Title: Generic Spin Model for Honeycomb Iridates Beyond the Kitaev Limit

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Abstract: Recently, realizations of Kitaev physics have been sought in the A2IrO3 family of honeycomb iridates, originating from oxygen-mediated exchange through edge-shared octahedra. However, for the J=1/2 Mott insulator in these materials exchange from direct d-orbital overlap is relevant, and it was proposed that a Heisenberg term should be added to the Kitaev model. Here we provide the generic nearest-neighbour spin Hamiltonian when both oxygen-mediated and direct overlap are present, containing a bond dependent off-diagonal exchange in addition to Heisenberg and Kitaev terms. We analyze this complete model using a combination of classical techniques and exact diagonalization. Near the Kitaev limit, we find new magnetic phases, 120 degree and incommensurate spiral order, as well as extended regions of zigzag and stripy order. Possible applications to Na2IrO3 and Li2IrO3 are discussed.

Generic spin model for the honeycomb iridates beyond the Kitaev limit

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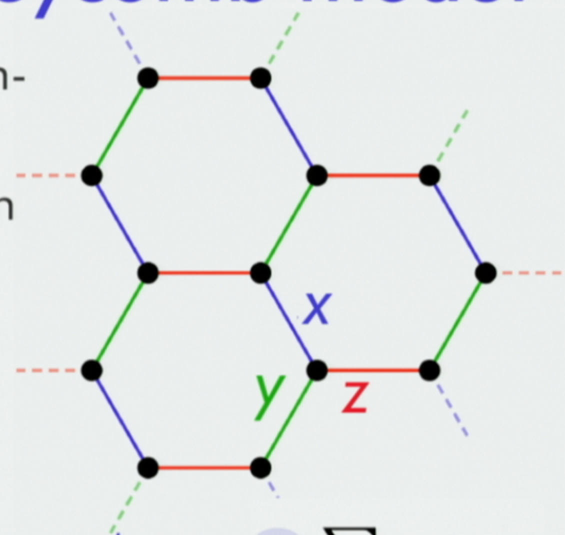
Four Corners Meeting, May 2014

Kitaev's honeycomb model

- Exactly solvable spin-½ model
- Highly anisotropic in spin and space
- Ground state is Z_2 spin liquid
- Gapless Majorana fermions



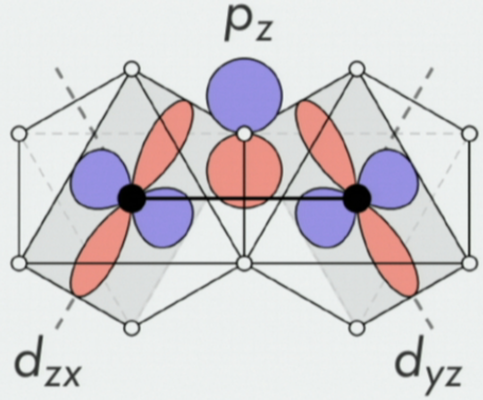
Kitaev exchange → K

$$K \sum_{\langle ij \rangle \in \gamma} S_i^\gamma S_j^\gamma$$

Can it be realized in a solid-state system?

A. Kitaev, Ann. Phys. (2005)

Spin-orbit Mott insulators



- Edge-shared oxygen octahedra
- Effective $j=1/2$ spin model
- Considers only oxygen mediated exchange

