Possible proximity of the Iridates $(Na,Li)_2IrO_3$ to a topologically ordered Mott insulator

Phase diagram of the Heisenberg-Kitaev model

APS March Meeting, Boston 2012

Simon Trebst
University of Cologne

Overview

honeycomb Iridates $(Na,Li)_2IrO_3$

microscopics – Heisenberg-Kitaev model

outlook / a theorist's wishlist

In collaboration with

Hong-Chen Jiang (KITP), Zheng-Chen Gu (KITP), Xiao-Liang Qi (Stanford),
Johannes Reuther (UC Irvine), Ronny Thomale (Stanford)

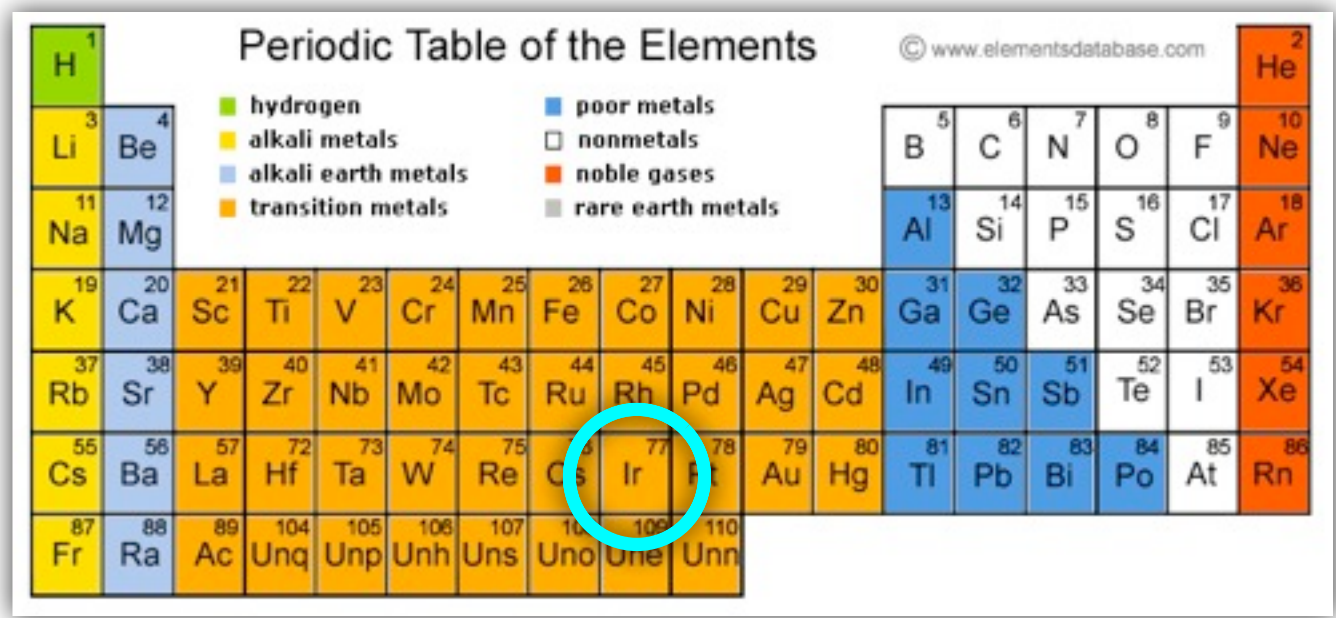
Spin-orbit entanglement

- Spin-orbit coupling has long been considered an afterthought, a relativistic correction.
- Recent years have seen an plethora of novel states that arise solely due to SOC in a variety of underlying electronic states:
  - SOC-driven band inversion → topological insulator
  - SOC in chiral magnet MnSi → skyrmion lattices
  - SOC in Sr_2RuO_4 → p_x+ip_y superconductor
  - This talk: SOC in correlated Mott insulators

Spin-orbit coupling in Mott insulators

Good candidate systems? – 5d transition metal oxides

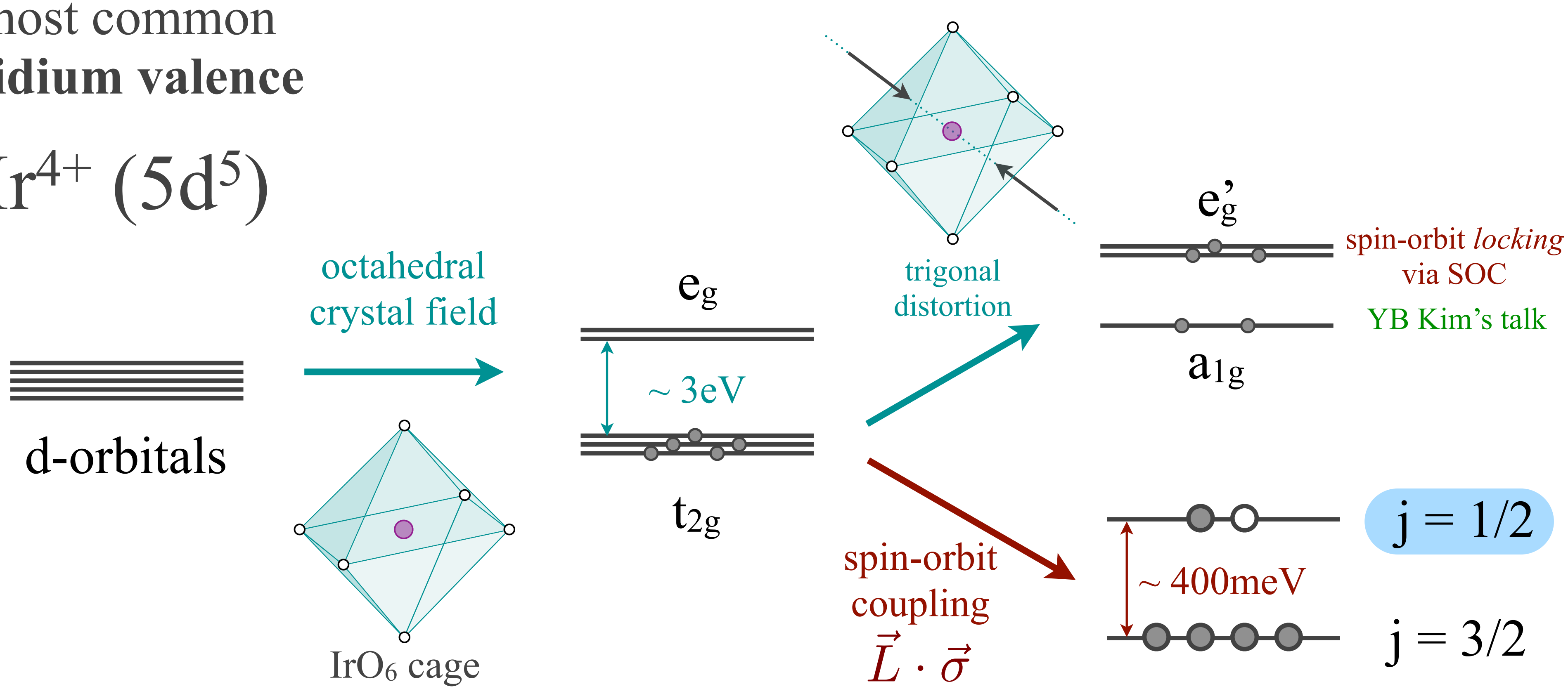
- *strong* spin-orbit coupling
- *weak* Mott insulators
- *enhanced sensitivity* to crystal fields



