Exploring New States of Matter in the *p*-orbital Bands of Optical Lattices

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C. Wu, D. Bergman, L. Balents, and S. Das Sarma, cond-mat/0701788.
C. Wu, W. V. Liu, J. Moore and S. Das Sarma, PRL 97, 190406 (2006).
W. V. Liu and C. Wu, PRA 74, 13607 (2006).

KITP, 02/01/2007.

Collaborators

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Outline

- **Introduction.**

  - Rapid progress of cold atom physics in optical lattices.

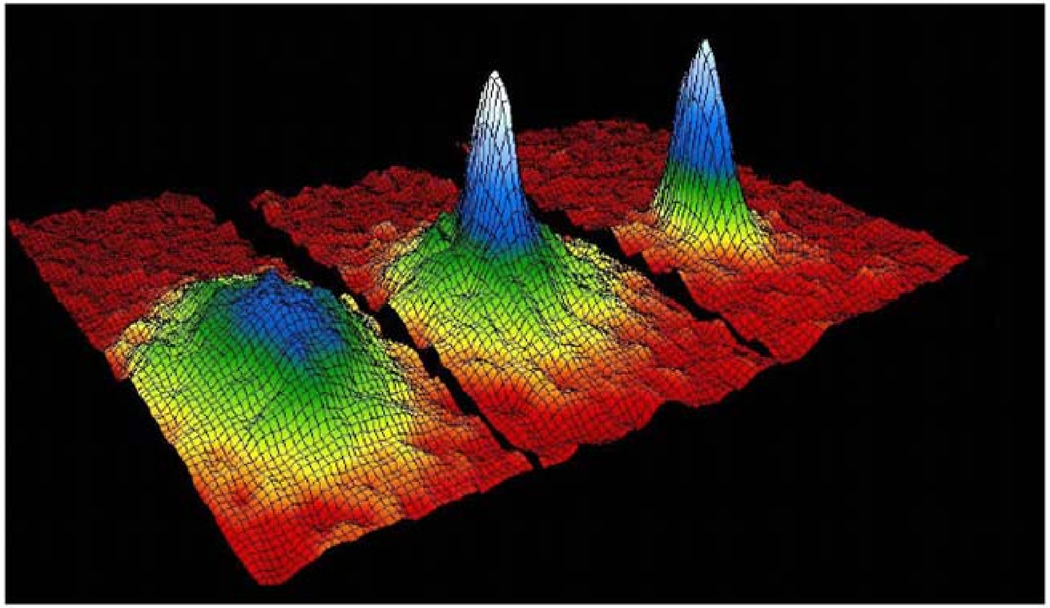
  - New direction: orbital physics in high orbital bands; several pioneering experiments.

- New features of orbital physics in optical lattices.

  Fermions: flat bands and crystallization in honeycomb lattice.

  Bosons: novel superfluidity with time-reversal symmetry breaking (square, triangular lattices).

Bose-Einstein condensation



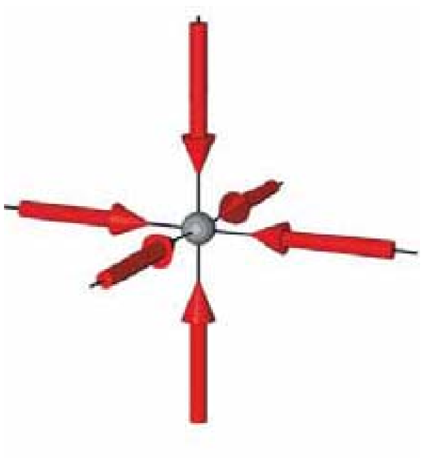
M. H. Anderson et al., Science 269, 198 (1995)

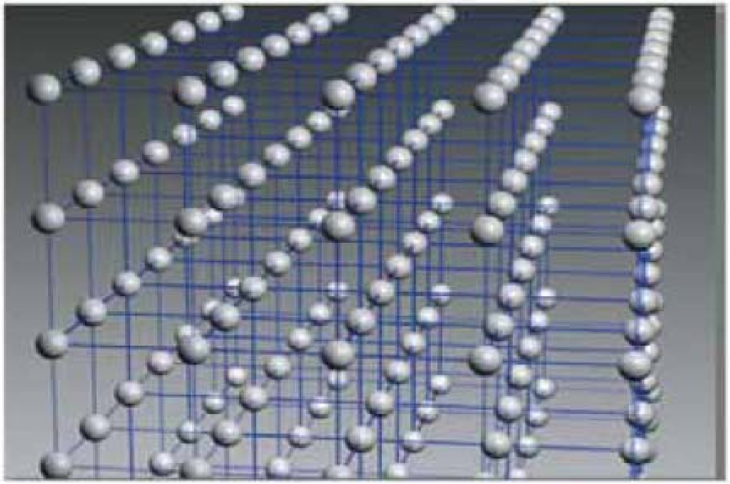
$$T_{BEC} \sim 1\mu K \quad n \sim 10^{14}\,\mathrm{cm}^{-3}$$

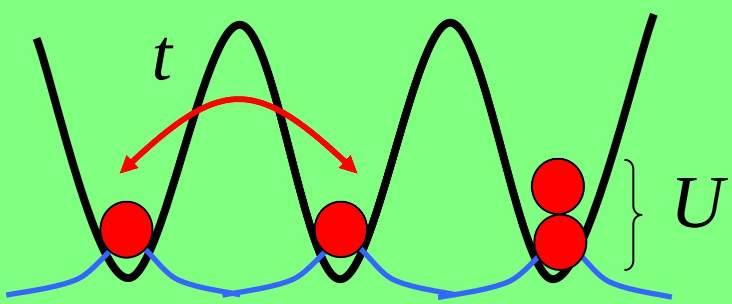
weakly interacting systems

New era: optical lattices

- New opportunity to study strongly correlated systems.
- Interaction effects are tunable by varying laser intensity.





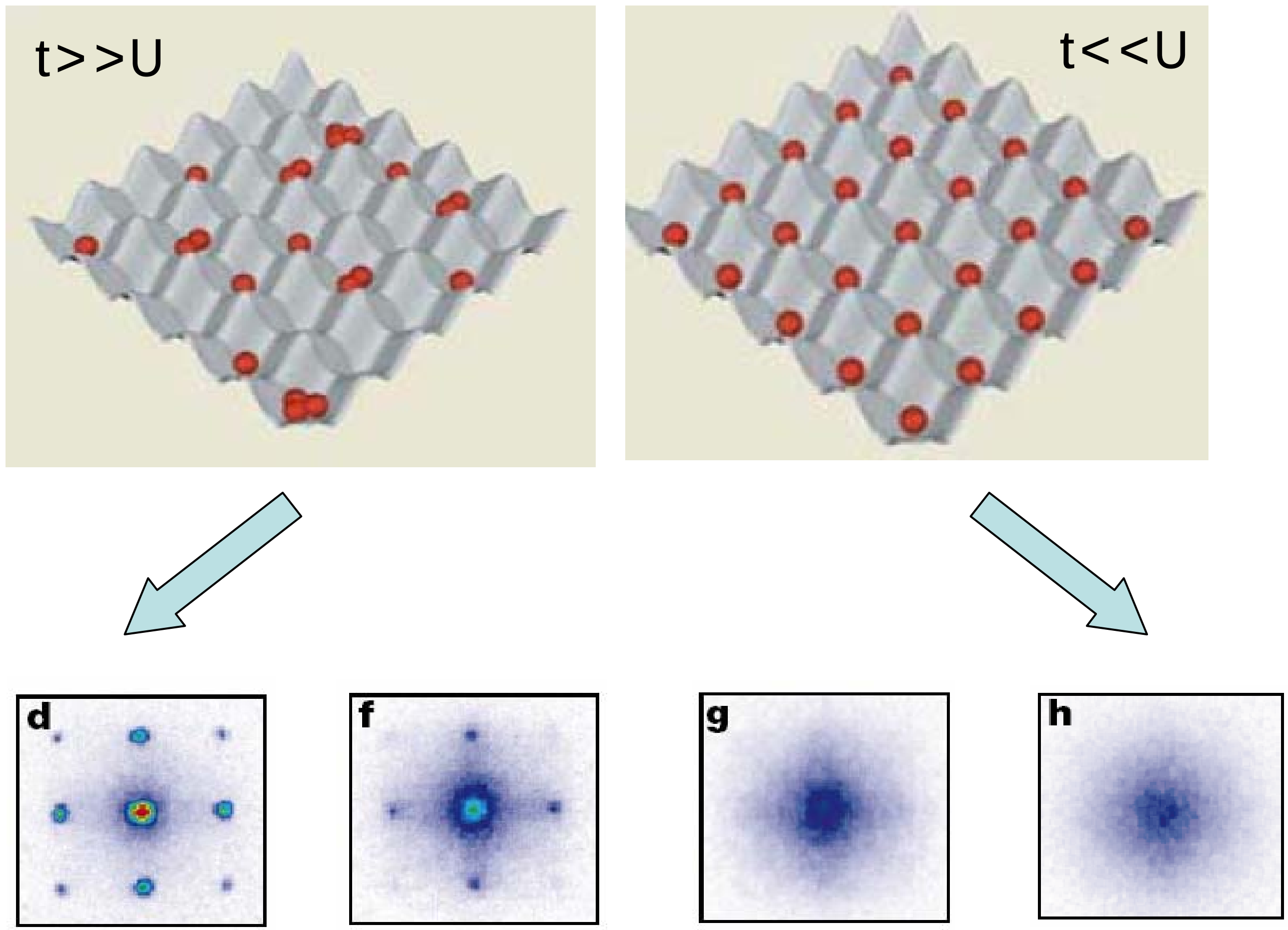


t: inter-site tunneling
U: on-site interaction

Superfluid-Mott insulator transition

Superfluid

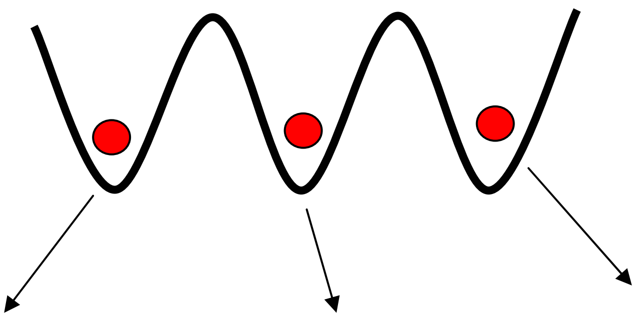
Mott insulator

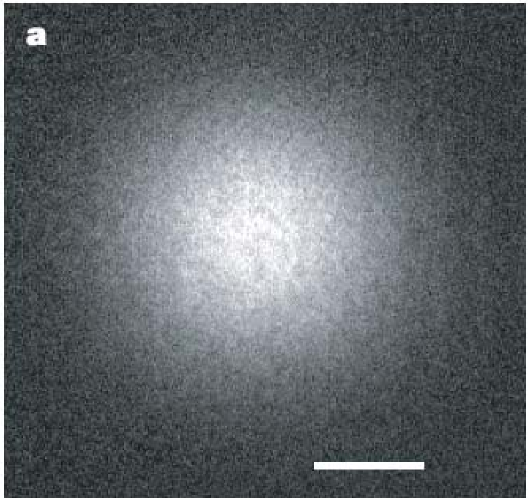


^{87}Rb

Greiner et al., Nature (2001).