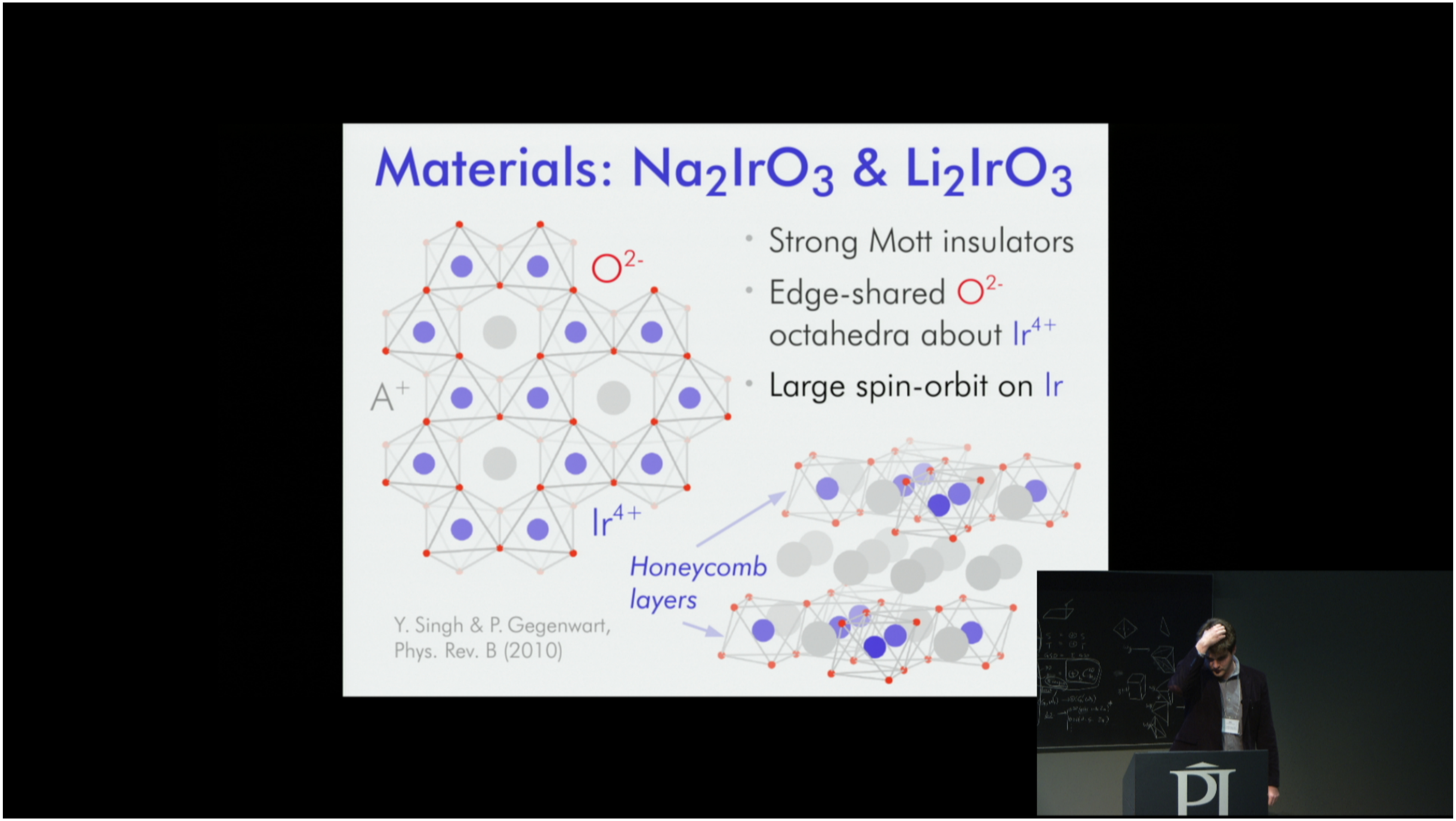
Ferromagnetic

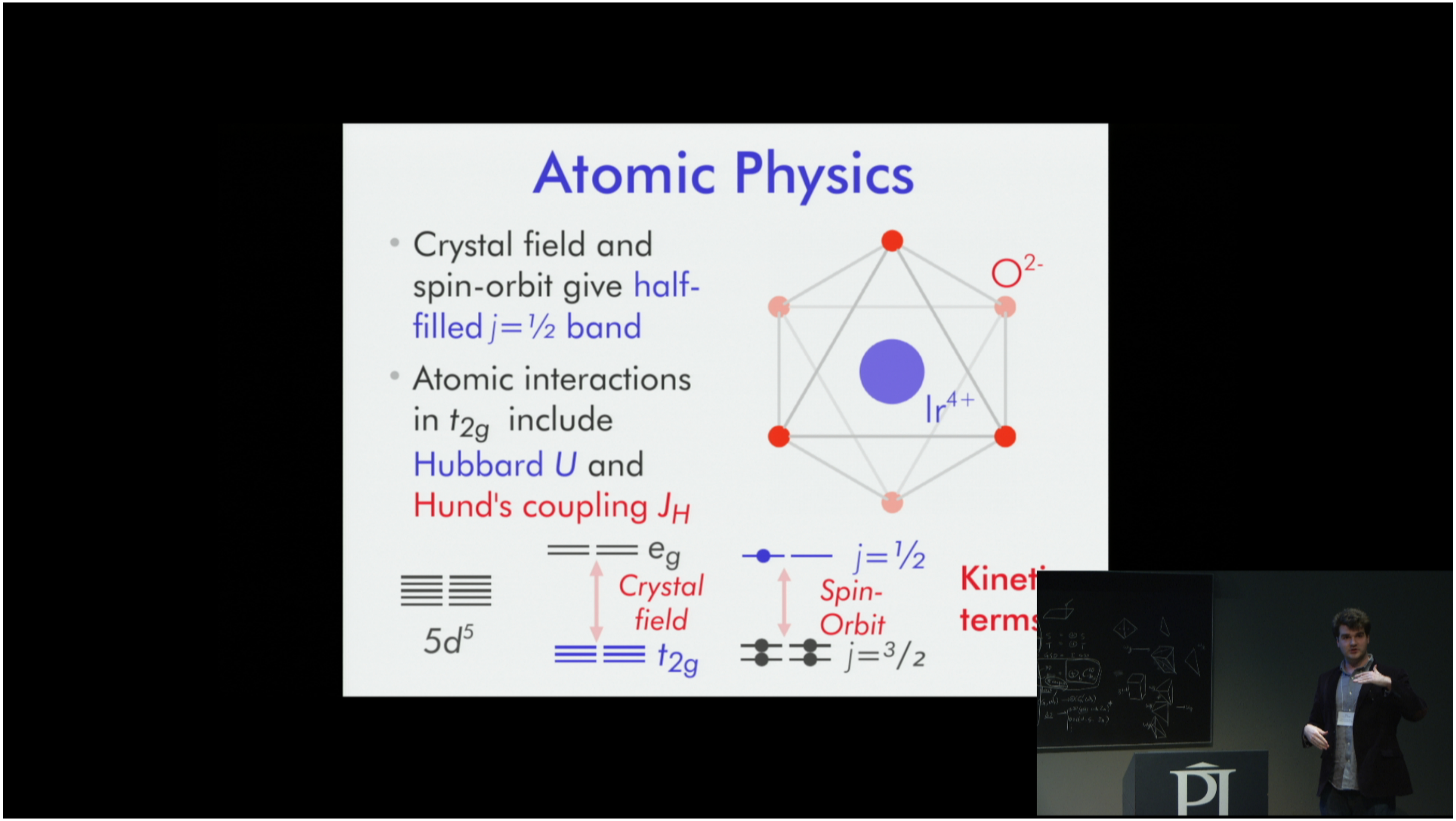
$$K \sim -\frac{8J_H}{3U^2}\left(\frac{t_{pd\pi}^2}{\Delta_{pd}}\right)^2$$

Hund's coupling

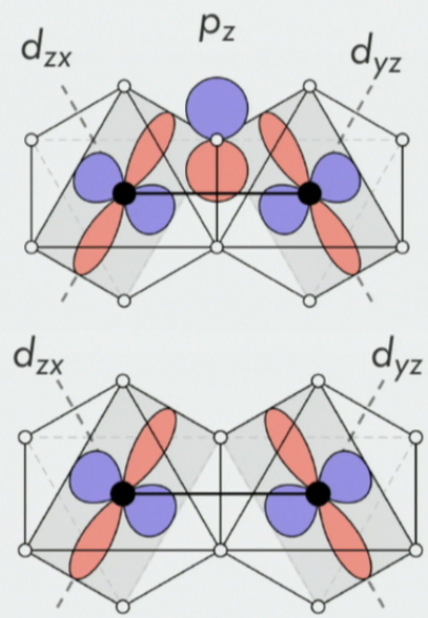
Candidate materials?