Spin-orbit entanglement in Iridates

most common
Iridium valence

Ir^{4+} $(5d^5)$



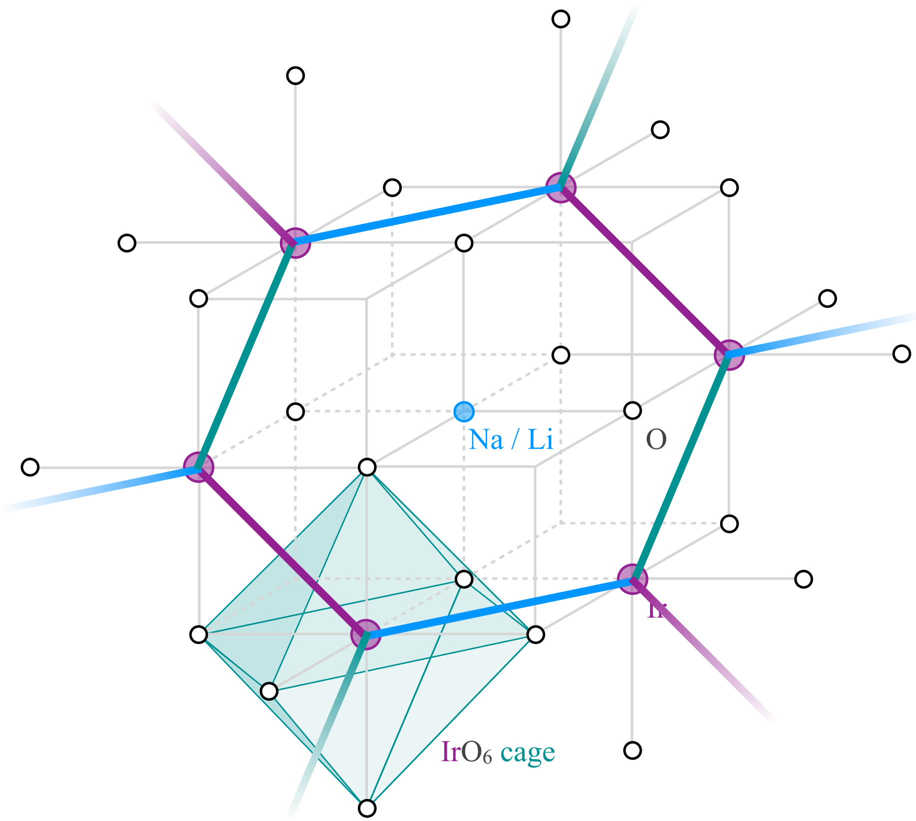
Sr_2IrO_4

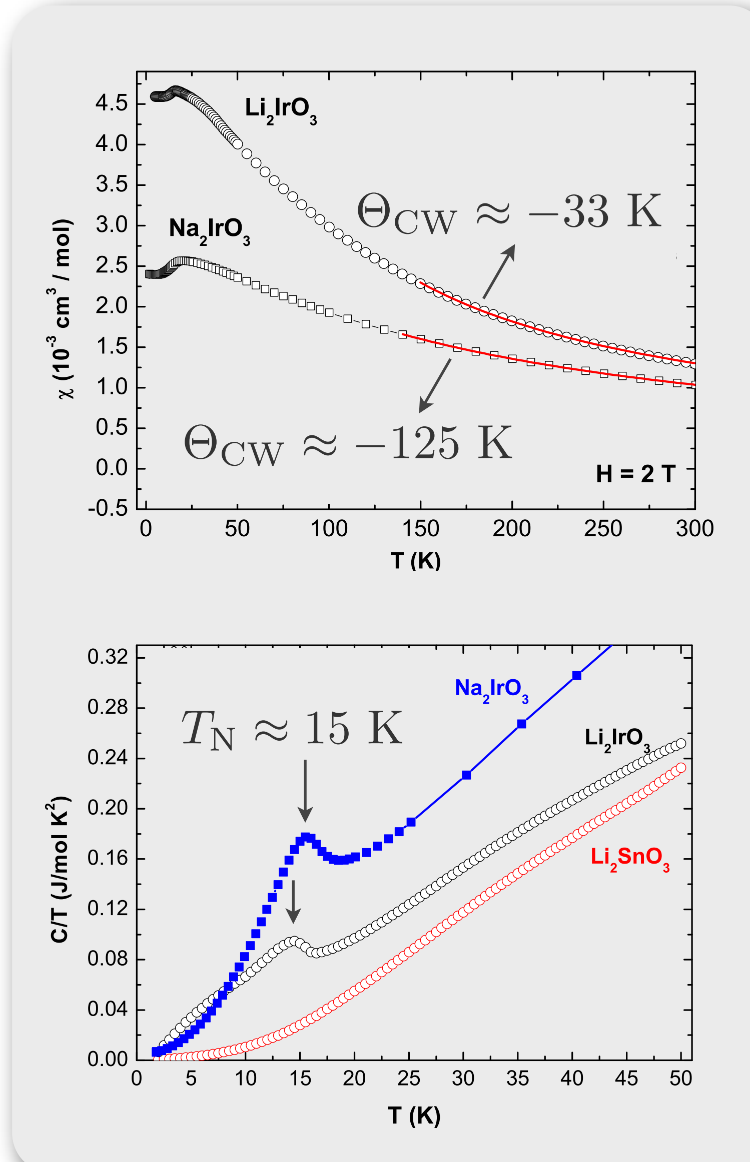
B.J. Kim *et al.* PRL **101**, 076402 (2008)
B.J. Kim *et al.* Science **323**, 1329 (2009)

$(Na,Li)_2IrO_3$?

honeycomb Iridates $(Na,Li)_2IrO_3$

$(Na,Li)_2IrO_3$ – spin-orbit Mott insulators



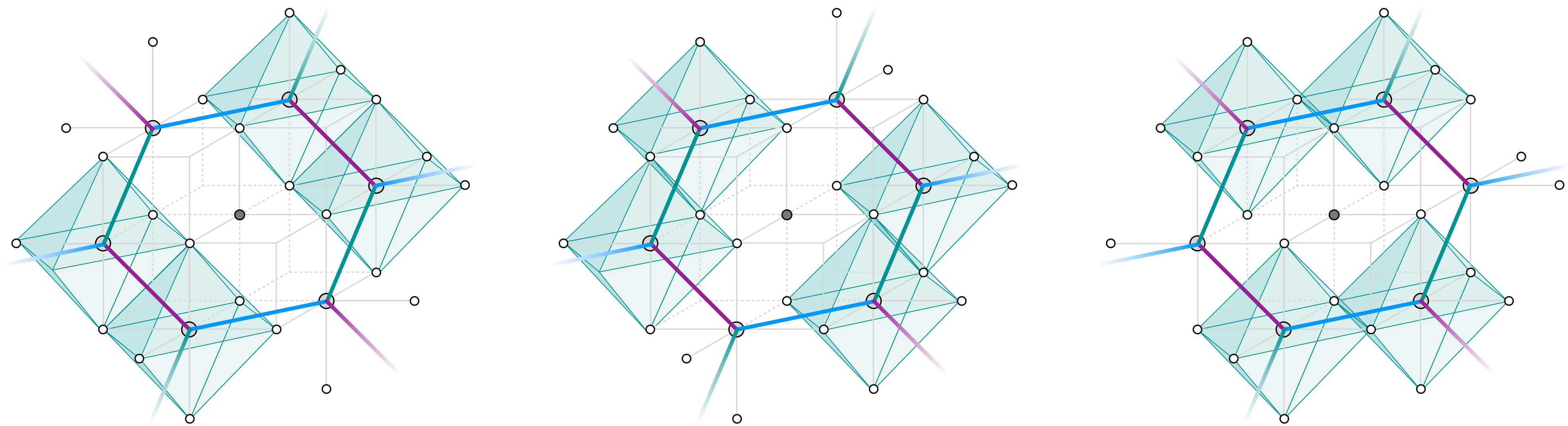


Experiments by Gegenwart group

Na_2IrO_3 $$\frac{|\Theta_{CW}|}{T_N} \approx 8$$

Li_2IrO_3 $$\frac{|\Theta_{CW}|}{T_N} \approx 1.7$$

Microscopic exchange



“x-bonds” “y-bonds” “z-bonds”

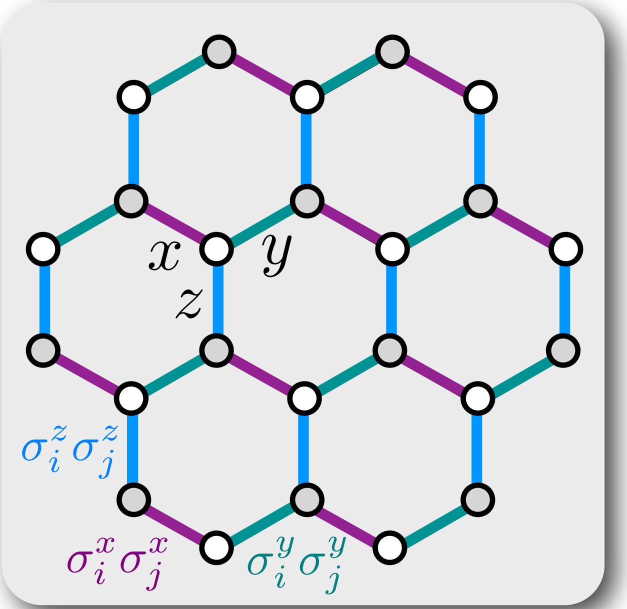
Exchange along all three bonds is mediated via **edge-sharing** IrO_6 octahedra, 90^o Ir-O-Ir path.