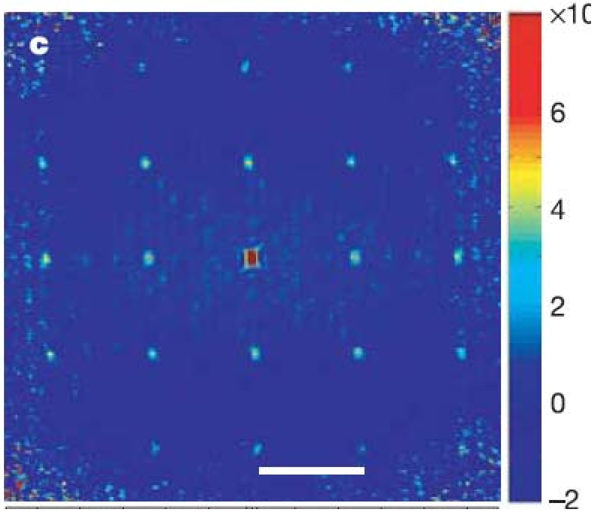
Noise correlation (time of flight) in Mott-insulators





- 1st order coherence $\langle n(\vec{k}) \rangle$ disappears in the Mott-insulating state.

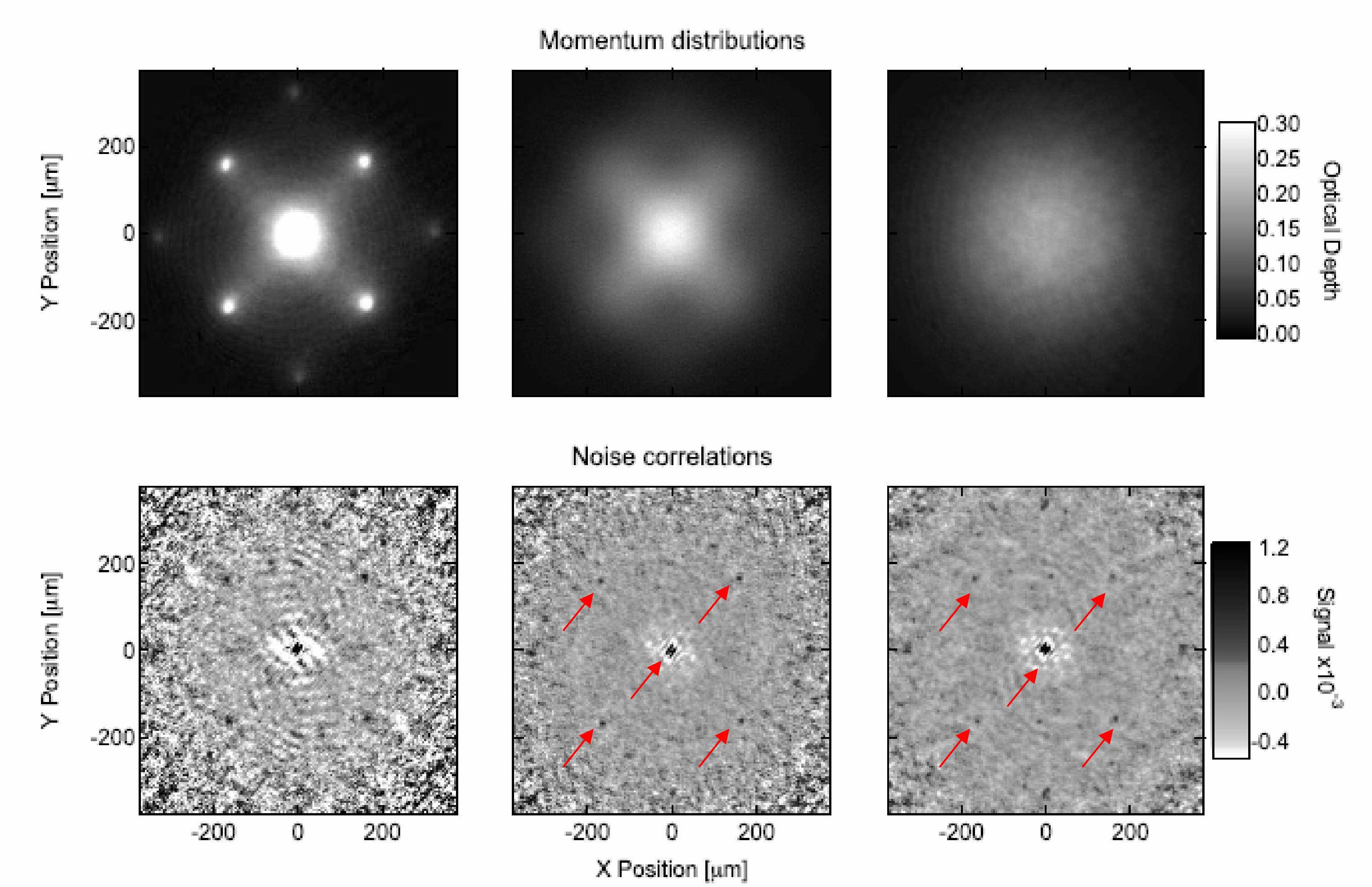
- Noise correlation function oscillates at the reciprocal lattice vectors; bunching effect for bosons.



$$\langle n(\vec{k}_1) n(\vec{k}_2) \rangle - \langle n(\vec{k}_1) \rangle \langle n(\vec{k}_2) \rangle \propto \sum_G \delta(\vec{k}_1 - \vec{k}_2 - \vec{G})$$

Folling et al., Nature 434, 481 (2005); Altman et al., PRA 70, 13603 (2004).

Two dimensional superfluid-Mott insulator transition

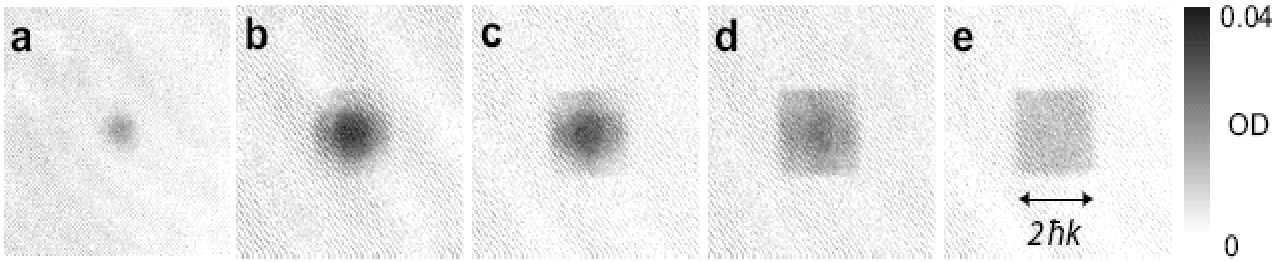


$V/E_R = 12$ $\qquad V/E_R = 20$ $\qquad V/E_R = 21$

I. B. Spielman et al., cond-mat/0606216.

Fermionic atoms in optical lattices

- Observation of Fermi surface. $^{40}K: \left|Fm\right\rangle = \left|\frac{9}{2}\frac{9}{2}\right\rangle, \left|\frac{9}{2}\frac{7}{2}\right\rangle$

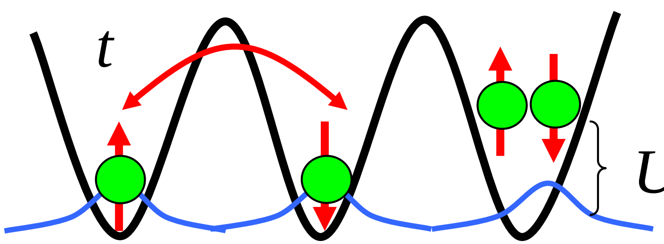


Esslinger et al., PRL 94:80403 (2005)

Low density: metal

high density: band insulator

$$H = -t\sum_{i,j,\sigma} c_{i\sigma}^{+} c_{j\sigma} + U\sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i} n_{i}$$



- Simulating strongly correlated condensed matter systems.

e.g. Can 2D Hubbard model describe high T_c cuprates?