G. Jackeli & G. Khalliliuin, Phys. Rev. Lett. (2009)


Materials: Na2IrO3 & Li2IrO3
O2-
A+
Ir4+
Strong Mott insulators
Edge-shared O2- octahedra about Ir4+
Large spin-orbit on Ir
Honeycomb layers
Y. Singh & P. Gegenwart, Phys. Rev. B (2010)
PI

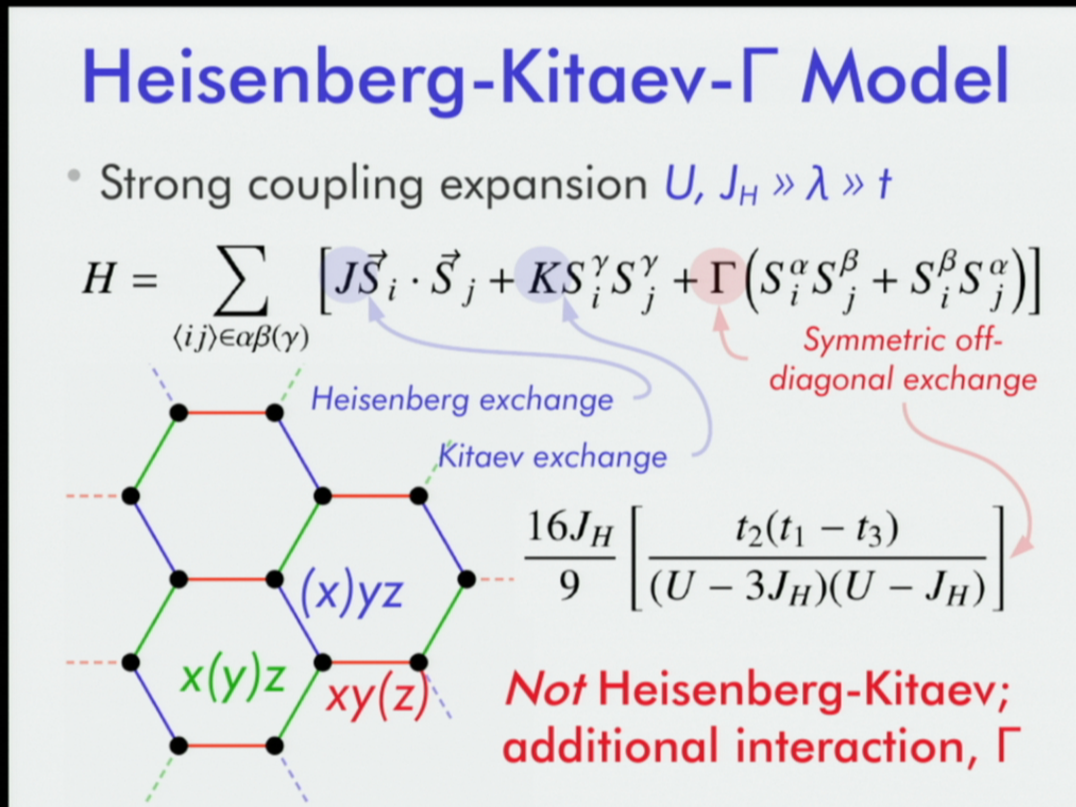

Atomic Physics
Crystal field and spin-orbit give half-filled j=½ band
Atomic interactions in t2g include Hubbard U and Hund's coupling JH
O2-
Ir4+
5d5
eg
Crystal field
t2g
j=½
Spin-Orbit
j=3/2
Kinet
terms

Inter-orbital hopping terms



- Focus on a z bond of the lattice
- Large *5d* orbitals
- Inter-orbital *yz*-*zx* hopping from oxygen and *dd*

$$t_2 = \frac{1}{2}(t_{dd\pi} - t_{dd\delta}) + \frac{t_{pd\pi}^2}{\Delta_{pd}}$$


Heisenberg-Kitaev-Γ Model
Strong coupling expansion $U, J_H \gg \lambda \gg t$
$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)\right]$$
Heisenberg exchange
Kitaev exchange
Symmetric off-diagonal exchange
$$\frac{16J_H}{9}\left[\frac{t_2(t_1 - t_3)}{(U - 3J_H)(U - J_H)}\right]$$
(x)yz
x(y)z
xy(z)
Not Heisenberg-Kitaev; additional interaction, Γ

HKΓ Model: cont.

