



**The Abdus Salam
International Centre for Theoretical Physics**



2252-S-6

Advanced Workshop on Non-Standard Superfluids and Insulators

18 - 22 July 2011

p-band superfluid and insulator phases in optical lattices

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Advanced Workshop on Non-standard Superfluids and Insulators, ICTP Trieste, 18-22 July 2011

p-orbital band superfluid and insulator phases in optical lattices

W. Vincent Liu

University of Pittsburgh, Pennsylvania, USA

[View of Pittsburgh---source: PittsburghSkyline.com]



Acknowledgement

Our Work:

- PRA 2006
- PRL 2006
- PRL 2008a
- PRL 2008b
- PRL 2010
- PRA 2010
- PRA 2011
- Nature Phys (news & view, 2011)
- arXiv:1011.4301
- arXiv:1103.5964

group members on p-band:

Students: Chiu-Man Ho (→UC Berkeley →Vanderbilt)
H. H. Hung (→UCSD →UIUC)
Xiaopeng Li (*current*)
Vladimir Stojanovic (*Carnegie-Mellon* → *U Basel*)
Zixu Zhang (*current*)

Postdoc: Chungwei Lin (*moving to UT Austin/2nd postdoc*),
Erhai Zhao (*now assistant professor at George Mason Univ, Fairfax, VA*)

External collaborators

Theory: Sankar Das Sarma, Ivan Deutsch, Kritika Goyal, Philipp Hauke, Maciej Lewenstein, Joel Moore, Kai Sun, Congjun Wu

Exp: Andreas Hemmerich



Thanks for Support by
U.S. ARO (individual) and
DARPA-OLE/ARO (Hulet/Rice team)



Outline

1. Introduction

- Beyond s-orbital, the basics of p-orbital? Why p-orbital?
- Recent experimental progress

2. p-band bosons (including examples of no prior analogue in solids).

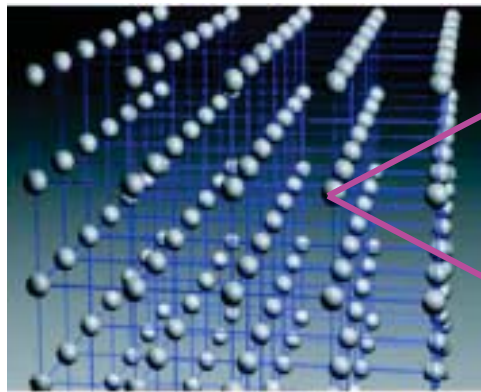
- Finite momentum BEC with $p_x + ip_y$ orbital order
- Mott insulator phases and orbital order
- Elongated Orbitals and mapping to quantum dimer model

3. p-band fermions

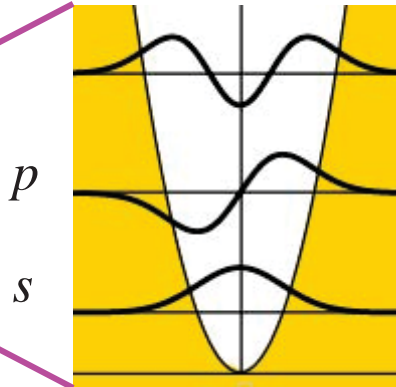
- Single species. Mott states. Orbital-only model. Realization of Kitaev-like model?
- Topological states (quantum Hall like). Topological semimetal (non-interacting), and topological insulator (turn on interaction). Time reversal breaking driven by interaction, no magnetic field!

Part 1. Introduction:
What is the p-band, Why?

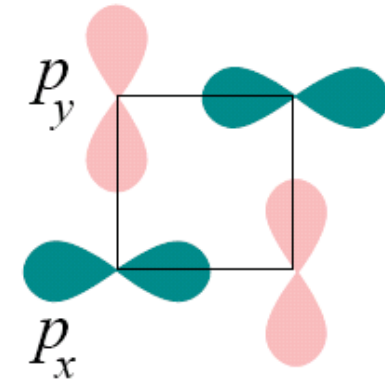
p-band of an optical lattice (1D illustration)



[lattice picture from web]



Top view



- Bose-Hubbard model**

$$H = -t \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{1}{2} U \sum_i b_i^\dagger b_i^\dagger b_i b_i$$

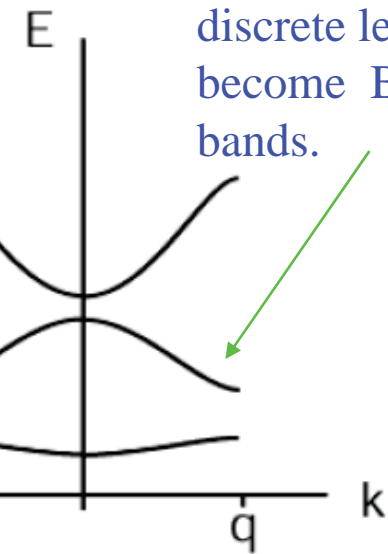
theory: Jaksch et al, PRL 1998

exp.: Bloch et al, Nature 2002

- This talk**

p-band

s-band



With tunneling,
discrete levels
become Bloch
bands.

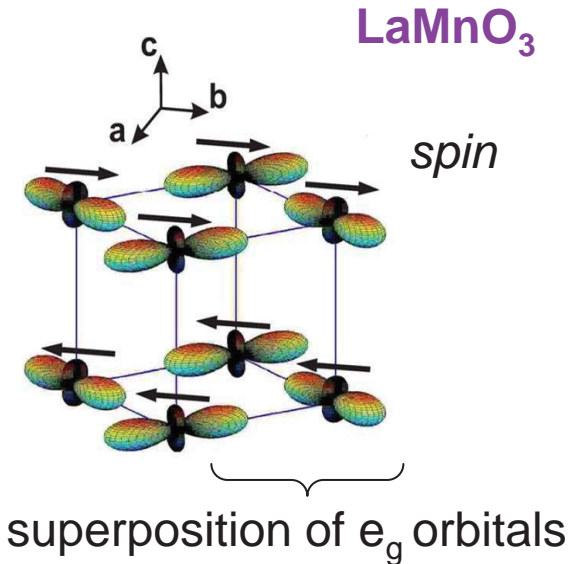
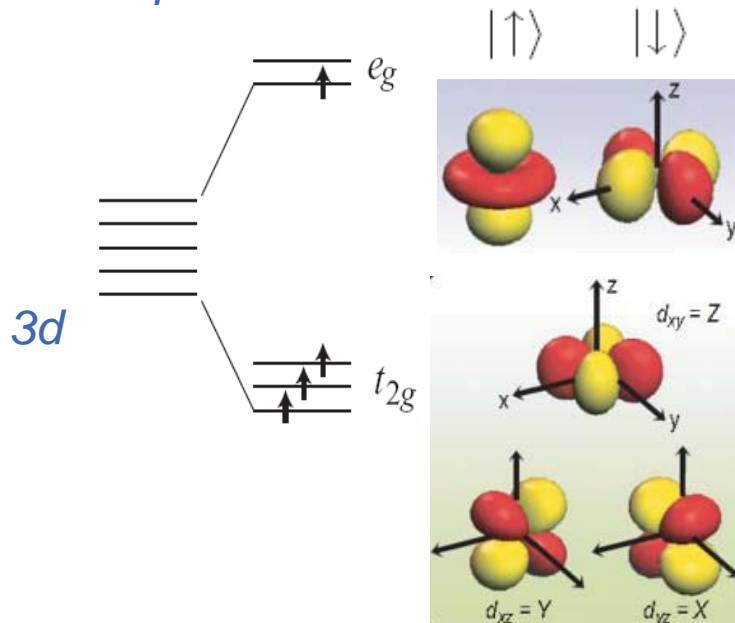
Orbital ordering of d-electrons

[see, for example, review by Tokura and Nagaosa, science 288, 462, (2000).]

orbital: shape of the electron cloud

Orbital degeneracy in transition metal oxides:

pseudospin 1/2:



Kugel-Khomskii superexchange

$$H = \sum_{\langle i,j \rangle} \hat{J}_{ij}^{(\gamma)} (\vec{S}_i \vec{S}_j + \frac{1}{4}),$$

$$\hat{J}_{ij}^{(\gamma)} = J(T_i^{(\gamma)} T_j^{(\gamma)} - \frac{1}{2} T_i^{(\gamma)} - \frac{1}{2} T_j^{(\gamma)} + \frac{1}{4})$$

$$T_i^{(a/b)} = \frac{1}{4} (-\sigma_i^z \pm \sqrt{3} \sigma_i^x), \quad T_i^{(c)} = \frac{1}{2} \sigma_i^z$$

- Charge, spin, orbital, and lattice degree of freedom entangled together
- Complex phase diagrams

A new direction: p-orbital physics in optical lattices

- **Orbital degeneracy** (px, py, pz orbitals) is considerably less understood in comparison. Implies emergent symmetry.
- **Similar to spin physics** but is different fundamentally.
- **Strong anisotropy:** Anisotropy is an interesting new feature, not a problem!
- **p -orbitals are different than d -orbital in solids:** Parity ODD. New possibility--- p -orbital bosons as opposed to d -electrons (fermions) in solids
- **unique** to cold atom systems, “non-standard” condensed matter systems. For instance, Orbital physics of bosons has no prior analogue in CM physics?!



new quantum phases (a main motivation of our study).

Theoretical studies on the excited bands An incomplete list!! [red=our work]

On multi-orbital

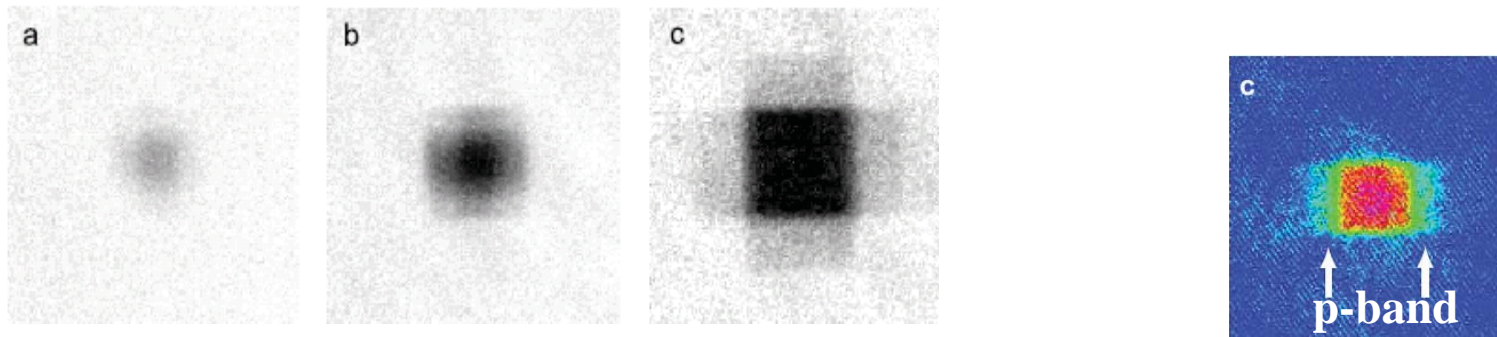
- V. Scarola, S. Das Sarma, *Phys. Rev. Lett.* (2005)
- O. E. Alon, A. I. Streltsov, L. S. Cederbaum, *Phys Rev Lett* (2005)
- ...

On p-orbital

- A. Isacsson and S. Girvin, *Phys. Rev. A* 72, 053604 (2005).
- A. B. Kuklov, *Phys. Rev. Lett.* (2006)
- WVL and C. Wu, *Phys. Rev. A* (2006)
- C. Wu, WVL, J. Moore, and S. Das Sarma, *Phys. Rev. Lett.* (2006).
- A. F. Ho, arXiv:cond-mat/0603299
- C. Xu and M. P. A. Fisher, *Phys. Rev. B* 75, 104428 (2007)
- C. Wu, D. Bergman, L. Balents, and S. Das Sarma, *Phys. Rev. Lett.* (2007)
- A. Kantian, A. J. Daley, P. Törmä and P. Zoller, *New J. Phys.* (2007)
- L. Guo, Y. Zhang, and S. Chen, *Phys. Rev. A* (2007)
- E. Zhao and WVL, *Phys. Rev. Lett.* (2008);
- R. O. Umucallar and M. Ö. Oktel, *Phys. Rev. A* (2008)
- K. Wu and H. Zhai, *Phys. Rev. B* (2008)
- L. Wang, X. Dai, S. Chen, X. C. Xie, arXiv:0805.2719 (2008)
- R. M. Lutchyn, S. Tewari, S. Das Sarma, arXiv:0812.0815 (2008)
- V. Stojanovic, C. Wu, WVL and S. Das Sarma, *Phys. Rev. Lett.* (2008)
- ...
- K. Sun, E. Zhao, WVL, *Phys. Rev. Lett.* (2010)
- Z. Zhang, H. H. Hung, C.M. Ho, E. Zhao, WVL, *Phys. Rev. A* (2010)
- A. Collin, J. Larson, and J.-P. Martikainen, *Phys. Rev. A* (2010)
- ...