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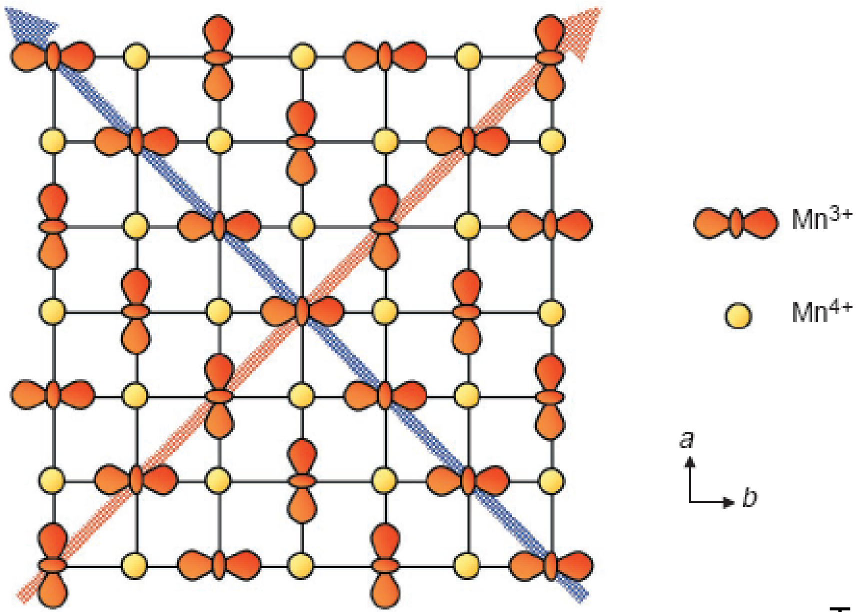
Orbital physics

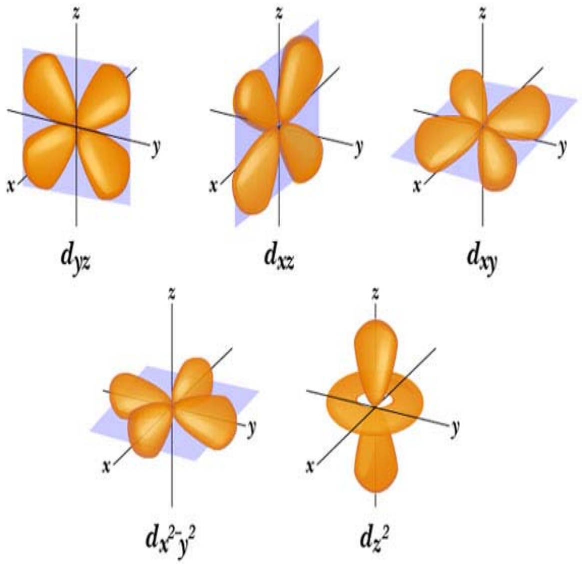
- Orbital: a degree of freedom independent of charge and spin.

- Orbital band degeneracy and spatial anisotropy.

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

Charge and orbital ordering in $La_{1-x}Sr_{1+x}MnO_4$

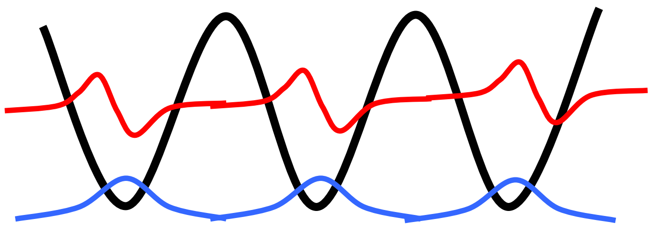


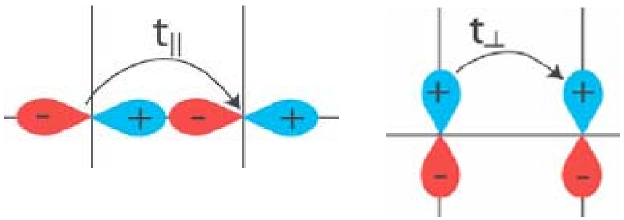


Tokura, et al., science 288, 462, (2000).

New features of orbital physics in optical lattices

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





σ-bond **π-bond**

- *p*-orbital physics using cold atoms.

  strong anisotropy: flat band, novel orbital ordering ... ...

  bosons in excited bands: frustrated superfluidity with translational and time-reversal symmetry breaking ... ...

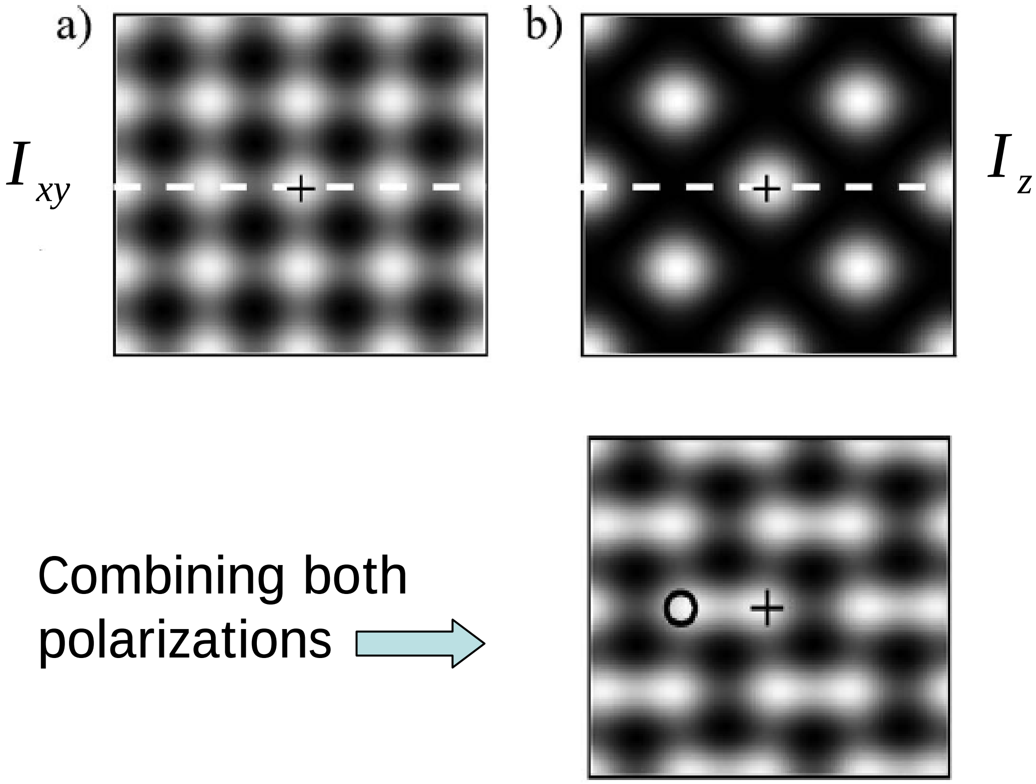
- Fermions: *s*-band is fully-filled; *p*-orbital bands are active.

- Bosons: pumping bosons from *s* to *p*-orbital bands.

Double-well optical lattices

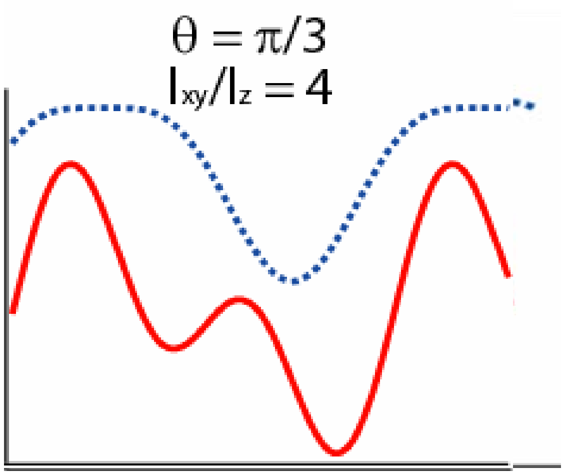
J. J. Sebby-Strabley, et al., PRA 73, 33605 (2006).

- Laser beams of in-plane and out-of-plane polarizations.



White spots=lattice sites.
Note the difference in lattice period!

Combining both polarizations

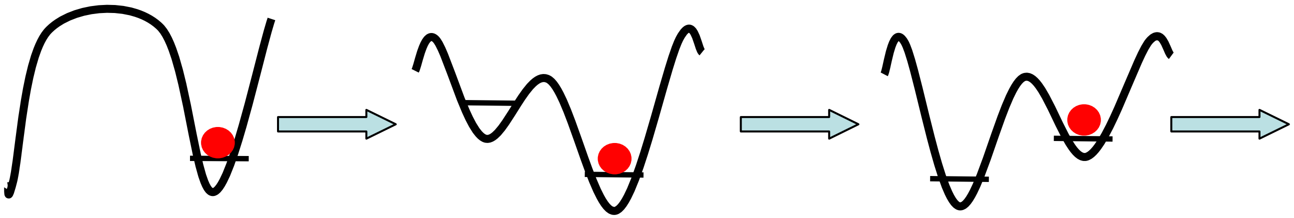


- The potential barrier height and the tilt of the double well can be tuned.