Spin-orbit entangled degrees of freedom suggested to interact via **“Heisenberg-Kitaev” model**.

$$H_{\mathrm{HK}} = (1-\alpha)\sum_{\langle i,j\rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - 2\alpha \sum_{\gamma-\mathrm{links}} \sigma_i^\gamma \sigma_j^\gamma$$

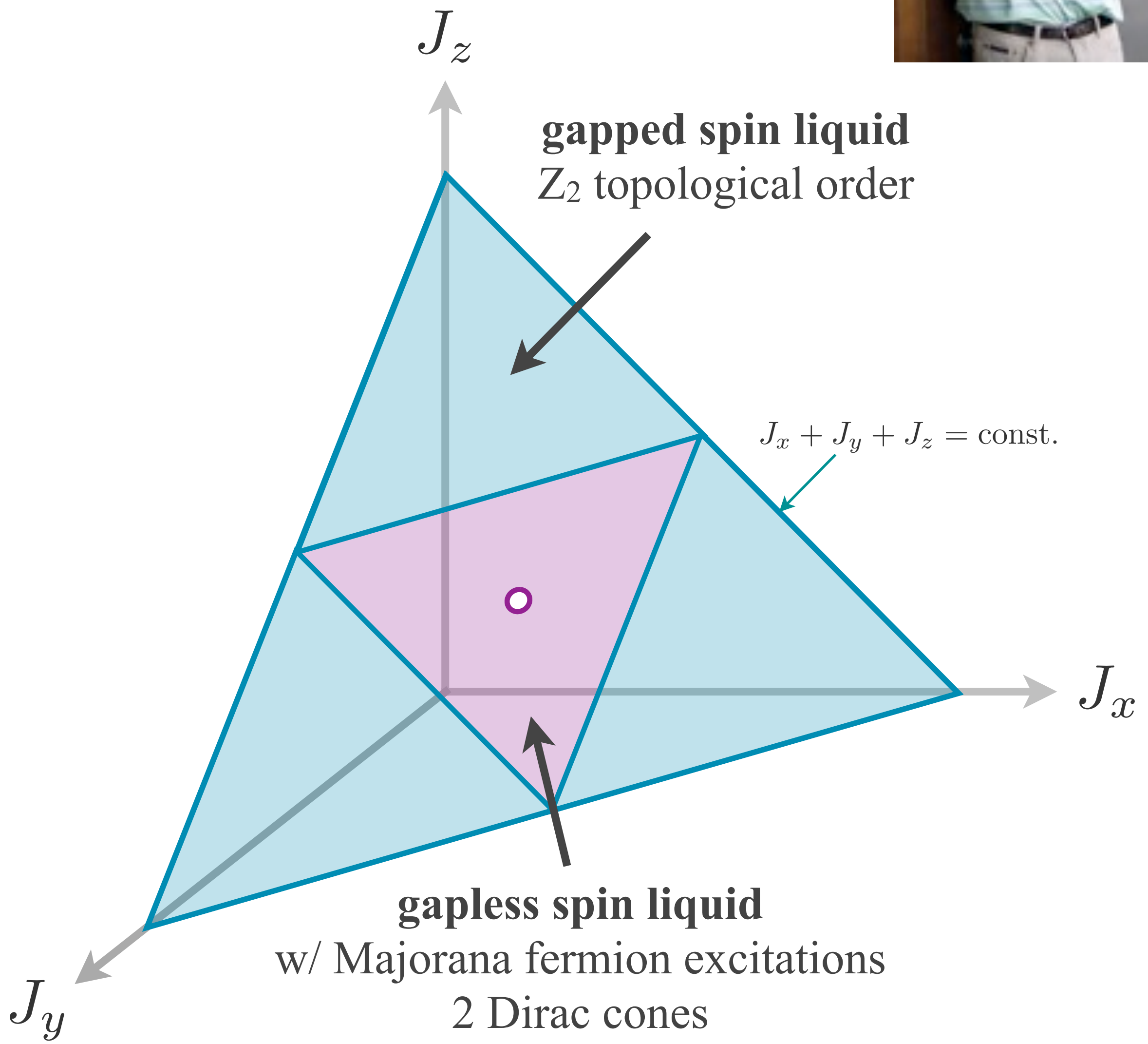
G. Jackeli and G. Khaliullin, PRL **102**, 017205 (2009)
J. Chaloupka, G. Jackeli, and G. Khaliullin, PRL **105**, 027204 (2010)

The Kitaev model



$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma \sigma_i^\gamma \sigma_j^\gamma$$

Rare combination of a model of fundamental conceptual importance and an *exact* analytical solution.

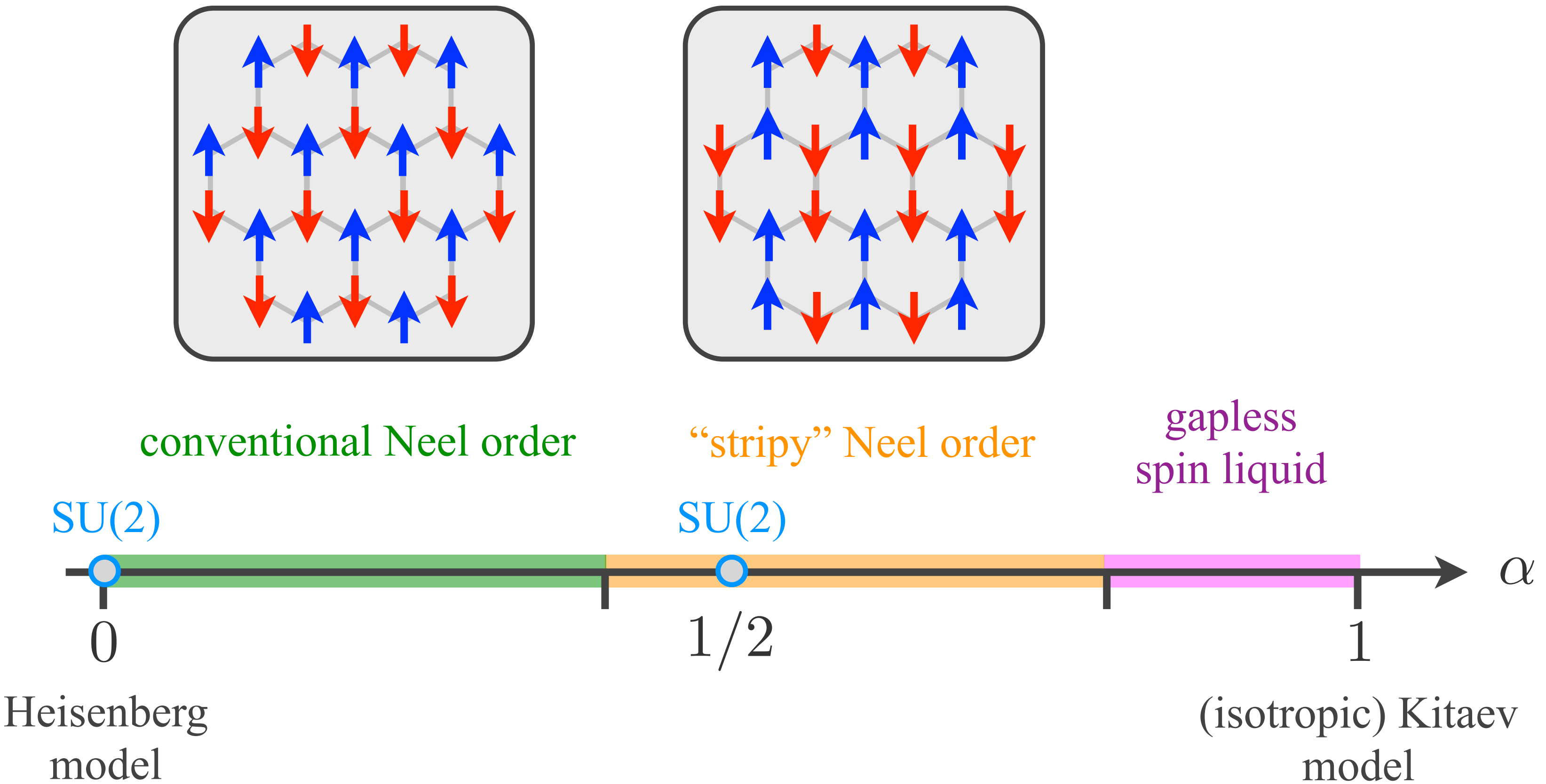


A. Kitaev, Ann. Phys. **321**, 2 (2006)

The Heisenberg-Kitaev model

The zero-temperature phase diagram

$$H_{\mathrm{HK}} = (1-\alpha)\sum_{\langle i,j\rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - 2\alpha \sum_{\gamma-\mathrm{links}} \sigma_i^\gamma \sigma_j^\gamma$$



The Heisenberg-Kitaev model

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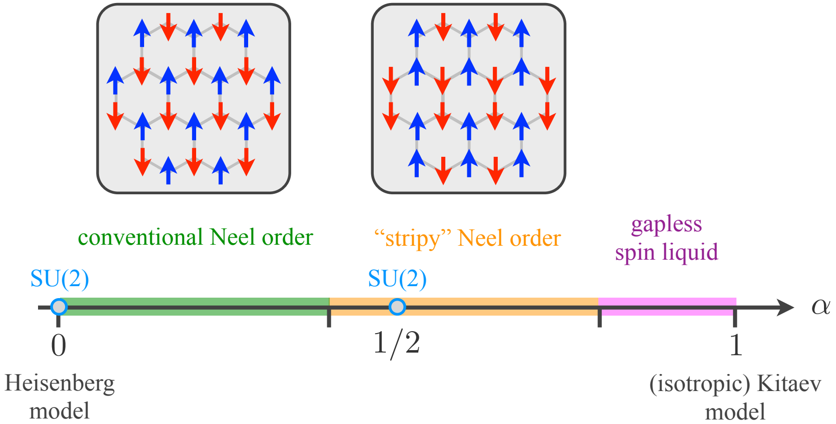


