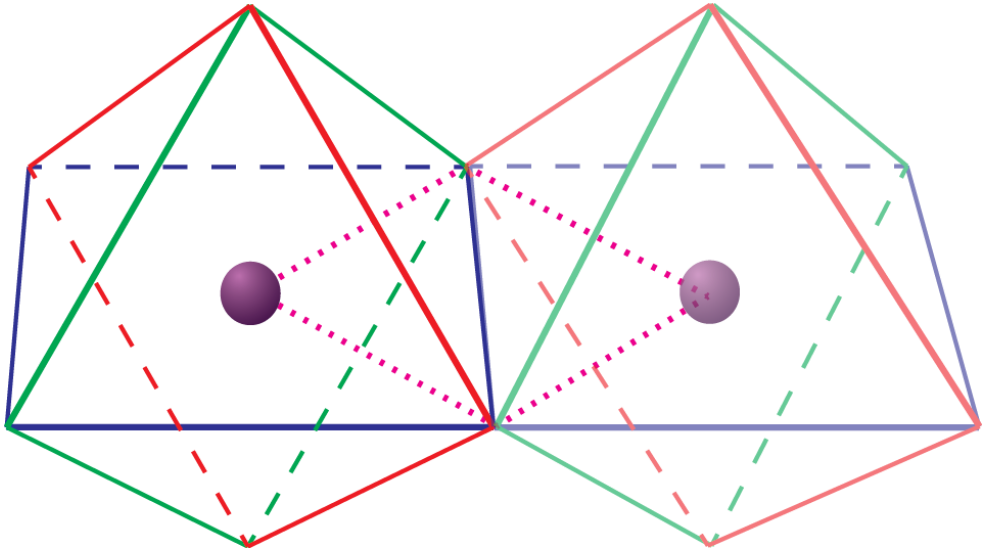
Honeycomb Iridates



Itamar Kimchi

UC Berkeley (& KITP)

Spin models for iridates with spin-orbit coupling

iridium (Ir, 77)

- Correlations + spin-orbit coupling

$$\sim (\alpha Z)^4 L \cdot S$$

Spin models for iridates with spin-orbit coupling

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- Opens portal through space in *The Avengers (2012)*

Spin models for iridates with spin-orbit coupling

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No SU(2) constraint -> new spin Hamiltonians

Interesting?

Describe honeycomb iridates?

Other iridates?

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Interesting?

Describe honeycomb iridates?

Other iridates? (Yes! ask me later for full story)

Kitaev honeycomb model

Summer 2005: Kitaev writes down a seemingly-artificial spin-1/2 Hamiltonian

Exactly solvable!

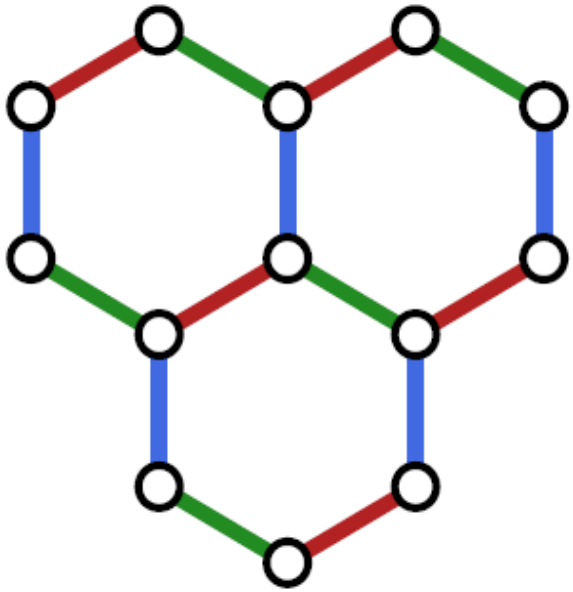
Ground state is quantum spin liquid

with **Majorana fermions** and $\mathbb{Z}_2$ gauge **visons**

Spin component coupling x,y,z depends on bond

↓

Inherently spin-orbit coupled



Kitaev, Ann.Phys. 321, 2 (2006)

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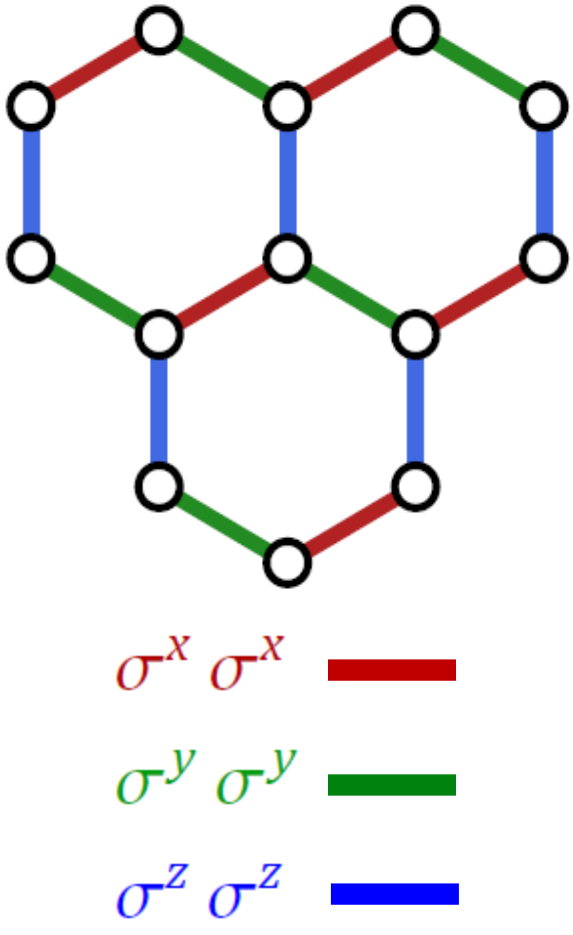


Kitaev, Ann.Phys. 321, 2 (2006)

Magnetic frustration in Na_2IrO_3 , Li_2IrO_3

Mott insulators

Ir on honeycomb layers

- Magnetic susceptibility χ(T):

Curie-Weiss

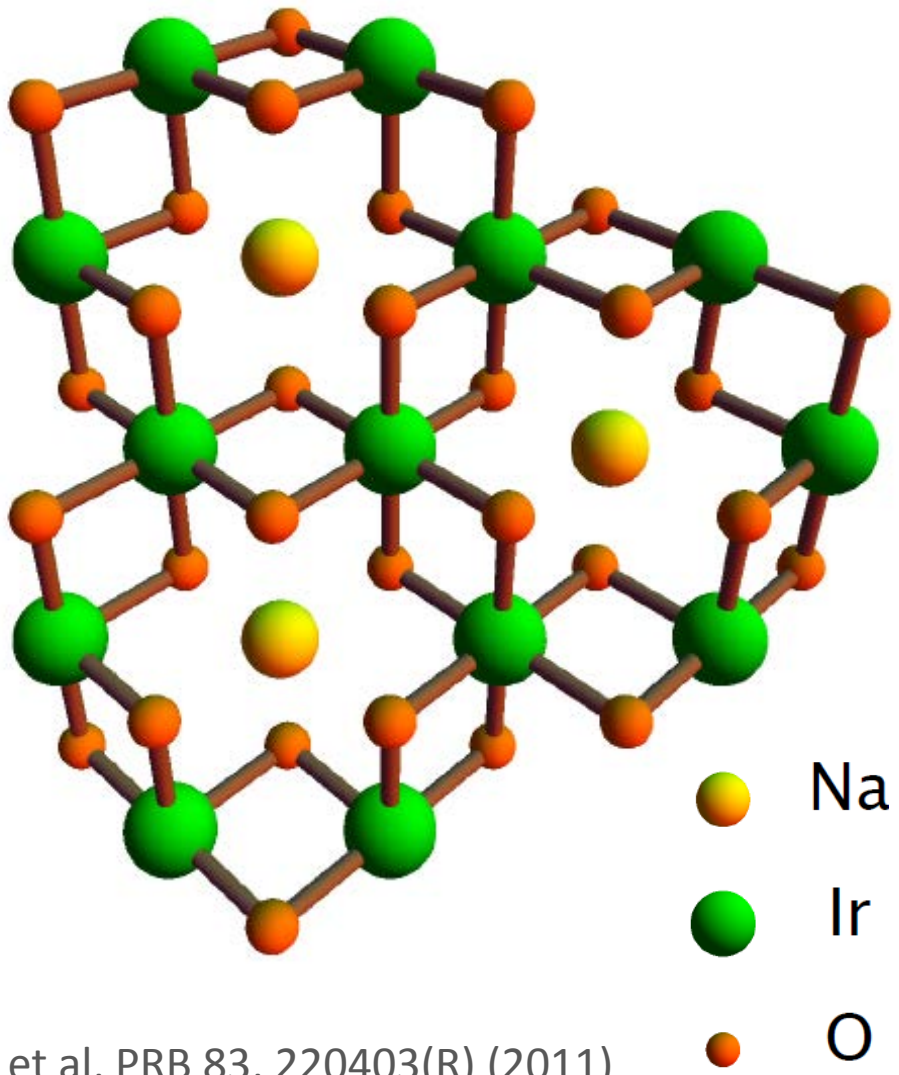
θ_{cw} = -125K Na, -33K Li

Local moments *j*=1/2 on Ir

- Order at low T = 15K

  frustrated (at least Na. Li?)