Orbital physics of interacting cold atoms

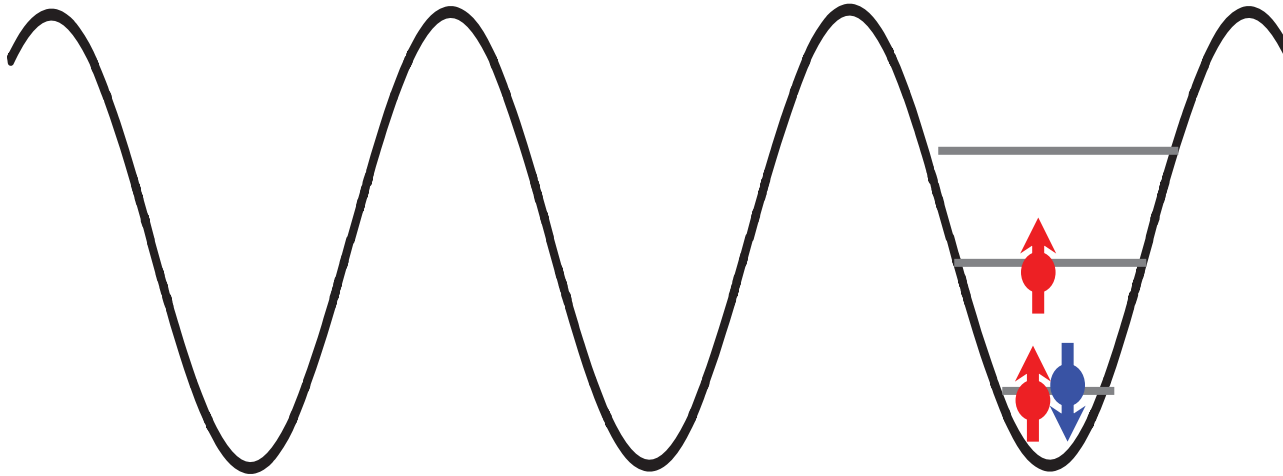
- **Fermions in p-band** M. Köhl et al, PRL **94**, 080403 (2005)



Fermi Surface vs band filling

Fermions are transferred into the p-band using a sweep across the Feshbach resonance, i.e., by strong interaction.

Preparation of p-band fermions

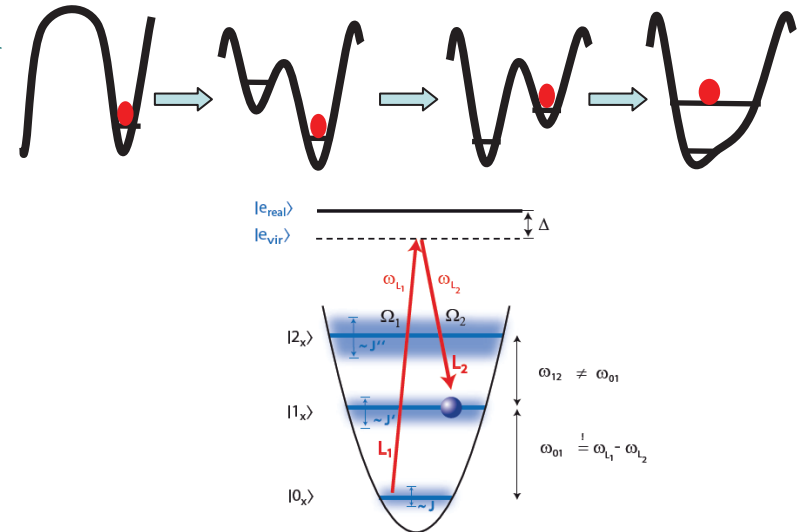
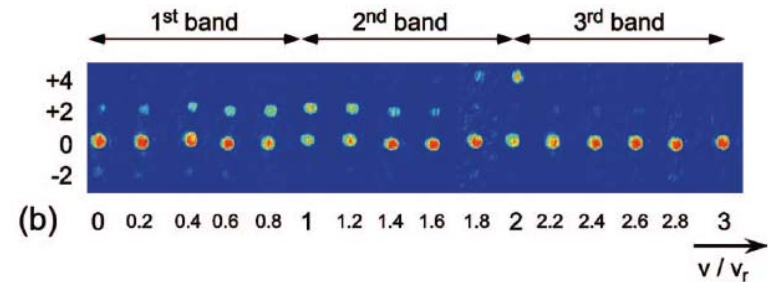


- ***Even simpler:*** Fill the lowest s-band with the specific species (say **spin up**). Just by having more than 2 particles/site for two-components
- p-band fermions should have no problem in lifetime (Pauli exclusion principle)

Bosons in the optical lattice p-band

Experiments

- By moving lattices [A. Browaeys, W. D. Phillips, et al, PRA **72**, 053605 (2005)]
- Dynamically deforming the double-well lattice [NIST Porto/Phillips groups: PRA (2006); J. Phys. B (2006); PRL 2007; Nature 2007; ...]
- Pumping bosons by Raman transition [T. Mueller, I. Bloch et al., PRL 2007]



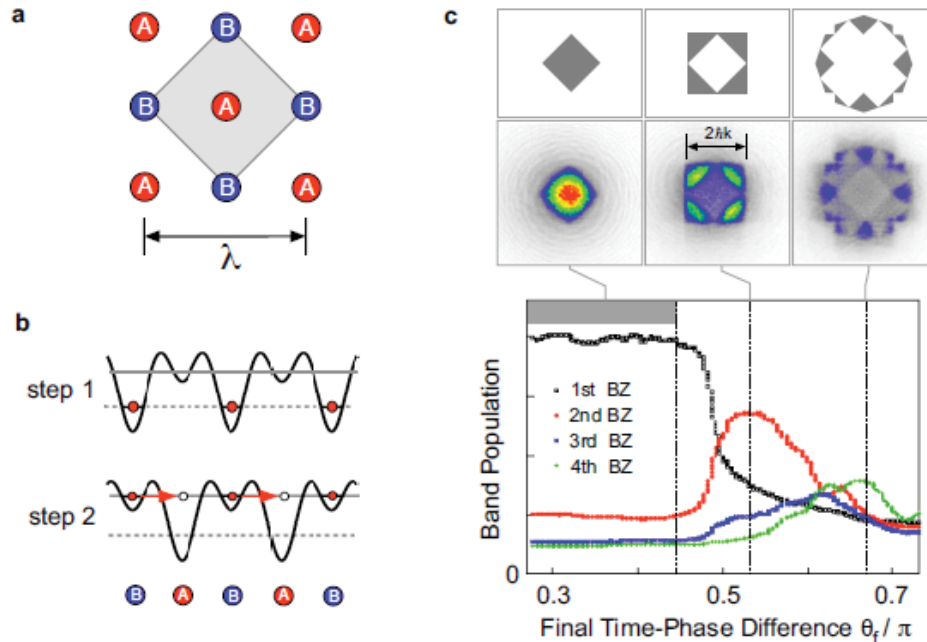
Theories:

- Isacson & Girvin, PRA 05
- Kuklov, PRL 06
- WVL & Wu, PRA 06

Lifetime issue: to be discussed.

New p- and f-band experiments – double well lattices

Hamburg/Hemmerich group



- “P-band superfluidity+orbital order in checkerboard (double well) lattice”, long life time [G. Wirth, M. Olschlager, A. Hemmerich, *Nature Physics* 2011]
- “F-band” [M. Olschlager, G. Wirth, A. Hemmerich, PRL 2011]

Another recent exp: hexagonal lattice

- Reported “Unconventional (complex) multi-orbital superfluidity” [P. Soltan-Panahi, D. Luhmann, J. Struck, P. Windpassinger, and K. Sengstock, arxiv:1104.3456]

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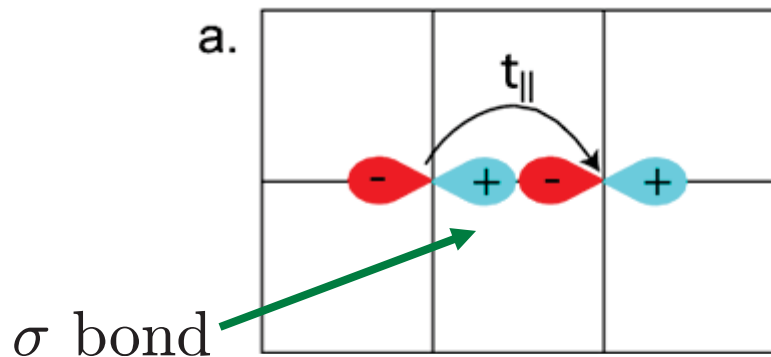
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p-orbital Bose-Hubbard model: 3D cubic lattice

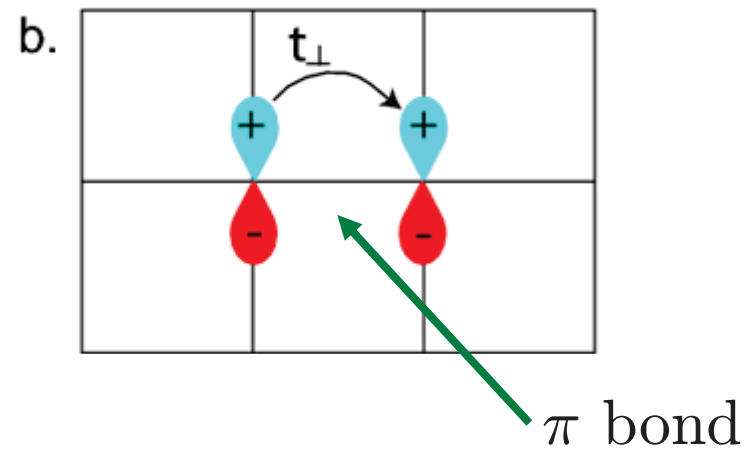
[derived in WVL and C. Wu, PRA (2006)]

$$H = \sum_{\mathbf{r}\mu} [t_{\parallel} \delta_{\mu\nu} - t_{\perp} (1 - \delta_{\mu\nu})] (b_{\mu, \mathbf{r} + a\mathbf{e}_{\nu}}^{\dagger} b_{\mu\mathbf{r}} + h.c.) + \frac{1}{2} U \sum_{\mathbf{r}} [n_{\mathbf{r}}^2 - \frac{1}{3} \mathbf{L}_{\mathbf{r}}^2]$$



$$\mu, \nu = x, y, z$$

or



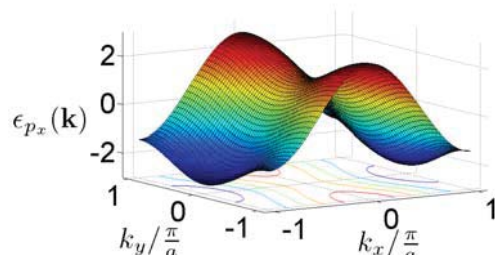
$$p_x, p_y, p_z$$

Density field operator $n_{\mathbf{r}} = \sum_{\mu} b_{\mu\mathbf{r}}^{\dagger} b_{\mu\mathbf{r}}$

Angular momentum operator: $L_{\mu\mathbf{r}} = -i \sum_{\nu\lambda} \epsilon_{\mu\nu\lambda} b_{\nu\mathbf{r}}^{\dagger} b_{\lambda\mathbf{r}}$

Weak coupling theory

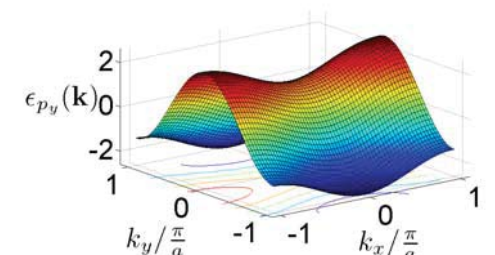
-p_x orbital band

$$\epsilon_{p_x} = 2t_{\parallel} \cos(k_x) - 2t_{\perp} \cos(k_y)$$


$\mathbf{Q}_x = (-\frac{\pi}{a}, 0)$ ← **band minima** → $\mathbf{Q}_y = (0, -\frac{\pi}{a})$

$\langle p_x(\mathbf{r}) \rangle = \varphi_x(\mathbf{r}) \sim \sqrt{n_x} e^{i\theta} e^{i\Delta/2} \mathbf{e}^{i\mathbf{Q}_x \cdot \mathbf{r}}$

-p_y orbital band

$$\epsilon_{p_y} = -2t_{\perp} \cos(k_x) + 2t_{\parallel} \cos(k_y)$$


$\mathbf{Q}_x = (-\frac{\pi}{a}, 0)$ ← **band minima** → $\mathbf{Q}_y = (0, -\frac{\pi}{a})$

$\langle p_y(\mathbf{r}) \rangle = \varphi_y(\mathbf{r}) \sim \sqrt{n_y} e^{i\theta} e^{-i\Delta/2} \mathbf{e}^{i\mathbf{Q}_y \cdot \mathbf{r}}$

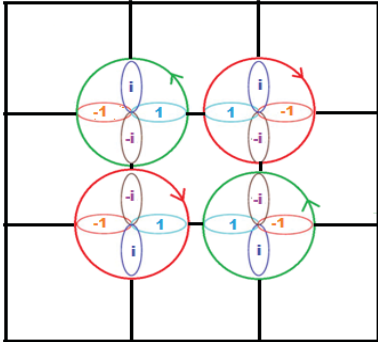
-inter-band phase locking

$$E(\Delta) \sim 2n_x n_y U \cos(2\Delta)$$

Gives a Bose-Einstein condensate of:

$$p_x \pm ip_y$$

-pattern of TSO superfluidity in real space



M. A. Lewenstein and WVL, Nat. Phys 7, 101(2011)

The p -orbital BEC (p -OBEC)

Parameterization of Order parameter:

$$\begin{pmatrix} \langle b_{x\mathbf{k}=\mathbf{Q}_x} \rangle \\ \langle b_{y\mathbf{k}=\mathbf{Q}_y} \rangle \\ \langle b_{z\mathbf{k}=\mathbf{Q}_z} \rangle \end{pmatrix} = \rho e^{i\varphi - i\vec{T}\cdot\vec{\theta}} \begin{pmatrix} \cos \chi \\ i \sin \chi \\ 0 \end{pmatrix}$$

U(1)
phase
SO(3)
orbital
T-reversal

For a dilute lattice gas of $U > 0$, the condensate is found to be a **non-zero-momentum $p_x + ip_y$ BEC**.

