Spin-Orbit Coupling in Mott Insulators: Unusual Interactions and Possible Exotic Phases

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In collaboration with

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GNSF

FRAGNETS12 @ KITP

Outline

- Possibility of a spin liquid phase in A_2IrO_3

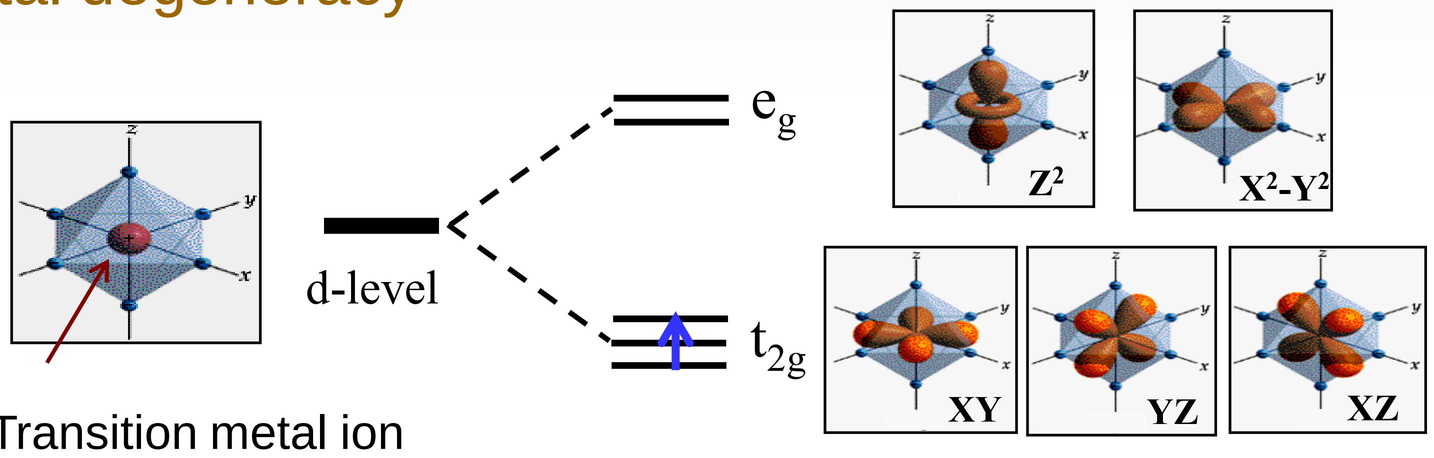
  GJ & G.Khaliullin, PRL 102, 017205, (2009)
  J.Chaloupka, GJ & G.Khaliullin, PRL 105, 027204, (2010)
  J.Chaloupka, GJ & G.Khaliullin, arXiv:1209.5100

- Magnetically hidden octupolar order in Sr_2VO_4

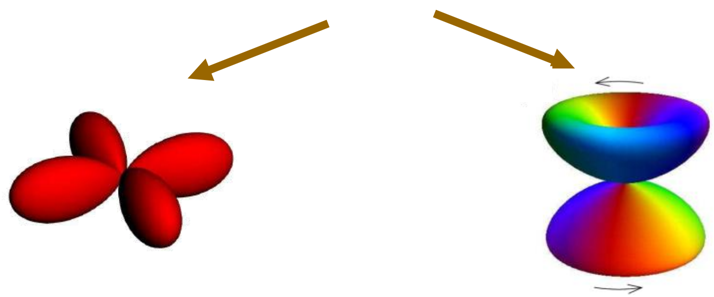
  GJ & G.Khaliullin, PRL 103, 067205, (2009)

Mott Insulators with t_{2g} orbital degeneracy

Orbital degeneracy



Unquenched angular momentum $L = -l_{eff} = 1$

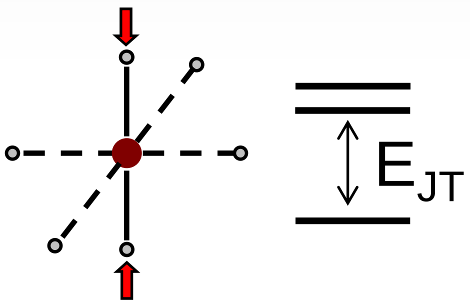


$|l_z\!=\!0\rangle \equiv |xy\rangle$

$|l_z\!=\!\pm1\rangle \equiv -\frac{1}{\sqrt{2}}(i|xz\rangle \pm |yz\rangle)$

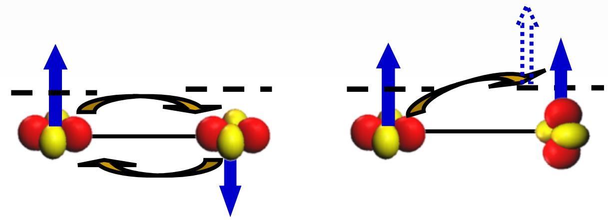
Three different couplings & regimes in spin-orbital systems

Jahn-Teller coupling- E_{JT}

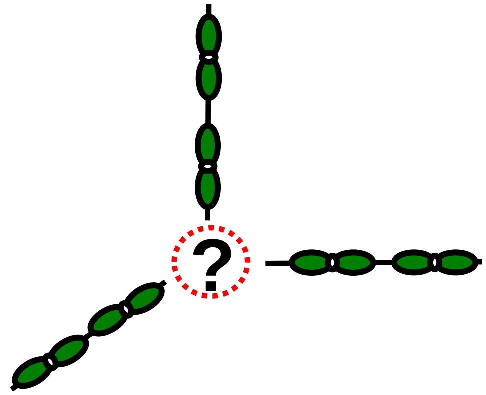


orbitals are rigidly ordered:
spin-only Heisenberg model

exchange interactions- J



spin exchange depends on orbital occupancy:
directional character of orbitals induces frustration



spin-orbit coupling-λ

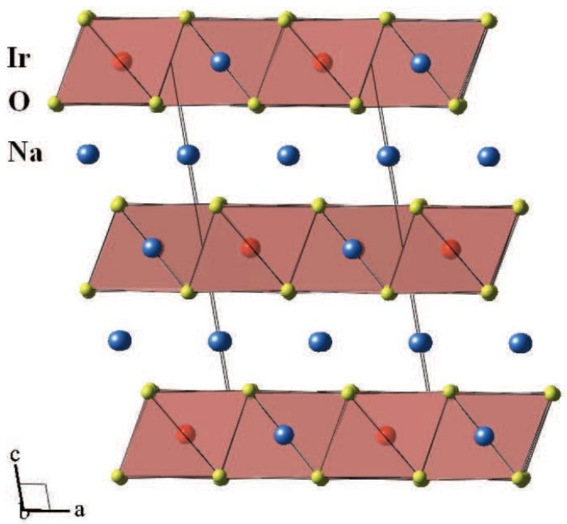
$$\lambda \vec{l} \cdot \vec{s}$$

spins & orbitals locally entangled:
orbital frustration & directional character are converted to iso-spins