  Na_2IrO_3: non-Neel AF



Singh & Gegenwart, PRB 82, 064412 (2010); Liu et al, PRB 83, 220403(R) (2011)

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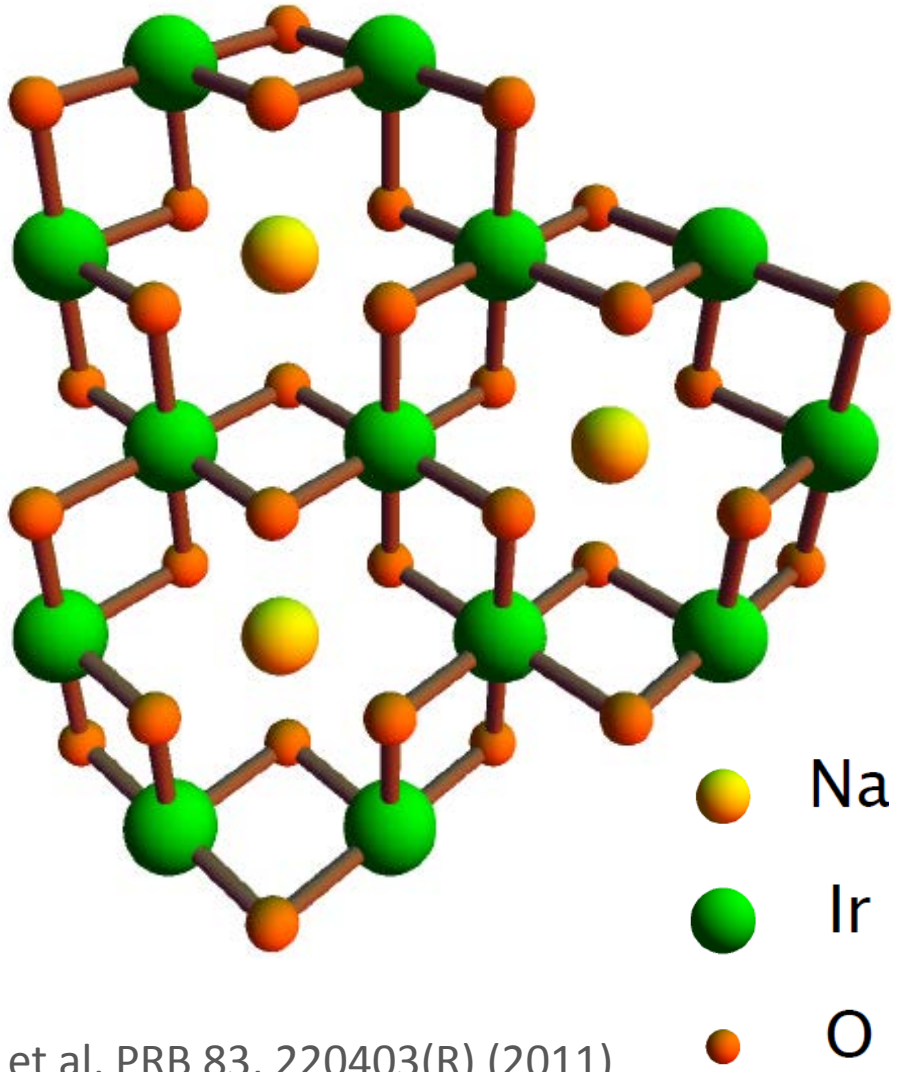

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Magnetic Hamiltonian admits Kitaev exchange

Octahedral coordination

spin-orbit coupling (SOC)

90^o Ir-O-Ir bonds

Ir^{4+} 5d

t_{2g}, e_g

j=1/2, j=3/2

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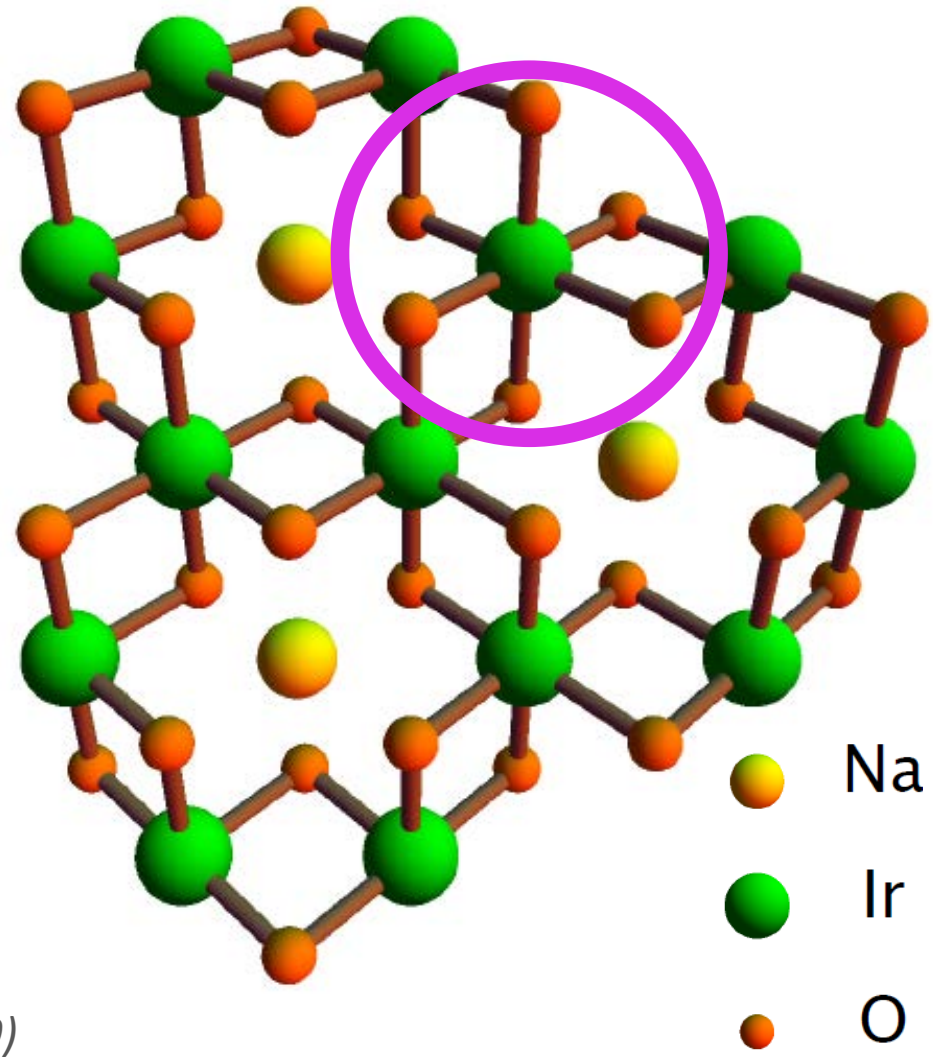