- In previous work only the Heisenberg and Kitaev terms were derived – no Γ term

Problem #1: Zigzag hard to find in HK model – if oxygen mediated hopping dominates K has wrong sign

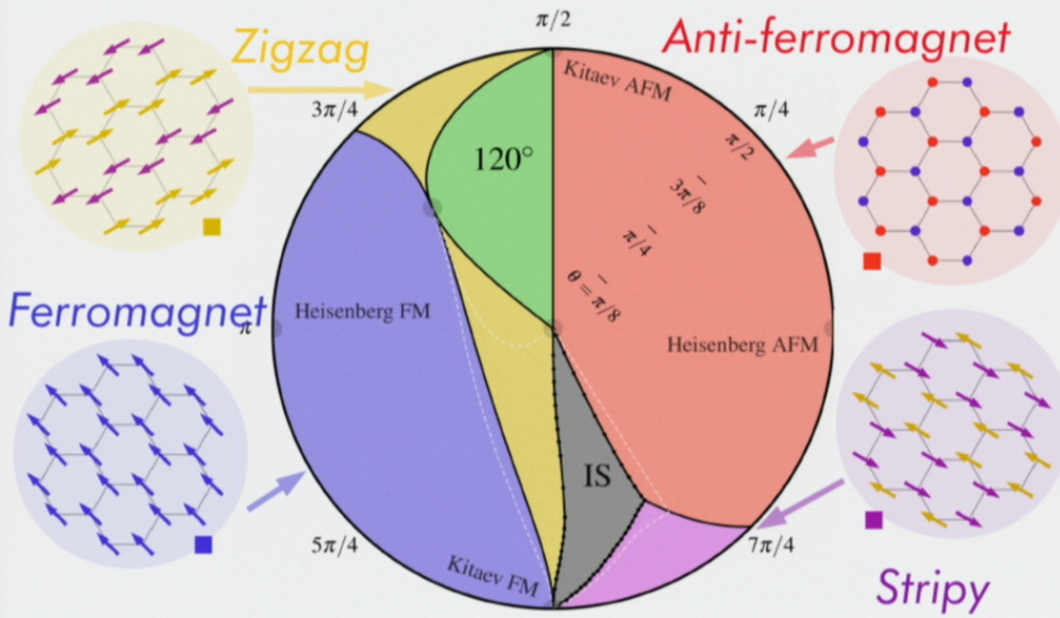
Problem #2: No incommensurate spiral

- Some proposed solutions: Strong e_g-t_{2g} contribution to K to change sign, further neighbour J_2 and J_3, etc.

