QUANTUM MAGNETISM IN EXCITED BANDS OF OPTICAL LATTICES

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Based on: Fernanda Pinheiro, J. Larson and J.-P. Martikainen, PRA 85, 033638 (2012)
Fernanda Pinheiro, G. M. Bruun, J.-P. Martikainen and J. Larson, PRL 111 205302 (2013)

CONCLUSIONS

The physics of excited bands of optical lattices reveal many interesting phenomena due to an additional orbital degree of freedom..

- The Hamiltonian of the Mott-I phase can be mapped into different types of spin models, and with different symmetries depending on the choice of the the atoms (if bosons or fermions)

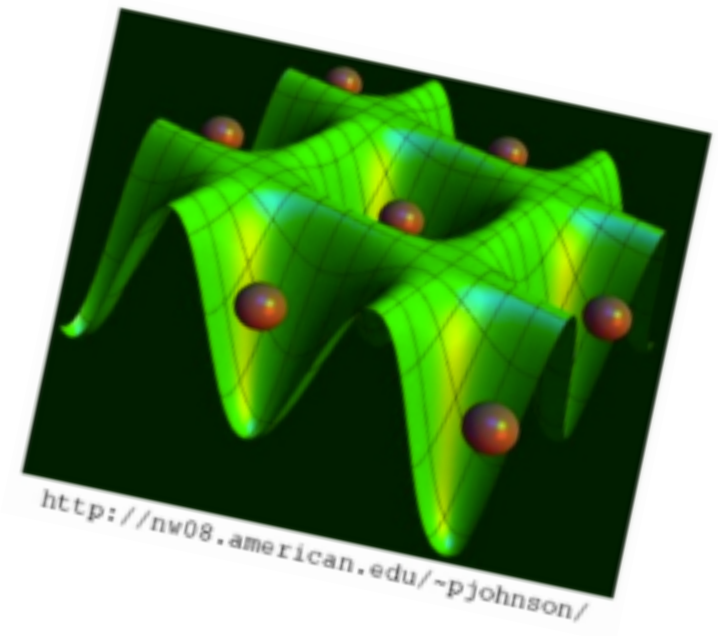
allows for simulation of non-integrable spin models with cold atoms in optical lattices!

OUTLINE

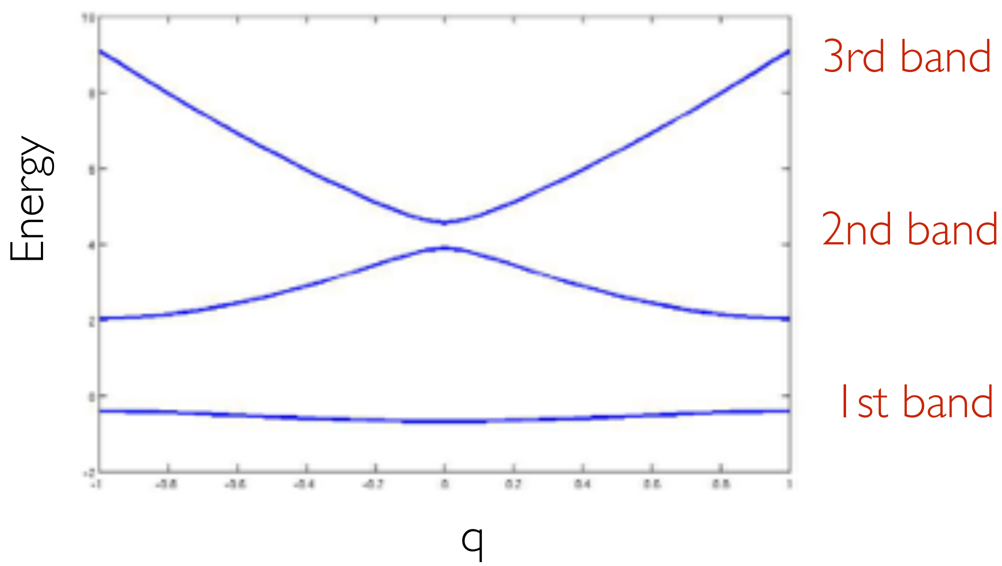
1. Putting things in context..
2. What happens in excited bands & p-orbitals..
3. Generic features of p-orbital bosonic systems..
4. From p-orbital bosons to XYZ quantum Heisenberg models..
5. 3D lattices and simulation of SU(3) Heisenberg models..

OPTICAL LATTICES & BAND STRUCTURE

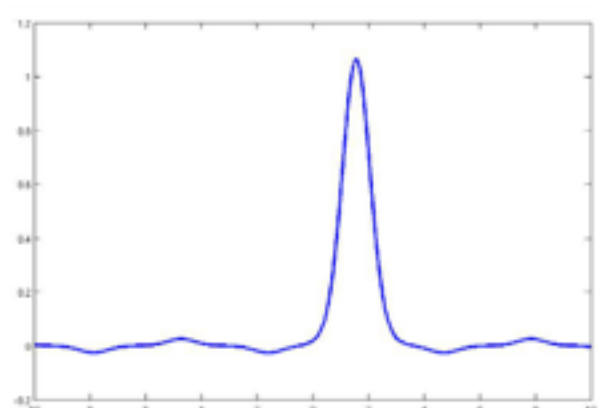
From superposition of beams of linearly polarized light it is possible to create spatially periodic potentials that can be used to trap atoms



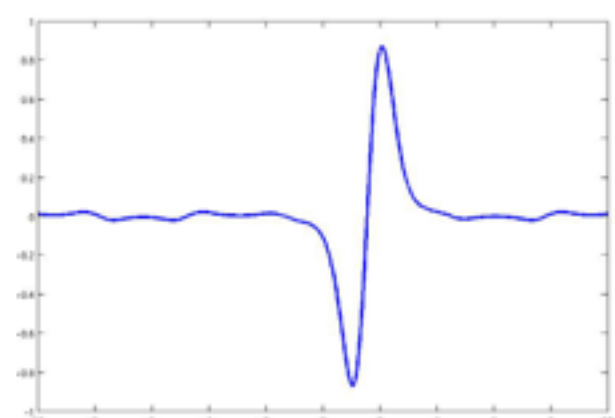
1 particle in a periodic potential



- A site localized basis can be constructed in terms of the Wannier functions



lattice sites

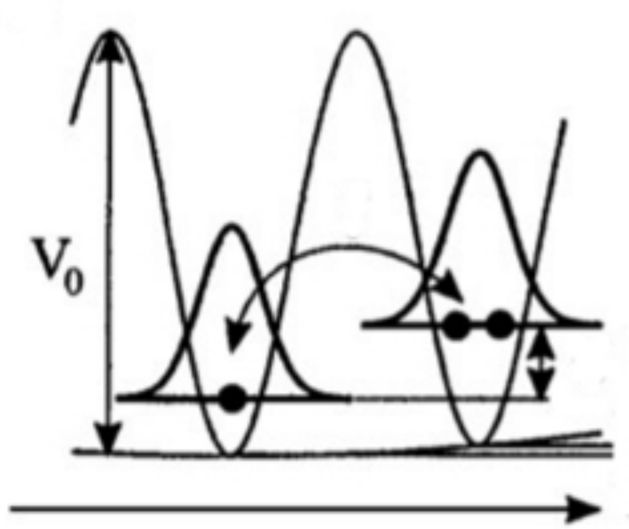


lattice sites

MANY PARTICLES IN AN OPTICAL LATTICE

(bosonic)

- Boson localization to superfluid insulator transition
  Fisher et. al. Phys. Rev. B 40, 546-570 (1989)



$$H = -t\sum_{\langle i,j\rangle}\hat{a}_i^{\dagger}\hat{a}_j + \sum_i \epsilon_i \hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1)$$

nearest neighbors tunneling | on-site energy | density-density interactions

- Cold bosonic atoms in optical lattices
  Jaksch et. al. Phys. Rev. Lett. 81, 15 (1998)

- Mott-insulator to superfluid transition was experimentally verified in 2002!
  Greiner et. al. Nature, 415, 39-44, 3, January 2002

Since then the experiments have gone beyond the first band..