Why hexagonal Iridates A_2IrO_3 (A=Na, Li) are interesting

A) Strong spin orbit coupling in Ir^{4+}

B) Honeycomb layers of spins 1/2 Ir^{4+}



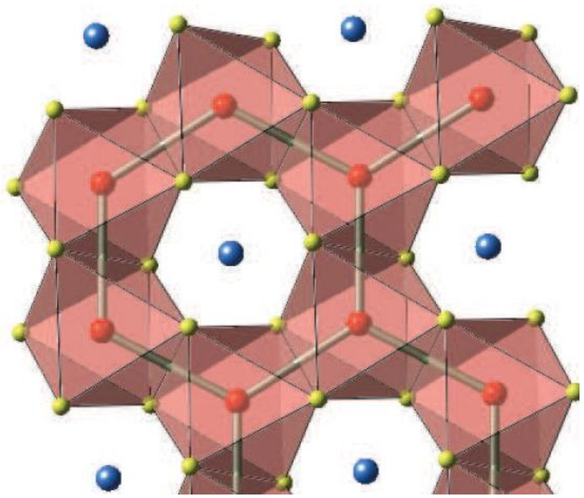


figure from: Singh & Gegenwart, PRB10

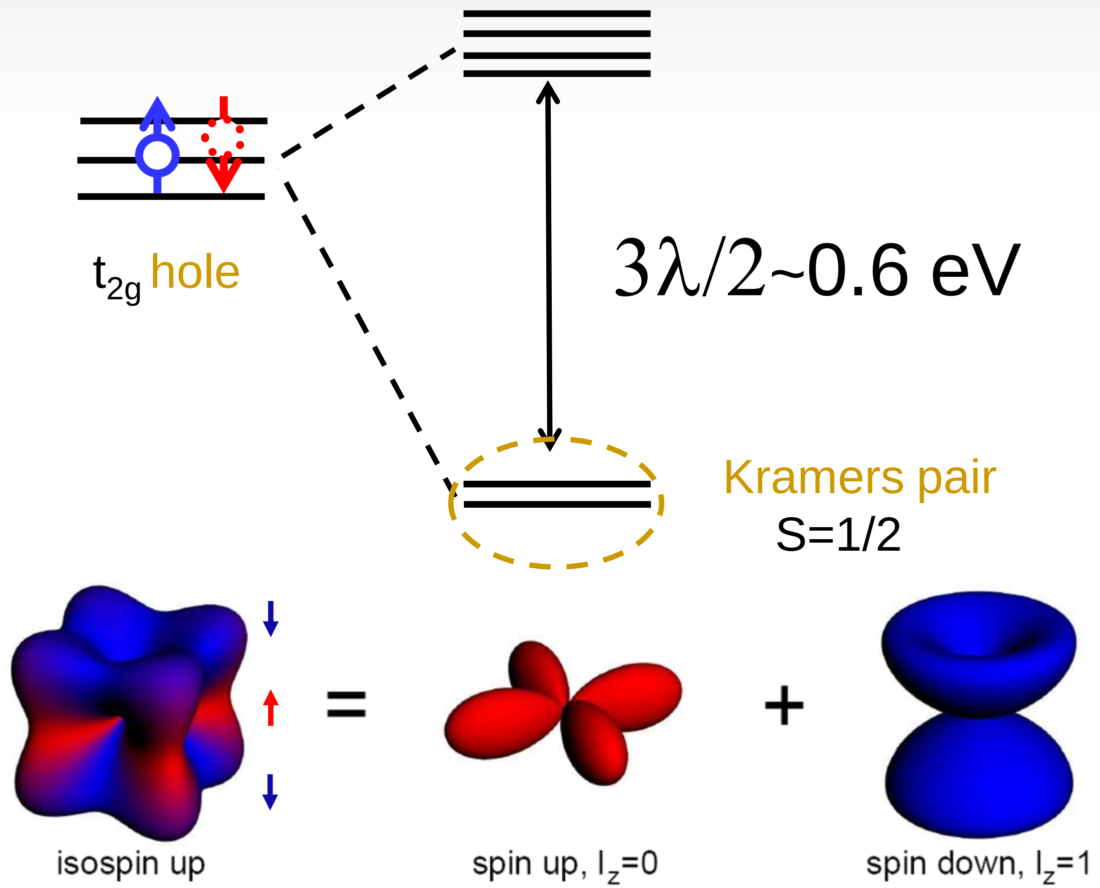
Why hexagonal Iridates A_2IrO_3 (A=Na, Li) are interesting

Two theory proposals based on above A) &B)

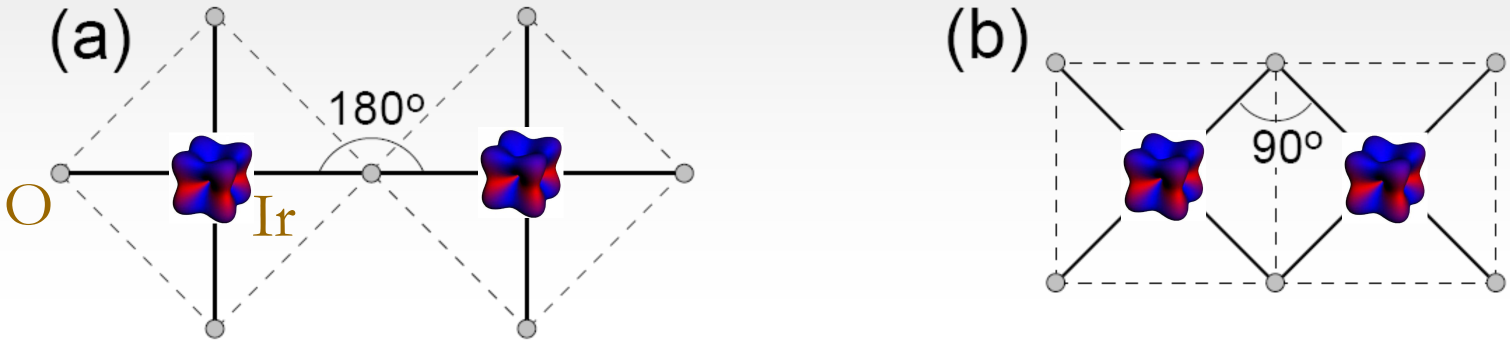
GJ & G.Khaliullin, PRL 102, 017205, (2009)
from Mott side:
As a candidate for a spin liquid phase

A.Shitade et al, PRL 102, 256403, (2009)
from itinerant side:
As a candidate for a topological insulator and QSH effect

Low energy Kramers doublet of Ir^{4+}



Super-exchange between Isospins



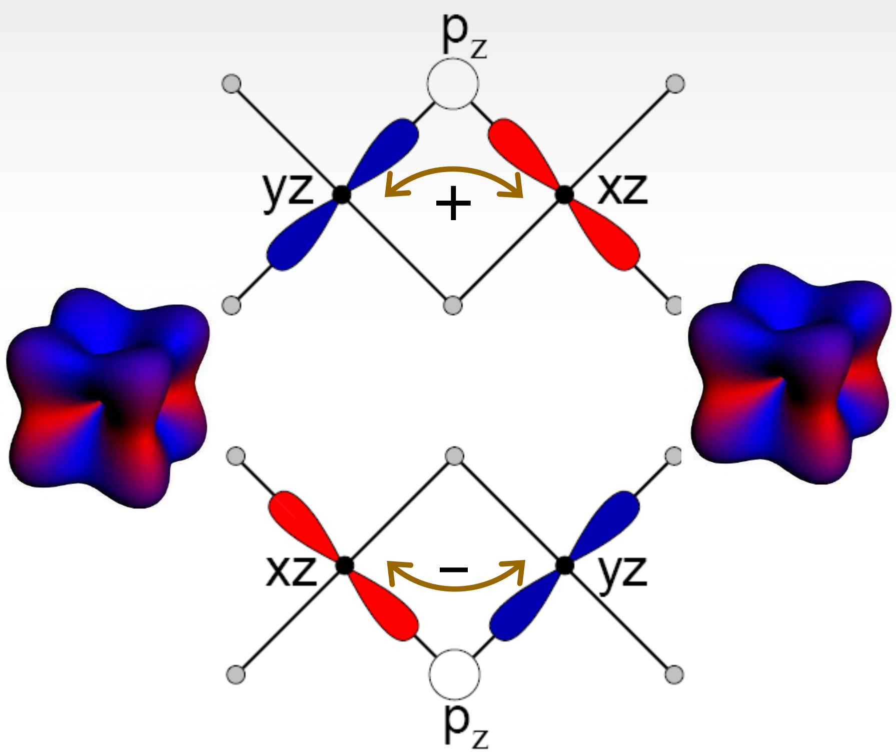
$$\mathcal{H}_{ij} = J_1 \vec{S}_i \cdot \vec{S}_j + J_2 (\vec{S}_i \cdot \vec{r}_{ij})(\vec{r}_{ij} \cdot \vec{S}_j)$$