Transfer bosons to the excited band

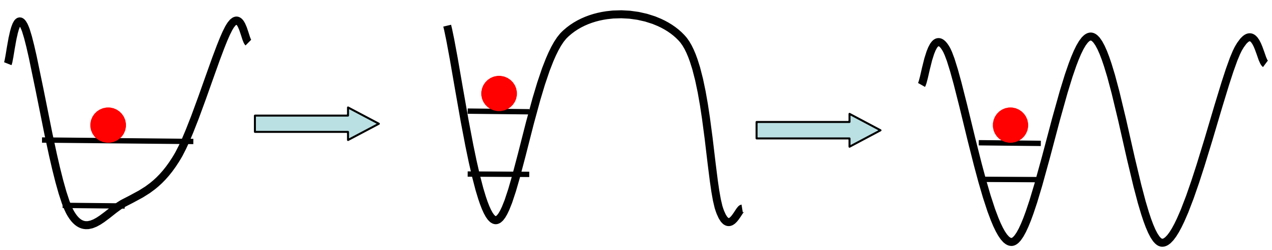
Grow the long period lattice

Avoid tunneling (diabatic)

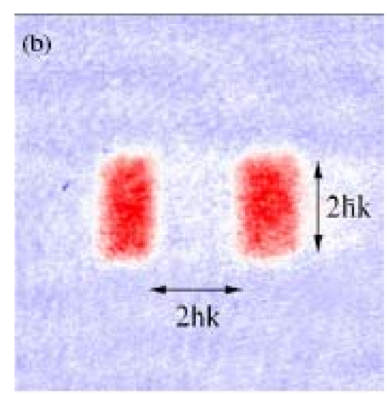


Create the excited state (adiabatic)

Create the short period lattice (diabatic)



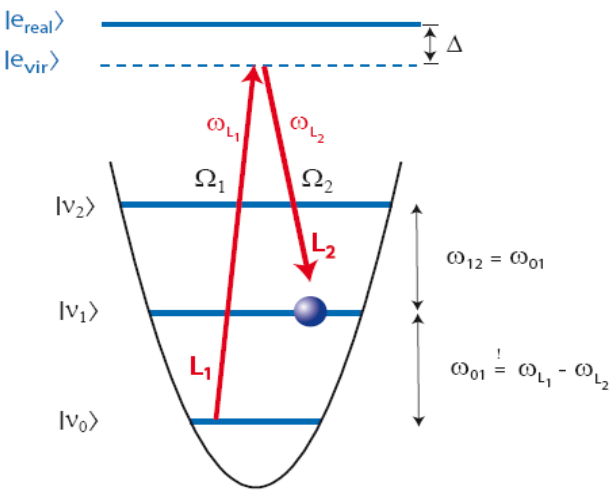
- Band mapping.
- Phase incoherence.

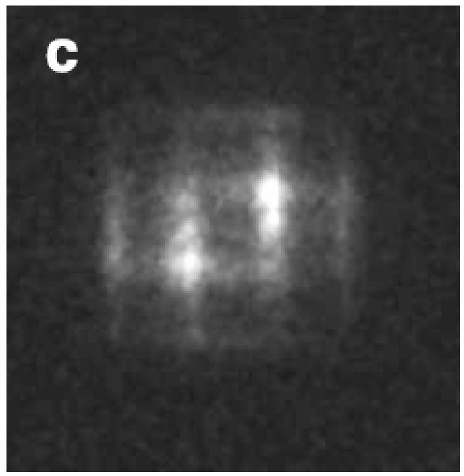


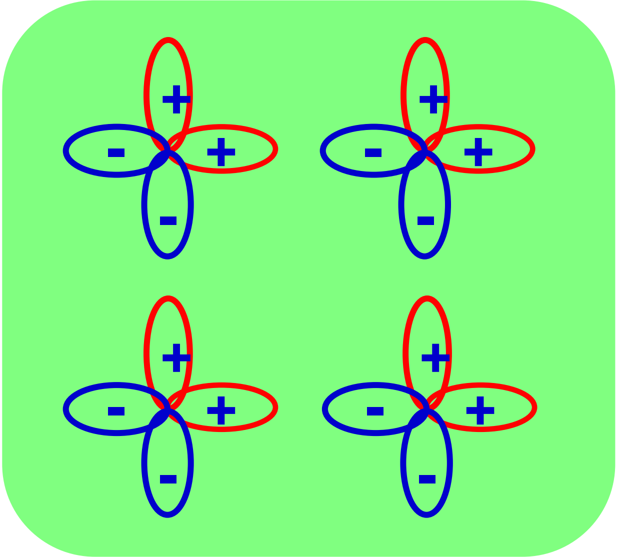
M. Anderlini, et al., J. Phys. B 39, S199 (2006).

Ongoing experiment: pumping bosons by Raman transition

- Long life-time: phase coherence.
- Quasi-1d feature in the square lattice.



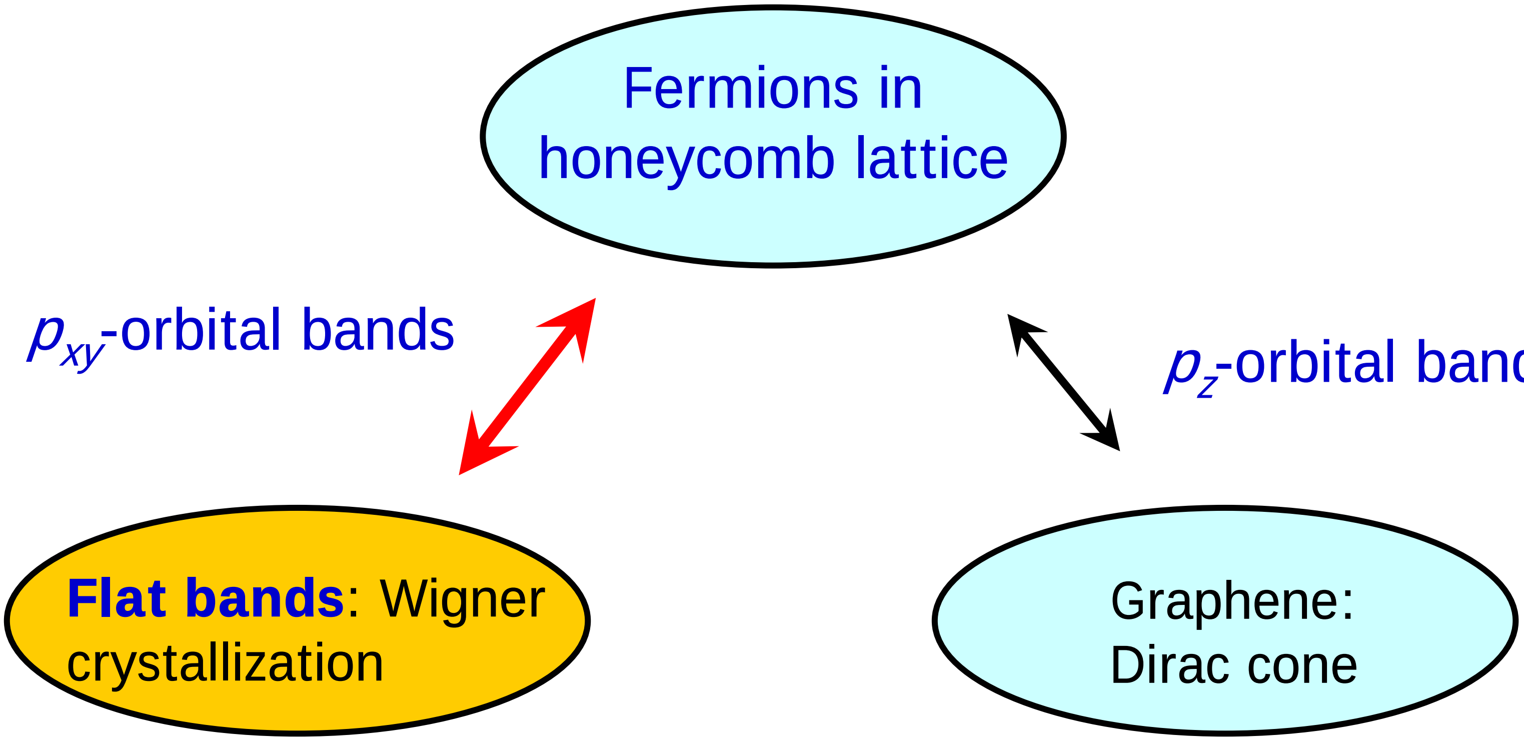




T. Mueller, I. Bloch et al.

Outline

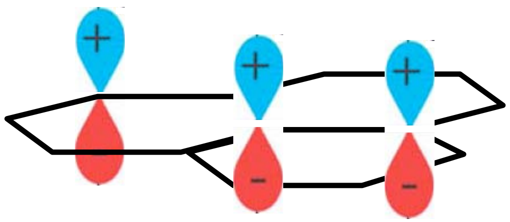
- Introduction.
- **New features of orbital physics in optical lattices.**

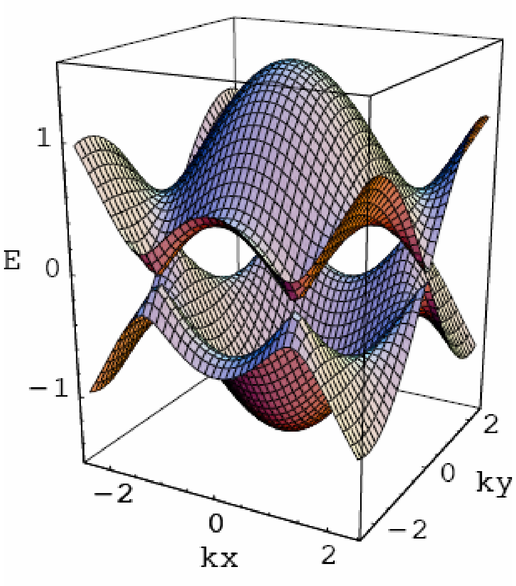


C. Wu, D. Bergman, L. Balents, and S. Das Sarma, cond-mat/0701788

Honeycomb lattice: a surge of research interest

- Graphene: $2p_z$-orbital band; Dirac cone; isotropic and non-degenerate.

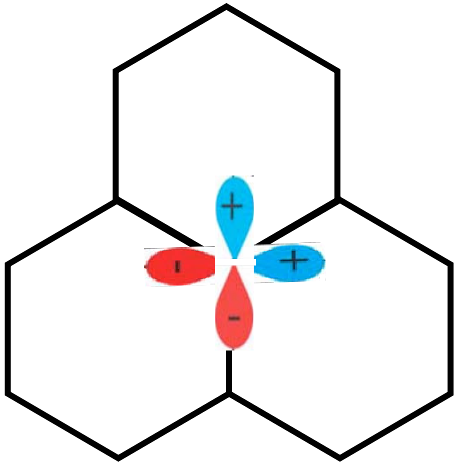




- Even more interesting physics in the px, py-orbital bands.

However, in graphene, $2p_x$, $2p_y$-orbital bands hybridize with $2s$.