COLD ATOMS IN EXCITED BANDS OF OPTICAL LATTICES (what is going on in the labs?)

PRL 99, 200405 (2007) PHYSICAL REVIEW LETTERS week ending 16 NOVEMBER 2007

State Preparation and Dynamics of Ultracold Atoms in Higher Lattice Orbitals

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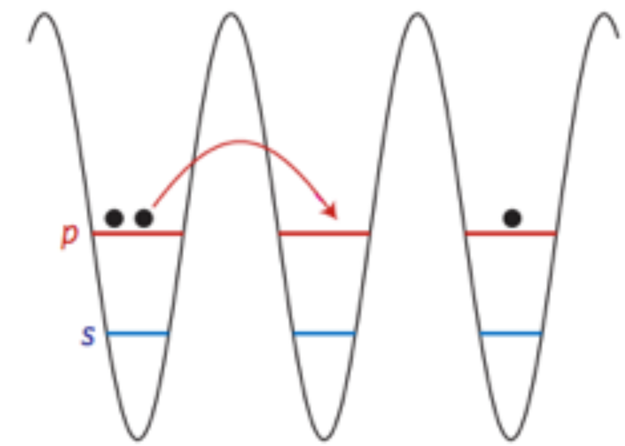
(Received 22 March 2007; published 16 November 2007)



(Nature Physics, Vol. 7, Feb. 2011)

decaying rates depend on:

- number of particles per site (because of collisions)
- depth of the lattice sites (because of rate of tunneling)

lifetimes in the p band can be hundreds of times larger than the time scale for intersite tunneling!

also..

nature physics ARTICLES
PUBLISHED ONLINE: 12 DECEMBER 2010 | DOI: 10.1038/NPHYS1857

Evidence for orbital superfluidity in the *P*-band of a bipartite optical square lattice

Georg Wirth, Matthias Ölschläger and Andreas Hemmerich*

- by using a superlattice it was possible to verify the establishment of coherence in the p band..

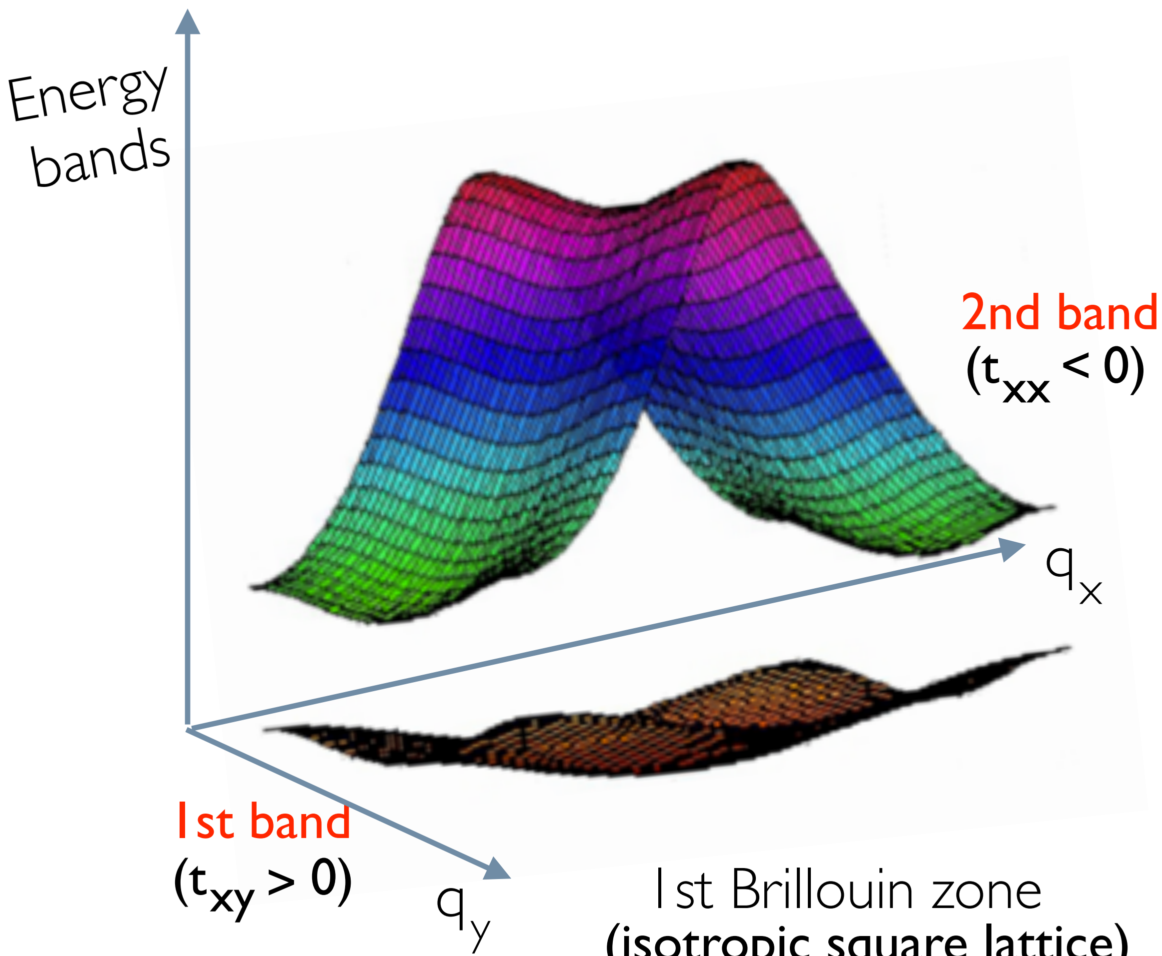
WHAT ARE THE P-BAND OR P-ORBITAL BOSONS?