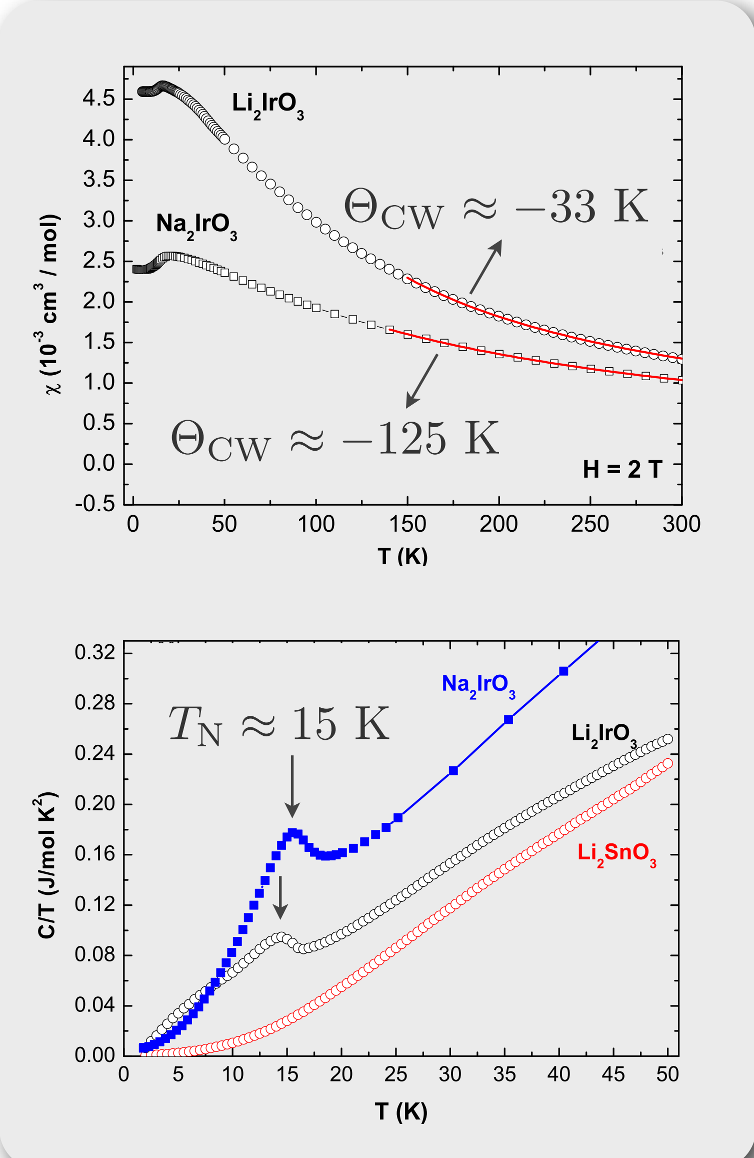
Open questions

T=0: Does this model reproduce the experimentally observed magnetic ordering?

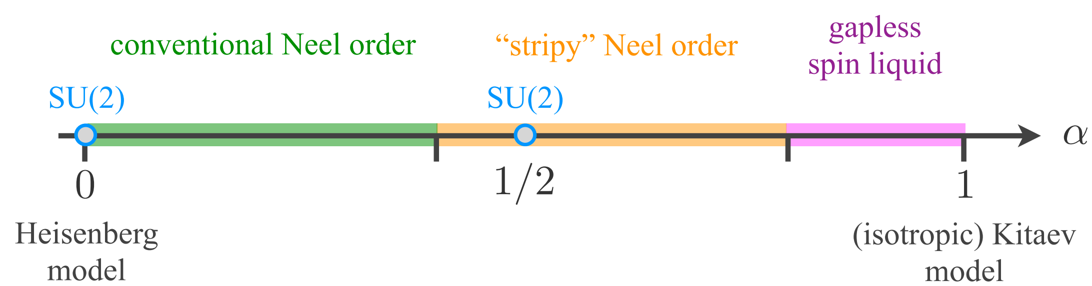
Finite T: Can we explain thermodynamic properties such as the ratio of Curie-Weiss and ordering temperature?

Magnetic field: How close are the experimental systems to even more exotic, topologically ordered ground states?

Thermodynamic properties



$$H_{HK} = (1-\alpha)\sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - 2\alpha \sum_{\gamma-\text{links}} \sigma_i^\gamma \sigma_j^\gamma$$



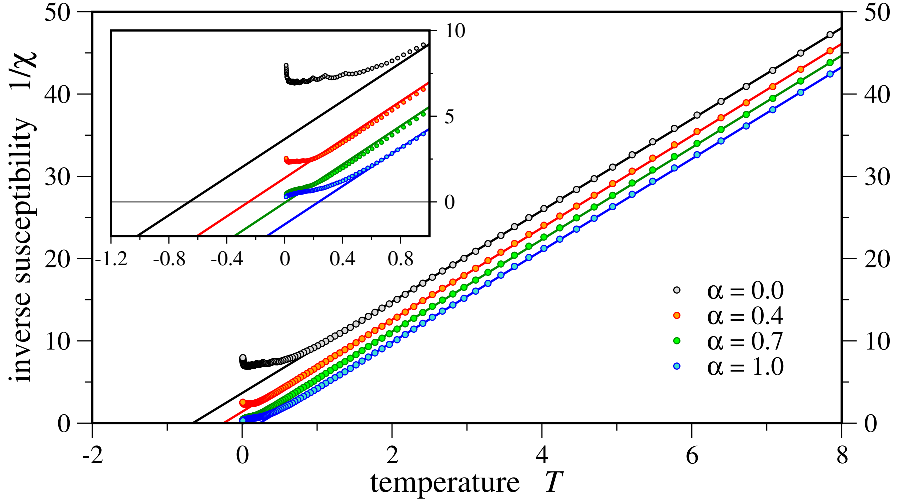
Our approach: functional renormalization group
We access finite-temperature physics by identifying the RG flow parameter with a temperature scale.

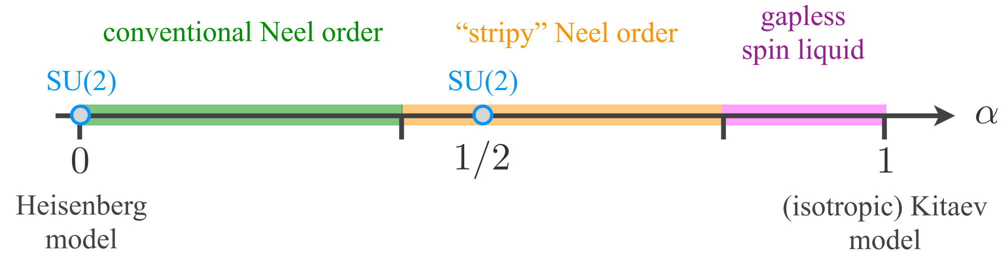
For details of this approach:
talk by Johannes Reuther Z8.00011
Friday afternoon 1:15pm

Thermodynamic properties

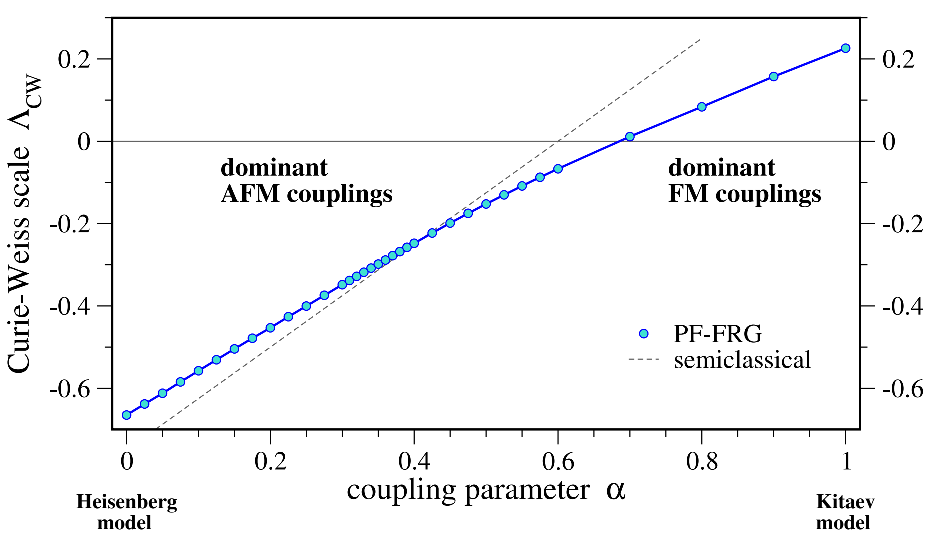
J. Reuther, R. Thomale, ST, PRB **84**, 100406(R) (2011).

$$H_{\mathrm{HK}} = (1-\alpha)\sum_{\langle i,j\rangle}\vec{\sigma}_i\cdot\vec{\sigma}_j - 2\alpha\sum_{\gamma-\mathrm{links}}\sigma_i^\gamma\sigma_j^\gamma$$





increasing frustration?