$$\mathcal{H}_{ij}^{(\gamma)} = -J S_i^{\gamma} S_j^{\gamma}$$

AF-Heisenberg and weaker “dipolar”

FM-Ising, γ-axis out of plane

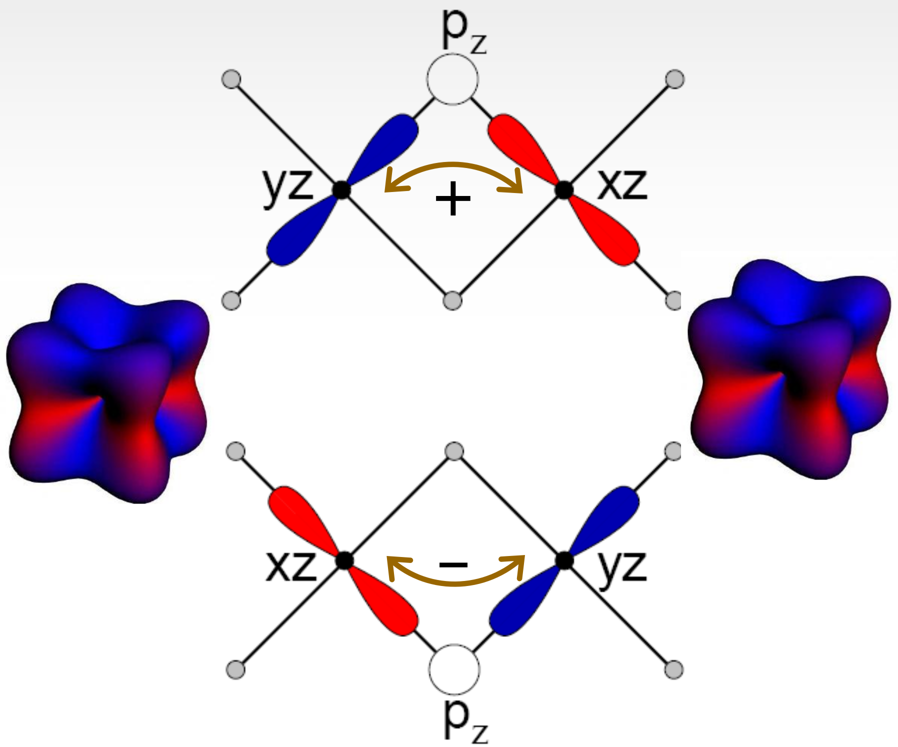
Superexchange Hamiltonian: 90º-bonds

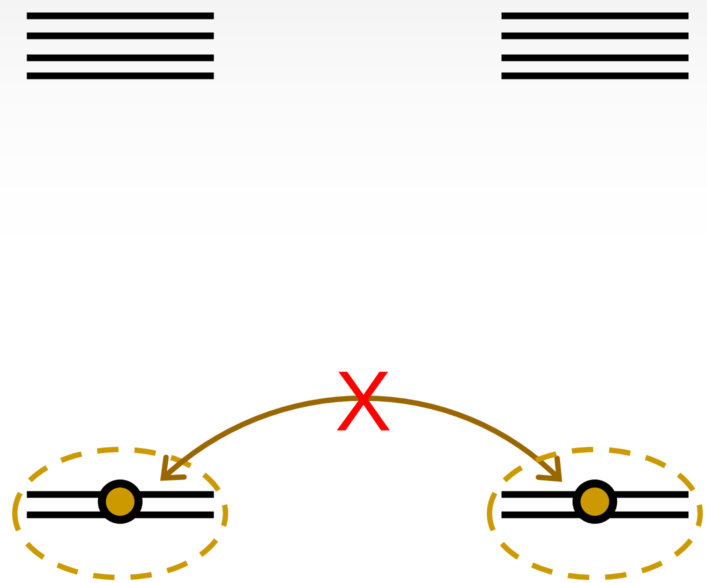


Destructive quantum interference between two channels

No conventional Heisenberg term

Superexchange Hamiltonian: 90º-bonds





$$\mathcal{H}_{ij}^{(\gamma)} = -J S_i^\gamma S_j^\gamma$$

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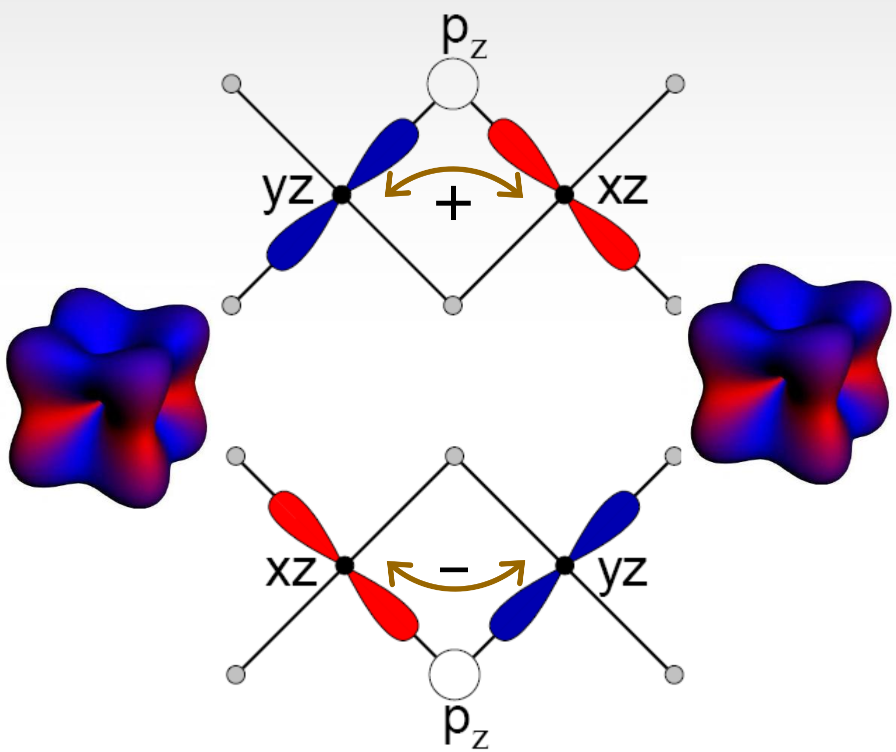
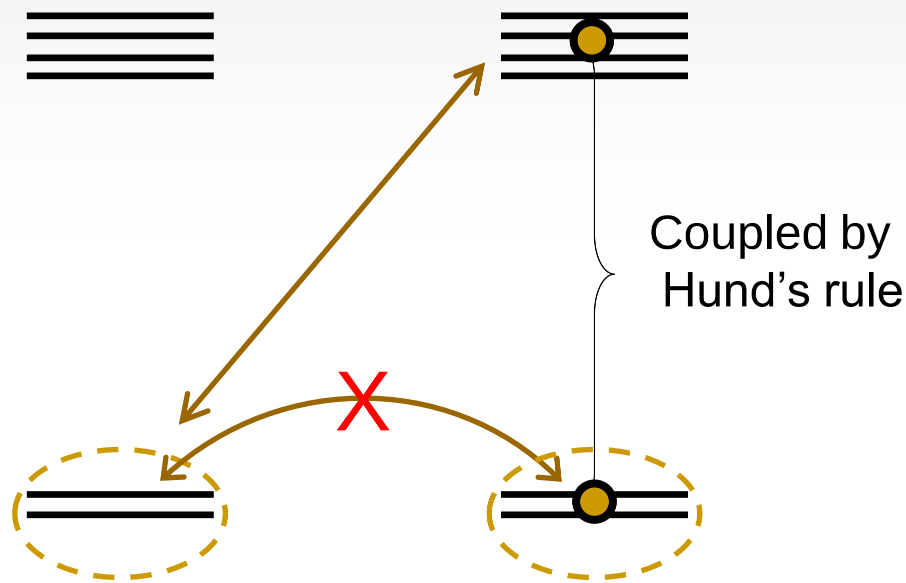
γ=(x,y,z) perp. of plaquet