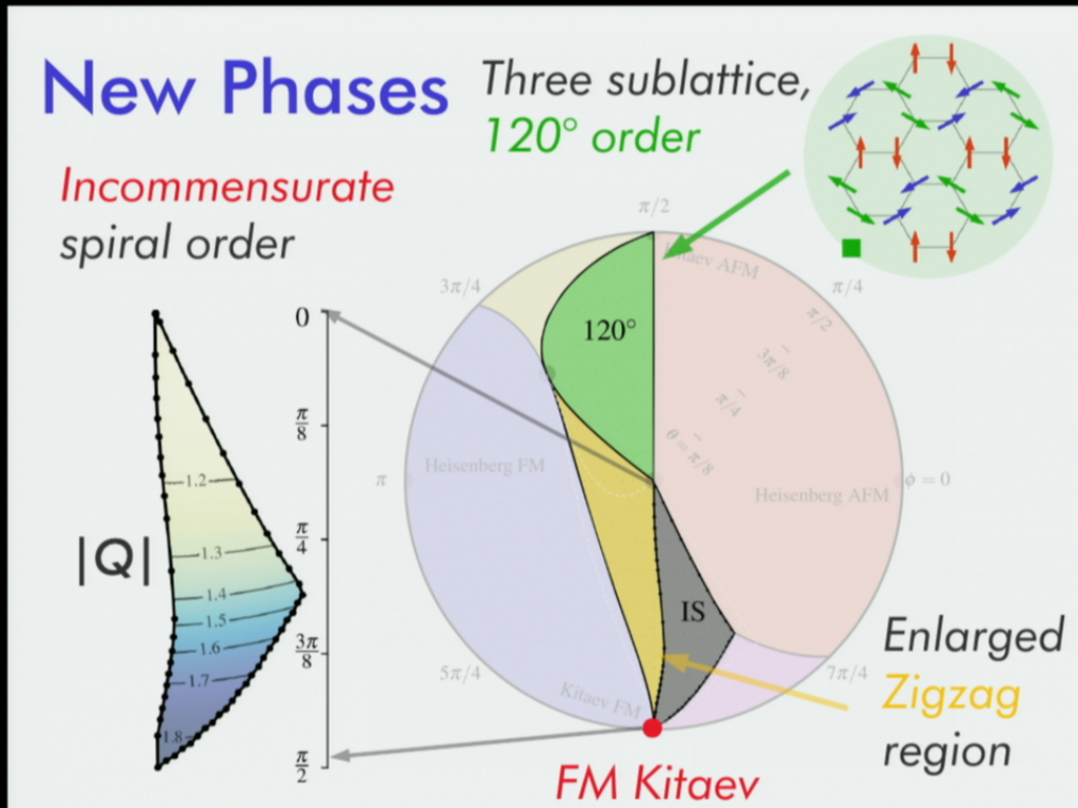
Chaloupka et al. Phys. Rev. Lett.(2010), (2013); Kimchi & You, Phys. Rev. B (2011), etc

What happens when is Γ finite?

Classical Phase Diagram Γ>0

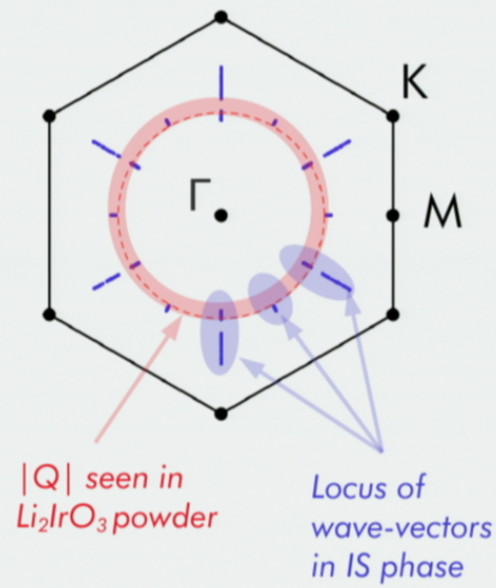


$$J = \sin\theta\cos\phi, \quad K = \sin\theta\sin\phi, \quad \Gamma = \cos\theta$$


New Phases
Three sublattice,
120° order
Incommensurate
spiral order
|Q|
0
π/8
π/4
3π/8
π/2
1.2
1.3
1.4
1.5
1.6
1.7
1.8
120°
IS
Heisenberg FM
Heisenberg AFM
Kitaev FM
π/2
3π/4
π/4
π
φ = 0
5π/4
7π/4
Enlarged
Zigzag
region
FM Kitaev