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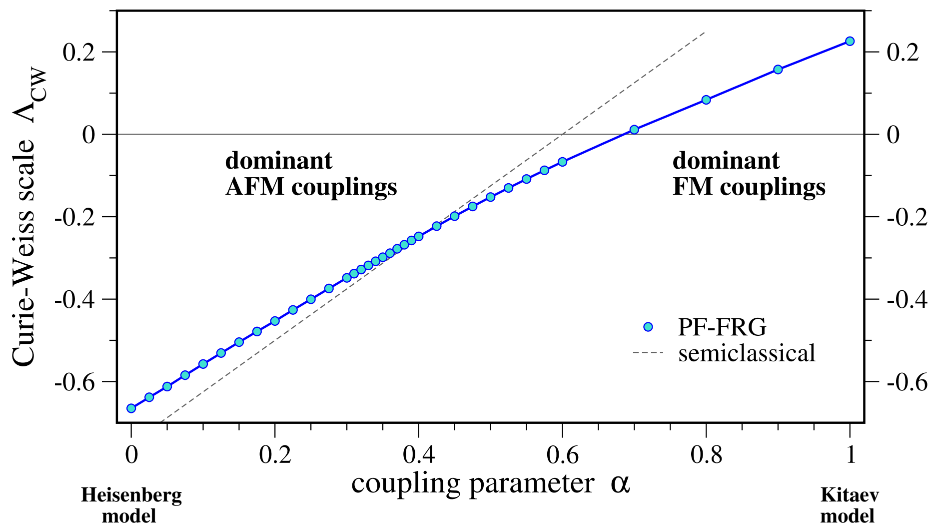
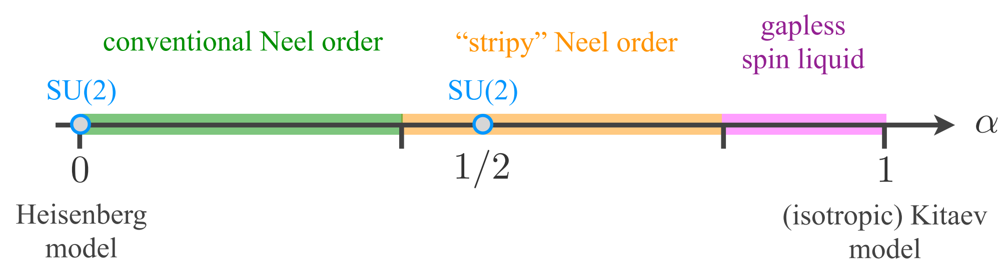
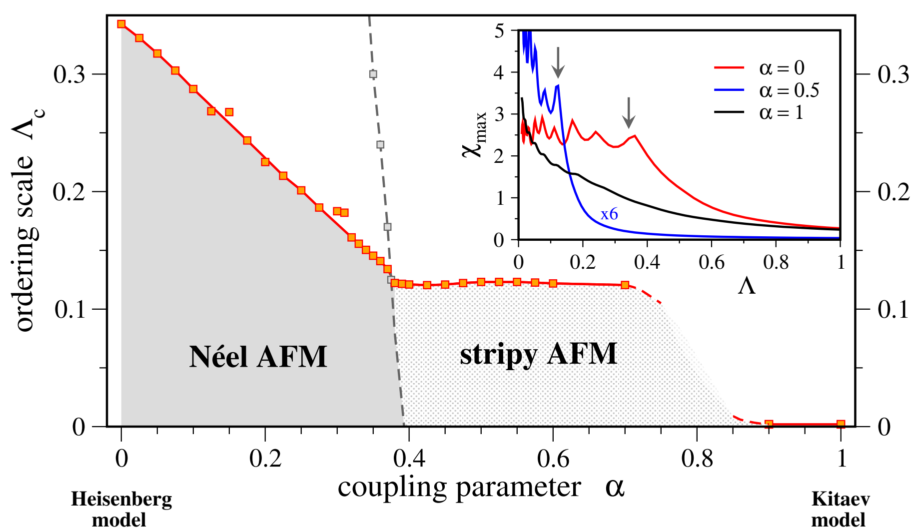
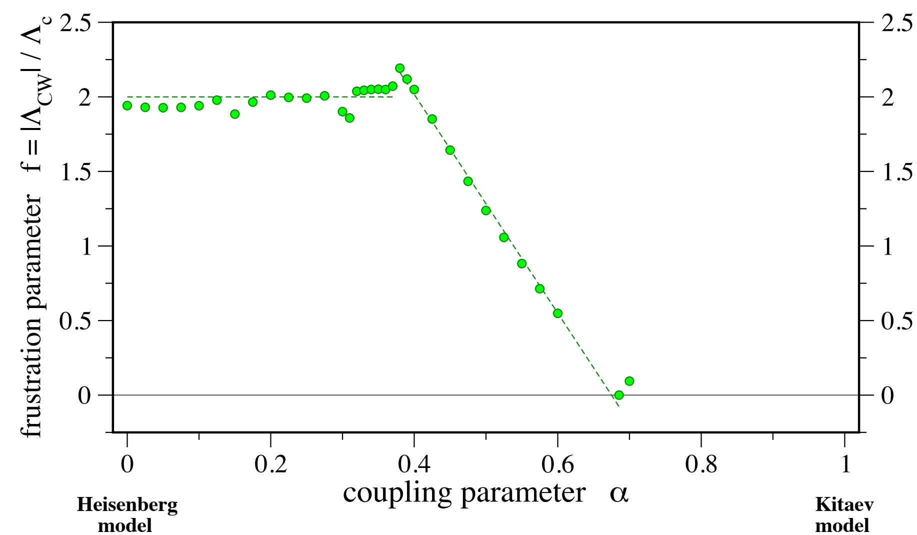




increasing frustration? **No!**

We need another mechanism to introduce frustration.

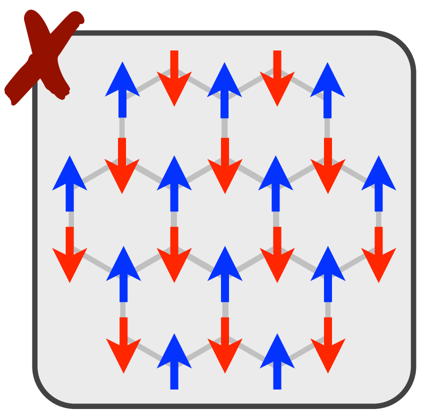




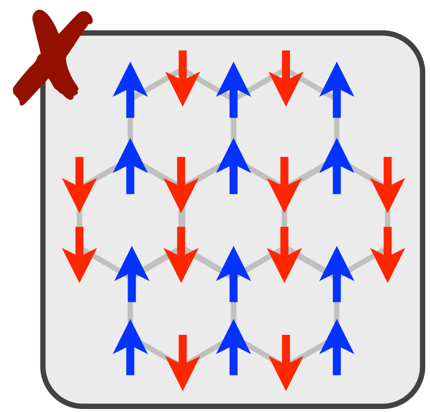
Magnetic order in experiments

X-ray and inelastic neutron scattering experiments on Na_2IrO_3 indicate **zig-zag** magnetic order.

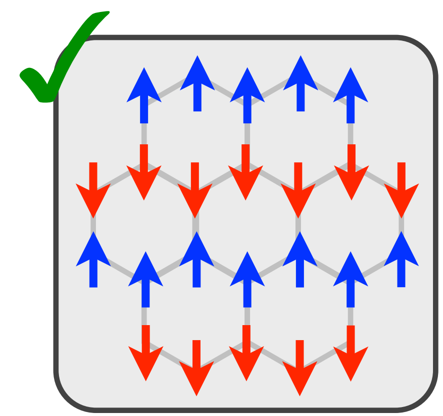
X. Liu *et al.*, PRB **83**, 220403(R) (2011)
S.K.Choi *et al.*, arXiv:1202.1268 (2012)
Y. Feng *et al.*, arXiv:1202.3995 (2012)