Superexchange Hamiltonian: 90º-bonds





$$\mathcal{H}_{ij}^{(\gamma)} = -J S_i^{\gamma} S_j^{\gamma}$$

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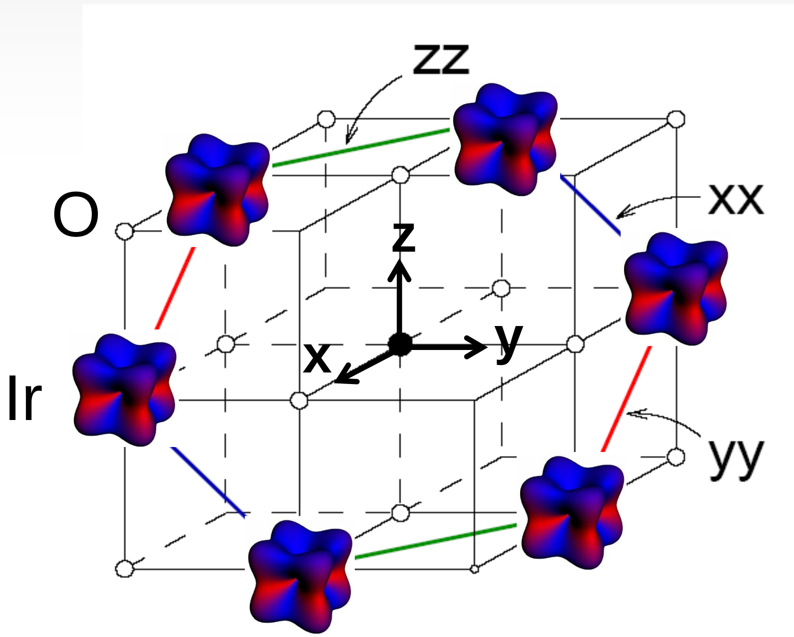
Isospins on a Honeycomb layer of A_2IrO_3 (A=Na, Li)



$$\mathcal{H}_{ij}^{(\gamma)} = -J_1 \; S_i^\gamma S_j^\gamma + J_2 \; \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

Kitaev term — Heisenberg term

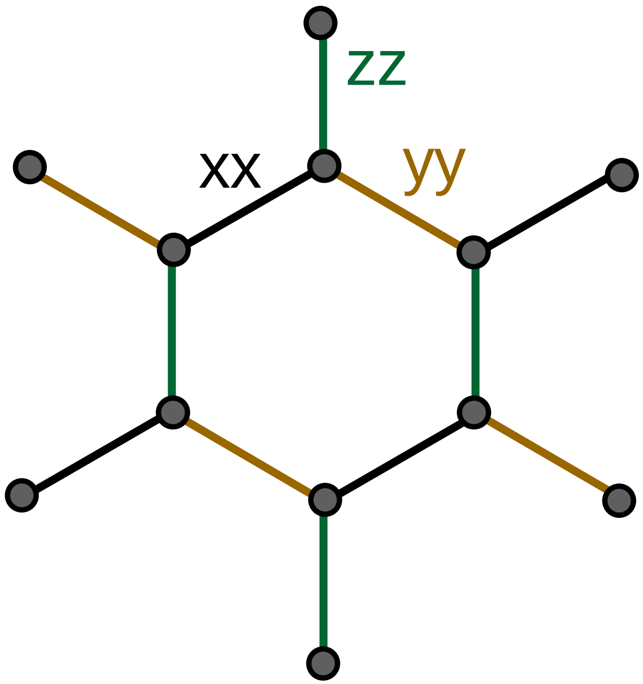
$$J_1 = 2\alpha \; , \quad J_2 = 1 - \alpha$$

Phases of Kitaev-Heisenberg Model

Frustration due to anisotropy: Kitaev model

A. Kitaev, Ann. Phys'06

$$\mathcal{H}_{ij}^{(\gamma)} = -J S_i^\gamma S_j^\gamma$$



- exactly soluble 2D quantum model
- spin liquid ground-state:
  with Majorana Fermions, Dirac spectrum
- only NN two-spin correlations
  (Baskaran et al PRL07)

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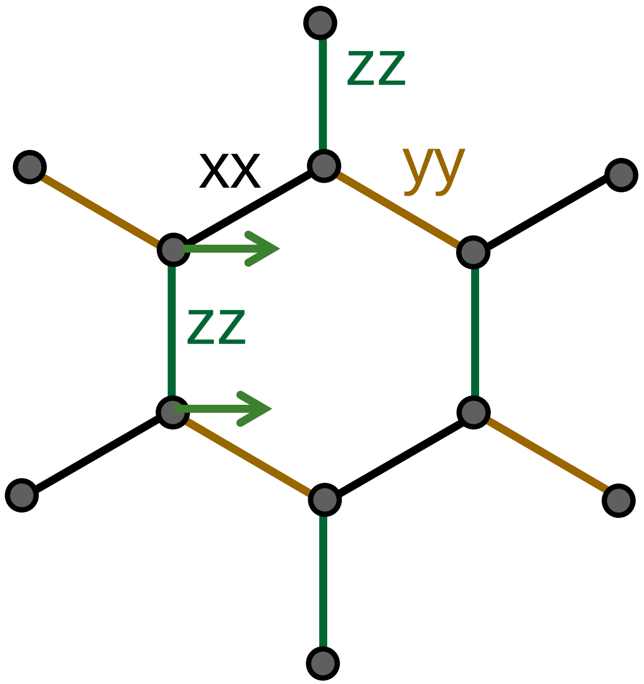