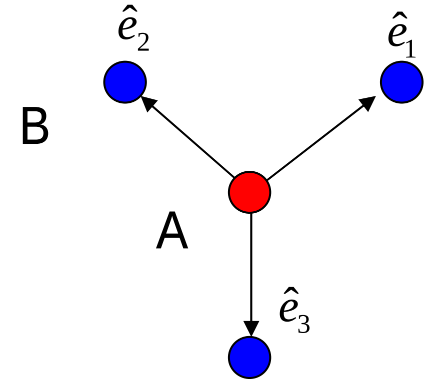
- In optical lattices, p_x and p_y-orbital bands are well separated from s.

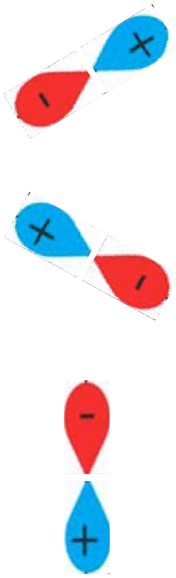


Artificial graphene in optical lattices

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

$$H_t = t_{//} \sum_{\vec{r} \in A} \{ p_i^+(\vec{r}) p_i(\vec{r} + \hat{e}_i) + h.c. \}$$

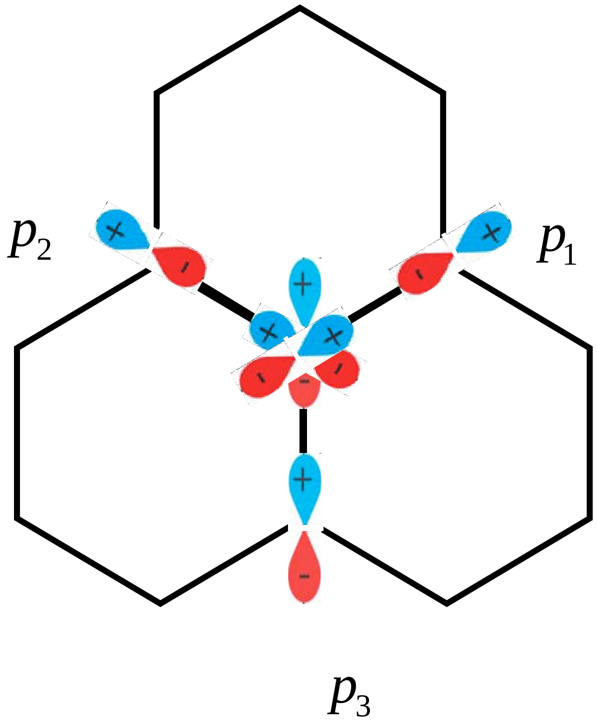




$$p_1 = \frac{\sqrt{3}}{2} p_x + \frac{1}{2} p_y$$

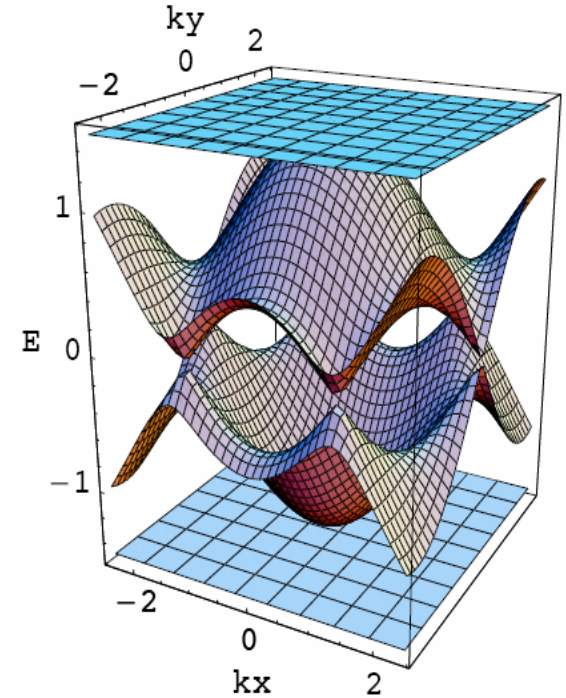
$$p_2 = \frac{\sqrt{3}}{2} p_x - \frac{1}{2} p_y$$

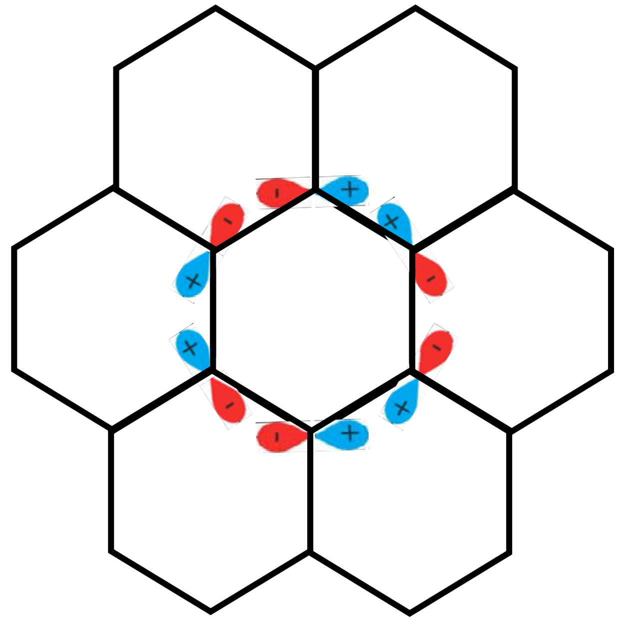
$$p_3 = -p_y$$



Only two are linearly-independent.

Flat bands in the entire Brillouin zone!

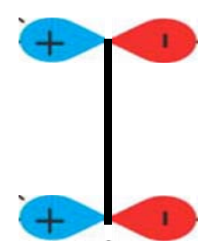




- Flat band + Dirac cone.

- localized eigenstates.

- If π-bonding is included, the flat bands acquire small width at the order of $t_\perp$.



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

π-bond

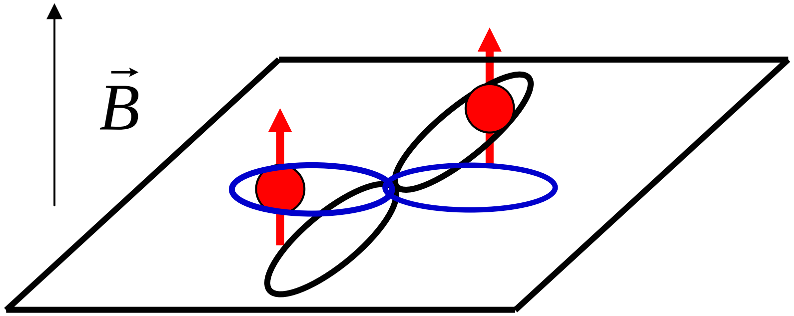
Enhance interactions among polarized fermions

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

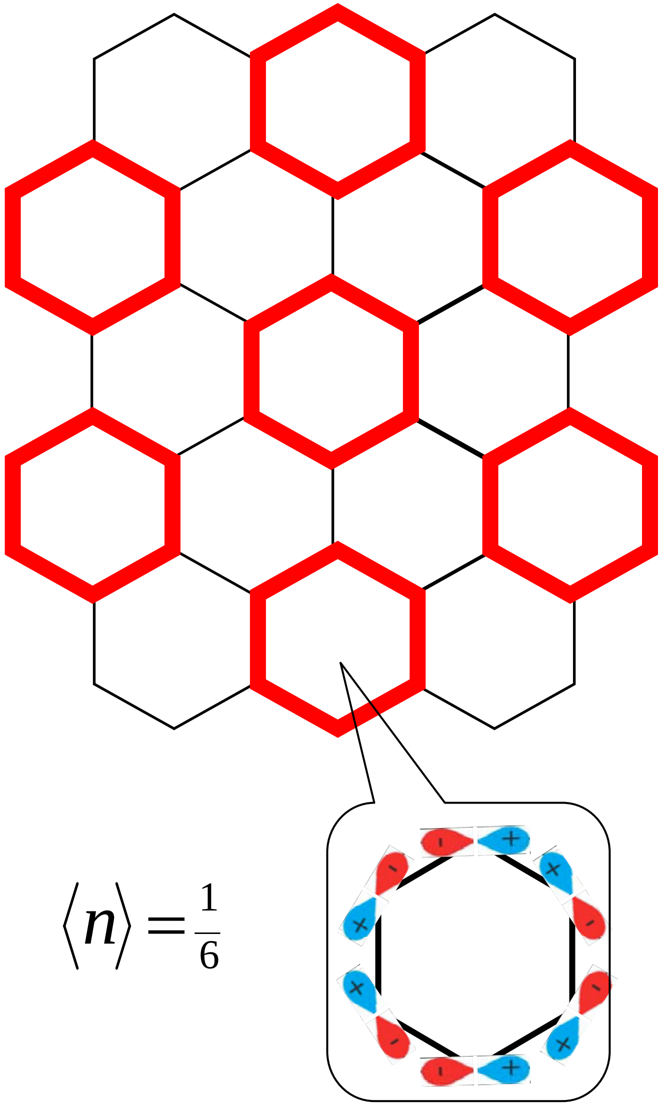
- Problem: contact interaction vanishes for spinless fermions.

- Use fermions with large magnetic moments. $$^{53}\text{Cr}\ (S=3, \mu=6\mu_B)$$

- Under strong 2D confinement, *U* is repulsive and can reach the order of recoil energy.