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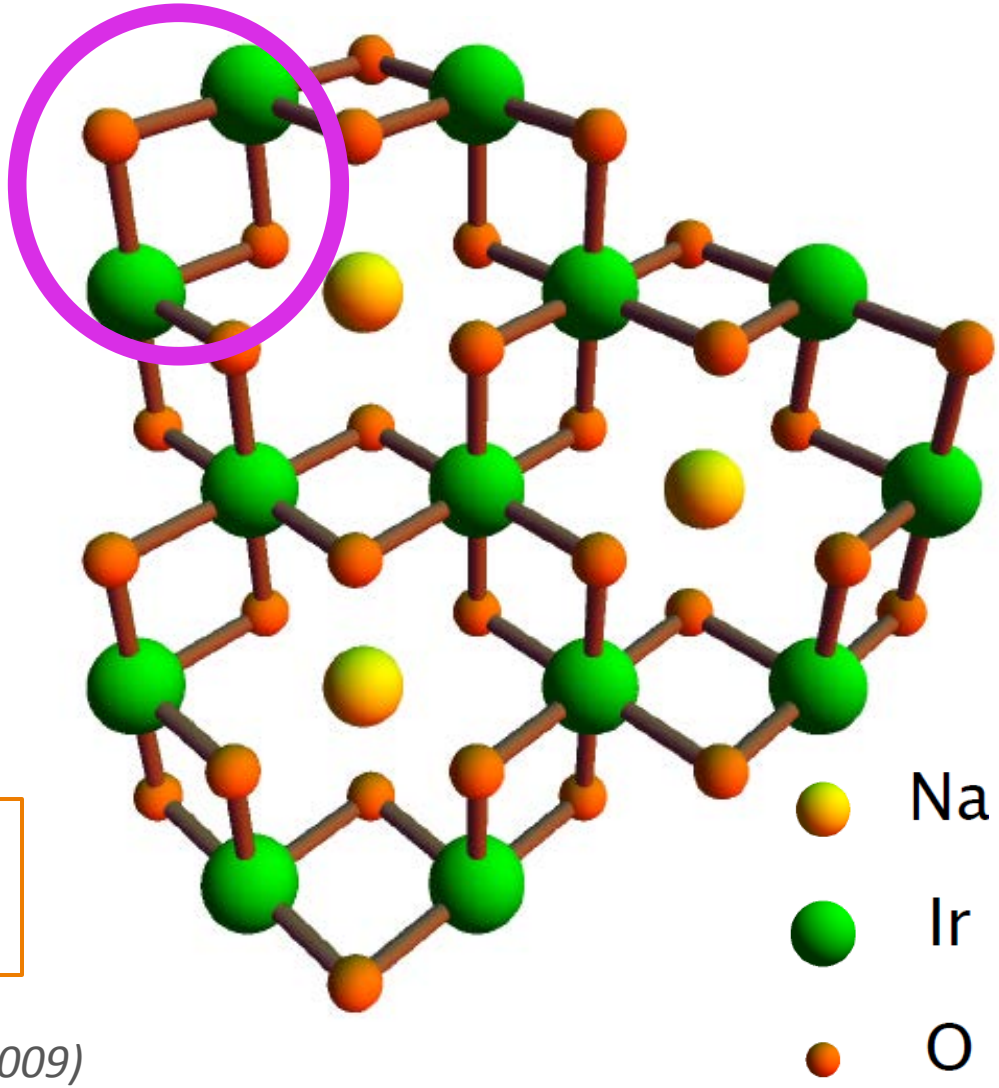

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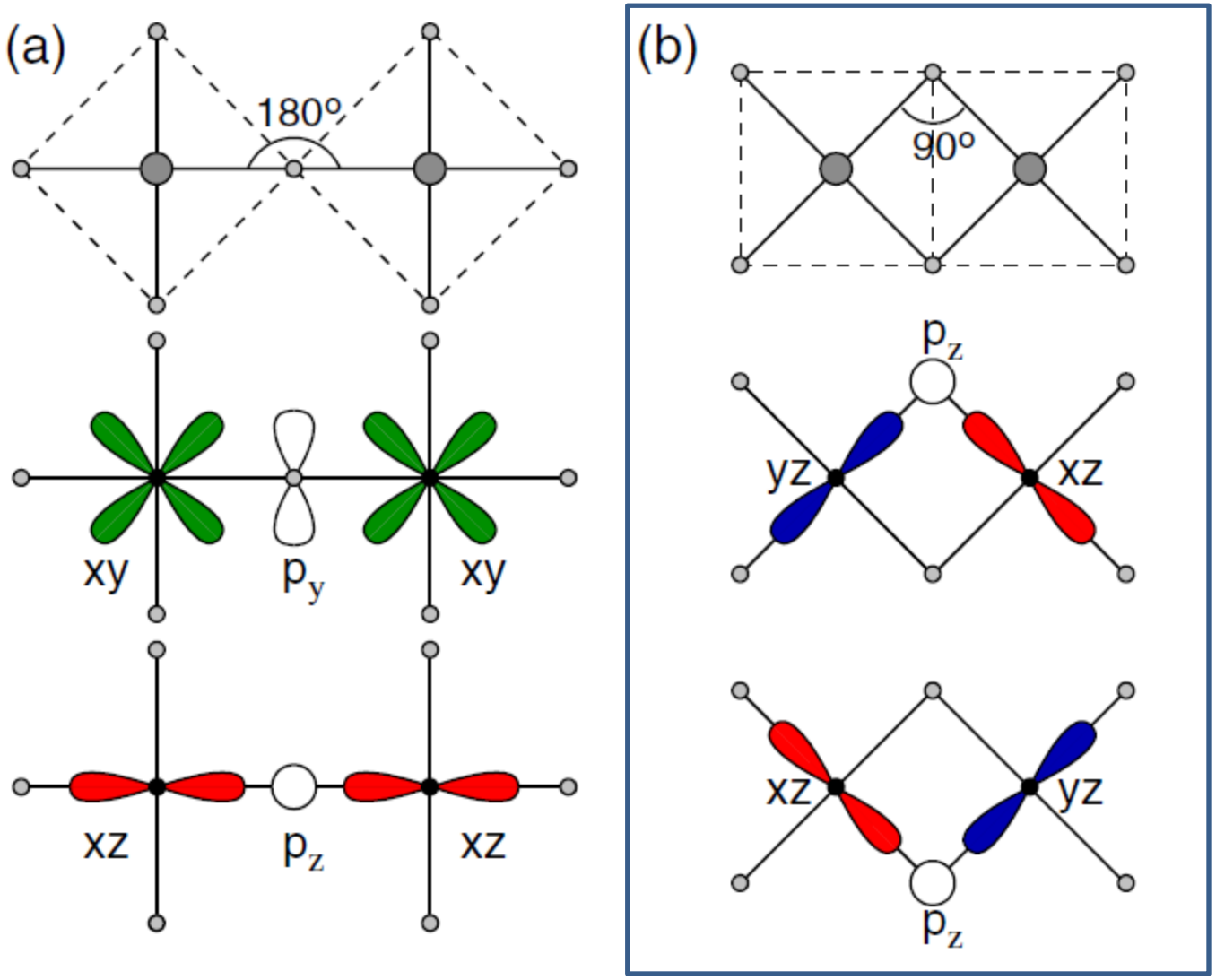