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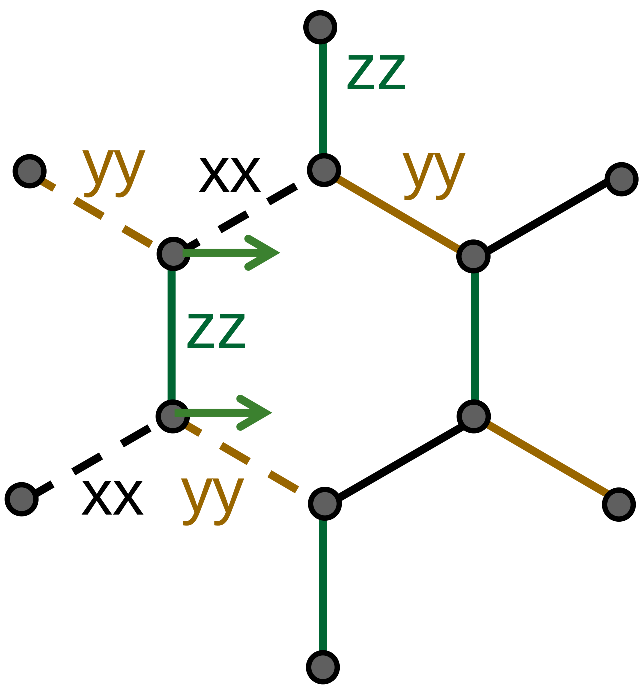

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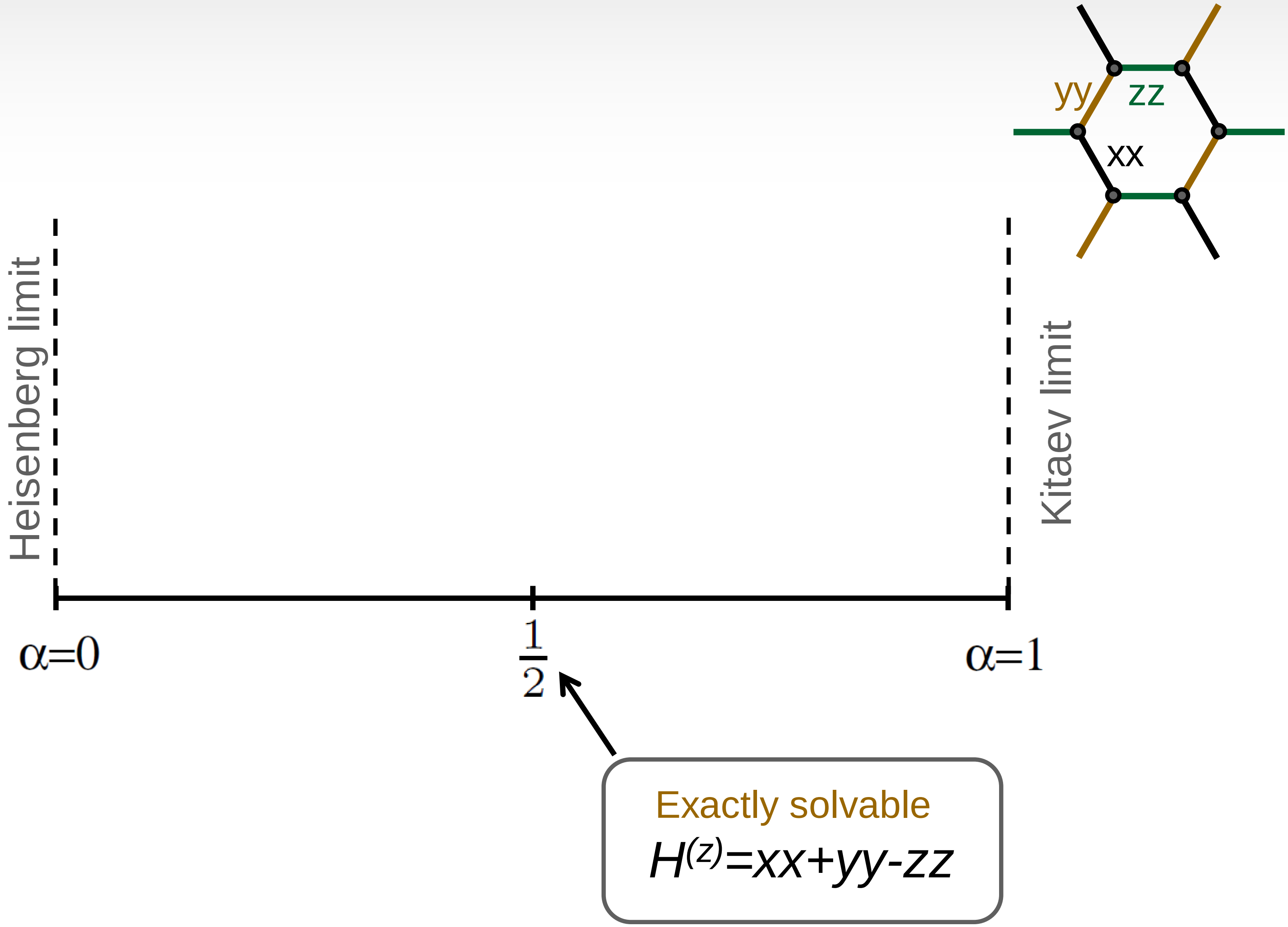
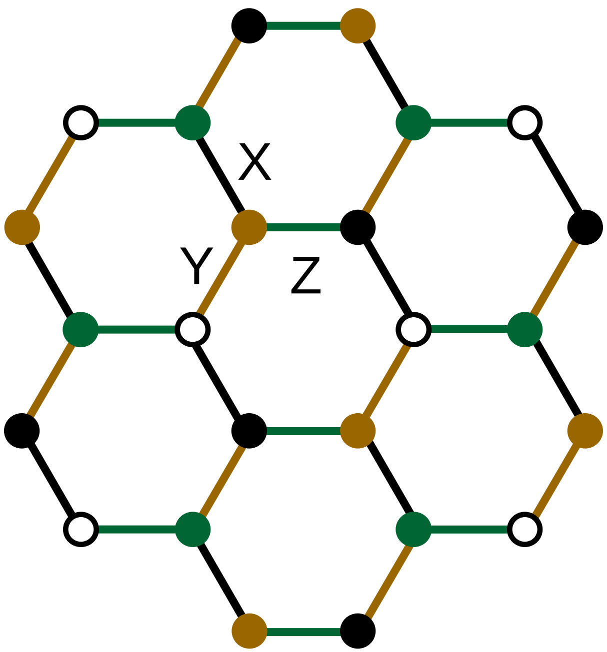


α=1/2: Hidden FM Heisenberg model

$$\mathcal{H}_{ij}^{(z)} = \frac{1}{2}(S_i^x S_j^x + S_i^y S_j^y - S_i^z S_j^z)$$