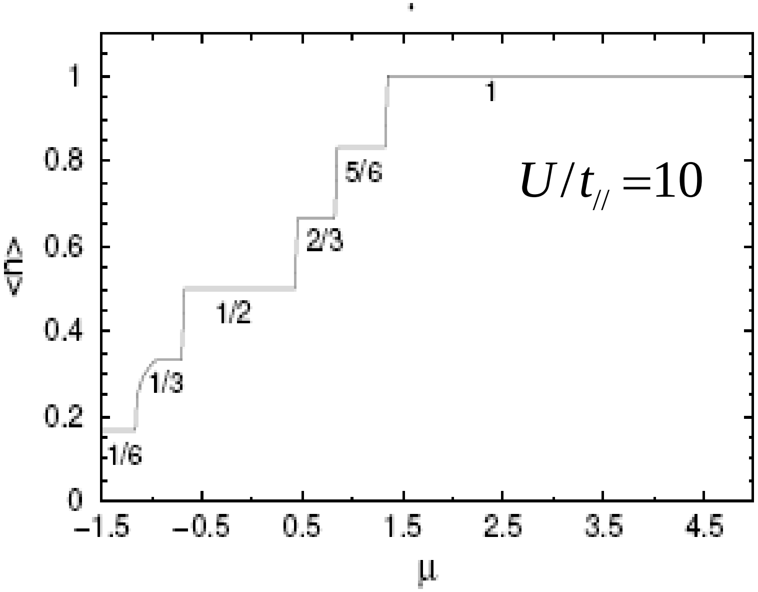
Exact solution with repulsive interactions!

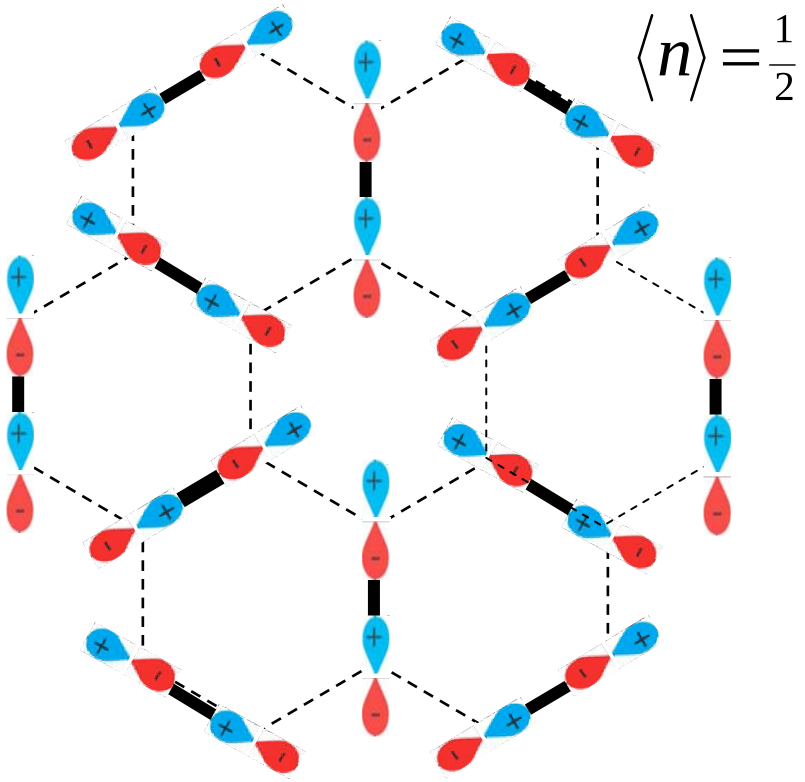


$\langle n \rangle = \frac{1}{6}$

- Crystallization with only on-site interaction!
- Closest packed hexagons; avoiding repulsion.
- The crystalline order is stable even with $t_\perp$ if $U >> t_\perp$.
- 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.

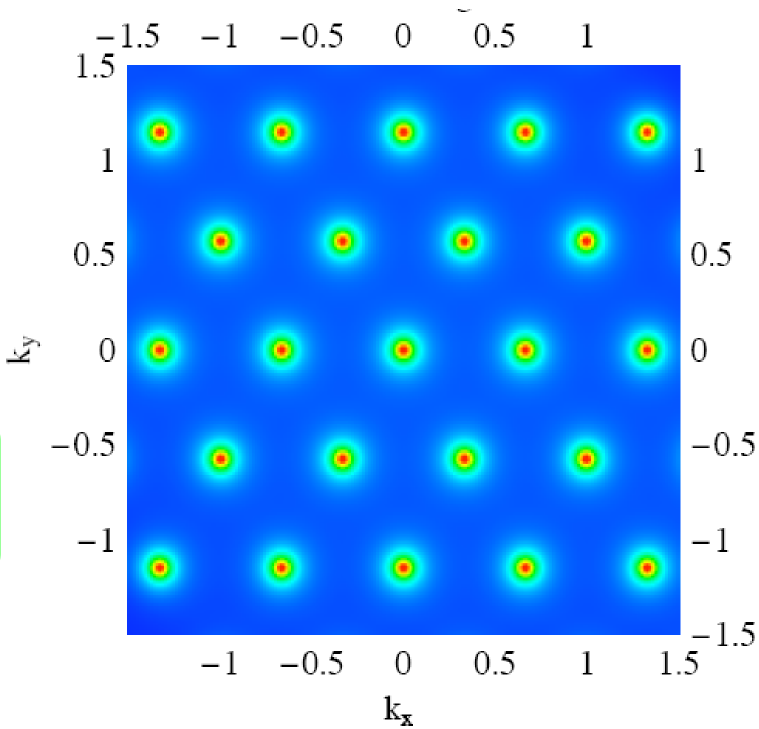
Experimental detection

- Transport: tilt the lattice and measure the excitation gap.

- Noise correlations of the time of flight image.

$$C(\vec{k}_1,\vec{k}_2)=\langle n(\vec{k}_1)n(\vec{k}_2)\rangle-\langle n(\vec{k}_1)\rangle\langle n(\vec{k}_2)\rangle$$

$$C(\vec{q})=\int d\vec{k}\,\frac{C(\vec{k}+\frac{\vec{q}}{2},\vec{k}-\frac{\vec{q}}{2})}{\langle n(\vec{k}+\frac{\vec{q}}{2})\rangle\langle n(\vec{k}-\frac{\vec{q}}{2})\rangle}\propto\pm\sum_G\delta(\vec{d}-\vec{G})$$



G: reciprocal lattice vector for the enlarged unit cells; '+' for bosons, '-' for fermions.

in unit of $2\pi/\sqrt{3}a$

Future work: exotic states of matter in the flat band; divergence of density of states.

- A wonderful **realistic** system for **flat band ferromagnetism (**fermions with spin**).**

- Pairing superfluidity in the flat band. BEC-BCS crossover? Is there the BCS limit?

- Bosons in the flat-band: highly frustrated system. **where to condense? Can they condense? Possible "Bose metal" phase?**

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Fermions: flat bands in honeycomb lattice.

Bosons: novel superfluidity with time-reversal symmetry breaking.

square lattice: **staggered** on-site orbital angular momentum (OAM) order.

triangular lattice: quantum **stripe** ordering of OAM.

W. V. Liu and C. Wu, PRA 74, 13607 (2006); C. Wu, W. V. Liu, J. Moore and S. Das Sarma, PRL 97, 190406 (2006).

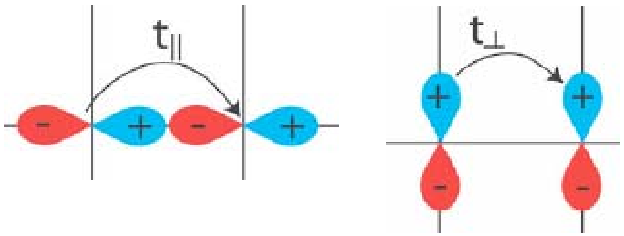
Other's related work: V. W. Scarola et. al, PRL, 2005; A. Isacsson et. al., PRA 2005; A. B. Kuklov, PRL 97, 2006; C. Xu et al., cond-mat/0611620 .

p-orbital Bose-Hubbard model (2D square lattice)

- Anisotropic hopping and odd parity:

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

$$H_t = t_{//} \sum_{\vec{r}} \{ p_x^+(\vec{r}) p_x(\vec{r} + \hat{e}_x) + h.c. + x \to y \}$$
$$- t_{\perp} \sum_{\vec{r}} \{ p_x^+(\vec{r}) p_x(\vec{r} + \hat{e}_y) + h.c. + x \leftrightarrow y \}$$

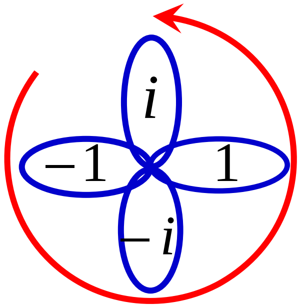


σ-bond π-bond

- On-site interaction → the orbital version of "Hund's rule".

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

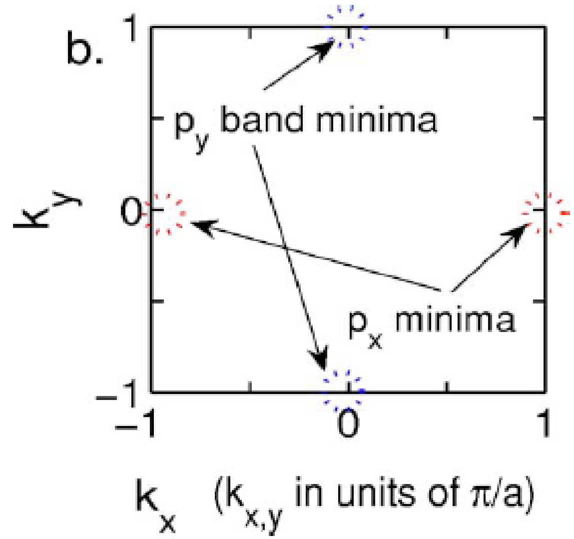
$$n = p_x^+ p_x + p_y^+ p_y, L_z = -i(p_x^+ p_y - p_y^+ p_x)$$



$|p_x\rangle \pm i |p_y\rangle$ are spatially more extended than polar states $|p_{x,y}\rangle$

Superfluidity with time-reversal symmetry breaking

- Band minima: $K_x=(\pi,0)$, $K_y=(0,\pi)$.