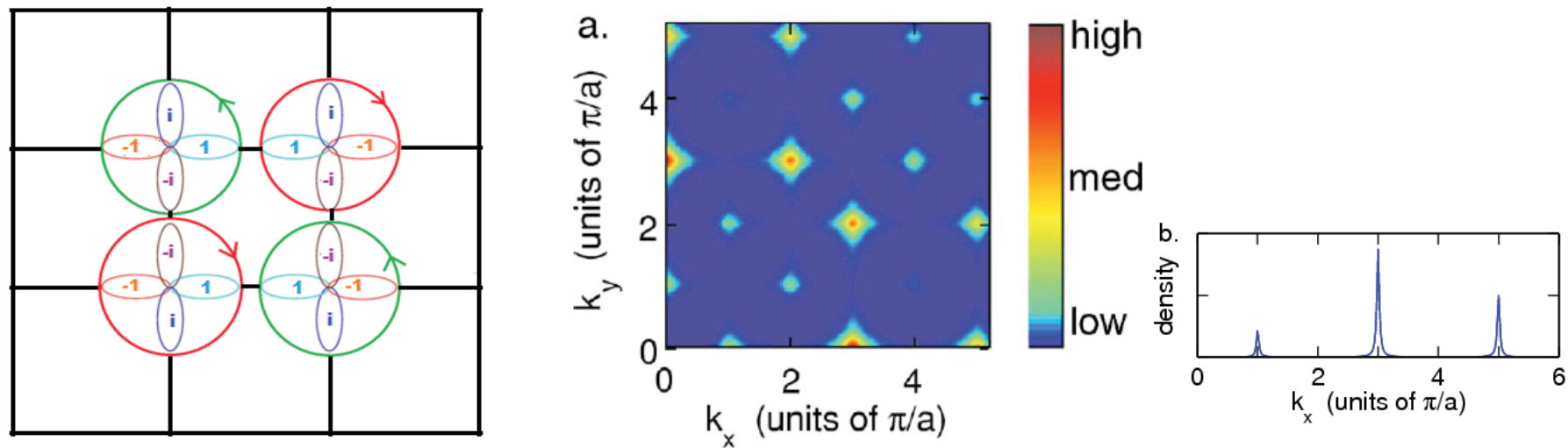
[\vec{T} 's are three 3x3 matrices]

$$\begin{pmatrix} \langle b_{x\mathbf{k}=\mathbf{Q}_x} \rangle \\ \langle b_{y\mathbf{k}=\mathbf{Q}_y} \rangle \\ \langle b_{z\mathbf{k}=\mathbf{Q}_z} \rangle \end{pmatrix} = \sqrt{\frac{\text{Vol.} \times n_0^b}{2}} \begin{pmatrix} 1 \\ \pm i \\ 0 \end{pmatrix}$$

- A **new concept** that defies the paradigm of BEC!
- A metastable BEC wavefunction with nodes---not contradict **Feynman's argument**.

Features of p-orbital BEC phase

- Spontaneous Time reversal symmetry breaking
- Transversely staggered orbital current in real space (TSOC)
- Coherent peaks at finite momenta (finite momentum BEC)
- Violation of Feynman “no-node theorem” but meta-stable

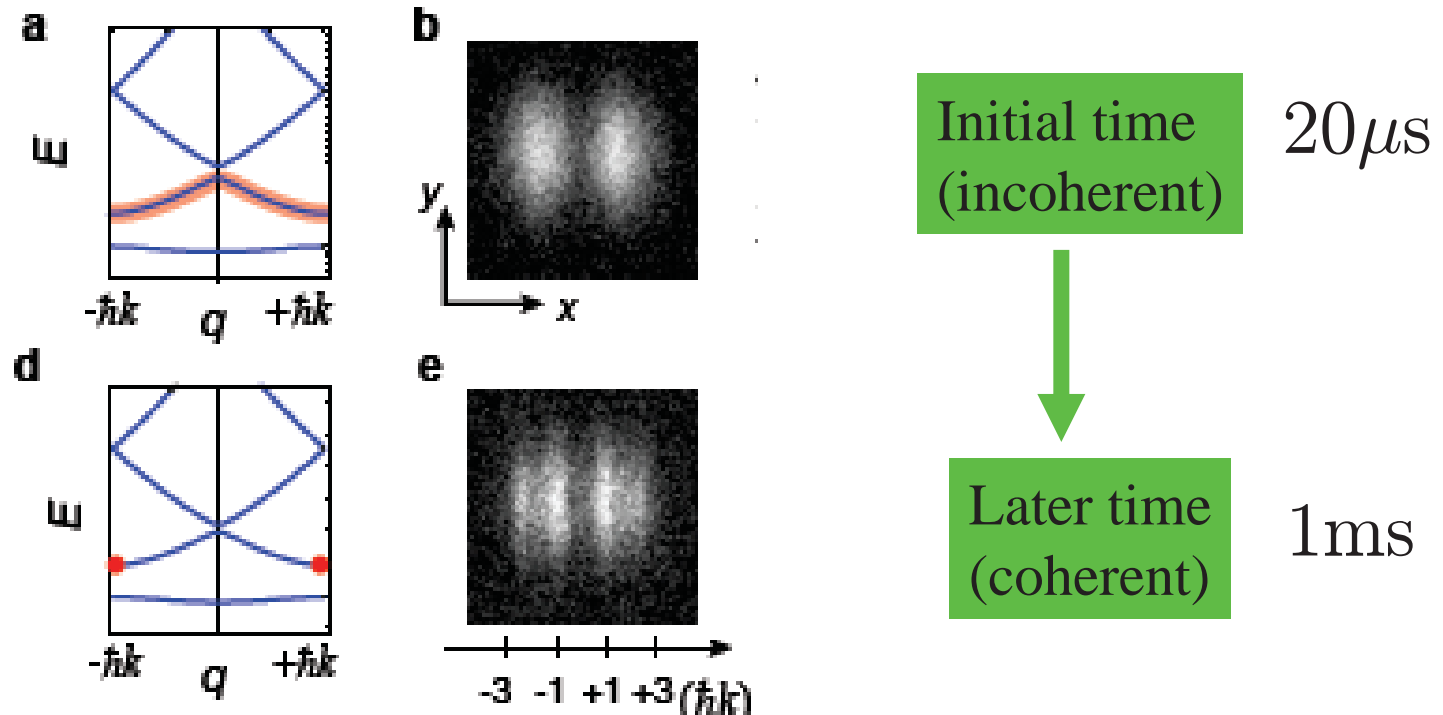


WVL and C. Wu Phys. Rev. A 74, 013607 (2006)

[Related results independently by: A. Isacsson, S. Girvin, PRA (2005); A. B. Kuklov, PRL 97, 110405 (2006)]

Experimental observation I: finite momentum BEC

by the Mainz/Bloch group [Mueller, Bloch, et al, PRL, 2007]

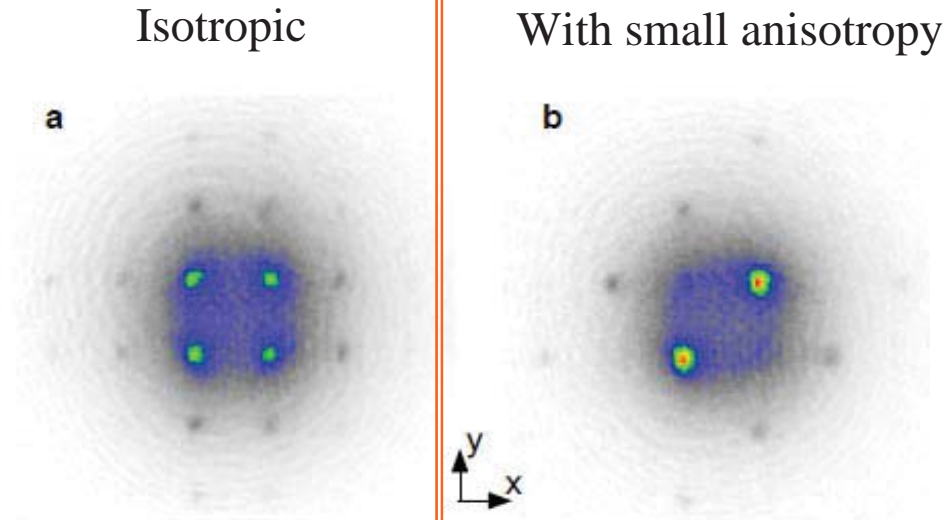


Mueller, Bloch et al [PRL 2007] and theoretical prediction [Isacson-Girvin, 2005; Kuklov, 2006; WVL, Wu 2006] **agrees!**

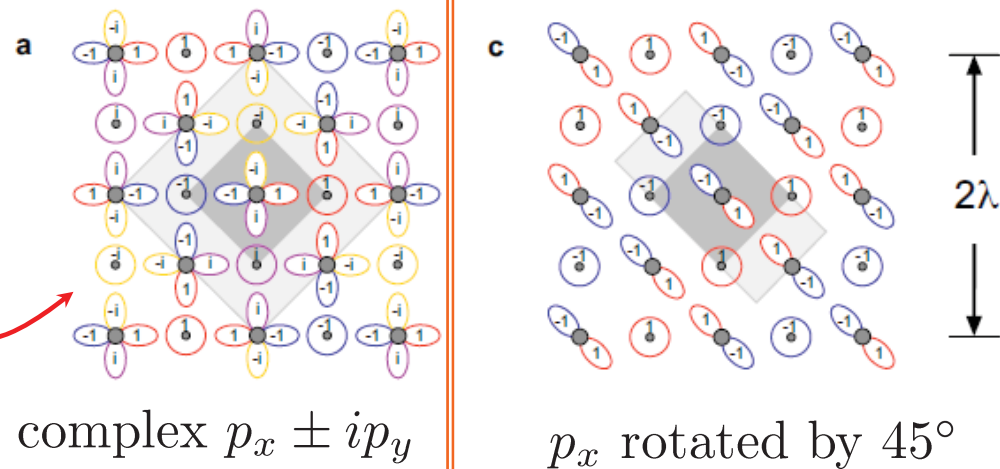
Experimental observation II: complex p-orbital superfluids

G. Wirth, M. Olschlager, A. Hemmerich, Nat. Phys. 2011

*Observed
momentum
distribution*



*Interpretation:
Nature of orbital
order*



Experimental finding consistent with prediction by [WVL, C. Wu, PRA 2006]

The decay problem of p-orbital bosons

The decay process where two p-bosons collide, promoting one to the 2nd excited band and bringing one down to the s-band.

My crude cartoon picture:

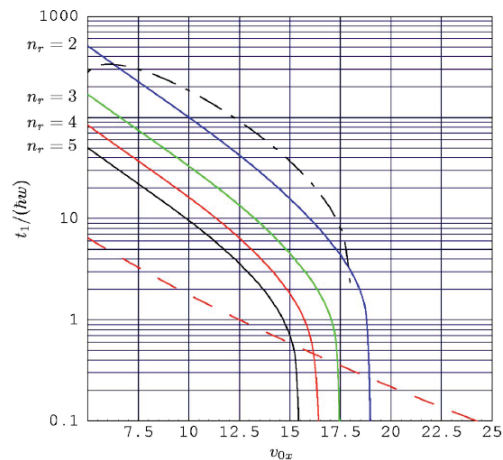
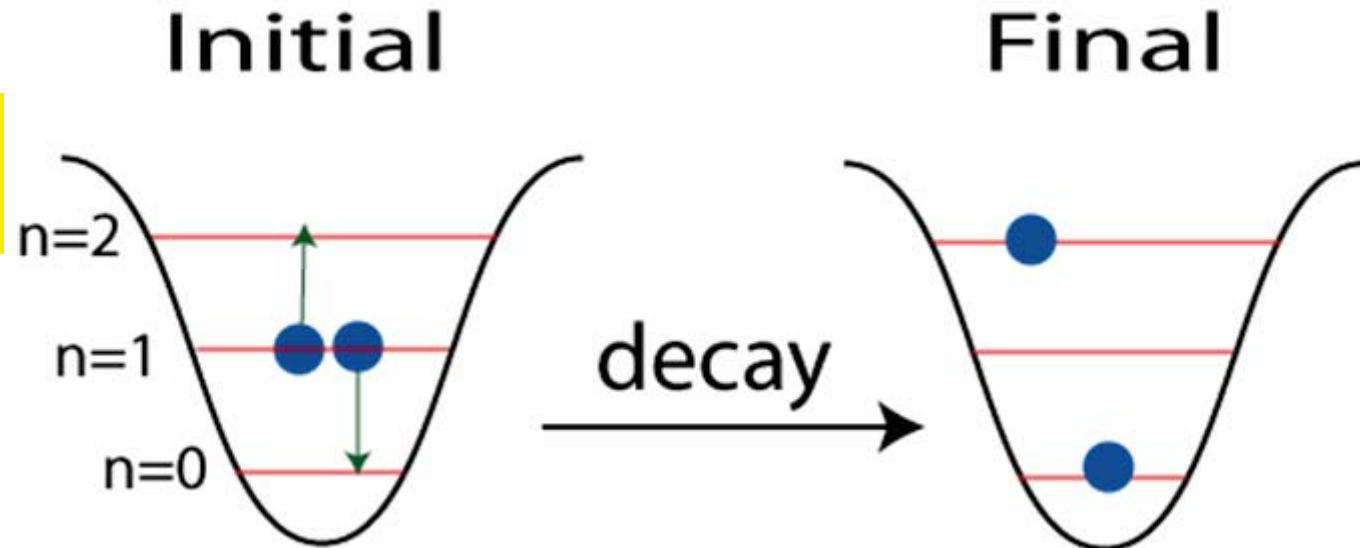