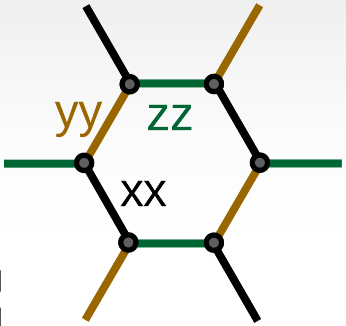


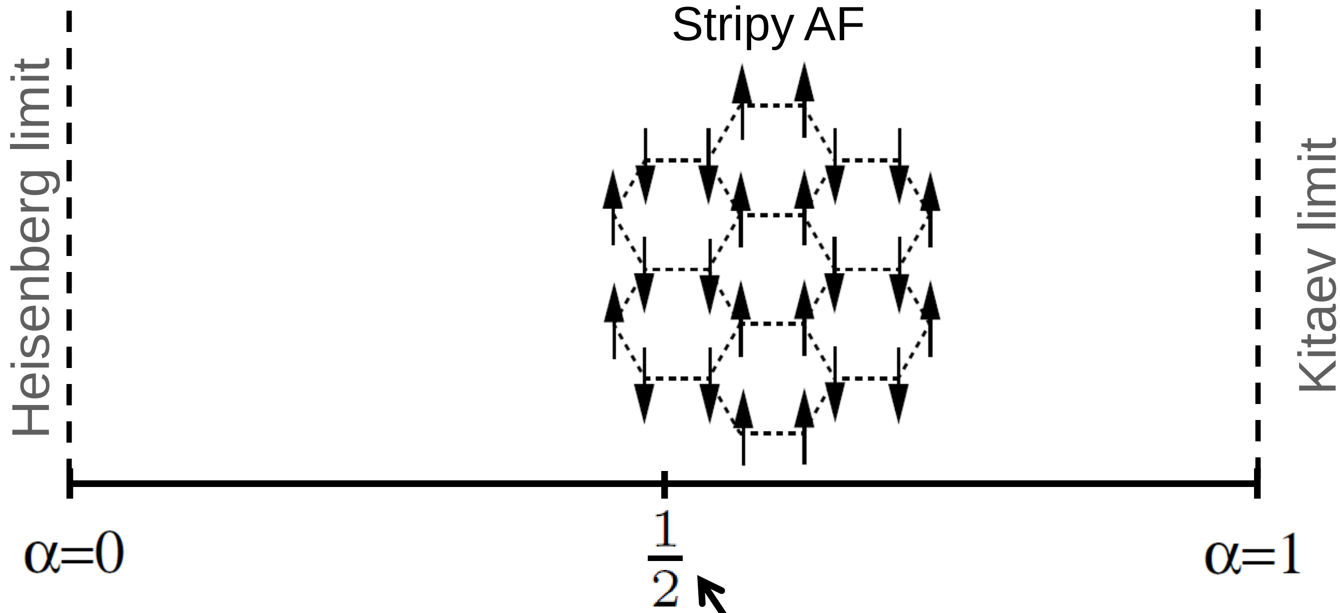
4-sublattice unitary transformation

- ○ original frame
- ● (black) $(S^x,S^y,S^z) \to (S^x,-S^y,-S^z)$
- ● (brown) $(S^x,S^y,S^z) \to (-S^x,S^y,-S^z)$
- ● (green) $(S^x,S^y,S^z) \to (-S^x,-S^y,S^z)$

$$\mathcal{H}_{ij}^{(\gamma)} = -\frac{1}{2}\ \tilde{\boldsymbol{S}}_i \cdot \tilde{\boldsymbol{S}}_j$$

Phases of Kitaev-Heisenberg Model

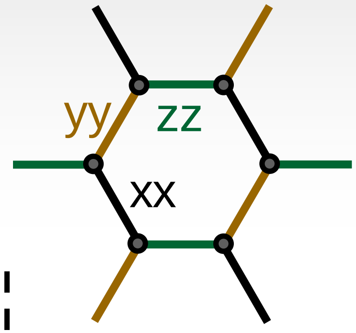


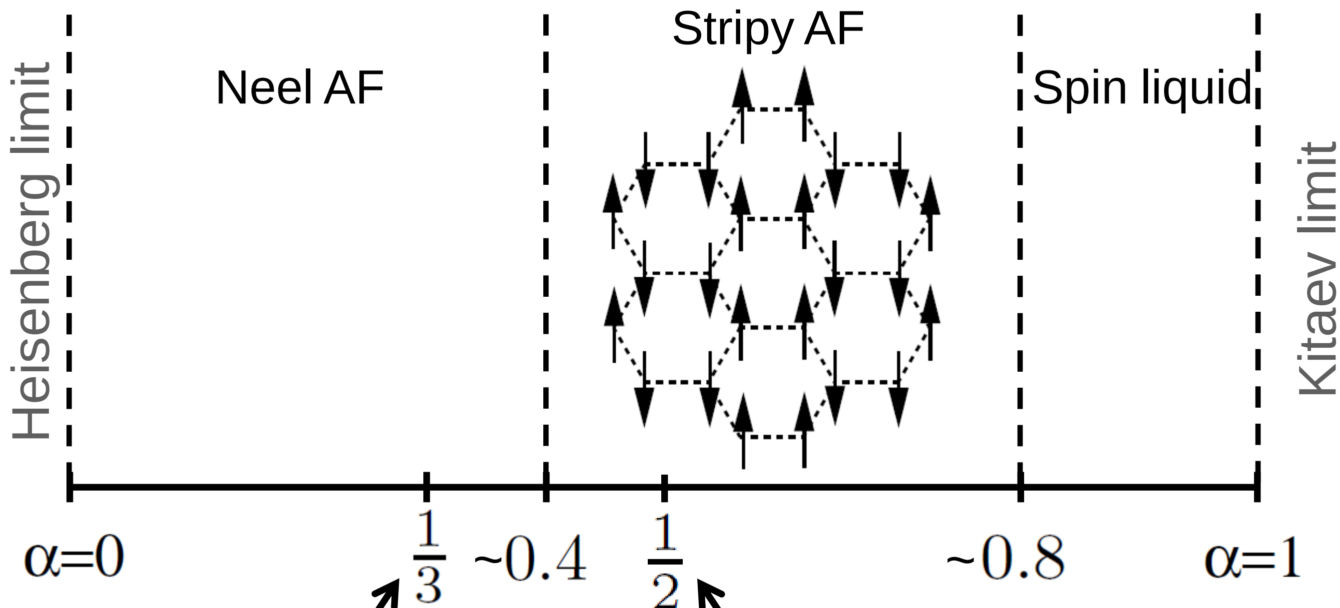


Exactly solvable

$H^{(z)}=xx+yy-zz$

Phases of Kitaev-Heisenberg Model





classical phase boundary
lines of zeros in SW spectra
$H^{(z)}=xx+yy$

Exactly solvable
$H^{(z)}=xx+yy-zz$

Recent Experimental Reports

Upcoming Talk by Radu Coldea

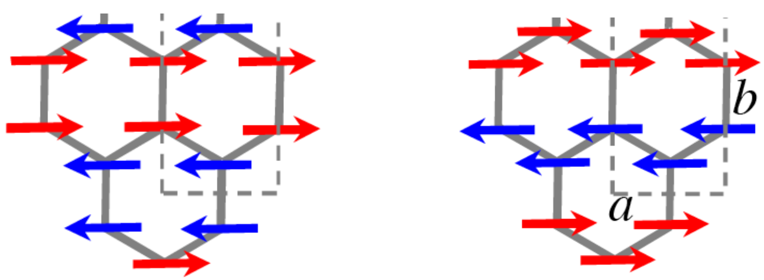
Susceptibility & Thermodynamics:

Singh and Gegenwart, PRB'10; Singh et al PRL'12

Ordering ~ 15K in both Na_2IrO_3 (θ=-125K) & Li_2IrO_3 (θ =-33K)

XRS : *Liu et al, PRB'11*

Stripy vs Zig-Zag order in Na_2IrO_3



INS: *Choi, Coldea et al, PRL'12; Ye et al PRB'12*

Trigonal distortion, deviation from 90º bond angle, Zig-Zag order

N&XR Difraction: *Ye et al PRB'12*

further neighbor interactions explains zigzag phase

PHYSICAL REVIEW B **84**, 180407(R) (2011)