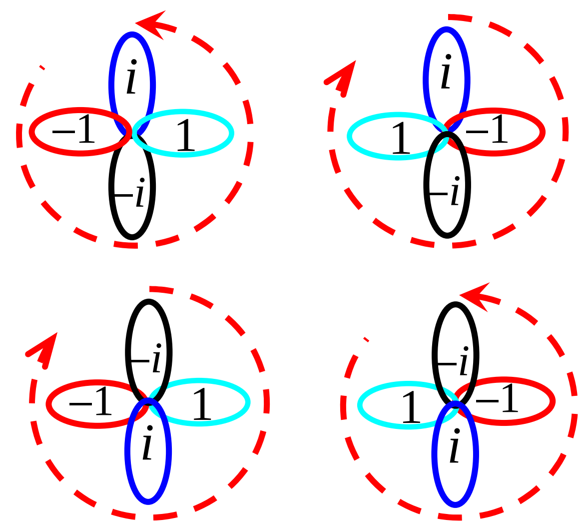


$$\varepsilon_x(k_x,k_y)=t_{//}\cos k_x - t_\perp \cos k_y$$

$$\varepsilon_y(k_x,k_y)=-t_\perp \cos k_x + t_{//}\cos k_y$$

- Interaction selects condensate as

$$|\psi\rangle_G = \frac{1}{\sqrt{N_0!}}\{\frac{1}{\sqrt{2}}(\psi^+_{Kx}+i\psi^+_{Ky})\}^{N_0}|0\rangle$$

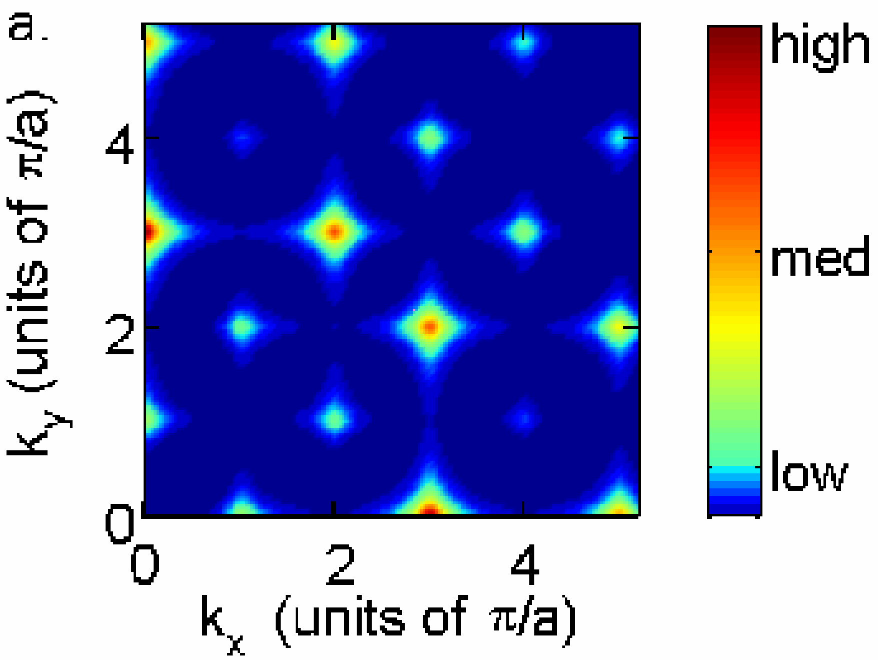


- Time-reversal symmetry breaking: staggered orbital angular momentum order.

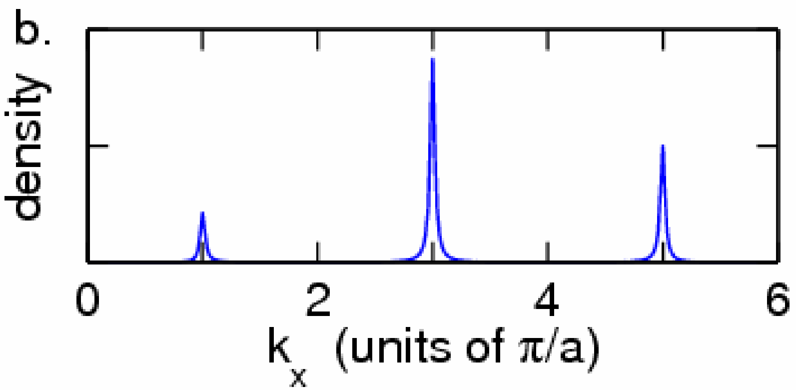
Time of flight signature of *p*-orbital BEC

- At zero temperate, 2D coherence peaks located at:

$$((m+\tfrac{1}{2})\frac{\pi}{a},0) \qquad (0,(n+\tfrac{1}{2})\frac{\pi}{a})$$



- *p*-orbital Wannier wavefunction imposes a *non-Gaussian* profile;

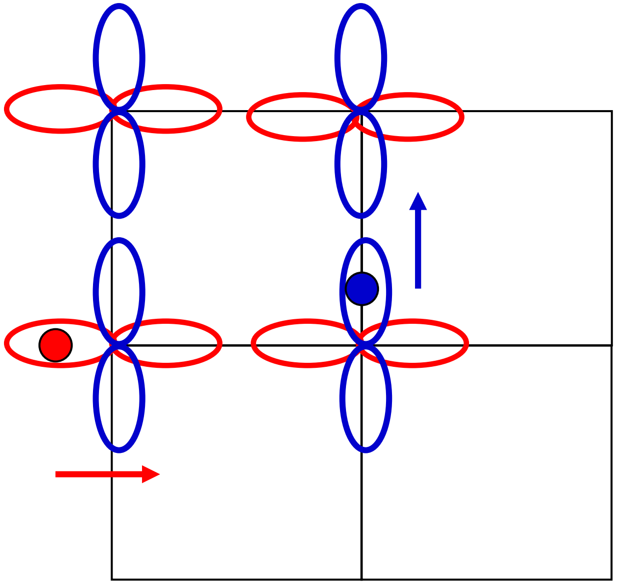


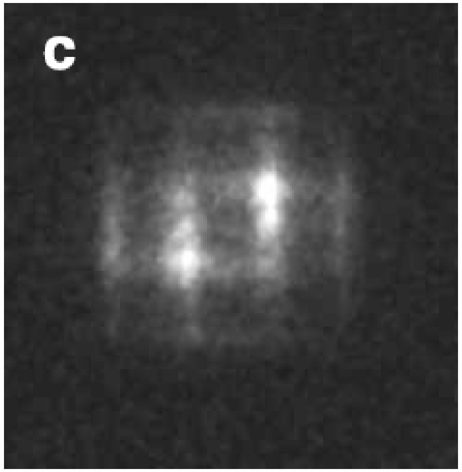
Quasi-1D behavior at finite temperatures

- Because $t_\perp << t_{//}$, p_x-particles can maintain phase coherence within the same row, but loose phase inter-row coherence at finite temperatures.

- Similar behavior also occurs for p_y-particles.

- The system effectively becomes 1D-like as shown in the time of flight experiment.



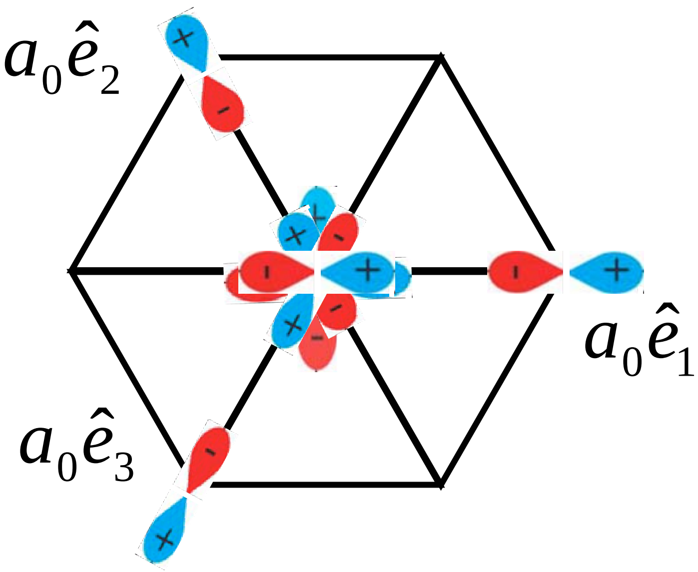


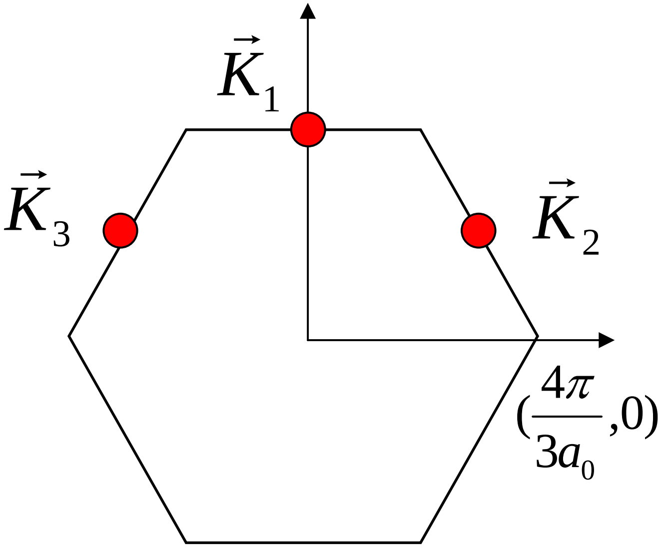
A. Isacsson et. al., PRA 72, 53604, 2005;

T. Mueller, I. Bloch et al.

p-band Bose-Hubbard model in triangular lattice

$$H_t = t_{//} \sum_{\vec{r}} \{ p_i^+(\vec{r}) p_i(\vec{r} \pm \hat{e}_i) + h.c. \} + \frac{U}{2} \sum_r \{ n_r^2 - \frac{1}{3} (L_r^z)^2 \}$$