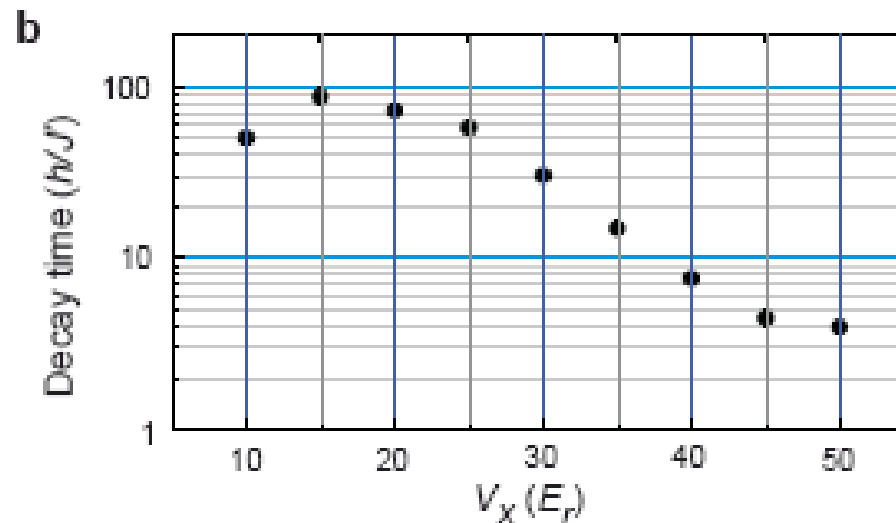
FIG. 15. (Color online) First-order lifetime τ_1^{-1} for a 1D system with filling factor $\nu_1=1$ and $(a_s/a)=1/100$ in the narrowband limit

First Studied by [Isacson and Girvin (2005).]

p-band decay time measured by the Mainz group

[T. Mueller, I. Bloch, et al, PRL 2007]

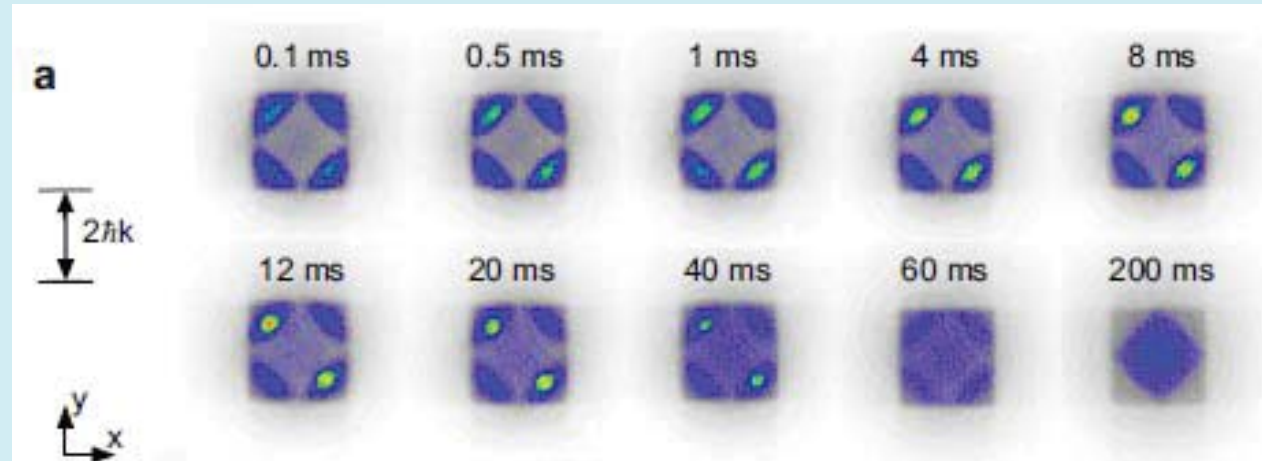
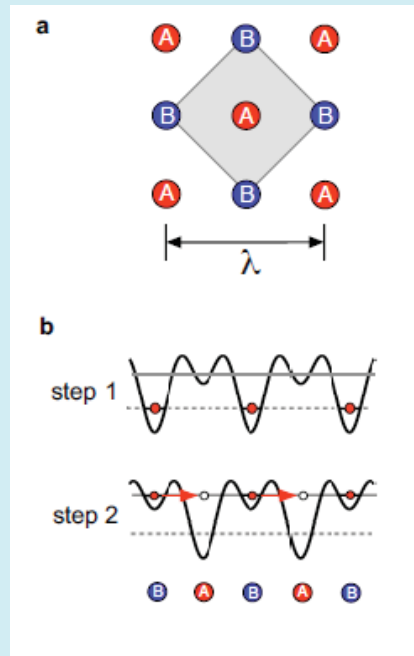
Decay time in units of tunneling time scale
vs
lattice depth



An idea to slow decay by Bloch et al: **anharmonicity**

p-band **long life** time observed in the double-well lattice

G. Wirth, M. Olschlager, A. Hemmerich, Nat. Phys. 2011



Note:

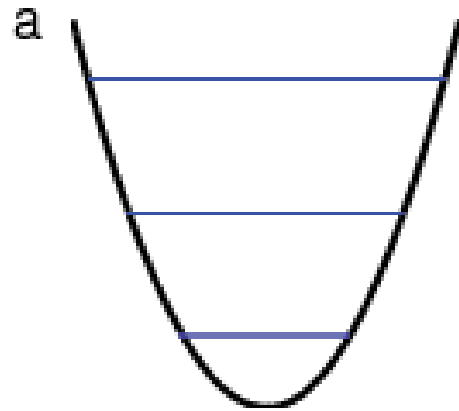
This **double-well lattice** exhibits a life-time of tens of milliseconds (and up to half second from private communication with A Hemmerich) with coherence.

Why? See possible explanation next slide

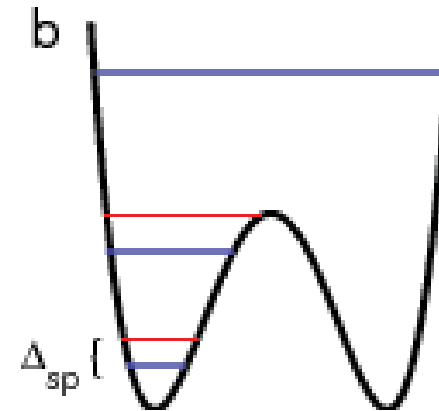
“Energy-blocking” mechanism to suppress the decay

[WVL and C. Wu, PRA (2006)]

single well lattice



double well lattice

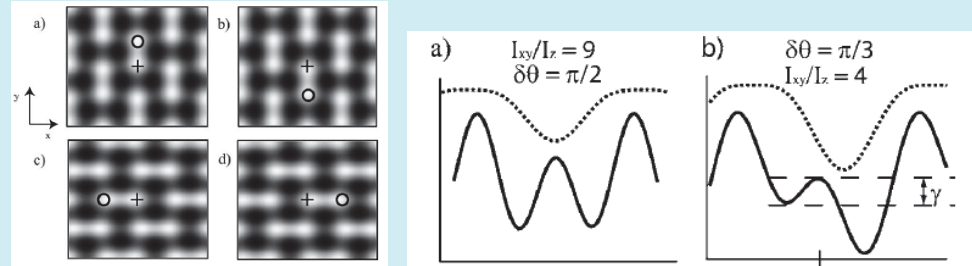


- Low energy motion of bosons is an effective two-band model;
- p -orbital bosons cannot decay to the “s” by energy conservation.

Early and recent experiments of double-well superlattices

NIST group (Porto/Phillips)

[J. Sebby-Strabley, et al, PRA (2006); M. Anderlini, et al, J. Phys. B (2006); Nature (2007); ...]



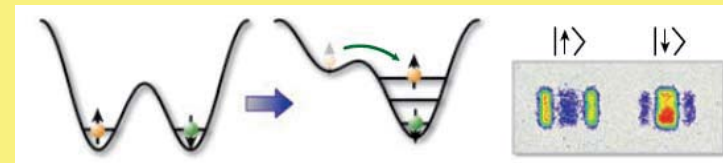
Does not preserved original geometric symmetry

Bloch group

[S. Trotzky et al, Science (2008); P. Cheinet et al, Phys. Rev. Lett. 101, 090404 (2008) ; Y. Chen et al, arXiv: 1003.4956 (2010); ...]

Time-Resolved Observation and Control of Superexchange Interactions with Ultracold Atoms in Optical Lattices

S. Trotzky, et al.
Science **319**, 295 (2008);



Stamper-Kurn group

Cf. his talk at this workshop

Superlattice (red and blue lattices overlapped)
→ Kagome

p-band Mott insulator and superfluid phases and finite temperature

- A. Isacsson and S. M. Girvin, PRA 72, 053604 (2005)
- A. Collin, J. Larson, and J.-P. Martikainen, Phys. Rev. A 81, 023605 (2010)
- X. Li, E. Zhao, WVL, Phys. Rev. A 83, 063626 (June 2011)

[different results on p-band Mott states]

Strong coupling theory

--physical picture

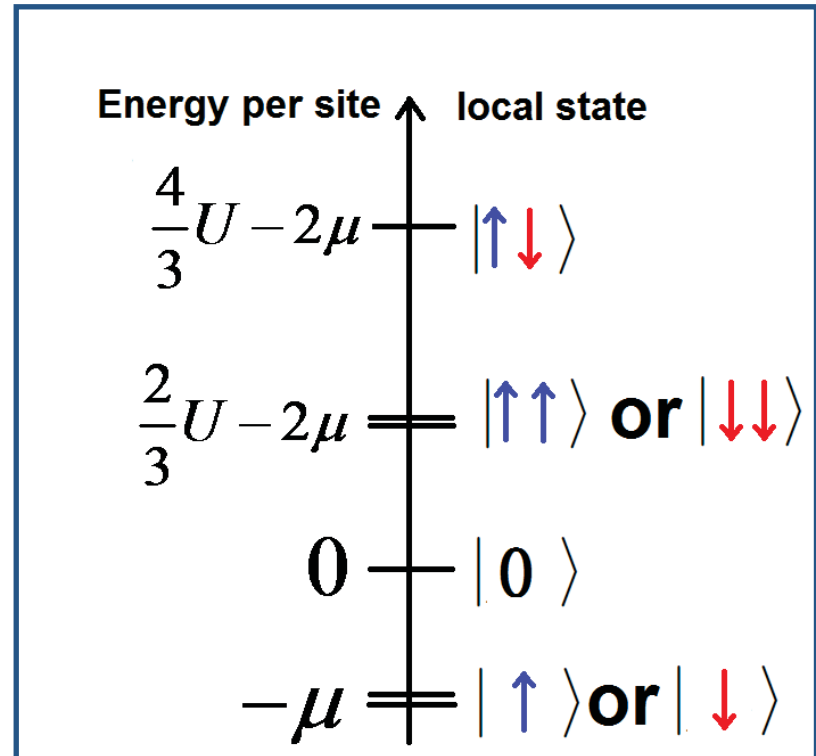
-Strong coupling limit

$$H_{\text{int}} = \frac{1}{2}U \sum_{\mathbf{r}} \left\{ n(\mathbf{r}) \left[n(\mathbf{r}) - \frac{2}{3} \right] - \frac{1}{3} L_z^2(\mathbf{r}) \right\}$$

$$\varepsilon(n, m) = \frac{U}{2} \left\{ (n+m) \left[(n+m) - \frac{2}{3} \right] - \frac{1}{3} (n-m)^2 \right\} - \mu(n+m)$$

- $\uparrow = p_x + ip_y$, $\downarrow = p_x - ip_y$
- n – the occupation number of $|\uparrow\rangle$
- m – the occupation number of $|\downarrow\rangle$

-Energy per site in the strong coupling limit



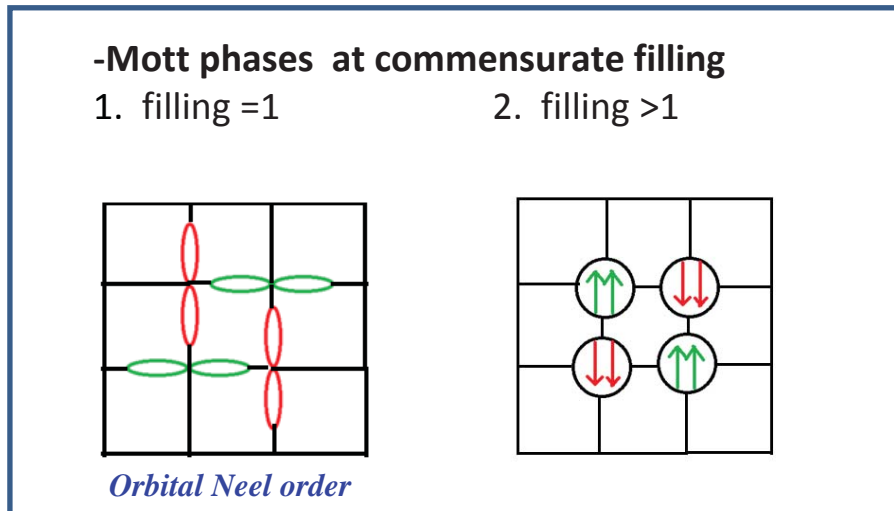
Single particle/hole gap $\sim U$

The particle/hole excitations are greatly suppressed by the gap in the strongly coupling regime.