Kitaev-Heisenberg-J_2-J_3 model for the iridates A_2IrO_3

Itamar Kimchi[1] and Yi-Zhuang You[1,2]

PRL **108,** 127204 (2012) PHYSICAL REVIEW LETTERS week ending 23 MARCH 2012

Spin Waves and Revised Crystal Structure of Honeycomb Iridate Na_2IrO_3

S. K. Choi,[1] R. Coldea,[1] A. N. Kolmogorov,[2] T. Lancaster,[1,*] I. I. Mazin,[3] S. J. Blundell,[1] P. G. Radaelli,[1] Yogesh Singh,[4,5] P. Gegenwart,[4] K. R. Choi,[6] S.-W. Cheong,[6,7] P. J. Baker,[8] C. Stock,[8] and J. Taylor[8]

PRL **108,** 127203 (2012) PHYSICAL REVIEW LETTERS week ending 23 MARCH 2012

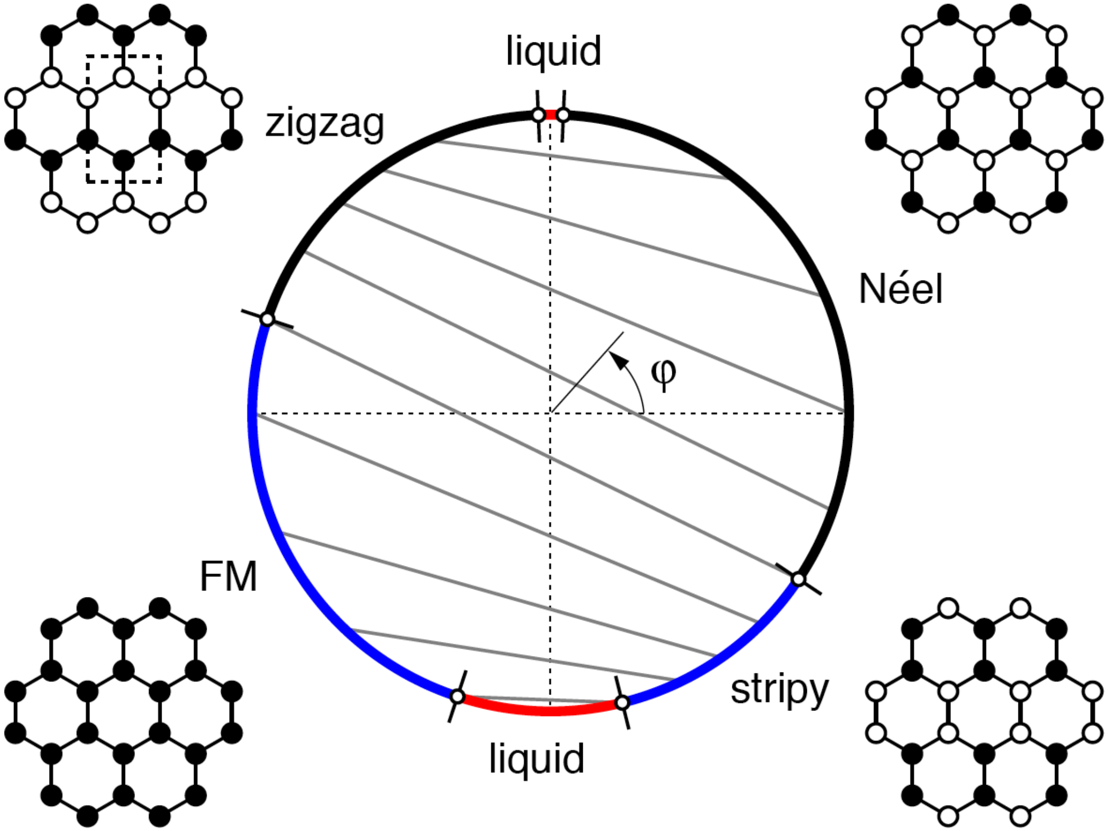
Relevance of the Heisenberg-Kitaev Model for the Honeycomb Lattice Iridates A_2IrO_3

Yogesh Singh,[1,2] S. Manni,[2] J. Reuther,[3,4] T. Berlijn,[5,6] R. Thomale,[7] W. Ku,[5,6] S. Trebst,[8] and P. Gegenwart[2]

Full Phase Diagram of Kitaev-Heisenberg Model

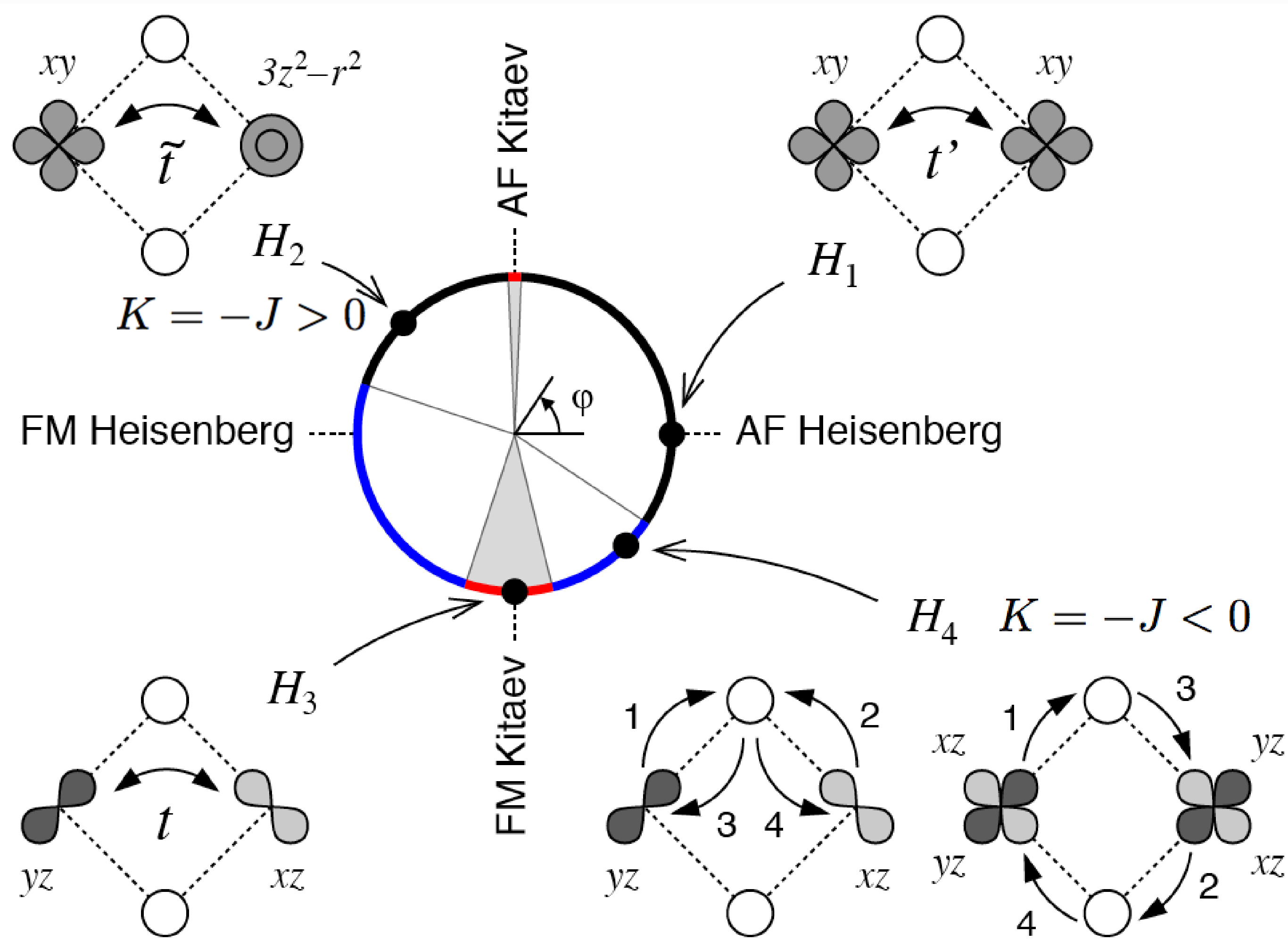
$$\mathcal{H}_{ij}^{(\gamma)} = 2K\ S_i^\gamma S_j^\gamma + J\ \mathbf{S}_i \cdot \mathbf{S}_j \qquad \tilde{\mathcal{H}}_{ij}^{(\gamma)} = 2[K+J]\ \tilde{S}_i^\gamma \tilde{S}_j^\gamma - J\ \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j$$