+ j = 1/2

+ Hund's J_H splitting on Ir

→ Kitaev

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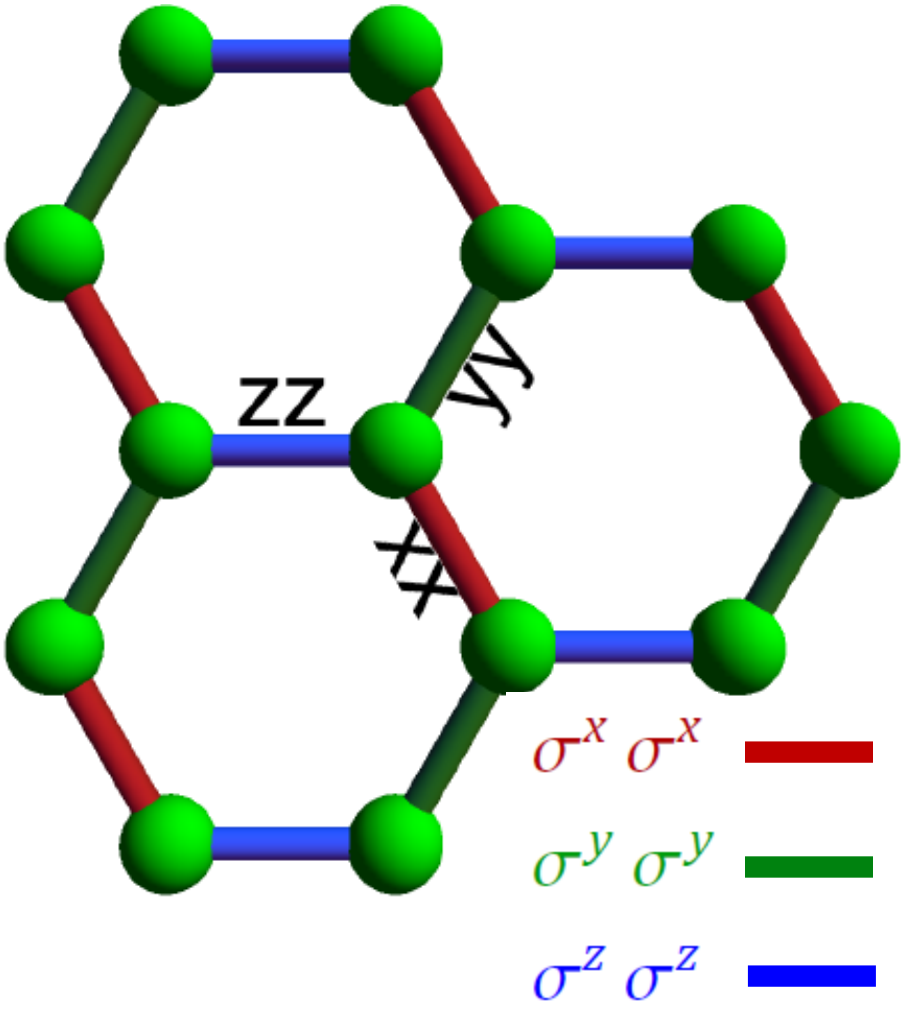

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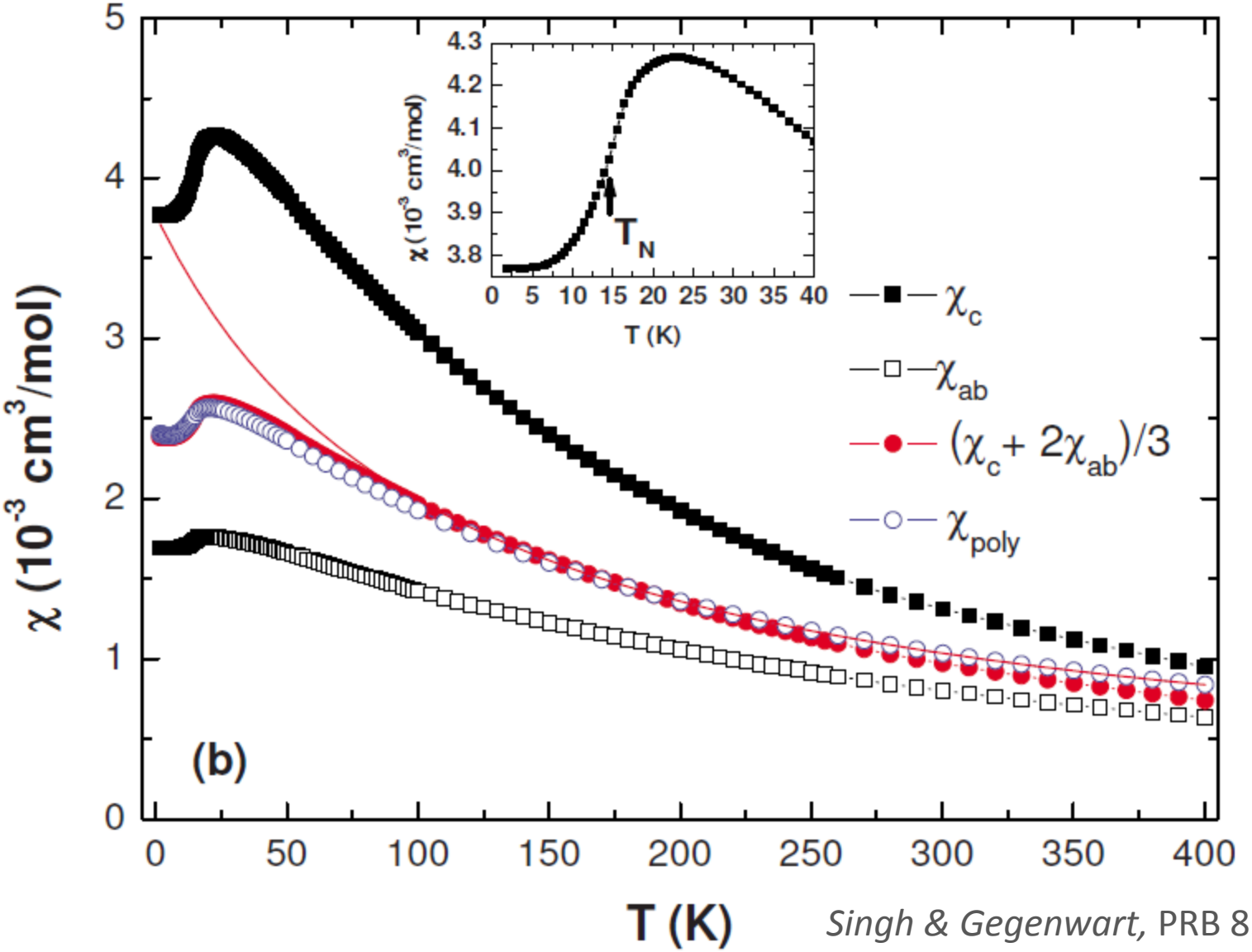
Na_2IrO_3 single crystals: Anisotropic susceptibility $\chi_c \sim 2\,\chi_{ab}$



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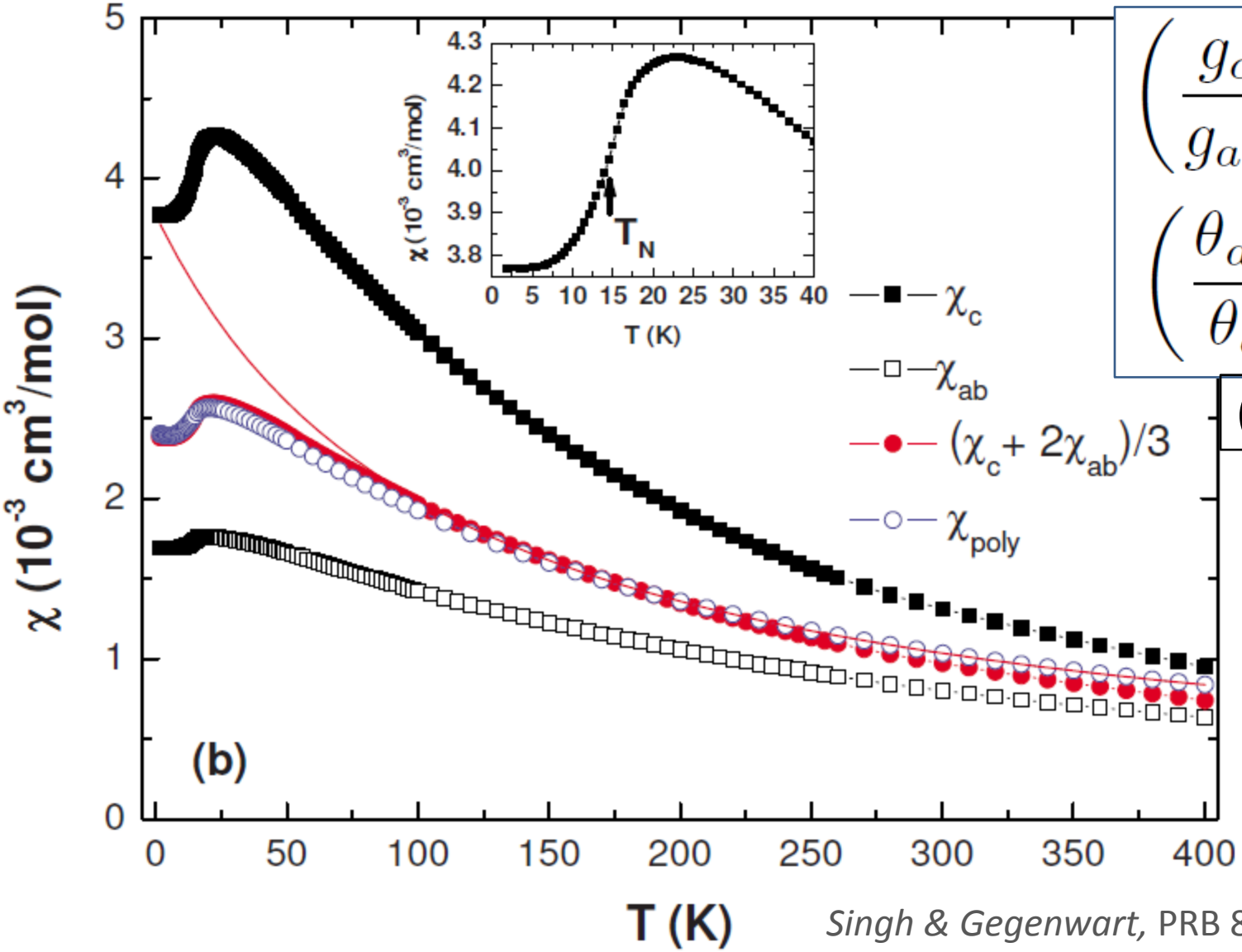