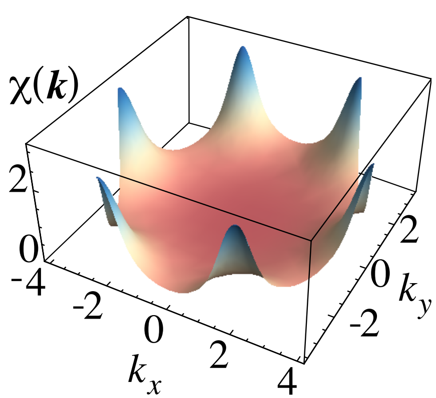
conventional Neel order

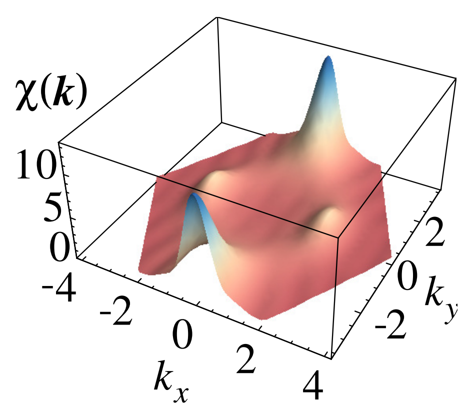


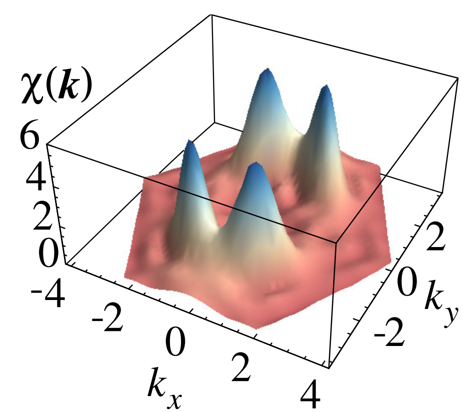
“stripy” order



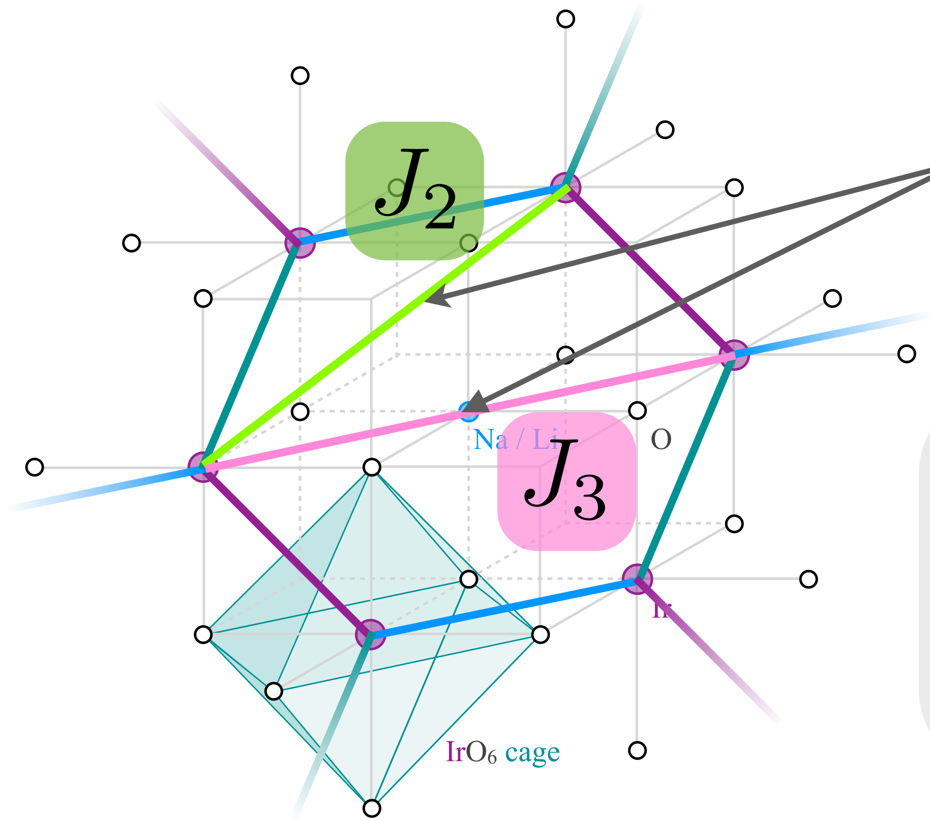
“zig-zag” order







Geometric frustration



Introduce **geometric frustration** by including next-nearest and 3rd-nearest neighbor interactions.

$$(1-\alpha)\left(\sum_{\langle ij\rangle} + J_2 \sum_{\langle\langle i,j\rangle\rangle} + J_3 \sum_{\langle\langle\langle i,j\rangle\rangle\rangle}\right) \vec{\sigma}_i \cdot \vec{\sigma}_j$$
$$-2\alpha \sum_{\gamma} \sigma_i^\gamma \sigma_j^\gamma$$

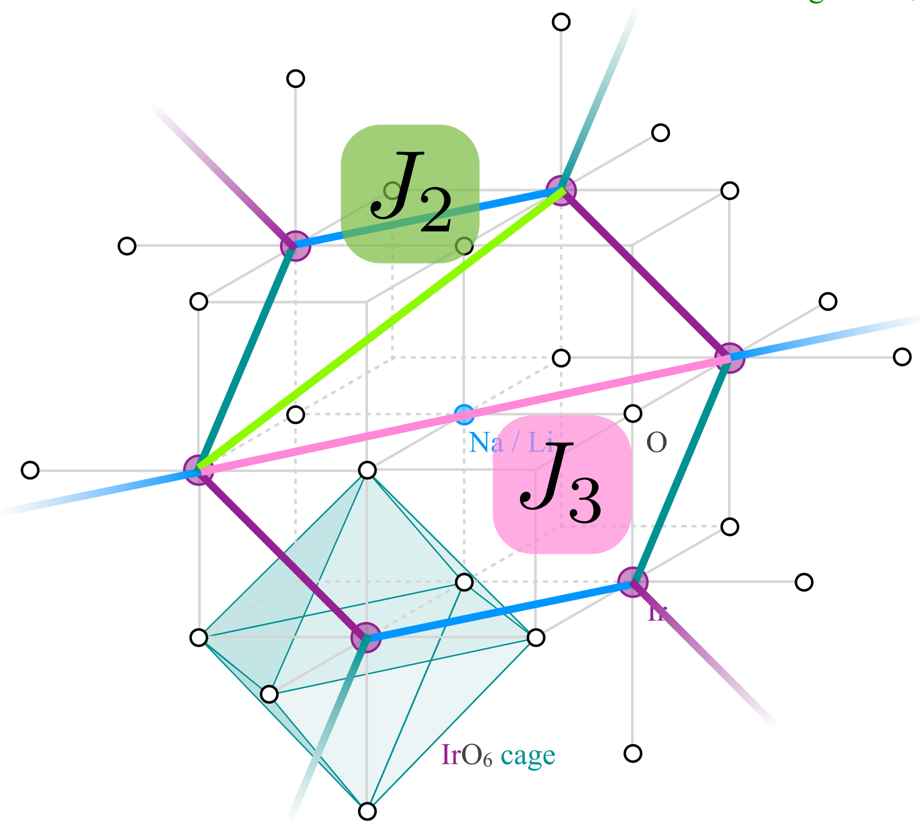
I. Kimchi and Y.-Z. You, PRB **84**, 180407(R) (2011)

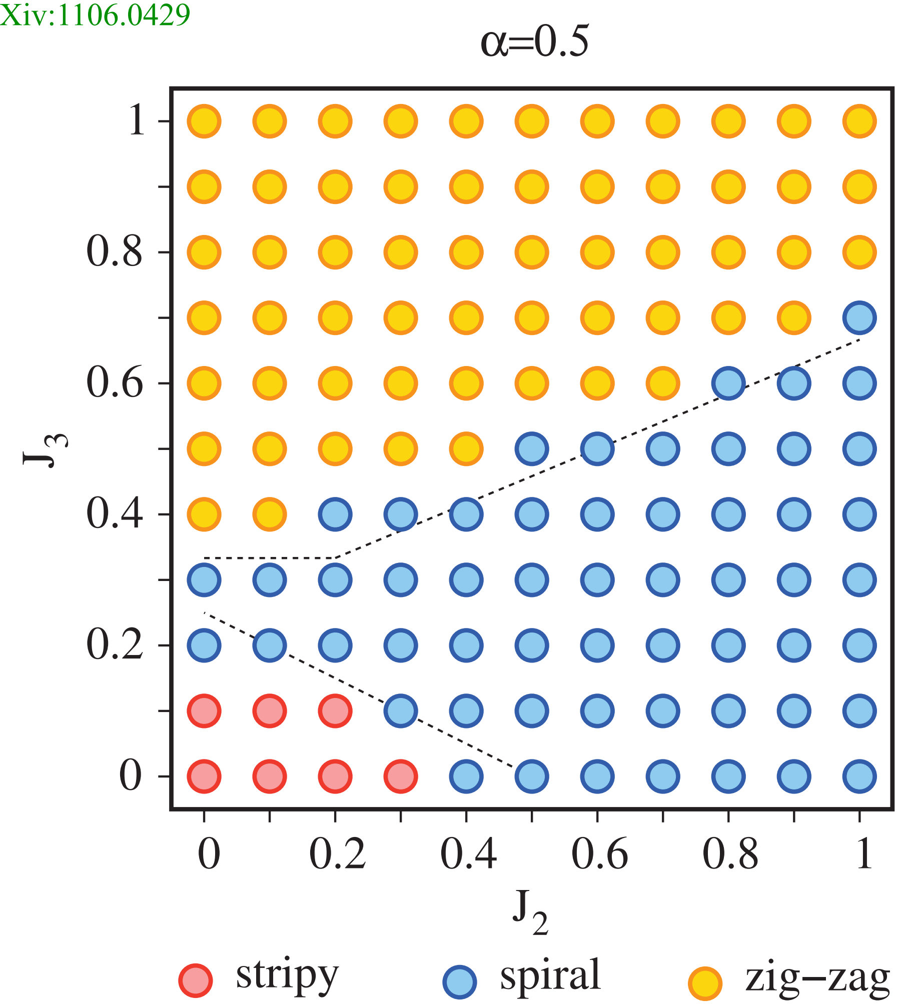
The next-nearest neighbor coupling J_2 destabilizes the Neel state in favor of **spin spiral** states.