$$K = A\sin\varphi \qquad J = A\cos\varphi$$

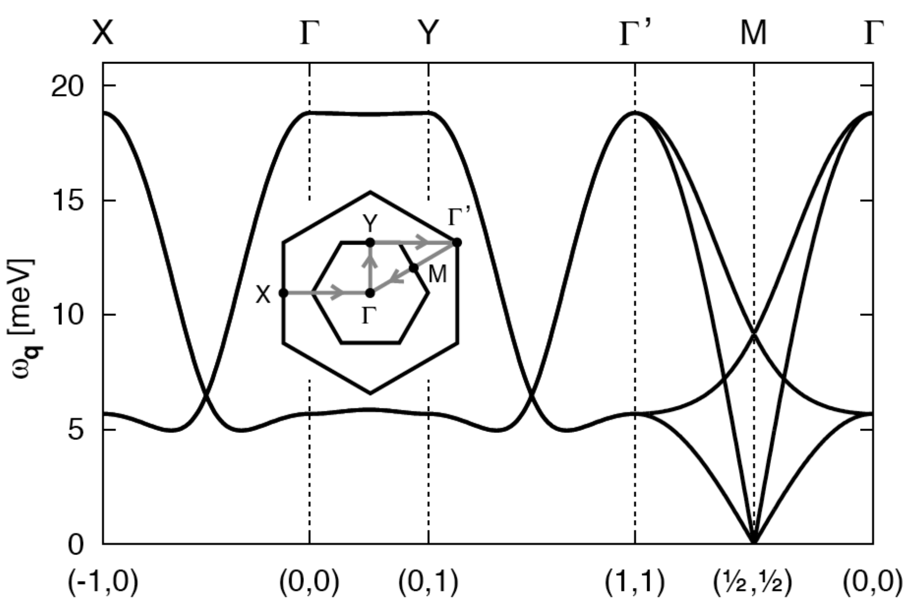


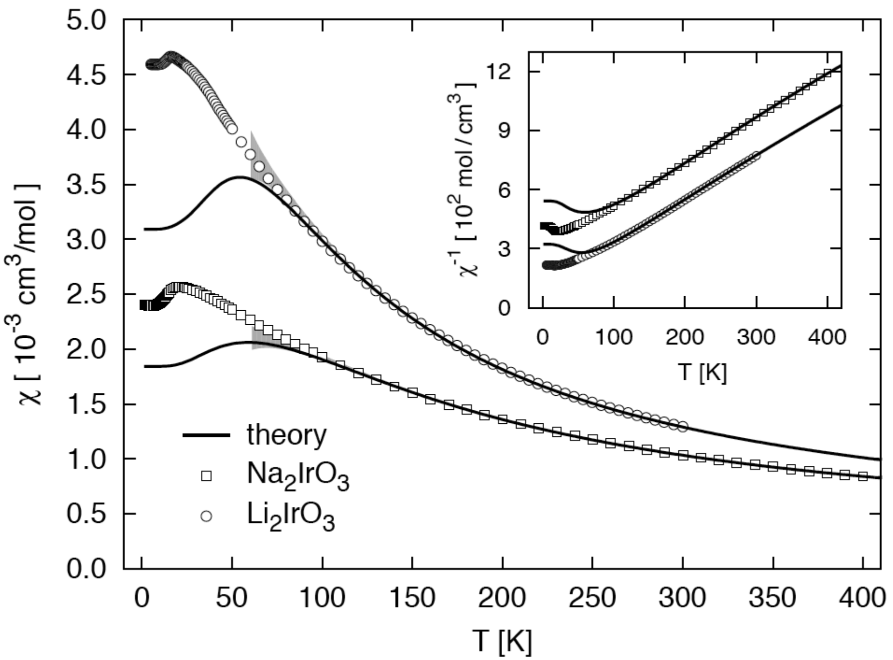
Examples of exchange processes

$$\mathcal{H}_{ij}^{(\gamma)} = 2K\ S_i^\gamma S_j^\gamma + J\ \mathbf{S}_i \cdot \mathbf{S}_j \qquad K = A\sin\varphi \qquad J = A\cos\varphi$$



Spin-wave dispersions and susceptibly of Zigzag phase





$$2K = 21.0\text{meV}, J = -4.0\text{meV} \quad g = 1.78 \quad \chi_0 = 0.16 \times 10^{-3}\text{cm}^3/\text{mol}$$

$$2K = 15.7\text{meV}, J = -5.3\text{meV} \quad g = 1.94, \ \chi_0 = 0.14 \times 10^{-3}\ \text{cm}^3/\text{mol}$$

Recent Experimental Reports

arXiv:1204.4471

Na_2IrO_3 as a Novel Relativistic Mott Insulator with a 350 meV Gap

R. Comin,[1] G. Levy,[1,2] B. Ludbrook,[1] Z.-H. Zhu,[1] C.N. Veenstra,[1] J.A. Rosen,[1] Yogesh Singh,[3] P. Gegenwart,[4] D. Stricker,[5] J.N. Hancock,[5] D. van der Marel,[5] I.S. Elfimov,[1,2] and A. Damascelli[1,2,*]

arXiv:1209.5424

Crystal field splitting and correlation effect on the electronic structure of A_2IrO_3

H. Gretarsson,[1] J. P. Clancy,[1] X. Liu,[2] J. P. Hill,[2] Emil Bozin,[2] Yogesh Singh,[3] S. Manni,[4] P. Gegenwart,[4] Jungho Kim,[5] A. H. Said,[5] D. Casa,[5] T. Gog,[5] M. H. Upton,[5] Heung-Sik Kim,[6] J. Yu,[6] Vamshi M. Katukuri,[7] L. Hozoi,[7] Jeroen van den Brink,[7] and Young-June Kim[1,*]

Summary

Mott insulators with strong spin-orbit coupling:
a new class of frustrated systems

⇩

Orbital frustration directly manifested in magnetic interactions

⇩

unusual interactions and exotic states

Optimistic Outlook

« IL EST BON DE SAVOIR QUE L'UTOPIE N'EST JAMAIS RIEN D'AUTRE QUE LA RÉALITÉ DE DEMAIN ET QUE LA RÉALITÉ D'AUJOURD'HUI ÉTAIT L'UTOPIE D'HIER »

LE CORBUSIER