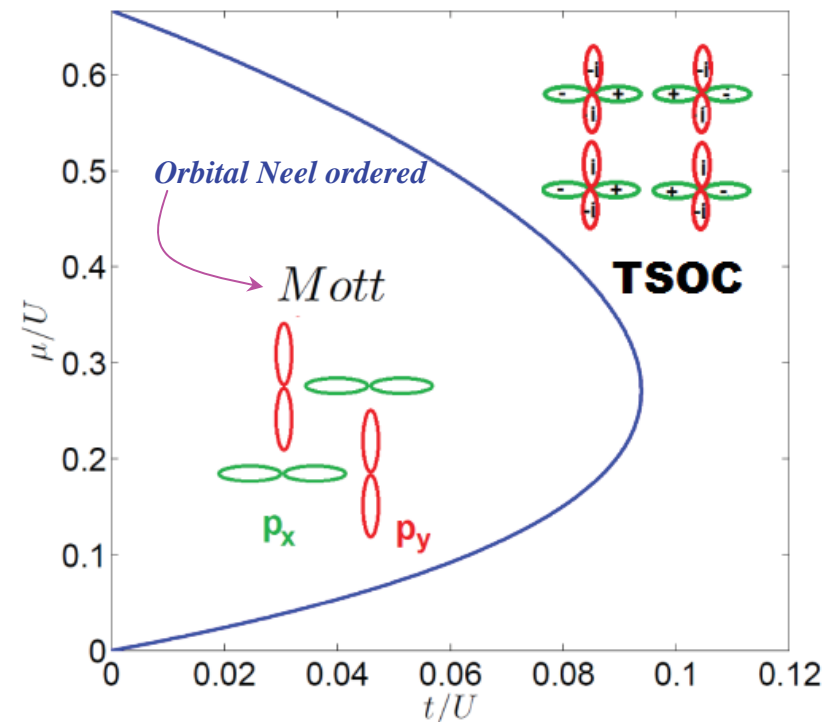
Phase diagram

[X. Li, E. Zhao and WVL, PRA 83, 063626 (2011)]

[See also early Mott phase results by A. Isacsson and S. M. Girvin, PRA 72, 053604 (2005); and A. Collin, J. Larson, and J.-P. Martikainen, Phys. Rev. A 81, 023605 (2010)]



-phase boundary of Mott with one particle per site



Compare Mott results

- Our theory agrees with Isacsson-Girvin MFT for filling=1
- Differs Isacsson-Girvin at higher integer fillings [who predicted p_x - p_y alternating]
- Collin-Larson-Martikainen disagrees with both Isacsson-Girvin and us

Compare: the usual s-band Mott phase is featureless.

Finite temperature phase transitions of the TSOC (p-orbital BEC) phase --- XY model plus Ising

$$\begin{bmatrix} \varphi_x(\mathbf{r}) \\ \varphi_y(\mathbf{r}) \end{bmatrix} = \sqrt{n_s/2} \begin{bmatrix} e^{i\theta(\mathbf{r})} (-)^{s_x(\mathbf{r})} \\ e^{i\theta(\mathbf{r}) + \frac{\pi}{2}} (-)^{s_y(\mathbf{r})} \end{bmatrix} \quad s_{x,y} = \text{even, odd}$$

$$E = -J_\theta \sum_{\mathbf{r}} [\cos(\theta(\mathbf{r}) - \theta(\mathbf{r} + x)) + \cos(\theta(\mathbf{r}) - \theta(\mathbf{r} + y))] + \sum_{\mathbf{r}} [-J_1 e^{i\pi s_y(\mathbf{r})} e^{i\pi s_y(\mathbf{r}+y)} - J_2 e^{i\pi s_y(\mathbf{r})} e^{i\pi s_y(\mathbf{r}+x)}] + \sum_{\mathbf{r}} [-J_1 e^{i\pi s_x(\mathbf{r})} e^{i\pi s_x(\mathbf{r}+y)} - J_2 e^{i\pi s_x(\mathbf{r})} e^{i\pi s_x(\mathbf{r}+x)}]$$

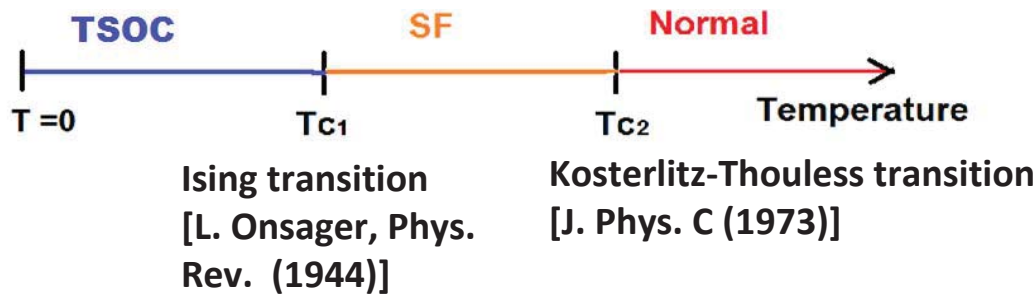
Isotropic XY

$J_\theta = (|t_{\parallel}| + |t_{\perp}|)n_s / 2$

Anisotropic Ising

$J_1 = \frac{1}{2} |t_{\parallel}| n_s$

$J_2 = \frac{1}{2} |t_{\perp}| n_s$



X. Li, E. Zhao and WVL, Phys. Rev. A 83, 063626 (2011)

Topological phase of dipolar bosons in elongated Wannier orbitals

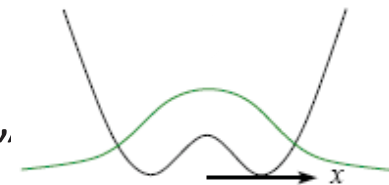
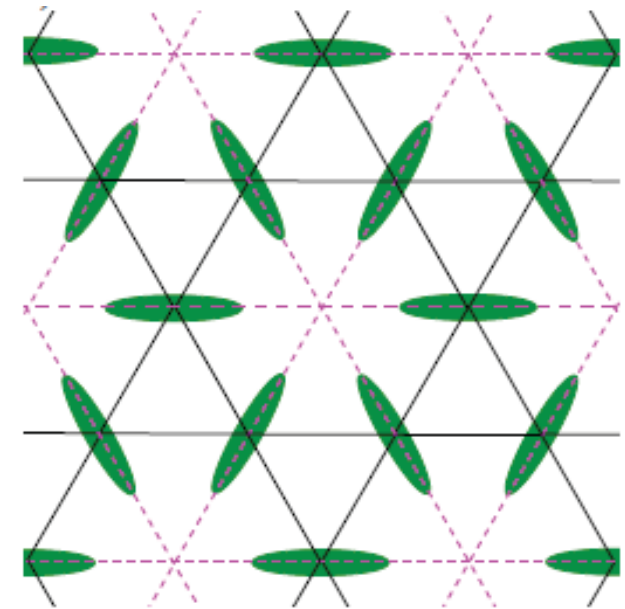
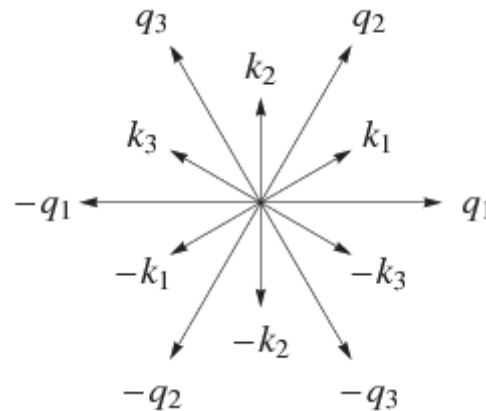
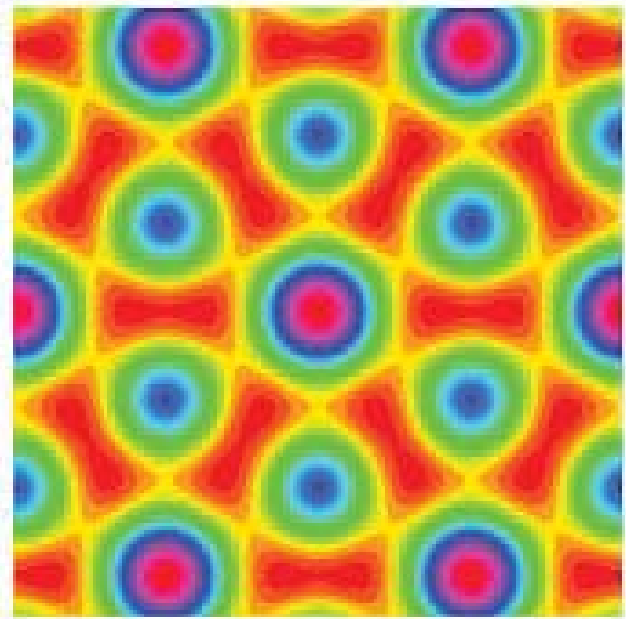
Orbital + Dipolar interaction to realize a quantum dimer model

[Kai Sun, Erhai Zhao, WVL, *Phys. Rev. Lett.* 104, 165303 (2010)]

2D Optical lattice with elongated orbital

$$I = I_1 \sum_{i=1,2,3} \cos^2(\mathbf{k}_i \cdot \mathbf{r}) + I_2 \sum_{j=1,2,3} \cos^2(\mathbf{q}_j \cdot \mathbf{r})$$

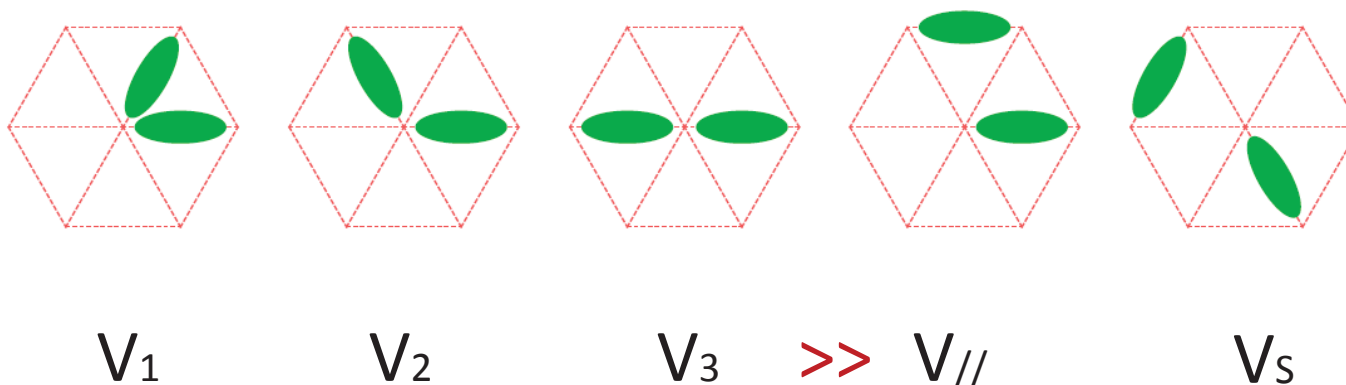
$$|\mathbf{q}_j| = \sqrt{3}|\mathbf{k}_i|, \theta_{\mathbf{q}_j} = 2j\pi/3, \theta_{\mathbf{k}_i} = (2i-1)\pi/6$$



- Elongated Wannier orbital wave-function is a “dimer”
 - use charge degree of freedom not spin
- Site of the Kagome lattice \longleftrightarrow bond of the triangular lattices
- Hard-core constraint? Polar molecules with dipolar interaction (next slide)

Polar Molecules

Dipoles aligned in z direction (2D $1/r^3$ repulsive interaction)



1/6 filling mapped to Orbital Quantum Dimer Model

- Energy scale: $1nk$ (by our estimate)
- Charge (no spin)
- Either **Fermion** or **Boson**? (Having fermionic dimers is new and unexplored.)