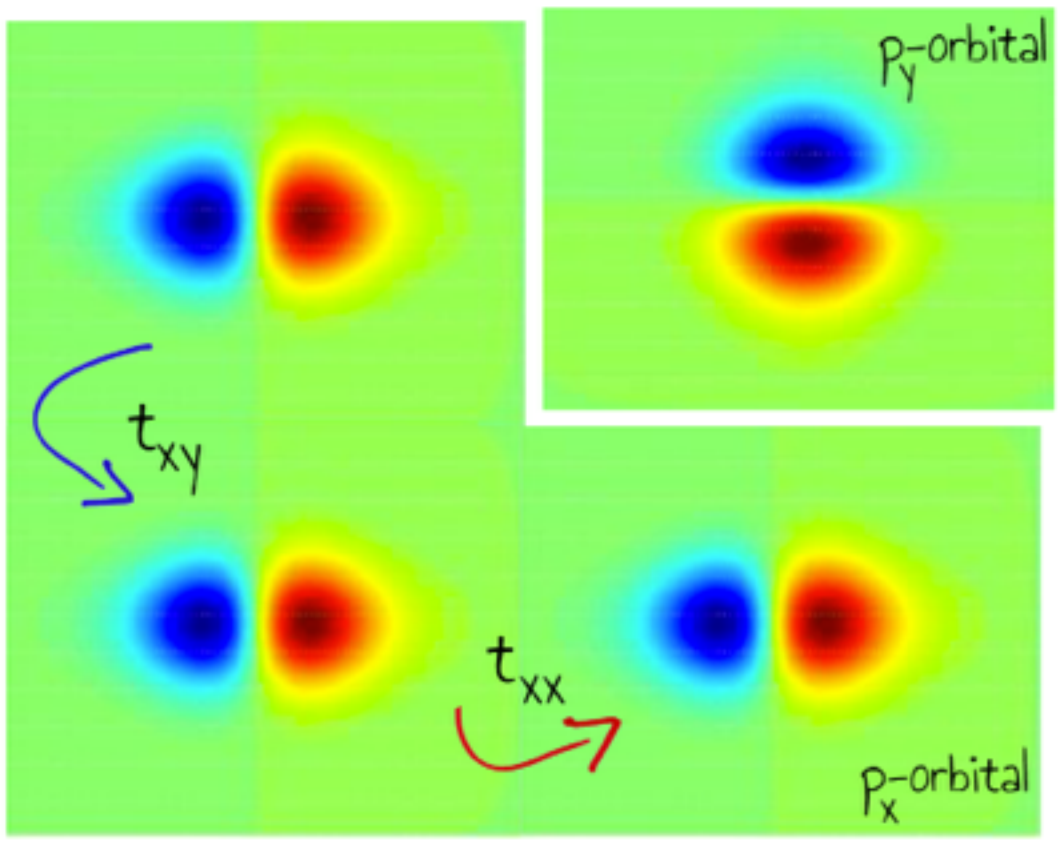
- p orbitals are the localized onsite single-particle states of the second bands..

First excited bands in 2D & 3D are degenerate!!

Like in the harmonic oscillator in 2D where
$|x, y\rangle = |1,0\rangle$ & $|0,1\rangle$ have the same energy!

p orbitals are anisotropic in magnitude and parity!





WHAT DOES THIS HAMILTONIAN LOOK LIKE?

$$H = H_0 + H_{nn} + H_{FD}$$

$$\mathbf{H_0} = -\sum_{\alpha,\beta}\sum_{\langle \mathbf{ij}\rangle_\beta} \mathbf{t}_{\alpha\beta}\, \hat{\mathbf{a}}^\dagger_{\alpha\mathbf{i}}\hat{\mathbf{a}}_{\alpha\mathbf{j}} + \sum_{\alpha}\sum_{\mathbf{j}} \mathbf{V_{trap}}(\mathbf{R_j})\hat{\mathbf{n}}_{\alpha\mathbf{j}}$$

anisotropic tunneling　　　　external potentials

$$\mathbf{H_{nn}} = \sum_{\alpha}\sum_{\mathbf{j}} \frac{\mathbf{U}_{\alpha\alpha}}{\mathbf{2}}\hat{\mathbf{n}}_{\alpha\mathbf{j}}(\hat{\mathbf{n}}_{\alpha\mathbf{j}} - \mathbf{1}) + \sum_{\alpha\beta,\alpha\neq\beta}\sum_{\mathbf{j}} \mathbf{U}_{\alpha\beta}\hat{\mathbf{n}}_{\alpha\mathbf{i}}\hat{\mathbf{n}}_{\beta\mathbf{j}}$$

density-density interactions

$$\mathbf{H_{FD}} = \sum_{\alpha\beta,\alpha\neq\beta}\sum_{\mathbf{j}} \frac{\mathbf{U}_{\alpha\beta}}{\mathbf{4}}\left(\hat{\mathbf{a}}^\dagger_{\alpha\mathbf{j}}\hat{\mathbf{a}}^\dagger_{\alpha\mathbf{j}}\hat{\mathbf{a}}_{\beta\mathbf{j}}\hat{\mathbf{a}}_{\beta\mathbf{j}} + \hat{\mathbf{a}}^\dagger_{\beta\mathbf{j}}\hat{\mathbf{a}}^\dagger_{\beta\mathbf{j}}\hat{\mathbf{a}}_{\alpha\mathbf{j}}\hat{\mathbf{a}}_{\alpha,\mathbf{j}}\right)$$

orbital-changing interactions

In 2D

$$\alpha, \beta = \{\mathbf{x}, \mathbf{y}\}$$

MEAN-FIELD PROPERTIES

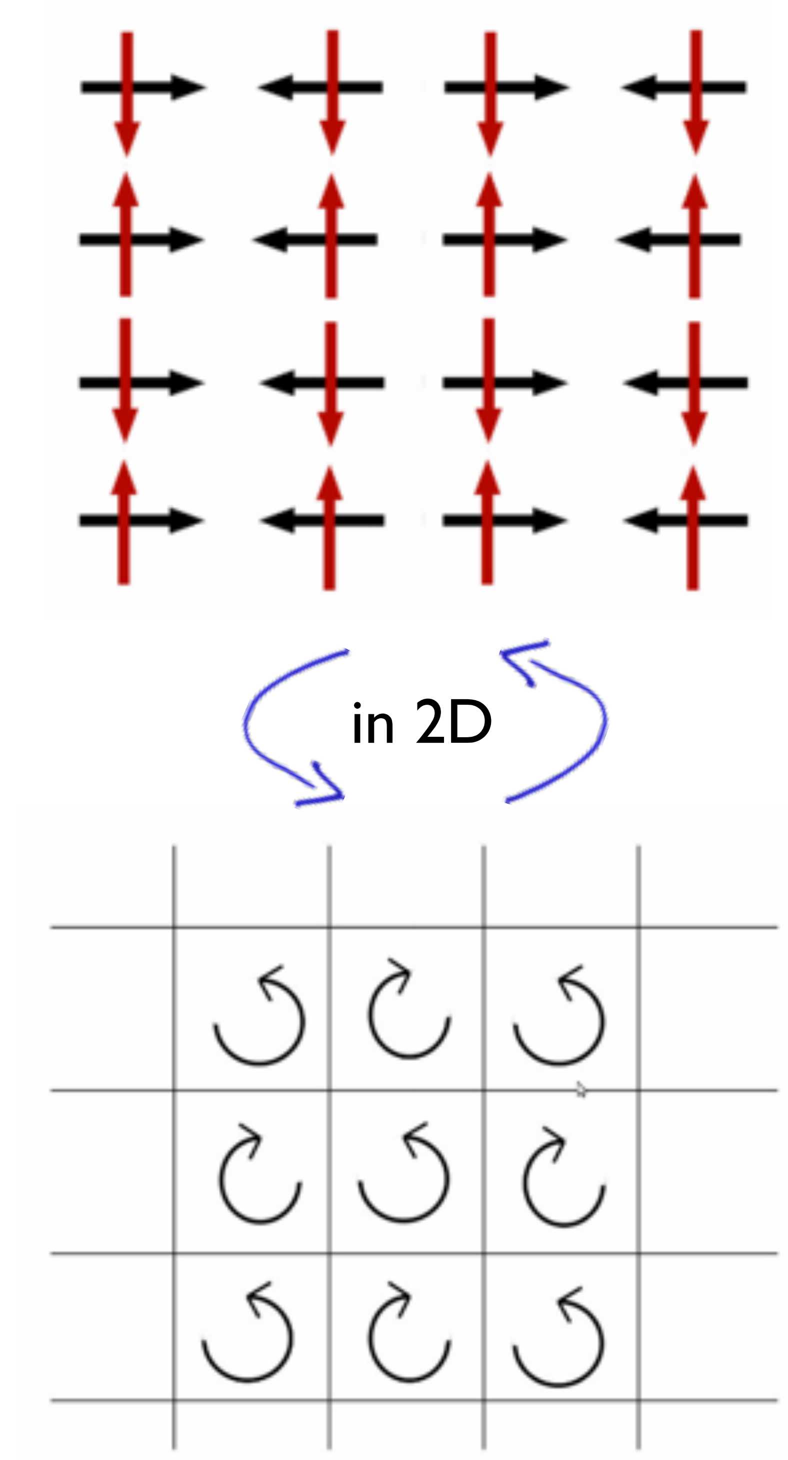
(isotropic lattice & homogeneous density)