$$\left(\frac{g_c}{g_{ab}}\right)^2 \sim 1.25$$

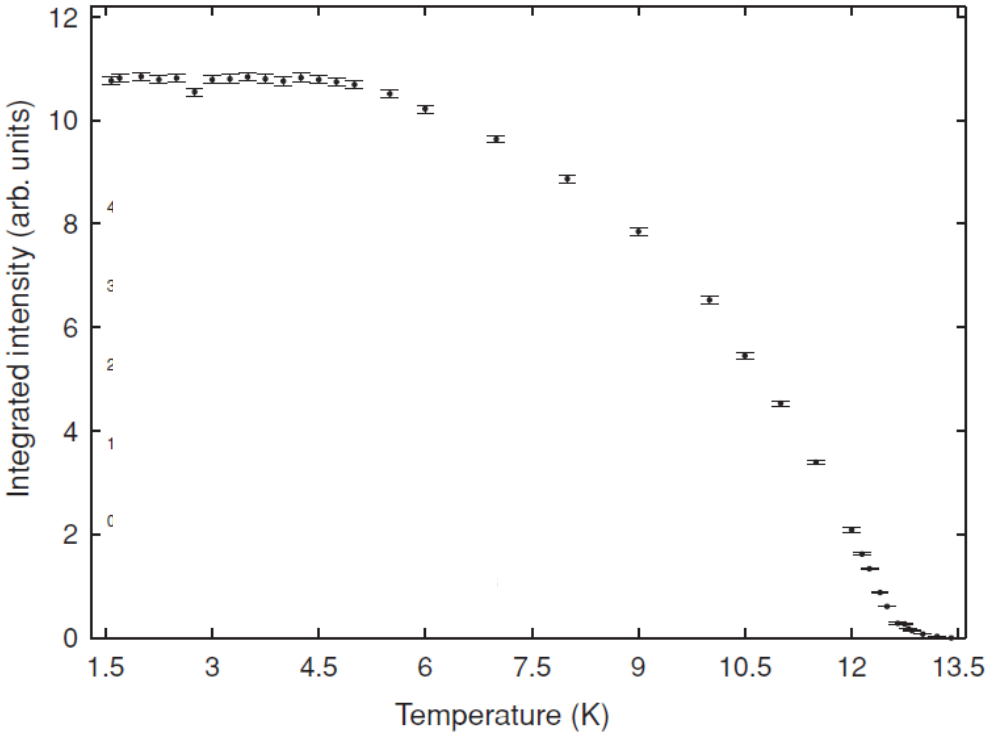
$$\left(\frac{\theta_{ab}}{\theta_c}\right) \sim 1.8$$

(my estimates)

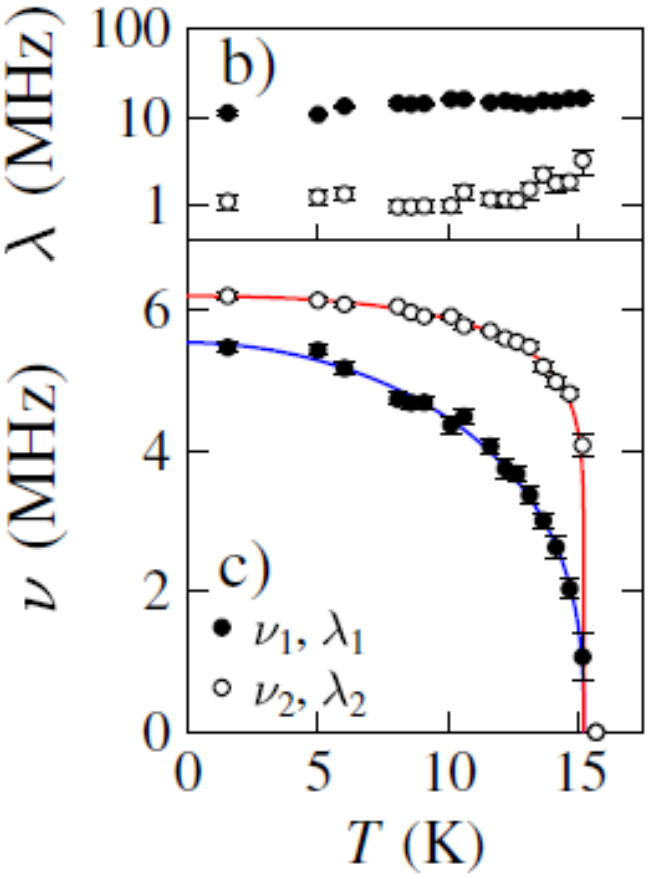
Singh & Gegenwart, PRB 82, 064412 (2010)

Na_2IrO_3 orders at T=15K

X-ray resonant magnetic scattering: *M* wavevector peak



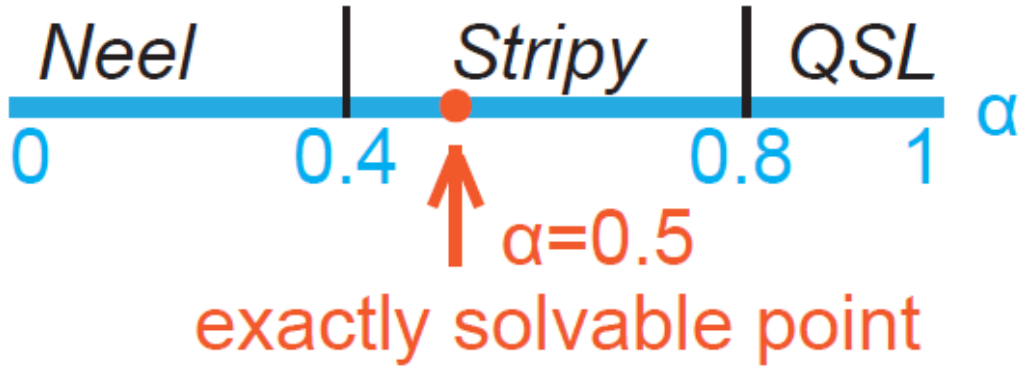
μ^+SR



Liu *et al*, PRB 83, 220403(R) (2011); Choi, Coldea *et al*, PRL 108, 127204 (2012)

Kitaev-Heisenberg model

$$H = (1-\alpha)\,\text{Heisenberg} - 2\,\alpha\,\text{Kitaev}$$



Chaloupka, Jackeli, Khaliullin, PRL 105, 027204 (2010)
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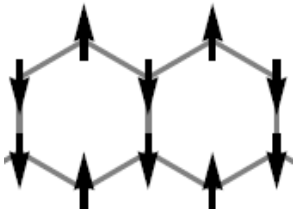
2. *Stripy* AF order, exact at α=1/2:



3. Majorana spin liquid (QSL), exact at α=1

- But cannot capture Na_2IrO_3 *zigzag* AF order

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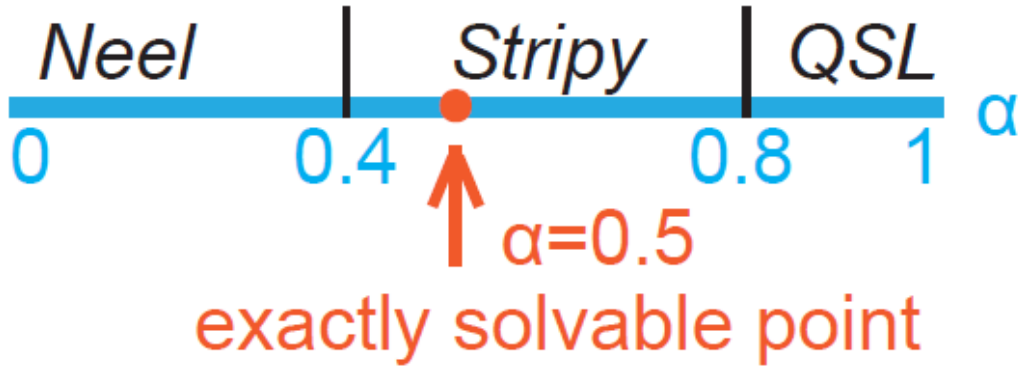