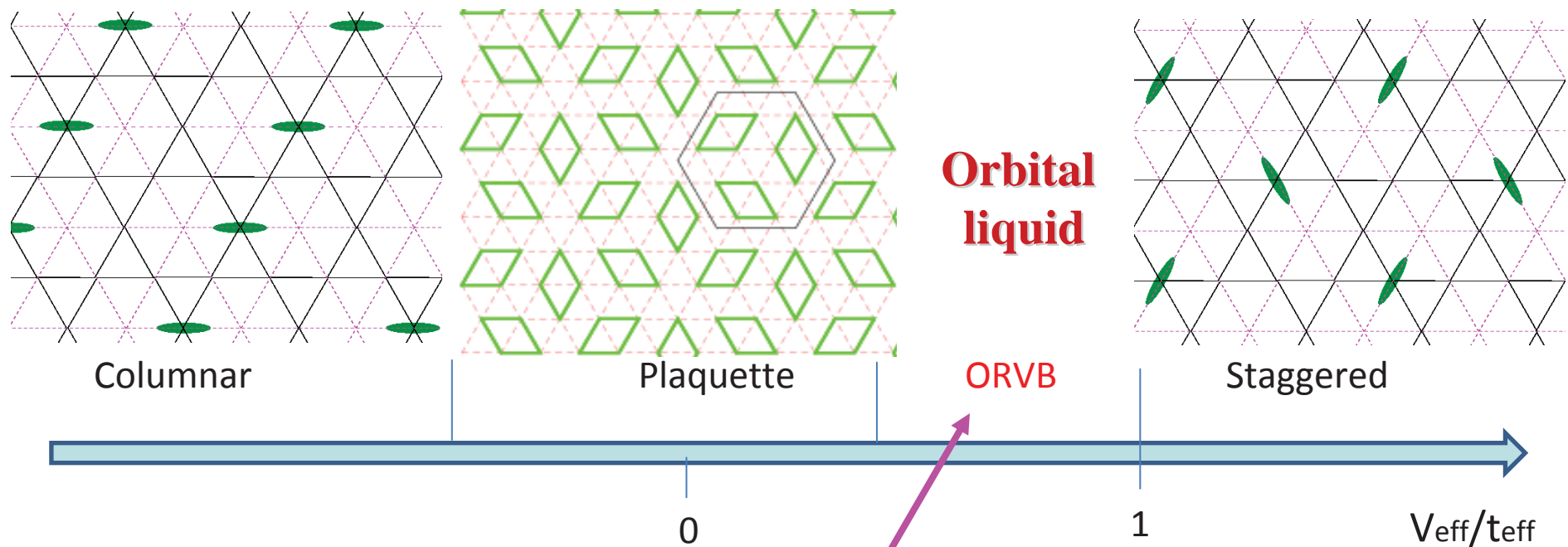
The dual effective Hamiltonian. Model of quantum dimers

$$H = -t_{\text{eff}} \sum \left(|\nabla\rangle\langle\nabla| + h.c. \right) \\ + V_{\text{eff}} \sum \left(|\nabla\rangle\langle\nabla| + |\nabla\rangle\langle\nabla| \right) \\ + \dots \text{ (perturbative terms)}$$

$$t_{\text{eff}} \sim \frac{t^2}{V_i} \quad \text{with } t = \text{molecule hopping amplitude}$$

$$V_{\text{eff}} \sim V_{\parallel} - V_S + O(t^2/V_i)$$

Phase Diagram for Bosons



- Breaks no symmetry (no local order parameter), outside the paradigm of Landau-Ginsburg-Wilson theory
 - No symmetry-related signature, c.f. other three phases
- Fractional excitation: **holons**
 - carries $\frac{1}{2}$ quantum number of the particle
 - can be **fermions** or **bosons** (microscopic details)
 - Fermionic quasiparticles in a bosonic system!
- Topological degeneracy

Unexplored Questions

- Phase transition to superfluid upon doping
- Fermionic dimers. use fermionic molecules.
- Dimers with polarity. Fill fermions onto the p-orbital?
- Challenge: Experimental detection of holons (for cold gases)

Outline

1. Introduction

- Beyond s-orbital, the basics of p-orbital? Why p-orbital?
- Recent experimental progress

2. p-band bosons (including examples of no prior analogue in solids).

- Finite momentum BEC with $p_x + ip_y$ orbital order
- Mott insulator phases and orbital order
- Elongated Orbitals and mapping to quantum dimer model

3. p-band fermions

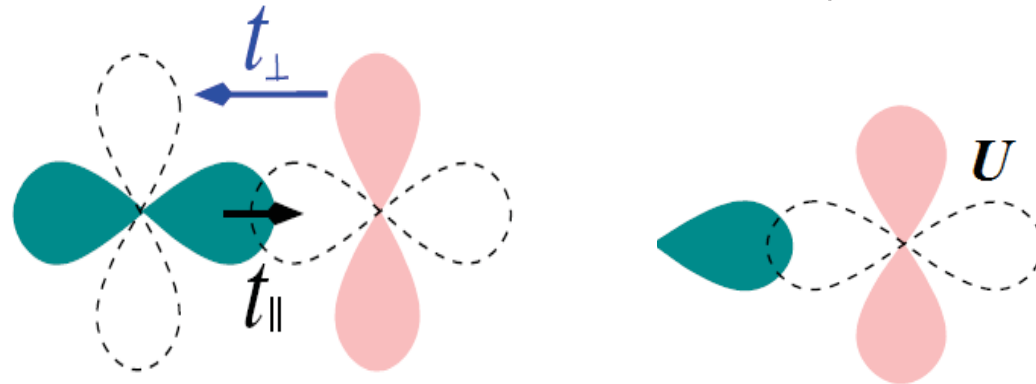
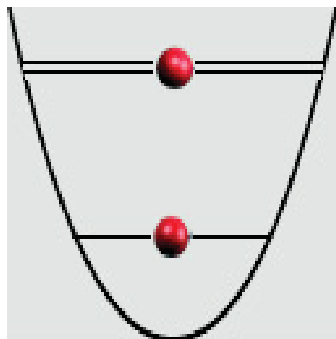
- Single species. Mott states. Orbital-only model. Realization of Kitaev-like model?
- Topological states (quantum Hall like). Topological semimetal (non-interacting), and topological insulator (turn on interaction). Time reversal breaking driven by interaction, no magnetic field!

Single species fermions in p-bands [E. Zhao and WVL, PRL (2008); C. Wu, PRL 2008.]

Motivation: Study the simplest possible case, without spin or lattice or charge effect
“plain-vanilla” orbital ordering & orbital only models

Single species (spinless) fermions interact in p-wave channel

Mott state: 2 fermion per site, one occupies the s-orbital, the other one occupies p-orbital (p_x or p_y , two fold degenerate for 2D lattice)



Strong coupling regime: U/t can be large by tuning close to a p-wave Feshbach resonance [e.g., talks of Leo Radzihovsky, G. Shlyapnikov]

Multiband (s and p) Hubbard \longrightarrow p-band Hubbard model with anisotropic hopping

Mott insulator phase - Effective orbital exchange

p-band Hubbard:

$$H_p = \sum_{i;\mu,\nu=x,y} t_{\mu\nu} [c_{i,\mu}^\dagger c_{i+\nu,\mu} + h.c.] + U \sum_i n_{ix} n_{iy}$$

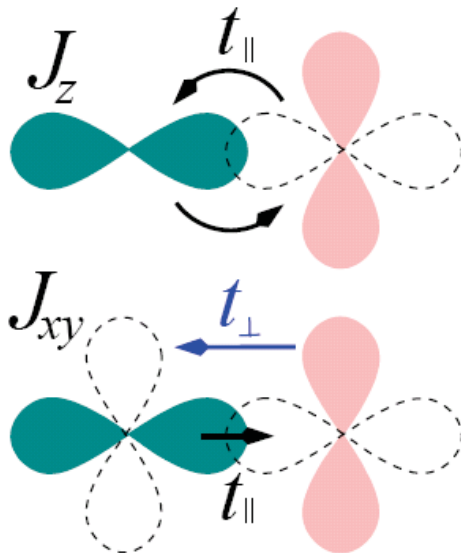
Hopping anisotropy: $t_{\mu\nu} = t_{\parallel} \delta_{\mu\nu} - t_{\perp} (1 - \delta_{\mu\nu})$

Virtual hopping \longrightarrow orbital exchange:

$$U \gg t_{\parallel}$$

$$H_{\text{orb}} = \sum_{\langle i,j \rangle} [J_{xy} (T_i^+ T_j^- + h.c.) + J_z T_i^z T_j^z]$$

$$J_{xy} \ll J_z$$



$$J_z = 2(t_{\perp}^2 + t_{\parallel}^2)/U$$

Antiferro-orbital Ising

$$J_{xy} = -2t_{\perp} t_{\parallel} / U$$

Ferro-orbital XY

$$H_{\text{orb}} \simeq J_z \sum_{\langle i,j \rangle} T_i^z T_j^z$$

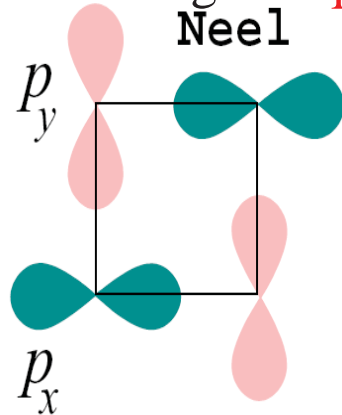
$$T^z = (c_x^\dagger c_x - c_y^\dagger c_y) / 2$$

$$T^+ = c_x^\dagger c_y, \quad T^- = (T^+)^\dagger$$

Neel orbital order and Frustration

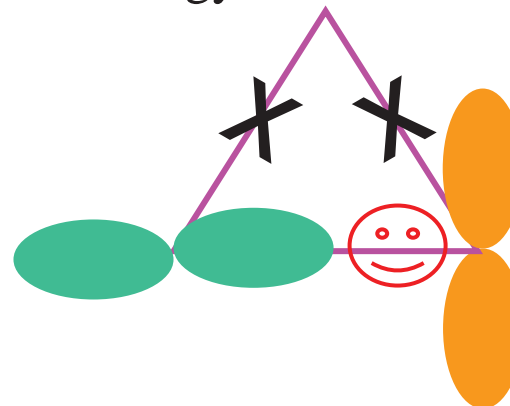
Antiferro-orbital exchange favors perpendicular alignment of nn orbitals along bonds

Neel ordering on **square** lattice



Triangle, honeycomb,
Kagome ...?

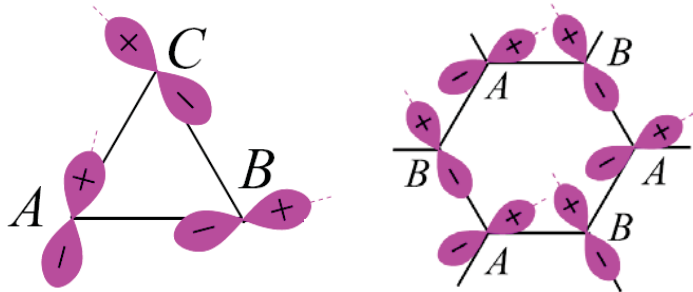
Non-orthogonal bonds can not achieve the
lowest energy simultaneously



Orbital quantum 120° model

[E. Zhao and WVL, PRL (2008); See also independent work by C. Wu, PRL 2008.]

Pseudo-spin operators on frustrated lattices (triangular, honeycomb, Kagome, ...)



$$T_\mu = \frac{1}{2} \begin{pmatrix} c_x^\dagger & c_y^\dagger \end{pmatrix} \sigma_\mu \begin{pmatrix} c_x \\ c_y \end{pmatrix}$$

$\mu, \nu = x, y, z$

The orbital exchange Hamiltonian is:

$$H_{120} = J_z \sum_{\mathbf{R}, j} T_j(\mathbf{R}) T_j(\mathbf{R} + \hat{e}_j)$$

lattice sites $j=1,2,3$

where

$$T_1 = T_z, T_2 = -\frac{1}{2}T_z - \frac{\sqrt{3}}{2}T_x$$

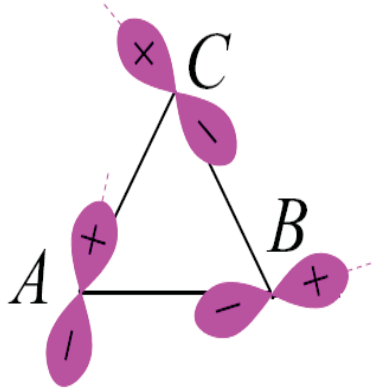
$$T_3 = -\frac{1}{2}T_z + \frac{\sqrt{3}}{2}T_x$$

This quantum 120° model is closely related to the **compass model** and **Kitaev model**.
 Quantum 120° model of electron e_g orbitals: van den Brink, New J. Phys. 6, 201 (2004).

(classical) Orbital phase on Kagome lattice

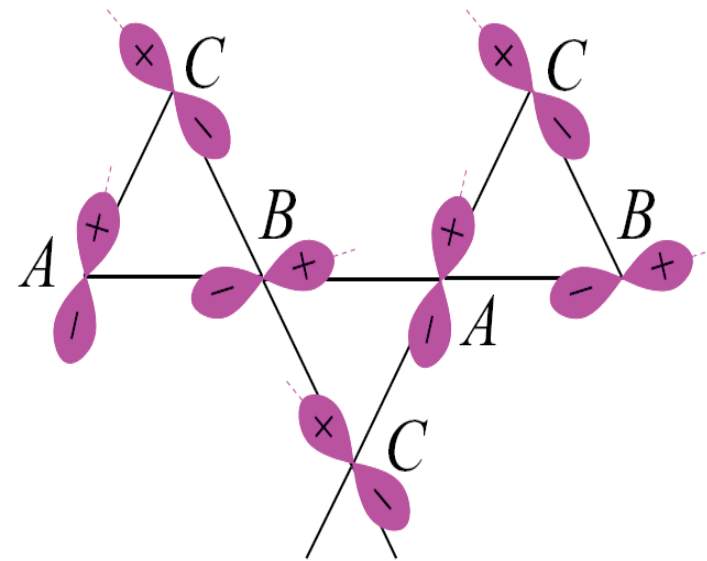
Strategy: large pseudospin T expansion, first solve the classical problem (mean field), then consider $1/T$ quantum fluctuation corrections.