The 3rd-nearest neighbor coupling J_3 indeed favors **zig-zag** magnetic order.

Geometric frustration

Y. Singh *et al.*, arXiv:1106.0429





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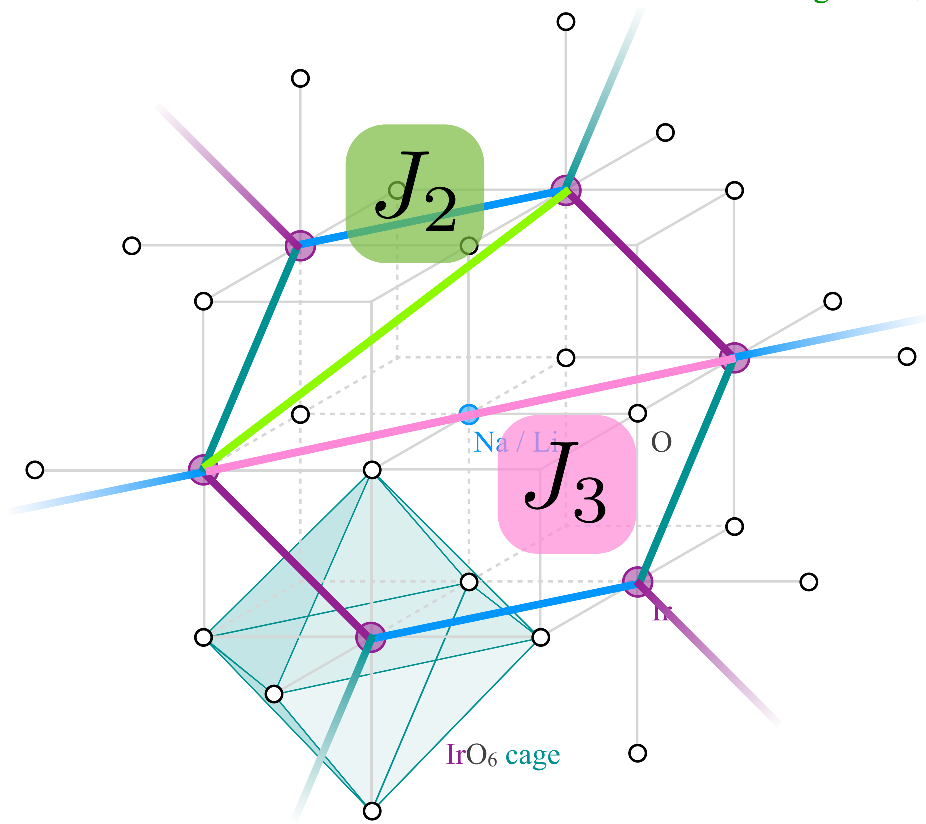

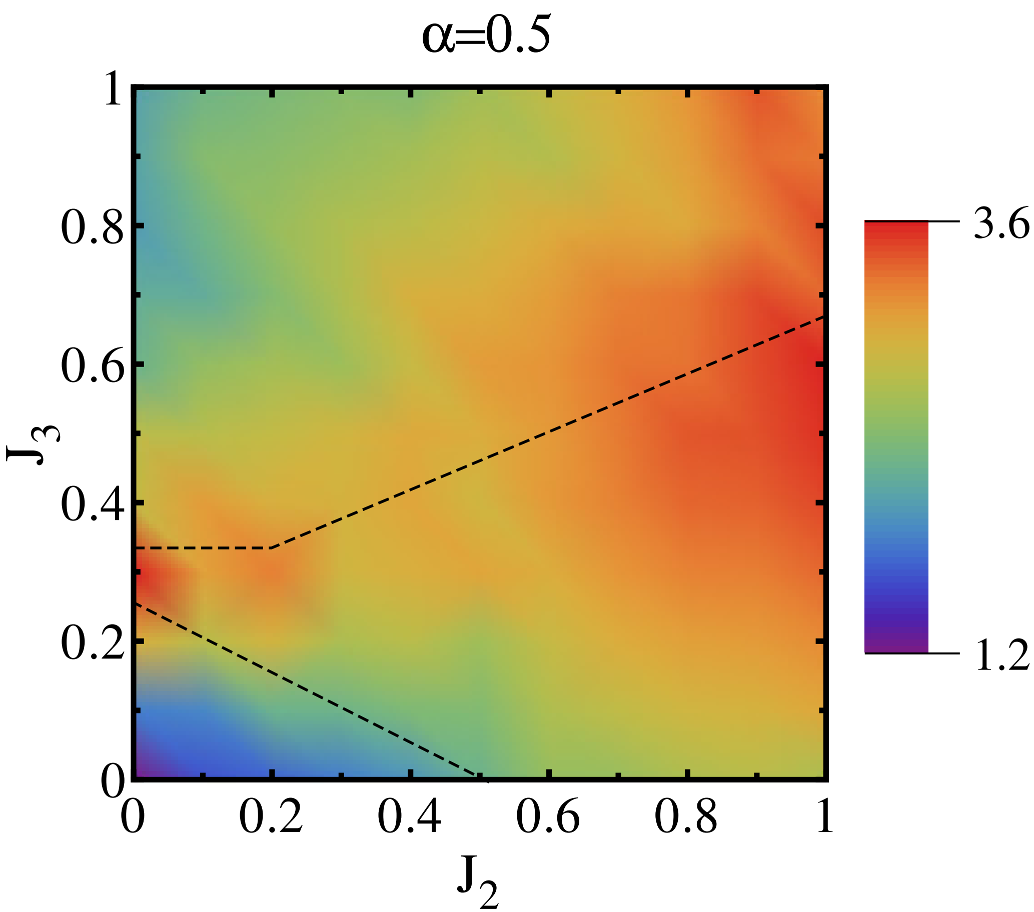

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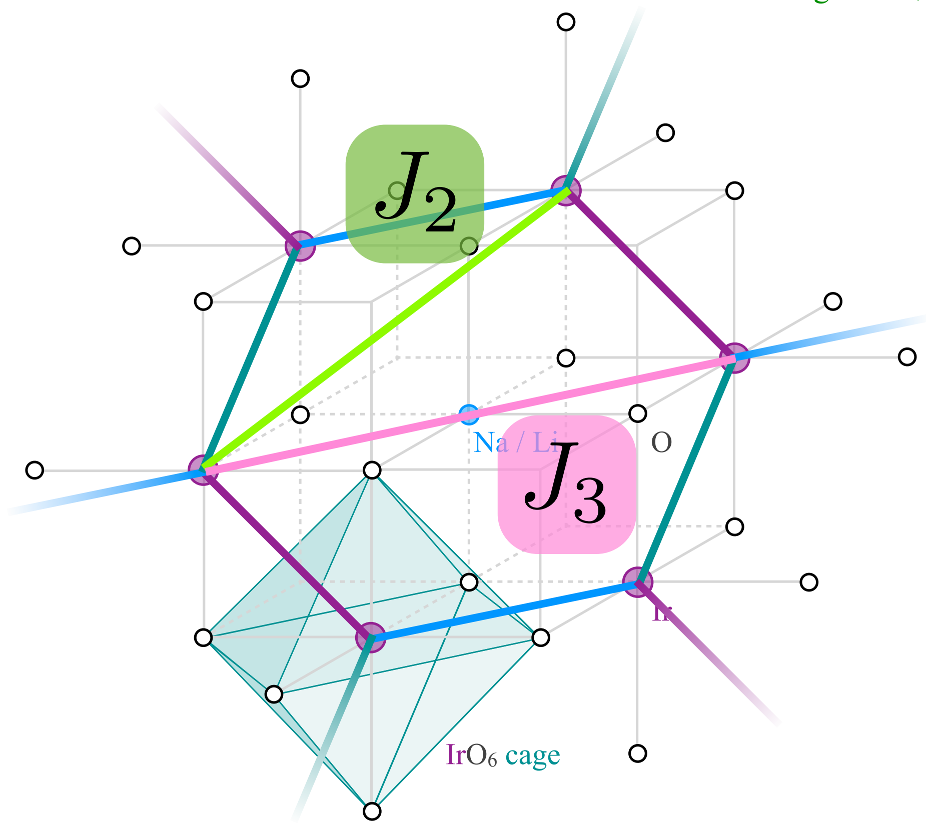