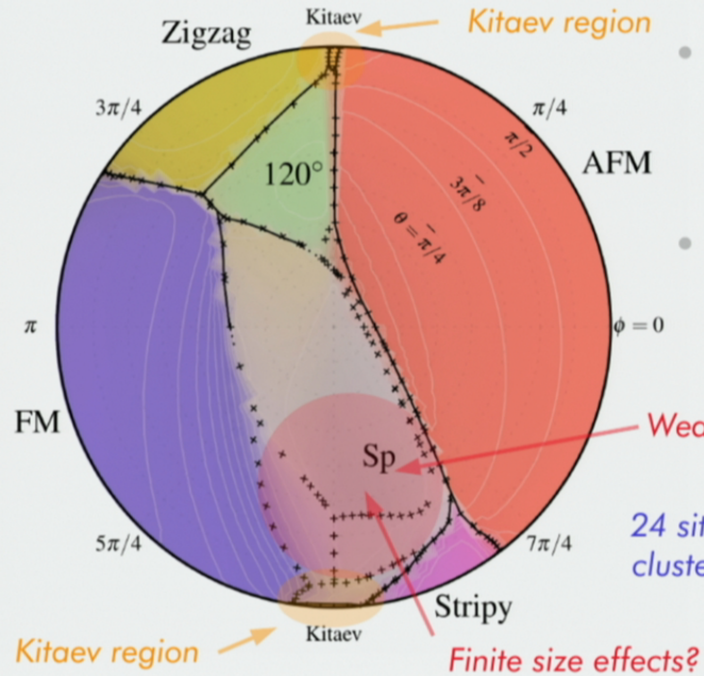
Incommensurate Spiral

- Appears near FM Kitaev limit
- Spiral wave-vector varies in phase
- Clusters with ~ fixed |Q| and along Γ-K lines
- Near wave-vector reported in Li_2IrO_3

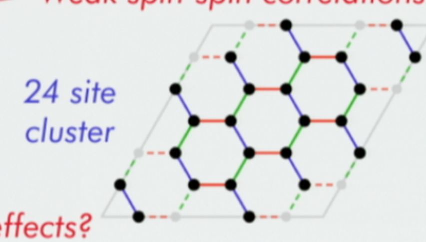


S.K. Choi, APS March Meeting Talk 2014

Exact Diagonalization: $\Gamma > 0$

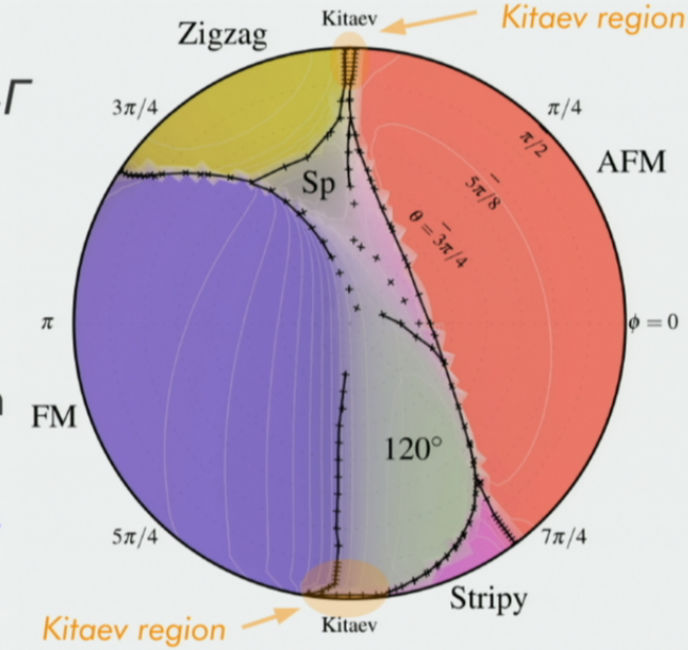


- Identify phases using static structure factor
- *Sp* phase? S_Q maximum at $K/2$



Exact Diagonalization: Γ<0

- Classical mapping Γ to -Γ *not* valid
- Qualitatively similar to mapped Γ>0 phase diagram
- Both Γ>0 and Γ<0 *consistent with classical results*



Conclusions

- Minimal $j=1/2$ spin model of edge-shared octahedra is

$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) \right]$$

Symmetric off-diagonal exchange

- Finite Γ gives new phases; 120° order and *incommensurate spiral* – relevant for Li_2IrO_3?
- New zigzag region for Γ>0 near the FM Kitaev limit – relevant for Na_2IrO_3?

Details in Phys. Rev. Lett. **112**, 077204 (2014)

Conclusions

- Minimal $j=½$ spin model of edge-shared octahedra is

$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) \right]$$

Symmetric off-diagonal exchange

- Finite Γ gives new phases; *120° order* and *incommensurate spiral* – relevant for Li_2IrO_3?
- New zigzag region for Γ>0 near the FM Kitaev limit – relevant for Na_2IrO_3?

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