Single triangle: minimize the classical energy



- Orbital at 15° with the bond
- Equivalent configuration: all orbitals rotated by 90°

Kagome lattice: corner shared triangles



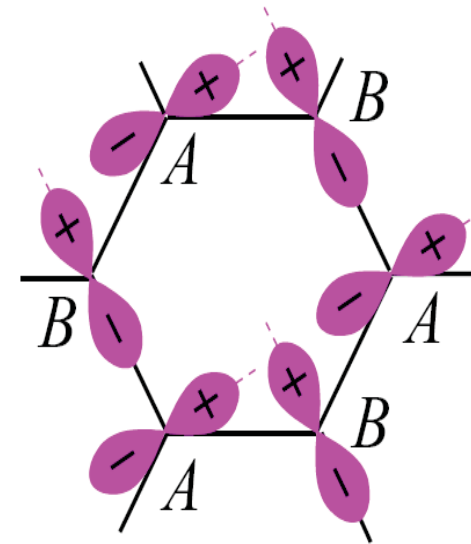
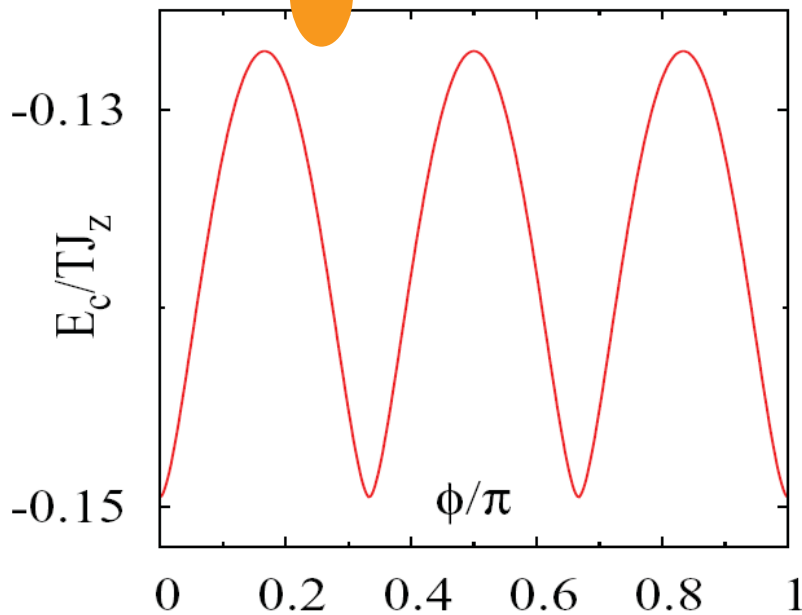
Order by disorder: honeycomb lattice

Classical energy is minimized for any Neel configuration, continuous degeneracy

Orbital wave fluctuations: correction to ground state energy

$$\frac{E_c(\phi)}{TJ_z} = \frac{1}{N} \sum_{\mathbf{k}, \lambda} \omega_\lambda(\mathbf{k}) \frac{\phi}{2}$$

or ...



Orbital at sublattice A at angle $n \cdot 30^\circ$

Mott phase of **3D** (*orbital only!*) lattice model

Interaction different for three p-wave channels

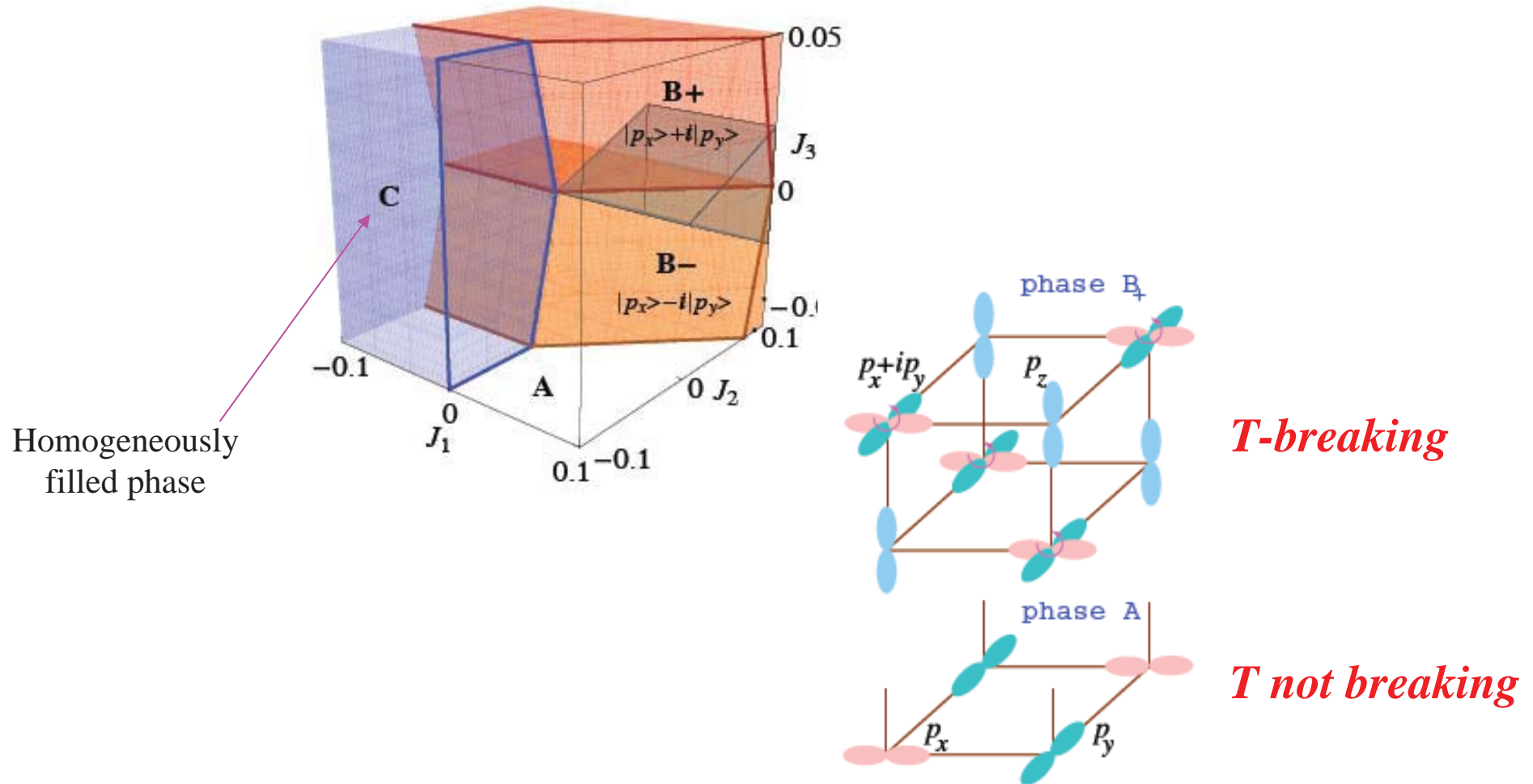
- 3D lattice
- 1/3 filling, three p-states per site

$$\begin{aligned}
 H_{\text{eff}} = & - \sum_{\mathbf{i}} \left[\sum_{\mu=x,y,z} \sum_{\delta=\pm\mathbf{e}_\mu} J_\mu n_{\mu,\mathbf{i}} (1 - n_{\mu,\mathbf{i}+\delta}) \right. \\
 & + \sum_{\mu=x,y} \sum_{\delta=\pm\mathbf{e}_\mu} (J_2 - J_1) n_{\mu,\mathbf{i}} n_{z,\mathbf{i}+\delta} \\
 & \left. + \sum_{\delta=\pm\mathbf{e}_z} J_3 (i c_{y,\mathbf{i}}^\dagger c_{x,\mathbf{i}} n_{z,\mathbf{i}+\delta} + h.c.) \right]
 \end{aligned}$$

$$J_x = J_y \equiv J_1, \quad J_z \equiv J_2$$

- Effective model for the system of Goyal-Reichenbach-Deutsch [PRA 2010] with optical p-wave Feshbach resonance (e.g., ^{171}Yb)
- $m = -1, 0, +1$ channels separate
- Explicit Time-Reversal breaking term

p-band fermions at 1/3 filling in 3D – Phase diagram



[with P. Hauke, E. Zhao, K. Goyal, I. Deutsch, M. Lewenstein, arXiv:1103.5964]

Topological Semimetal: a probable new state of cold gases in optical lattices

protected by D4 symmetry

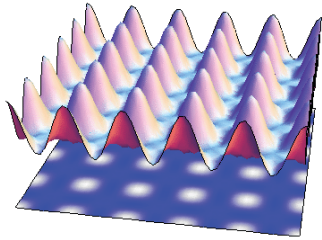
Work done (in collaboration) with:

- Kai Sun (Maryland)
- Sankar Das Sarma (Maryland)
- Andreas Hemmerich (Hamburg)

[[arXiv:1011.4301](https://arxiv.org/abs/1011.4301)]

Motivations and Summary of Results

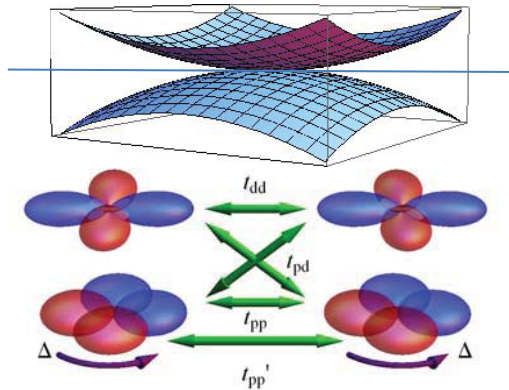
A. Fermions on a square lattice of double-wells



$$V(x, y) = -V_1[\cos(kx) + \cos(ky)] + V_2[\cos(kx + ky) + \cos(kx - ky)]$$

Will show how to experimentally realize [with Hemmerich]

B. Mixing of p and d orbitals: Semi-metal with topological winding number 2



- **Beyond Fermi liquid:** $k_F=0$
- **Graphene:** (Nobel Prize 2010)
- Here: a different example of semi-metal

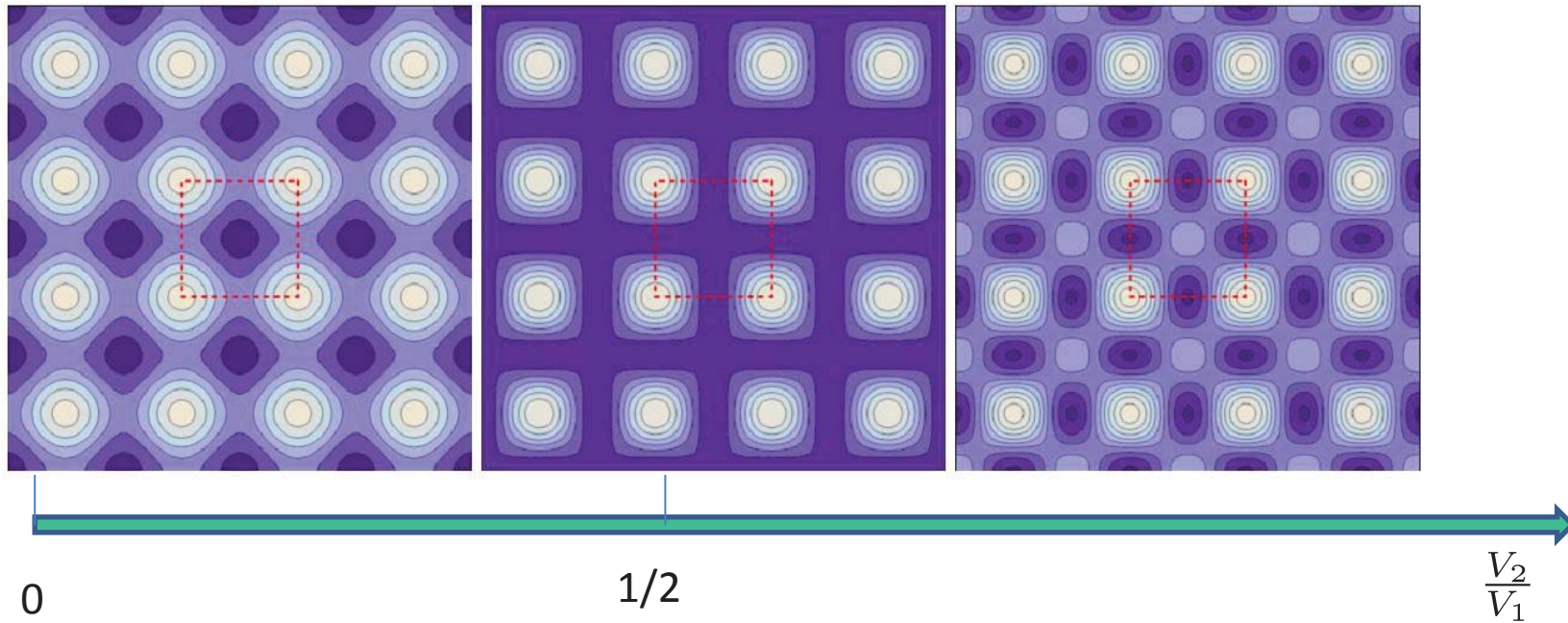
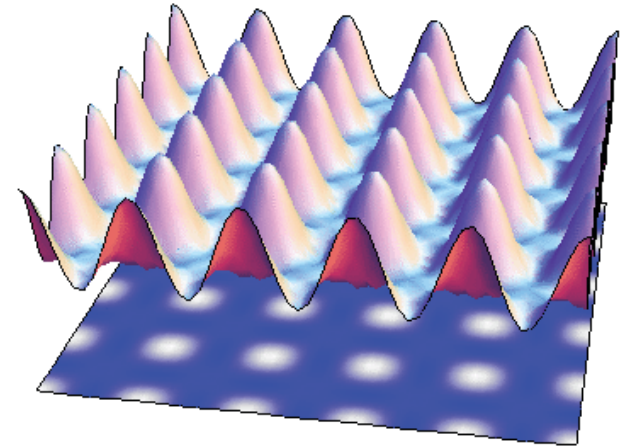


C. Interaction turns this topological semimetal into topological insulator. Mechanism differs from:

- Rotating fermions
- Synthetic gauge fields: I. B. Spielman (2009)