$$\psi_{\alpha\mathbf{j}} = e^{i\theta_{\alpha\mathbf{j}}}|\psi_{\alpha\mathbf{j}}|$$

The phase of the order parameter has a structure!

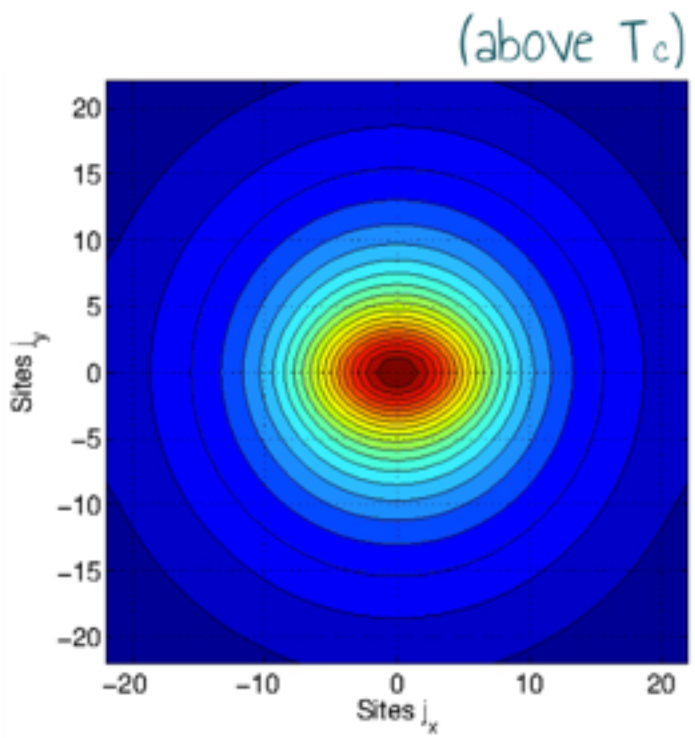
- tunneling terms establish inter-site phase relation
- orbital-changing interaction terms establish onsite phase relation

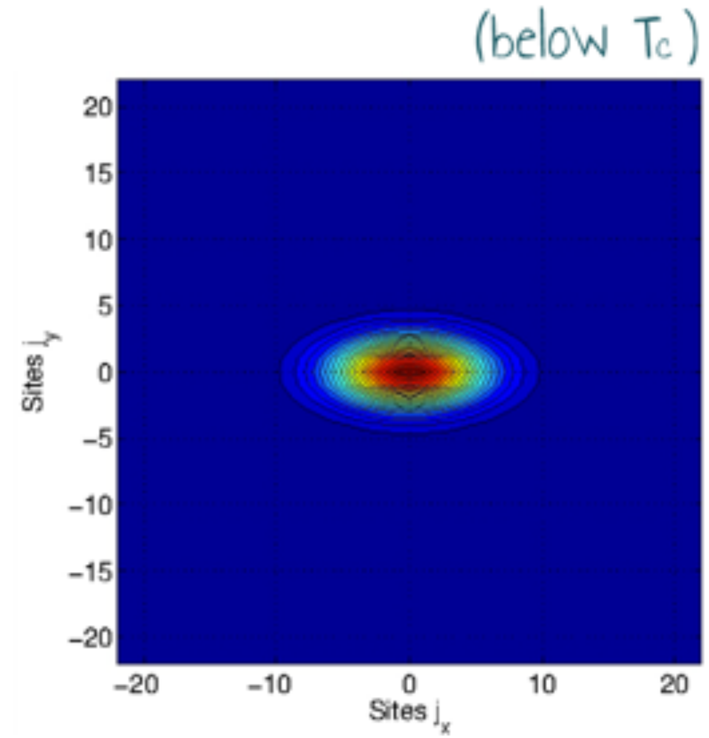
Staggered vortex solution!



A. Collin, J. Larson, J.-P. Martikainen, PRA 81, 023605 (2010)

IDEAL GAS IN THE CONFINED SYSTEM
(or condensation with anisotropic tunneling + inhomogeneous density)

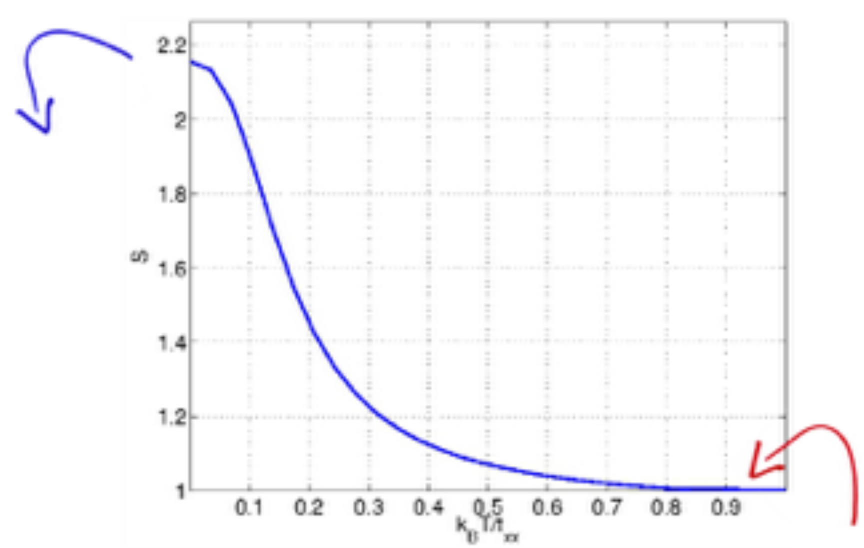




anisotropy parameter

$$S_x = \sqrt{\frac{(\Delta_x x)^2}{(\Delta_x y)^2}}$$

characterizes anisotropies of the density in the lattice



F. Pinheiro, J. Larson and J.-P. Martikainen, PRA 85, 033638 (2012)

Effective spin systems..