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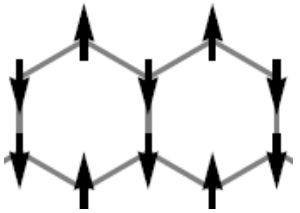

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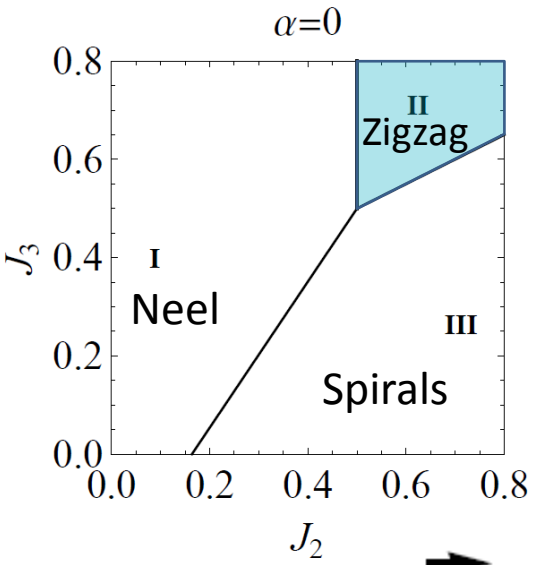
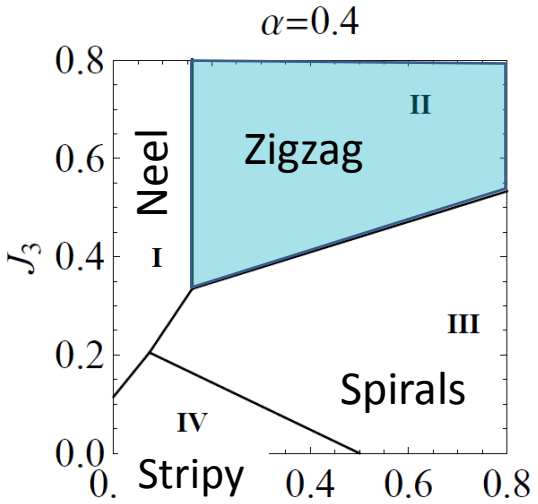
- But cannot capture Na_2IrO_3 *zigzag* AF order

Kitaev exchange + J_2 + J_3 : combined frustration stabilizes observed Na_2IrO_3 *zigzag* order

$$H = J\left[(1-\alpha)\left(\sum_{n.n} + J_2 \sum_{2^{\text{nd}}\, n.} + J_3 \sum_{3^{\text{rd}}\, n.}\right)\text{Heisenberg} \;\; -2\,\alpha\,\text{Kitaev}\right]$$

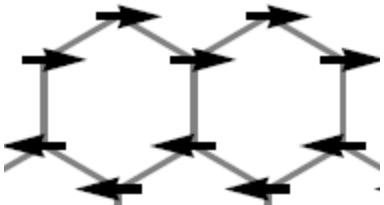


+ Kitaev

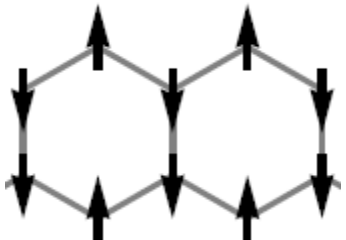


I.K. & Y.Z. You, PRB(**R**)(2011)

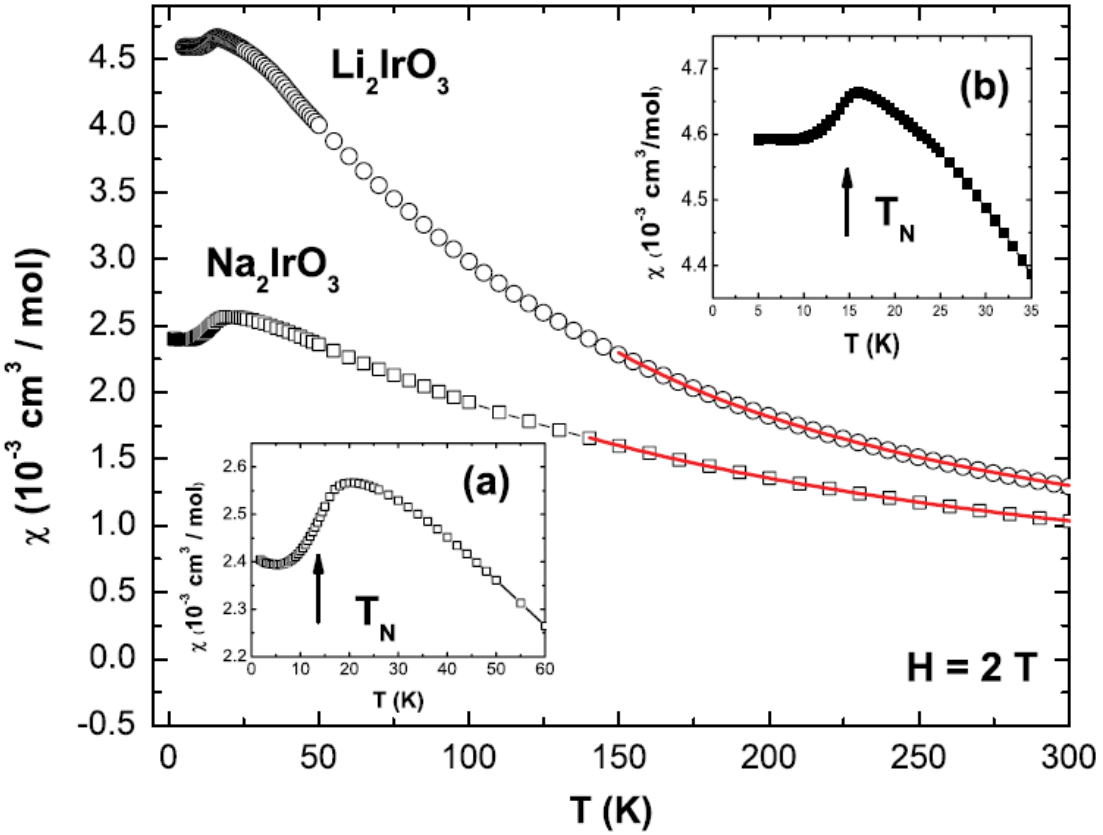
Zigzag:



Stripy:



Check model by fitting A_2IrO_3 susceptibility $\chi(T)$ measured by Singh & Gegenwart to $\chi(T)$ from exact diagonalization of H:



Singh & Gegenwart, *PRB* **82**, 064412 (2010)

Singh *et al*, *PRL* **108**, 127203 (2012)

Using eight or more spin clusters for ED, can fit medium+high temperature $\chi(T)$