Optical lattice and Band degeneracy

$$V(x, y) = -V_1[\cos(kx) + \cos(ky)] \\ + V_2[\cos(kx + ky) + \cos(kx - ky)]$$

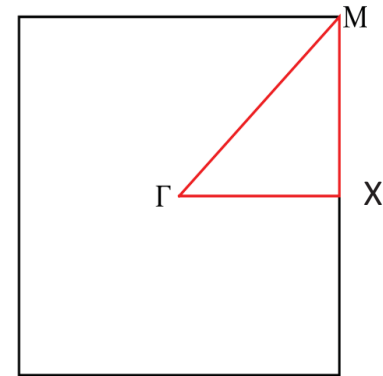


Band structure (from Numerical)

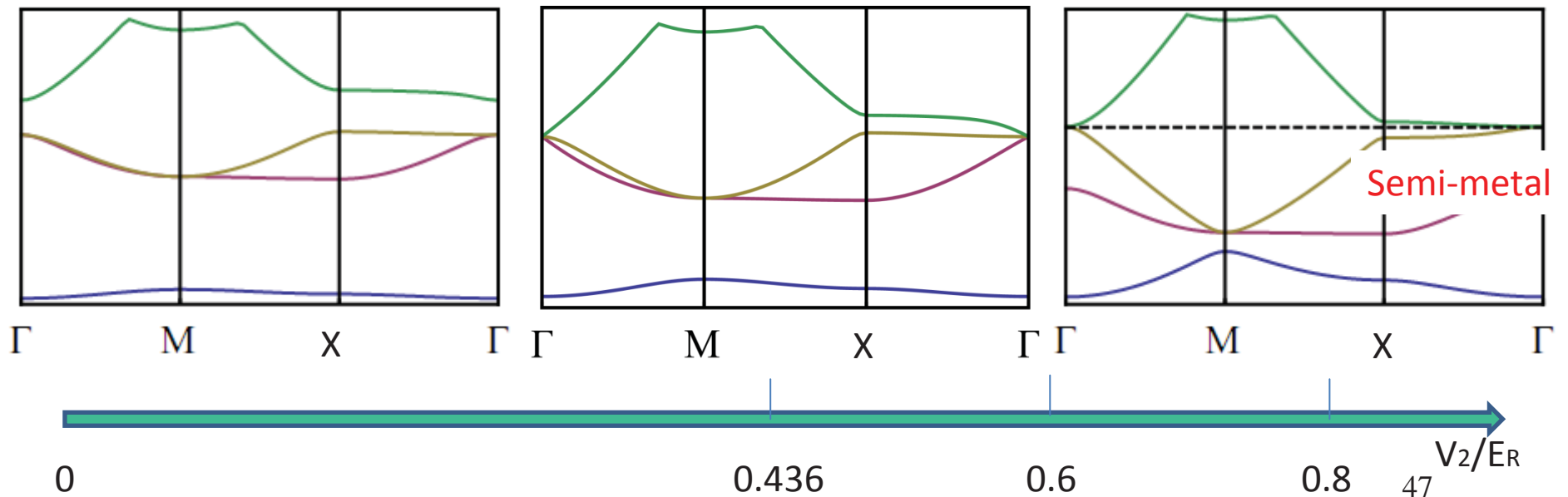
$$V(x, y) = -V_1[\cos(kx) + \cos(ky)] + V_2[\cos(kx + ky) + \cos(kx - ky)]$$

$$V_1 = 1.2 E_R$$

$$V_2 < 0.8 E_R$$



Band Degeneracy: Very stable (symmetry/ topologically protected)



Topology of the band degenerate point Γ

Expand momentum around point Γ :

$$\mathcal{H} = \frac{t_1 + t_2}{2}(k_x^2 + k_y^2)I + 2t_3k_xk_y\sigma_x + \frac{t_1 - t_2}{2}(k_x^2 - k_y^2)\sigma_z$$

$$t_1 = t_{pp} + \frac{4t_{pd}^2}{2t_{pp} - 2t'_{pp} + 4t_{dd} - \delta}, \quad t_2 = -t'_{pp}, \quad t_3 = \frac{2t_{pd}^2}{2t_{pp} - 2t'_{pp} + 4t_{dd} - \delta}$$

Map Hamiltonian to a planar vector

$$\vec{h} = \left(2t_3k_xk_y, \frac{t_1 - t_2}{2}(k_x^2 - k_y^2) \right)$$

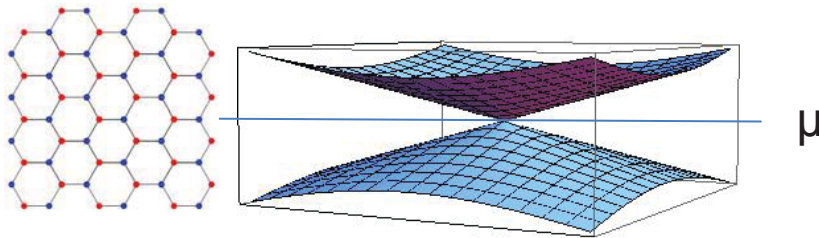
Winding number

$$W = \frac{1}{2\pi} \oint_C d\mathbf{k} \cdot \left[\epsilon_{ij} \frac{h_i}{|\vec{h}|} \nabla \left(\frac{h_j}{|\vec{h}|} \right) \right]$$

Found $W=2$ for Γ point

Interaction

Dirac Point (graphene)

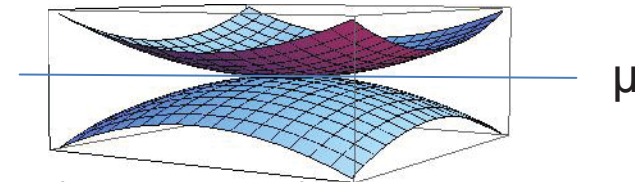


- Linear dispersion relation
- Appear in pairs at k and $-k$ (same energy)
- Observed in real systems

At low T

- **Stable against short-range interactions**

Semi-metal found here

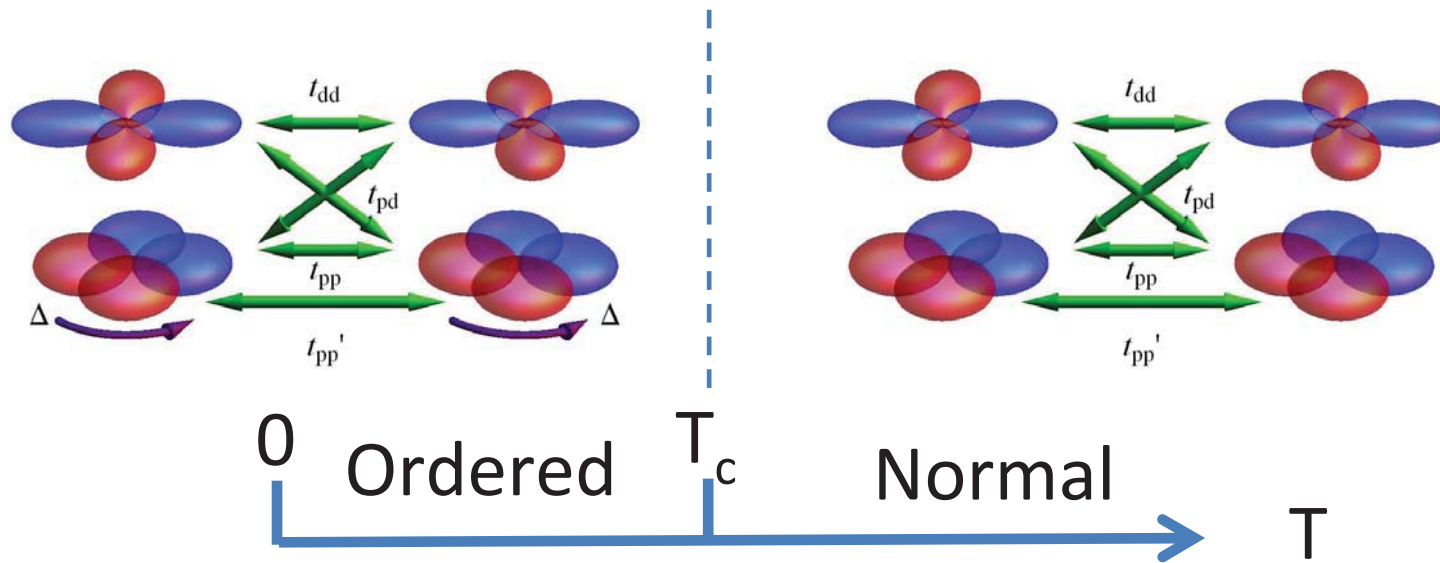


- Quadratic dispersion relation
- no pairs at $-k$ (can split into two Dirac point)
- Not observed in real systems

At low T

- **Unstable against short-range repulsions** (by usual Renormalization group analysis, applied to quadratic dispersion, time scaling $\text{dim}=2$ opposed to 1 in usual Fermi liquid)

Phase diagram



$$H_{\text{int}} = V \sum_{\vec{r}} p_{x,\vec{r}}^\dagger p_{x,\vec{r}} p_{y,\vec{r}}^\dagger p_{y,\vec{r}} = -\frac{V}{2} \sum_{\vec{r}} (L_{\vec{r}}^z)^2$$

$$L_{\vec{r}}^z = -i(p_{x,\vec{r}}^\dagger p_{y,\vec{r}} - p_{y,\vec{r}}^\dagger p_{x,\vec{r}})$$

$$L_{\vec{r}}^z |p_x + ip_y\rangle = |p_x + ip_y\rangle$$

$$L_{\vec{r}}^z |p_x - ip_y\rangle = -|p_x - ip_y\rangle$$

Low T ordered phase:

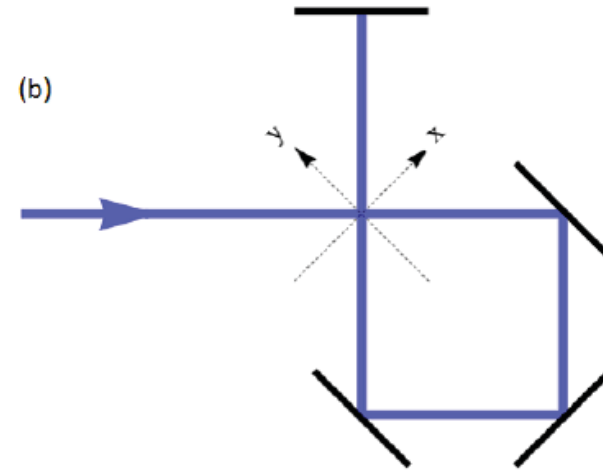
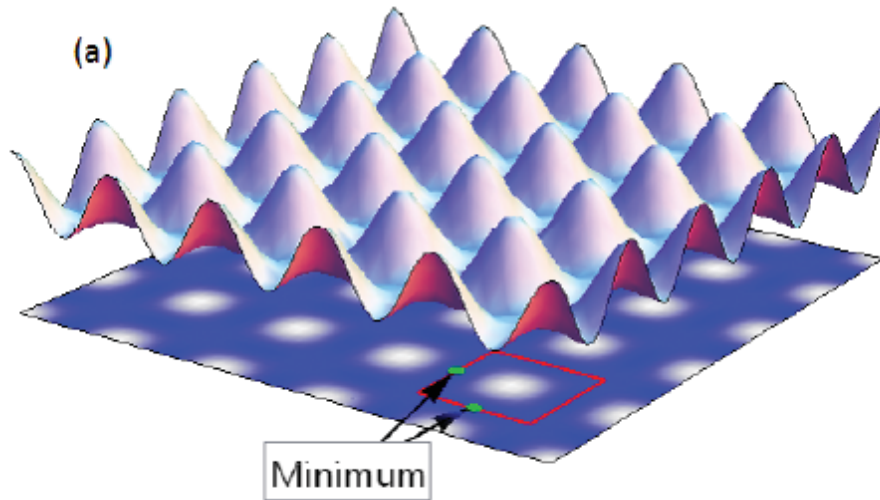
- Breaks Time-reversal symmetry
- Topological state of matter
- Quantum Hall induced by interaction
 - Anomalous Quantum Hall [1-2]
 - Chern number=1 [2]

1. Haldane PRL 1988; S. Raghu, et.al. PRL 2008.

2. K. Sun, et al. PRL 2009, PRB 2008. 50

How to realize the proposed lattice?

[due to A. Hemmerich]



$$E = \epsilon \begin{pmatrix} 0 \\ \sin \alpha \\ \cos \alpha \end{pmatrix} \cos [k(x + y)/2] - \epsilon \begin{pmatrix} \sin \alpha \\ 0 \\ \cos \alpha \end{pmatrix} \cos [k(x - y)/2]$$



by $U(x, y) = -\chi |E(x, y)|^2$

$$U(x, y) = -V_1 [\cos(kx) + \cos(ky)] + V_2 [\cos(kx + ky) + \cos(kx - ky)] + \chi \epsilon^2$$

$$V_1 = -\chi \epsilon^2 \cos^2 \alpha,$$

$$V_2 = -\chi \epsilon^2 / 2.$$

Conclusion

- Degenerate p-orbitals. Emergent symmetry. Orbital physics.
- Novel superfluid and Mott states – no prior analogue in condensed matter physics.
 - *Examples: T-breaking $px+ipy$ finite-momentum BEC. Real or complex orbital Neel order in Mott states. Topological semimetal. Interaction-driven quantum Hall-like topological insulator, etc.*
- Can also emulate condensed matter orbital models (*e.g., quantum 120° model*)

Interested? Perspectives in:

OPTICAL LATTICES

Orbital dance

Emulating condensed-matter physics with ground-state atoms trapped in optical lattices has come a long way. But excite the atoms into higher orbital states, and a whole new world of exotic states appears.

Maciej Lewenstein and W. Vincent Liu [Nature Phys. 7, 101 (Feb 2011) (news and views)]