COLD ATOMS CAN BE USED TO SIMULATE QUANTUM MAGNETISM

VOLUME 91, NUMBER 9 PHYSICAL REVIEW LETTERS week ending 29 AUGUST 2003

Controlling Spin Exchange Interactions of Ultracold Atoms in Optical Lattices

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[2]*Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA*
(Received 25 October 2002; published 26 August 2003)

All you need is

- an optical lattice
- 2 state bosonic or fermionic atom

Mott-1 phase maps into

Spin Hamiltonian!

the couplings in the spin model are given in terms of the lattice parameters

For bosonic systems we typically find:

- spin models with a continuous symmetry, as, e.g. the XXZ model
- couplings that favor ferromagnetic order

see also:

New J. Phys. 5, 113.1 - 113.19, (2003)
Nature 472, 307-312 (2011)

Other proposals:

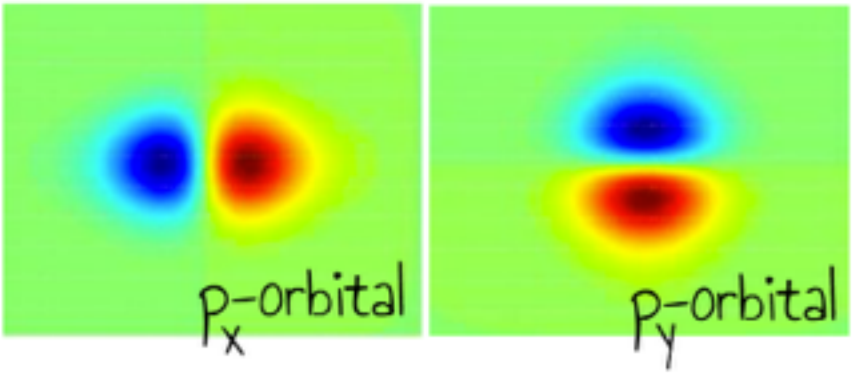
- polar molecules
- trapped ions

FROM BOSONS IN THE P BAND TO THE XYZ MODEL

(doing the math)

In the 2D lattice we have:

- 2 degenerate orbitals
- anisotropic tunneling
- dynamical processes that describe population dynamics within the orbital states



By using Schwinger bosons

$$\hat{S}_i^z = \frac{1}{2}(\hat{a}_{xi}^\dagger \hat{a}_{xi} - \hat{a}_{yi}^\dagger \hat{a}_{yi})$$
$$\hat{S}_i^+ = \hat{S}_i^x + i\hat{S}_i^y = \hat{a}_{xi}^\dagger \hat{a}_{yi}$$
$$\hat{S}_i^- = \hat{S}_i^x - i\hat{S}_i^y = \hat{a}_{yi}^\dagger \hat{a}_{xi}$$

The effective Hamiltonian describing the Mott phase with a unit filling can be mapped into a spin 1/2 model

of the XYZ type with an external field in the z-axis!

$$\hat{H}_{XYZ} = \sum_{\langle ij \rangle} J\left[(1+\gamma)\hat{S}_i^x\hat{S}_j^x + (1-\gamma)\hat{S}_i^y\hat{S}_j^y\right] + \sum_{\langle ij \rangle} \Delta \hat{S}_i^z\hat{S}_j^z + h\sum_i \hat{S}_i^z$$

-> Couplings depend on the lattice configuration!

* Mott regime justifies the perturbation in t/U

Fernanda Pinheiro, et. al., PRL 111 205302 (2013)

(in a more transparent language)

$$\hat{H}_{Mott} = -\sum_{\langle i,j\rangle}\left(J^{zz}\hat{S}_i^z\hat{S}_j^z + J^{xx}\hat{S}_i^x\hat{S}_j^x + J^{yy}\hat{S}_i^y\hat{S}_j^y\right) - \sum_i J^z\hat{S}_i^z$$

$$J^{xx} = 2\frac{t_x t_y}{U_{xy}}\left(1 - 4\frac{U_{xy}^2}{U^2}\right)$$

$$J^{yy} = 2\frac{t_x t_y}{U_{xy}}\left(1 + 4\frac{U_{xy}^2}{U^2}\right)$$

$$J^{zz} = 4\frac{|t_x|^2 U_{yy}}{U^2} + 4\frac{|t_y|^2 U_{xx}}{U^2} - \frac{|t_x|^2}{U_{xy}} - \frac{|t_y|^2}{U_{xy}}$$

$$J^z = \frac{4|t_x|^2 U_{yy}}{U^2} - \frac{4|t_y|^2 U_{xx}}{U^2} + (E_x^{os} - E_y^{os})$$

Therefore

$$\hat{\mathrm{H}}_{\mathrm{XYZ}} = \sum_{\langle \mathrm{ij}\rangle}\mathbf{J}\left[(1+\gamma)\hat{\mathrm{S}}_\mathrm{i}^\mathrm{x}\hat{\mathrm{S}}_\mathrm{j}^\mathrm{x} + (1-\gamma)\hat{\mathrm{S}}_\mathrm{i}^\mathrm{y}\hat{\mathrm{S}}_\mathrm{j}^\mathrm{y}\right] + \sum_{\langle \mathrm{ij}\rangle}\Delta\hat{\mathrm{S}}_\mathrm{i}^\mathrm{z}\hat{\mathrm{S}}_\mathrm{j}^\mathrm{z} + \mathbf{h}\sum_\mathrm{i}\hat{\mathrm{S}}_\mathrm{i}^\mathrm{z}$$

$$\gamma = -4U_{xy}^2/U^2$$

$$\Delta = -J^{zz}$$

$$h = -J^z$$

- no assumptions regarding the geometry of the lattice are required for deriving this effective Hamiltonian!