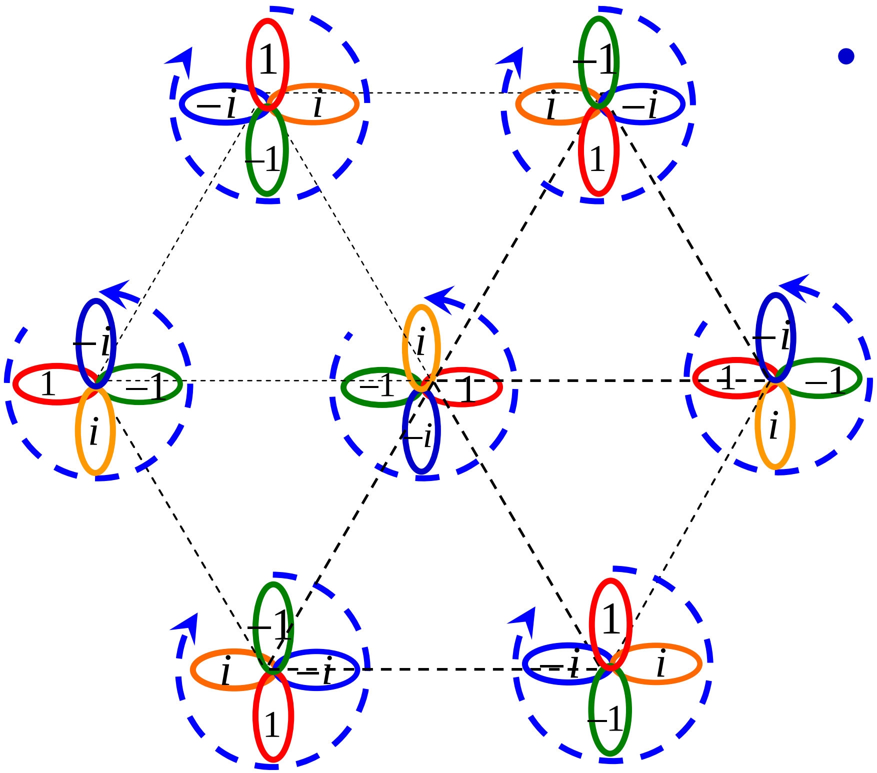


- Interactions select the condensate as (weak coupling analysis):

$$\frac{1}{\sqrt{N_0!}} \{ \frac{1}{\sqrt{2}} (\psi_{K_2}^+ + i \psi_{K_3}^+) \}^{N_0} |0\rangle$$

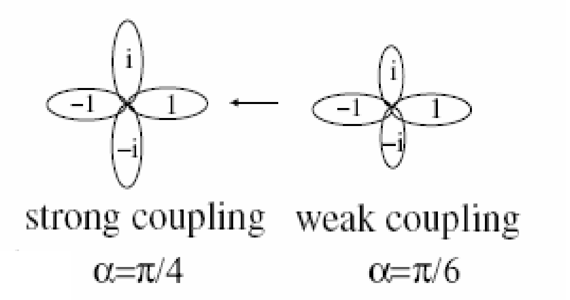
CW, W. V. Liu, J. Moore, and S. Das Sarma, *Phys. Rev. Lett.* (2006).

Quantum stripe ordering of orbital angular momentum moments



- Orbital configuration in each site:

$$e^{i\phi_r}(\cos\alpha|p_x\rangle + i\sigma_r \sin\alpha|p_y\rangle)\ (\sigma_r = \pm 1)$$



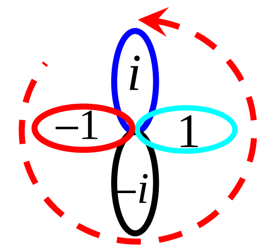
- Time-reversal, lattice translational, rotational symmetries are broken.

Strong coupling analysis

- Each site is characterized by a U(1) phase ϕ , and an Ising variable σ .

ϕ : the phase of the right lobe.

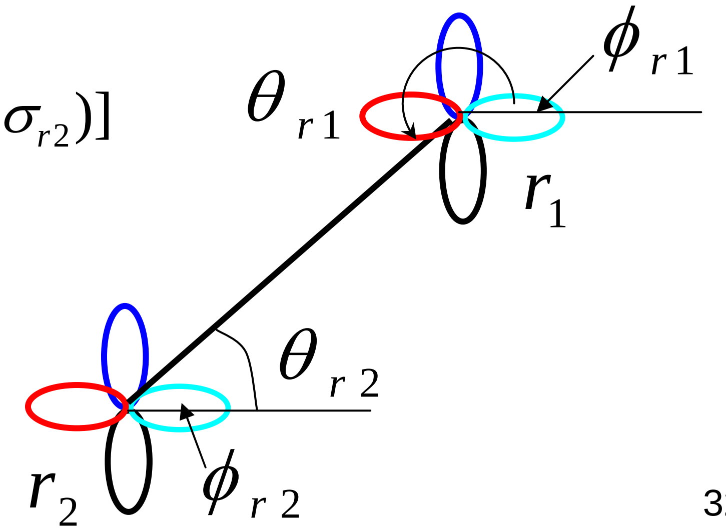
σ : direction of the Lz.



- Inter-site Josephson coupling: effective vector potential.

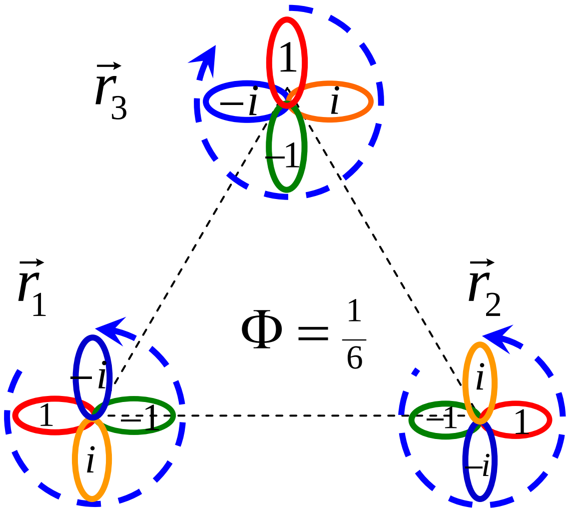
$$H_{eff} = -\frac{1}{2} n t_{//} \sum_{\langle r_1, r_2 \rangle} \cos[\phi_{r1} - \phi_{r2} + A_{r1,r2}(\sigma_{r1}, \sigma_{r2})]$$

$$A_{r1,r2}(\sigma_{r1}, \sigma_{r2}) = \sigma_{r1}\theta_{r1} - \sigma_{r2}\theta_{r2}$$



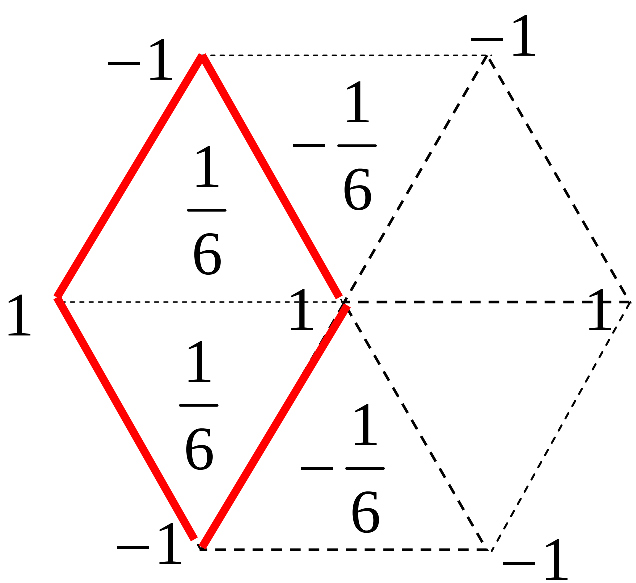
J. Moore and D. H. Lee, PRB, 2004.

Strong coupling analysis



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

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



- The stripe pattern minimizes the ground state vorticity.

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

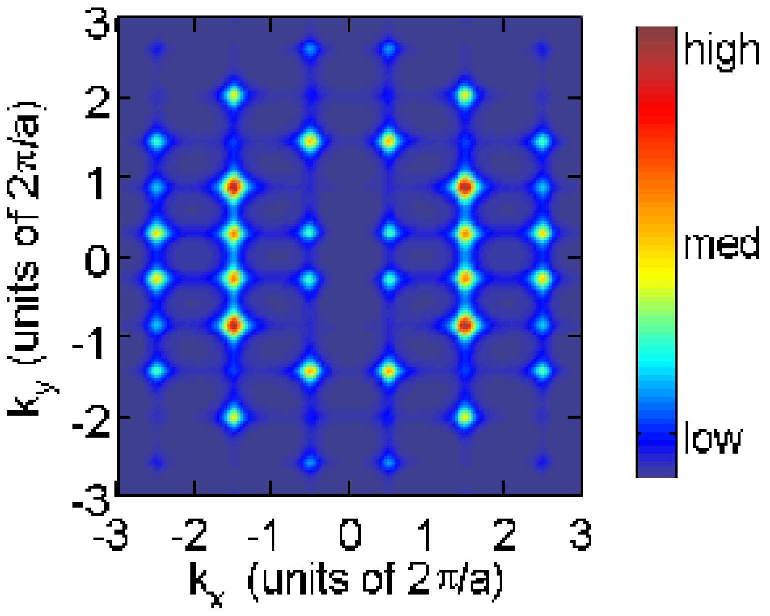
Time of flight signature

- Guzwiller mean field calculation also confirms the stripe ordering in the intermediate coupling regime.

- Stripe ordering occurs throughout all the coupling regimes.

- Predicted time of flight density distribution for the stripe-ordered superfluid.

- Coherence peaks occur at non-zero wavevectors.



Summary

- Current experiment progress has provided a wonderful opportunity to study orbital physics in optical lattices.

- Fermions: flat bands and crystallization in honeycomb lattice.

- Bosons: novel superfluidity with time-reversal symmetry breaking (square, triangular).