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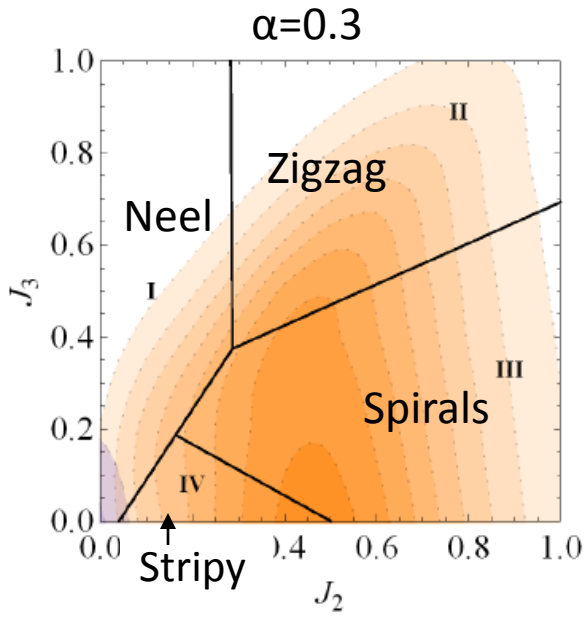
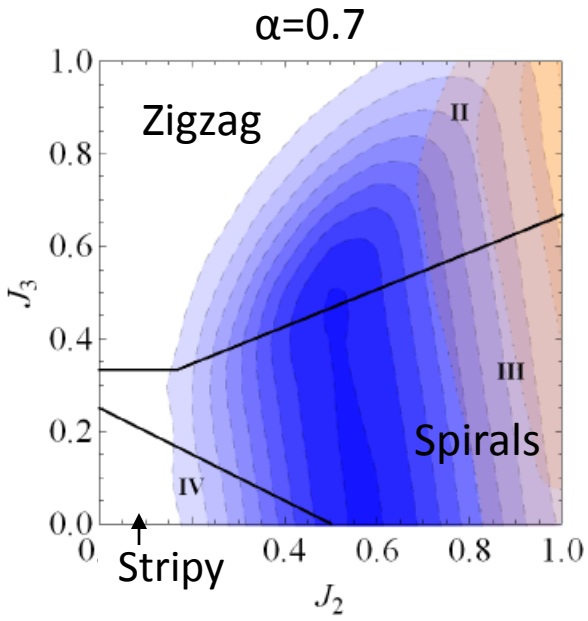




Dark color = good fit:

Na_2IrO_3

Li_2IrO_3

→ **Na, Li** both need **second+third neighbor couplings**

→ **Li** needs substantial **Kitaev exchange**, α≈0.7

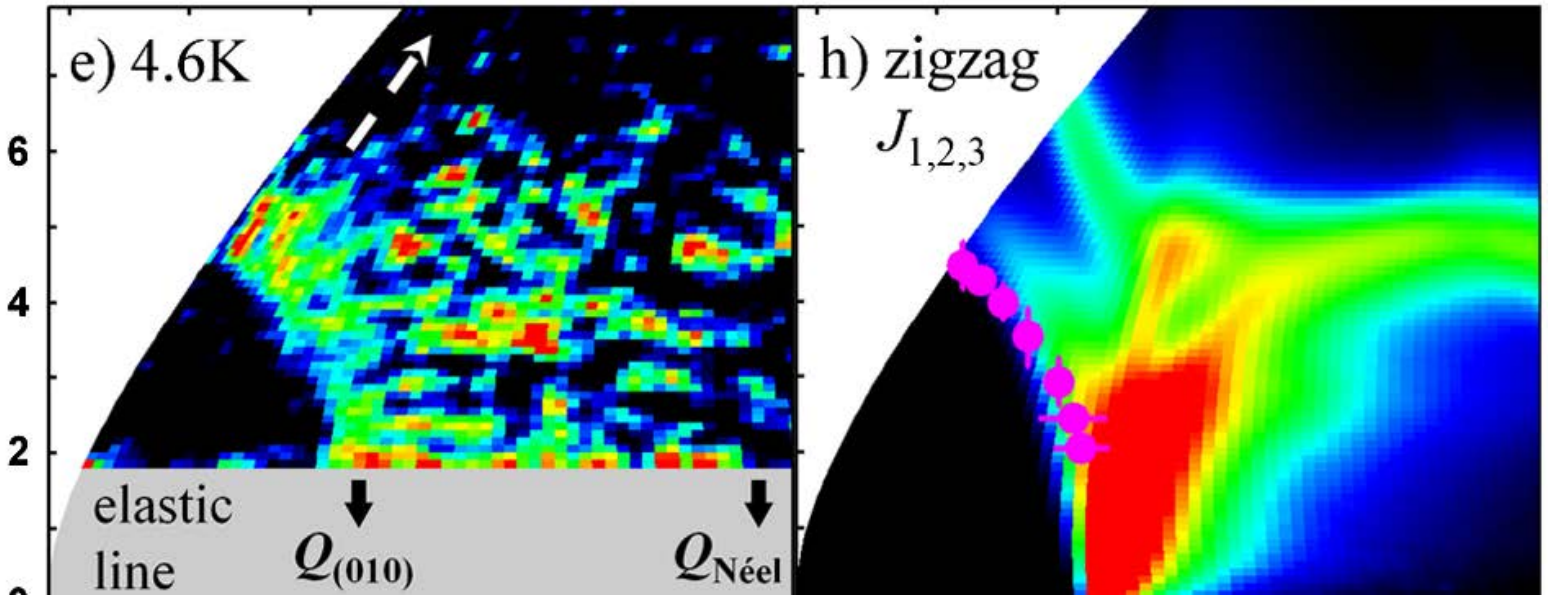
to fit susceptibility for *zigzag* order

I.K. & Y.Z. You, PRB(**R**)(2011)

Singh & Gegenwart, *PR*B (2010); Singh et al, *PRL* (2012).

Recent Na_2IrO_3 neutron scattering

Inelastic NS by Coldea (other work in Oak Ridge)



Consistent with our results:

Kitaev $\alpha \leq 0.4$, large $J_2, J_3 \sim J_1$

Choi, Coldea *et al*, PRL 108, 127204 (2012)

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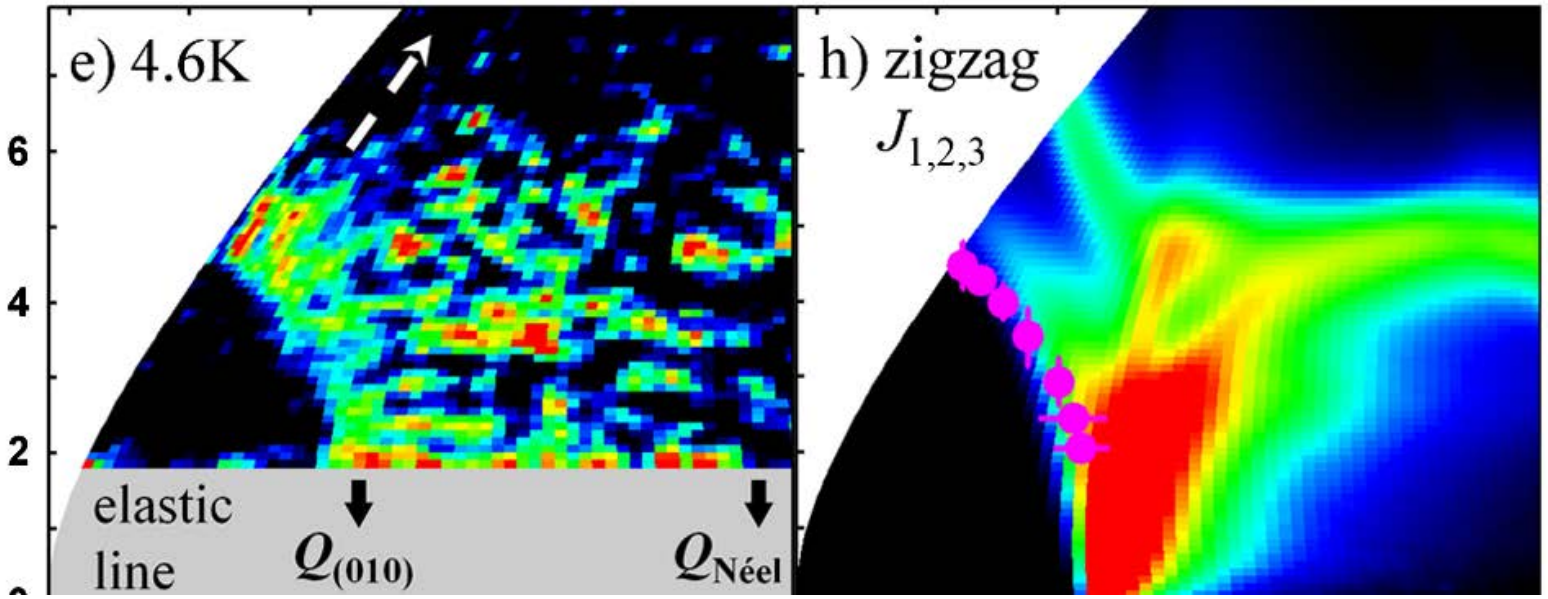

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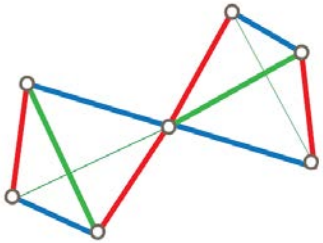
Li_2IrO_3 ?