LET US CONSIDER A 1D REALIZATION

(out of the 2D lattice)

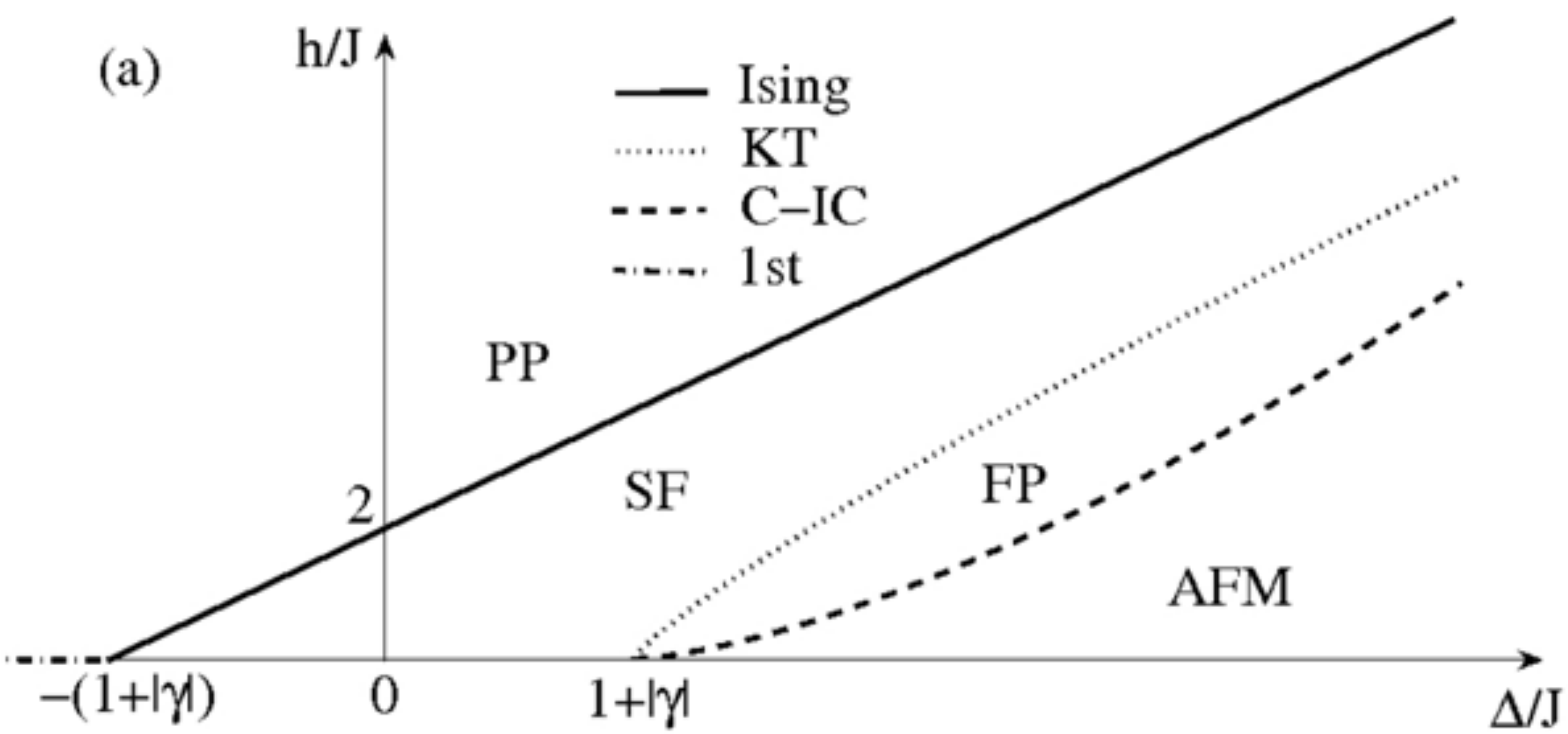
1. Make the wells much deeper in one of the directions..

$$|t_{xx}| \;\&\; |t_{yx}| \gg |t_{yy}| \;\&\; |t_{xy}|$$

2. Keep the degeneracy between the orbitals..

$$V_x k_x^2 = V_y k_y^2$$

(in the harmonic approximation)



- Highly magnetized phase (PP)
- Spin-Flop phase (SF)
- Floating phase (FP)
- Anti-ferromagnetic phase (AFM)

E. Sela et. al., PRB 84 085114 (2011)

F. Pinheiro, et. al., PRL 111 205302 (2013)

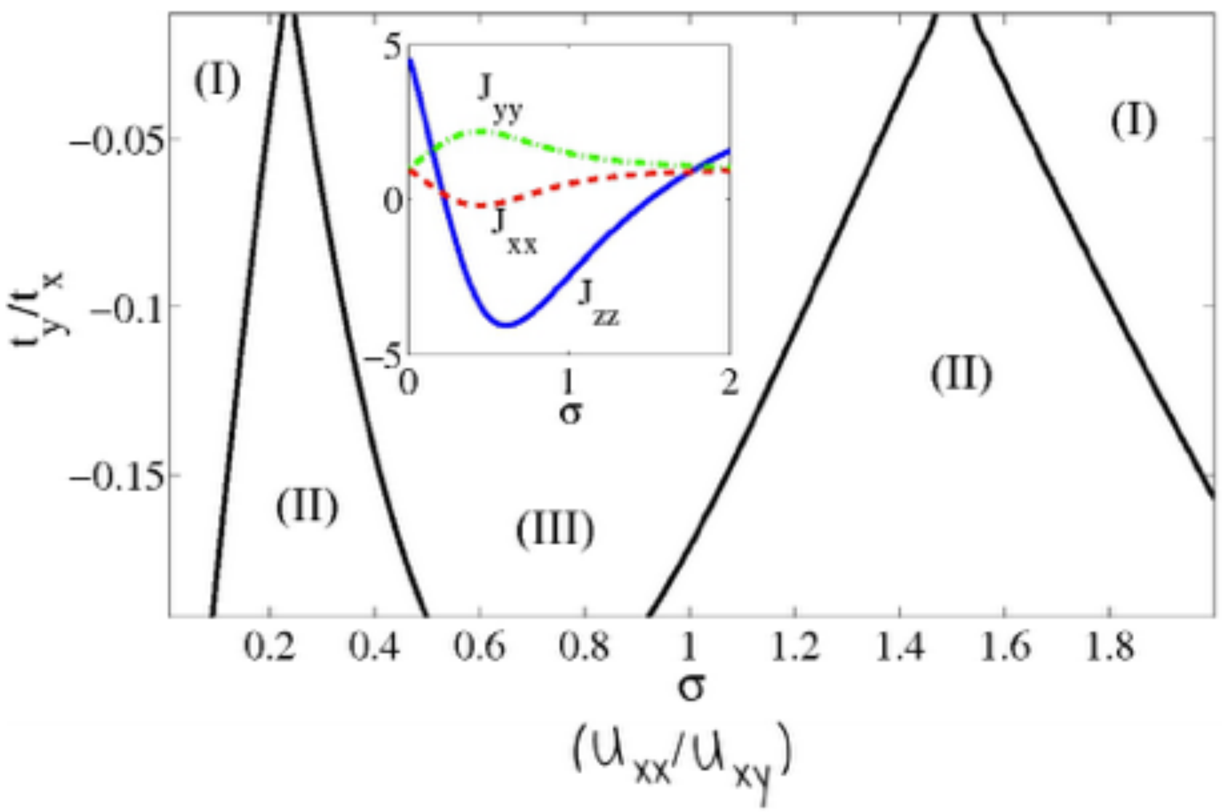
WITH DIFFERENT TYPES OF COUPLINGS

Since the spin is encoded in an spatial degree of freedom

- Trapped ion techniques can be used to manipulate the (shape of the) orbital states

couplings can be tuned

-> different types of XYZ models!

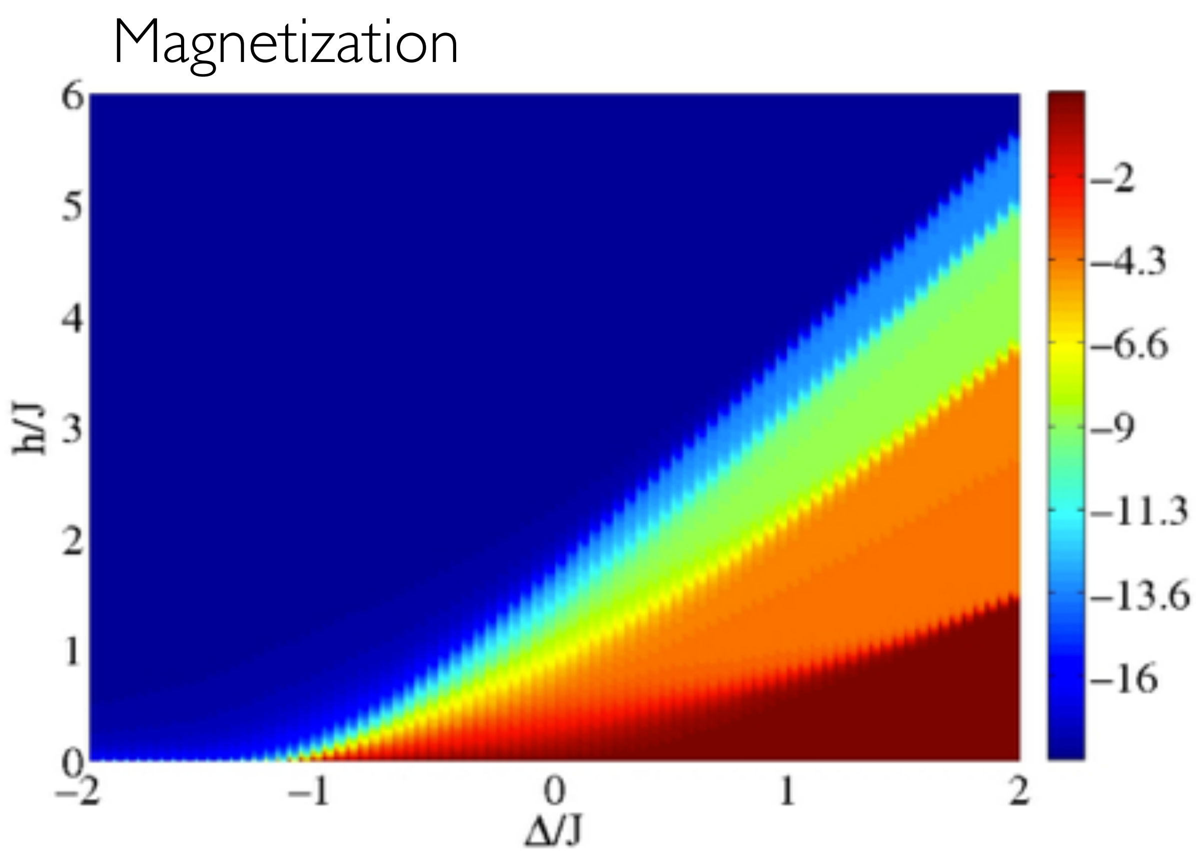


(I) Anti-ferromagnetic couplings in all the spin components

(II) Anti-ferromagnetic coupling in the y-component (Jxx > Jzz)

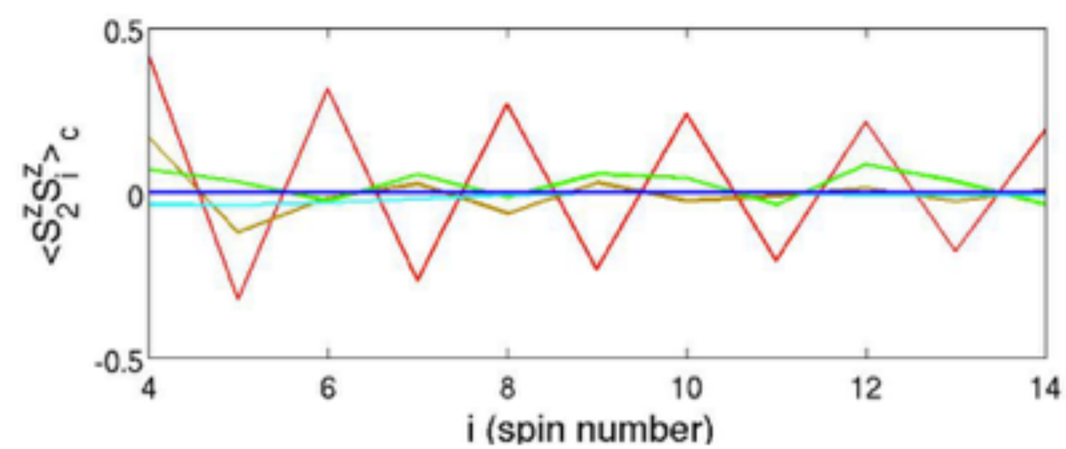
(III) Anti-ferromagnetic coupling in the y-component (Jxx < Jzz)

IN THE FINITE SYSTEM



Main finite size effects:

spin density waves

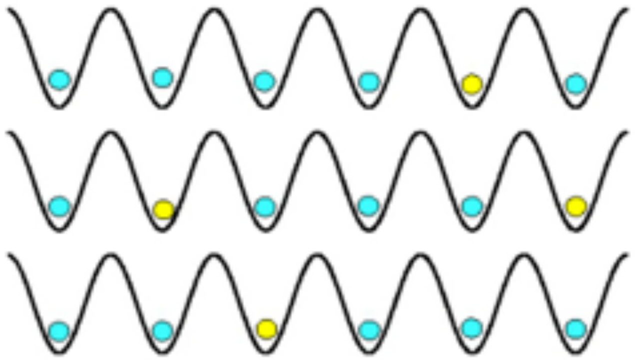


- Lifetimes are of the order of dozens tunneling times..
  (should allow for studies of the physics discussed here!)
- Required temperatures are of the order ~ $k_B T \lesssim t^2/U$
  (corresponds to the current frontier of experimental research!)

EXPERIMENTAL REALIZATION

Due to imperfections in loading the atoms to the p band

EFFECTIVE MODEL INCLUDING IMPERFECTIONS



Hamiltonian has the additional term:

$$-\frac{t_\alpha^2}{U_{ps}}\hat{a}^\dagger_{\alpha,i}\hat{a}^\dagger_{s,j}\hat{a}_{\alpha,i}\hat{a}_{s,j} = -\frac{t_\alpha^2}{U_{ps}}\hat{n}_{\alpha,i}$$

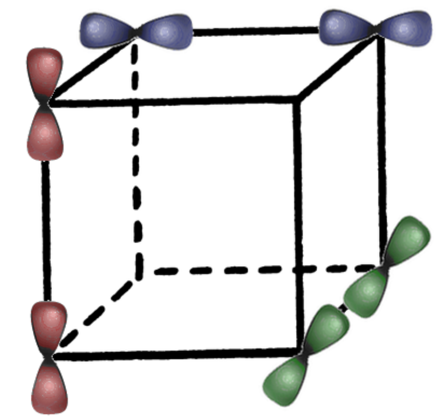
XYZ model with disorder in the field!