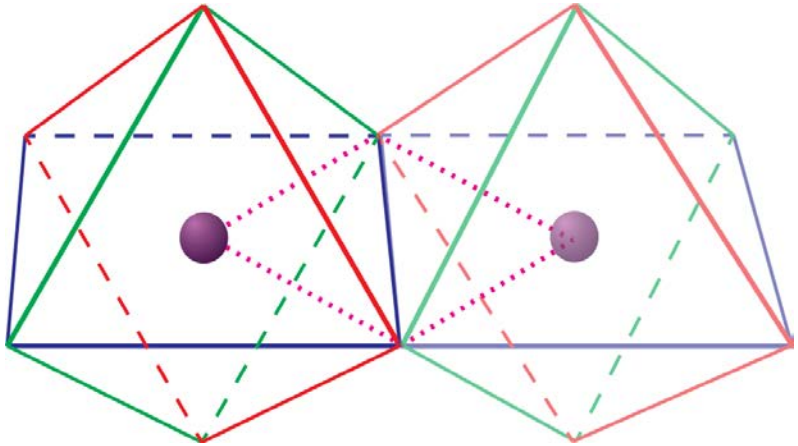
Choi, Coldea *et al*, PRL 108, 127204 (2012)

Kitaev exchange in other geometries

Pyrochlore

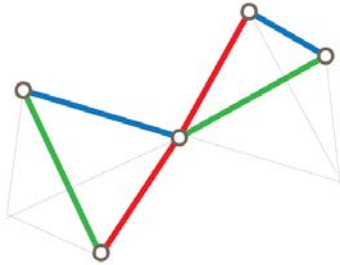
Ir_2O_4





Hyperkagome

$Na_4Ir_3O_8$



Exactly solvable point: AF magnetic order

Schwinger boson MFT finds likely spin liquid

and more! (manuscript in preperation)

Kitaev exchange in other geometries

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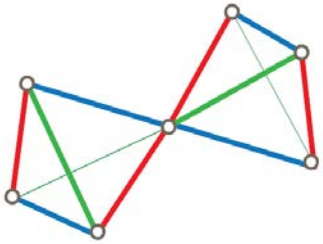

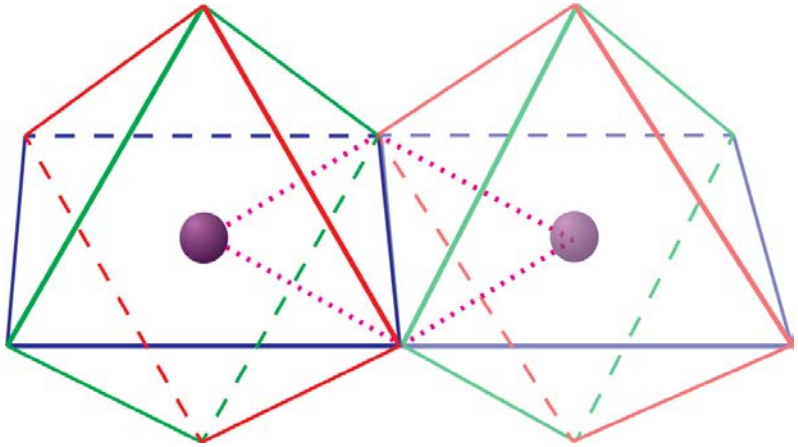

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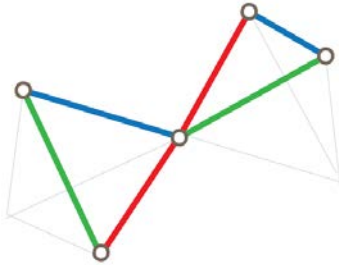

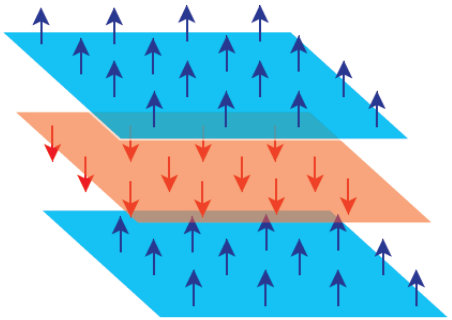

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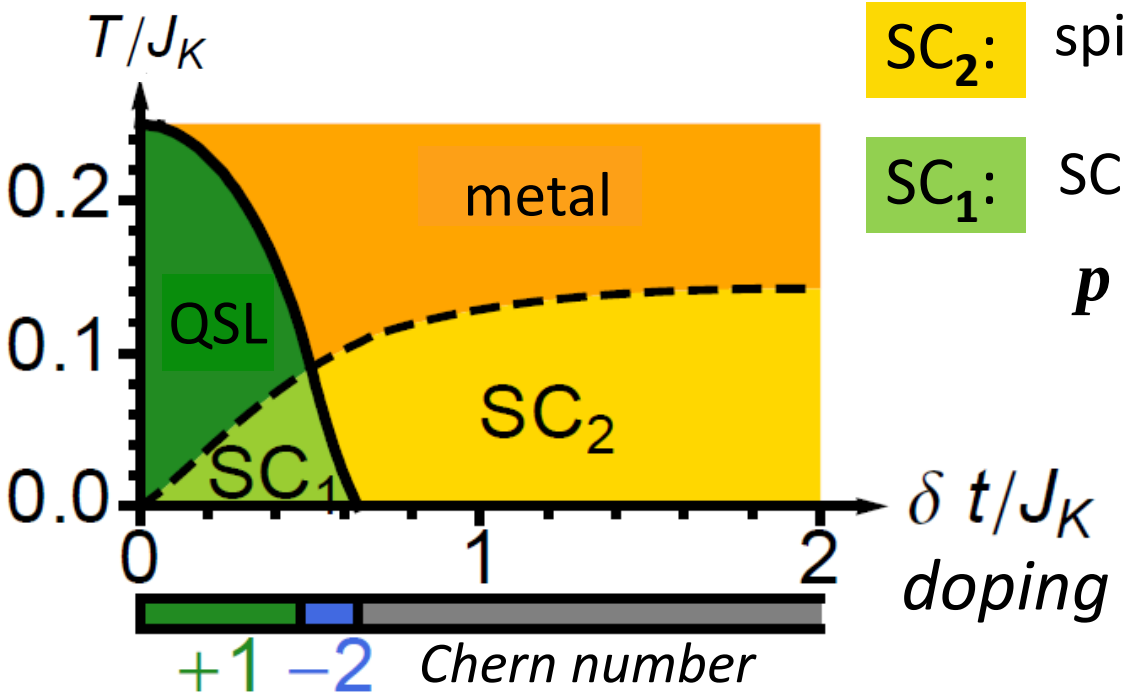
Doping Kitaev spin-liquid -> topological superconductor(s)

***t*-J_K model:** $H = H_{\text{Kitaev}} - t \sum_{\sigma \langle ij \rangle} \mathcal{P} c^{\dagger}_{i\sigma} c_{j\sigma} \mathcal{P}$

SU(2) slave boson mean field, exact at: T=0, doping δ=0



SC_2: spin-triplet BCS

SC_1: SC from spinons; holon BEC

$p + ip$ -> topological (chiral edge modes)

You, IK, Vishwanath
PRB **86**, 085145 (2012)

Outlook: Kitaev-Heisenberg models for iridates

- Honeycomb Kitaev-Heisenberg model with J_2, J_3 is likely realized in Li_2IrO_3 (awaiting more experiments)
- May be relevant for other materials: Ir_2O_4, $Na_4Ir_3O_8$

Work discussed:

- Jackeli & Khaliullin, PRL 102, 017205 (2009)
- Chaloupka, Jackeli, Khaliullin, PRL 105, 027204 (2010)
- Singh & Gegenwart, PRB 82, 064412 (2010)
- Singh *et al*, PRL 108, 127203 (2012)
- Liu *et al*, PRB 83, 220403(R) (2011)
- Choi, Coldea *et al*, PRL 108, 127204 (2012)
- Ye *et al*, PRB 85, 180403(R)(2012)
- IK & You, PRB 84, 180407(R) (2011)
- You, IK, Vishwanath PRB 86, 085145 (2012)