Fernanda Pinheiro, et. al., PRL 111 205302 (2013)

What about the 3-orbital system?

(or when the p band is 3-fold degenerate?)

BOSONS, FERMIONS & MODELS OF QUANTUM MAGNETISM



We use the orbital states to write the SU(3) ladder operators

$$\begin{aligned}
\frac{\hat{T}_{\mathbf{i}}^{\pm}}{2} &= \hat{a}^{\dagger}_{x,\mathbf{i}}\hat{a}_{y,\mathbf{i}} = \lambda^{1}_{z,\mathbf{i}} \pm \lambda^{2}_{z,\mathbf{i}} \\
\frac{\hat{V}_{\mathbf{i}}^{\pm}}{2} &= \hat{a}^{\dagger}_{x,\mathbf{i}}\hat{a}_{z,\mathbf{i}} = \lambda^{1}_{y,\mathbf{i}} \pm \lambda^{2}_{y,\mathbf{i}} \\
\frac{\hat{U}_{\mathbf{i}}^{\pm}}{2} &= \hat{a}^{\dagger}_{z,\mathbf{i}}\hat{a}_{y,\mathbf{i}} = \lambda^{1}_{x,\mathbf{i}} \pm \lambda^{2}_{x,\mathbf{i}}
\end{aligned}
\quad + \quad
\begin{aligned}
\hat{n}_{x,\mathbf{i}} &= \tfrac{1}{3} + \tfrac{1}{2}\lambda_{3,\mathbf{i}} + \tfrac{\sqrt{3}}{6}\lambda_{8,\mathbf{i}} \\
\hat{n}_{y,\mathbf{i}} &= \tfrac{1}{3} - \tfrac{1}{2}\lambda_{3,\mathbf{i}} + \tfrac{\sqrt{3}}{6}\lambda_{8,\mathbf{i}} \\
\hat{n}_{z,\mathbf{i}} &= \tfrac{1}{3} - \tfrac{\sqrt{3}}{6}\lambda_{8,\mathbf{i}}
\end{aligned}$$

- **Bosonic case:**

$$\begin{aligned}
H^{b}_{Mott_1} = & -\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\sum_{\alpha,\beta\neq\alpha}\left[2|t^{\alpha}_{\mathbf{ij}}|^{2}\left(\frac{U_{\beta\beta}U_{\sigma\sigma}-U^{2}_{\beta\sigma}}{\Lambda}\right)\hat{n}_{\alpha,\mathbf{i}}\hat{n}_{\alpha,\mathbf{j}} + \frac{|t^{\alpha}_{\mathbf{ij}}|^{2}}{U_{\alpha\beta}}\hat{n}_{\alpha,\mathbf{i}}\hat{n}_{\beta,\mathbf{j}}\right] \\
& -\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\sum_{\alpha,\beta\neq\alpha}\frac{t^{\alpha}_{\mathbf{ij}}t^{\beta}_{\mathbf{ji}}}{U_{\alpha\beta}}\left[(1+\gamma)\,\lambda^{1}_{\sigma,\mathbf{i}}\lambda^{1}_{\sigma,\mathbf{j}} + (1-\gamma)\,\lambda^{2}_{\sigma,\mathbf{i}}\lambda^{2}_{\sigma,\mathbf{j}}\right]
\end{aligned}$$

Here: $\alpha \neq \beta \neq \sigma$

$\Lambda = (U_{xx}U_{yy}U_{zz} - U^{2}_{xz}U_{yy} - U^{2}_{yz}U_{xx} - U^{2}_{xy}U_{zz} + 2U_{xy}U_{xz}U_{yz})$

F. Pinheiro, in preparation

- **Fermionic case:**

$$H^{f}_{Mott_1} = \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \sum_{\alpha,\beta\neq\alpha} \left[\frac{|t^{\alpha}_{\mathbf{ij}}|^2}{U_{\alpha\beta}} \hat{n}_{\alpha,\mathbf{i}} \hat{n}_{\beta,\mathbf{j}} + \frac{t^{\alpha}_{\mathbf{ij}} t^{\beta}_{\mathbf{ji}}}{U_{\alpha\beta}} \left(\lambda^1_{\sigma,\mathbf{i}} \lambda^1_{\sigma,\mathbf{j}} + \lambda^2_{\sigma,\mathbf{i}} \lambda^2_{\sigma,\mathbf{j}} \right) \right]$$

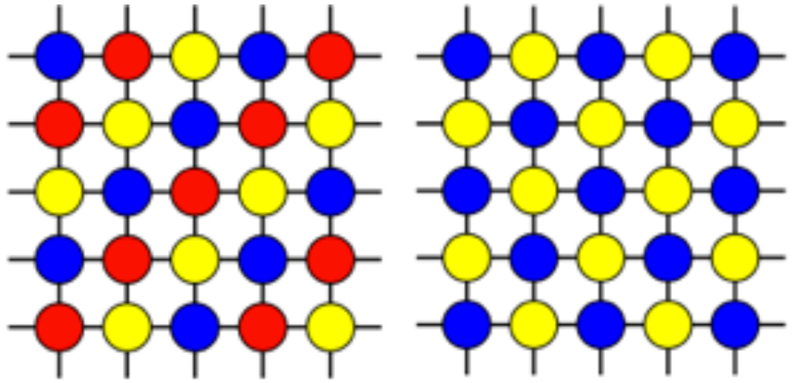
By loading fermions in the p band we recover the XXZ-like coupling isotropy..

the fermionic case will favor anti-ferromagnetic order!

Quantum fluctuations are very important in anti-ferro SU(3) XXZ-like models in the square lattice

It stabilizes the sublattice order against other competing states!

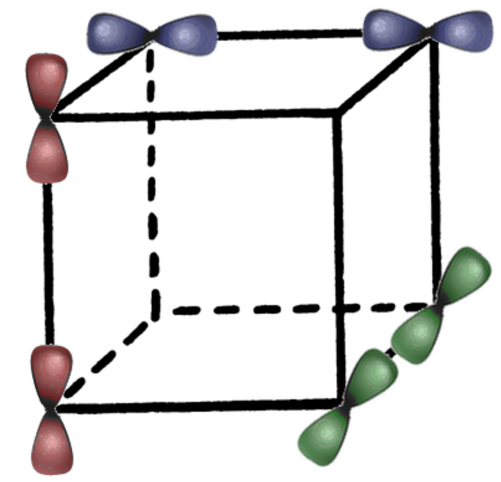
Two- & three-sublattice phases



T. A. Toth, et. al., PRL 105, 265301 (2010)

Now what happens

- In the cubic lattice?
- In the bosonic system?



Next in the to-do list:

How does the XYZ-like anisotropy changes the physics for bosons?

(study via linear flavor wave theory)

Can we use this system to study (orbital) frustration?

TAKE HOME MESSAGE

The physics of excited bands of optical lattices reveal many interesting phenomena due to an additional orbital degree of freedom..

- The Hamiltonian of the Mott-1 phase can be mapped into different types of spin models, and with different symmetries depending on the choice of the the atoms (if bosons or fermions)

allows for simulation of non-integrable spin models with cold atoms in optical lattices!

Thank you for attention! :)