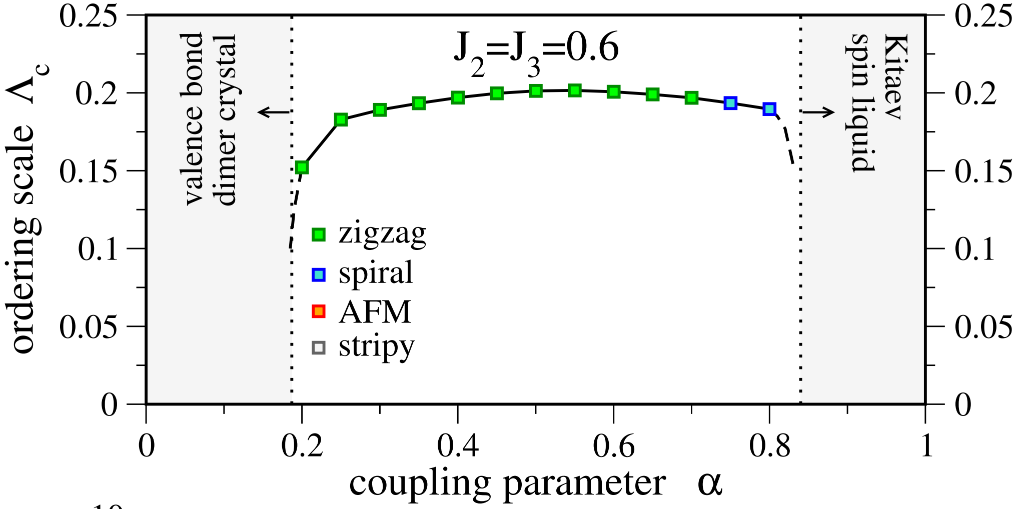

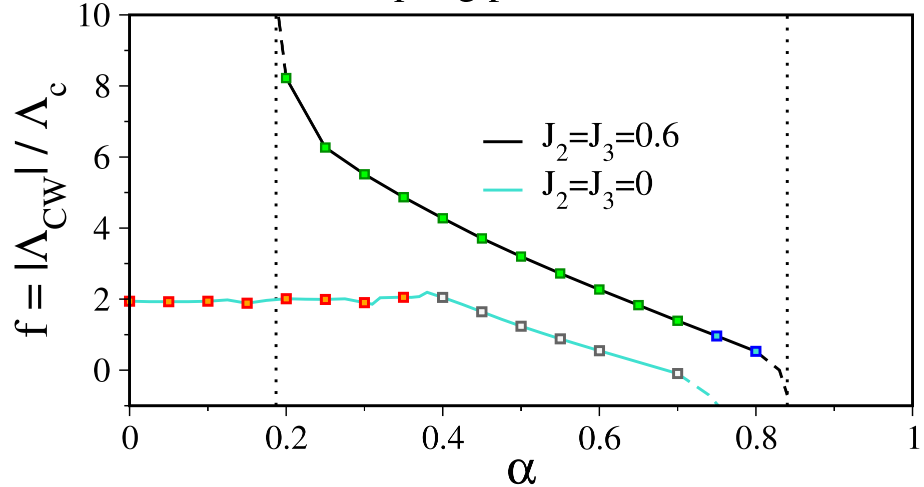

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The 3rd-nearest neighbor coupling J_3 indeed favors **zig-zag** magnetic order.

Microscopic parameter estimates

Y. Singh *et al.*, arXiv:1106.0429

Na_2IrO_3

$\Theta_{\mathrm{CW}} \approx -125$ K

$T_{\mathrm{N}} \approx 15$ K

zig-zag order

$J_2/J_1 \approx 0.6$

$J_3/J_1 \approx 0.6$

$\alpha \approx 0.25$

Heisenberg : Kitaev ~ 3 : 2

Li_2IrO_3

$\Theta_{\mathrm{CW}} \approx -33$ K

$T_{\mathrm{N}} \approx 15$ K

zig-zag order

$J_2/J_1 \gtrsim 0.6$

$J_3/J_1 \gtrsim 0.6$

$\alpha \gtrsim 0.65$

Heisenberg : Kitaev ~ 1 : 4


What next?
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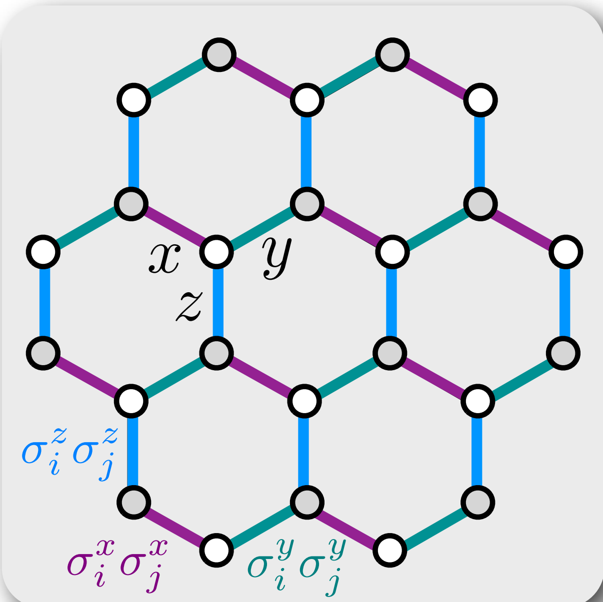
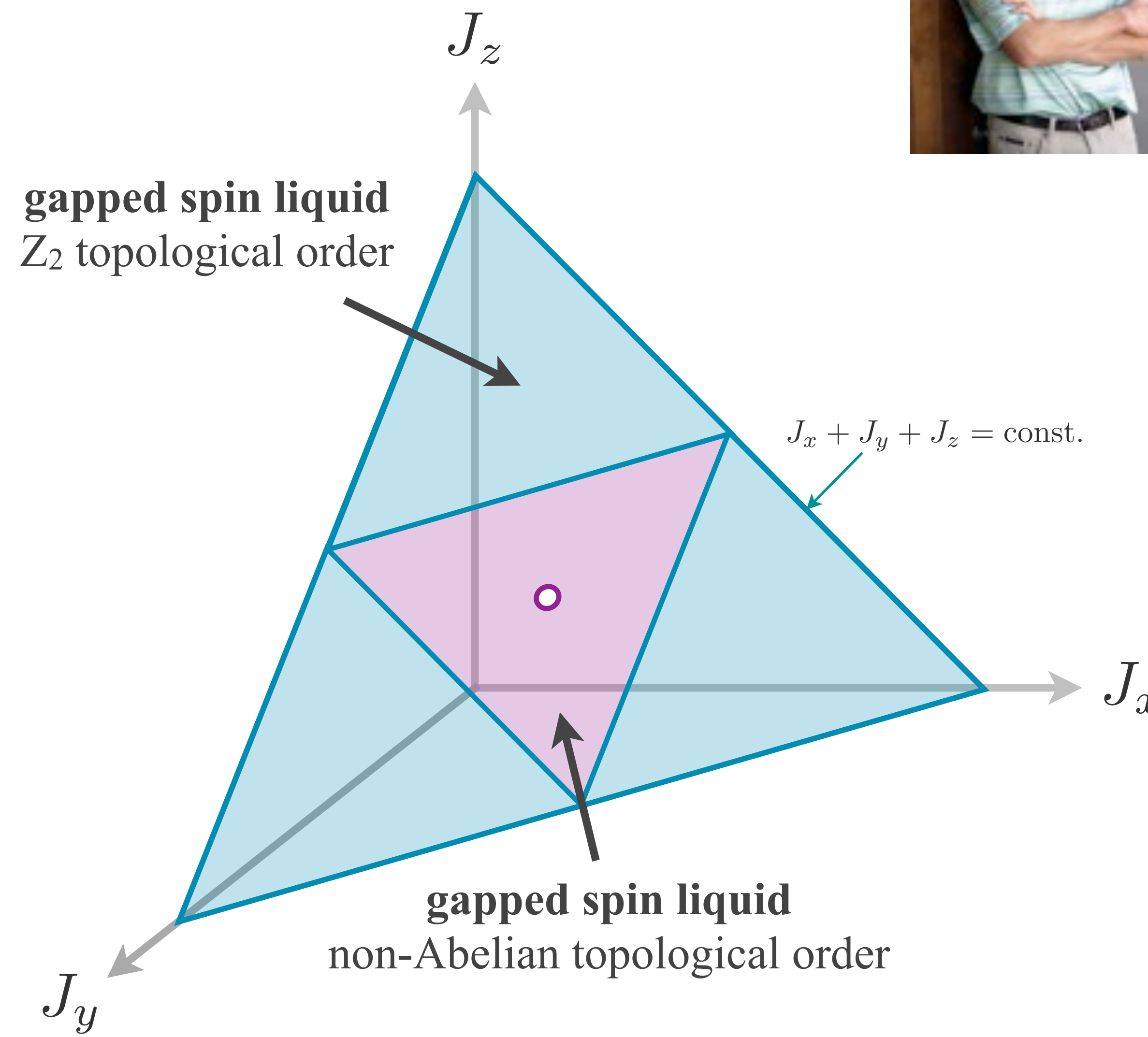
The Kitaev model + field



$$H_{\text{Kitaev+h}} = \sum_{\gamma-\text{links}} J_\gamma \sigma_i^\gamma \sigma_j^\gamma - \sum_i \vec{h} \cdot \vec{\sigma_i}$$

$\vec{h} = h\,(1, 1, 1)$

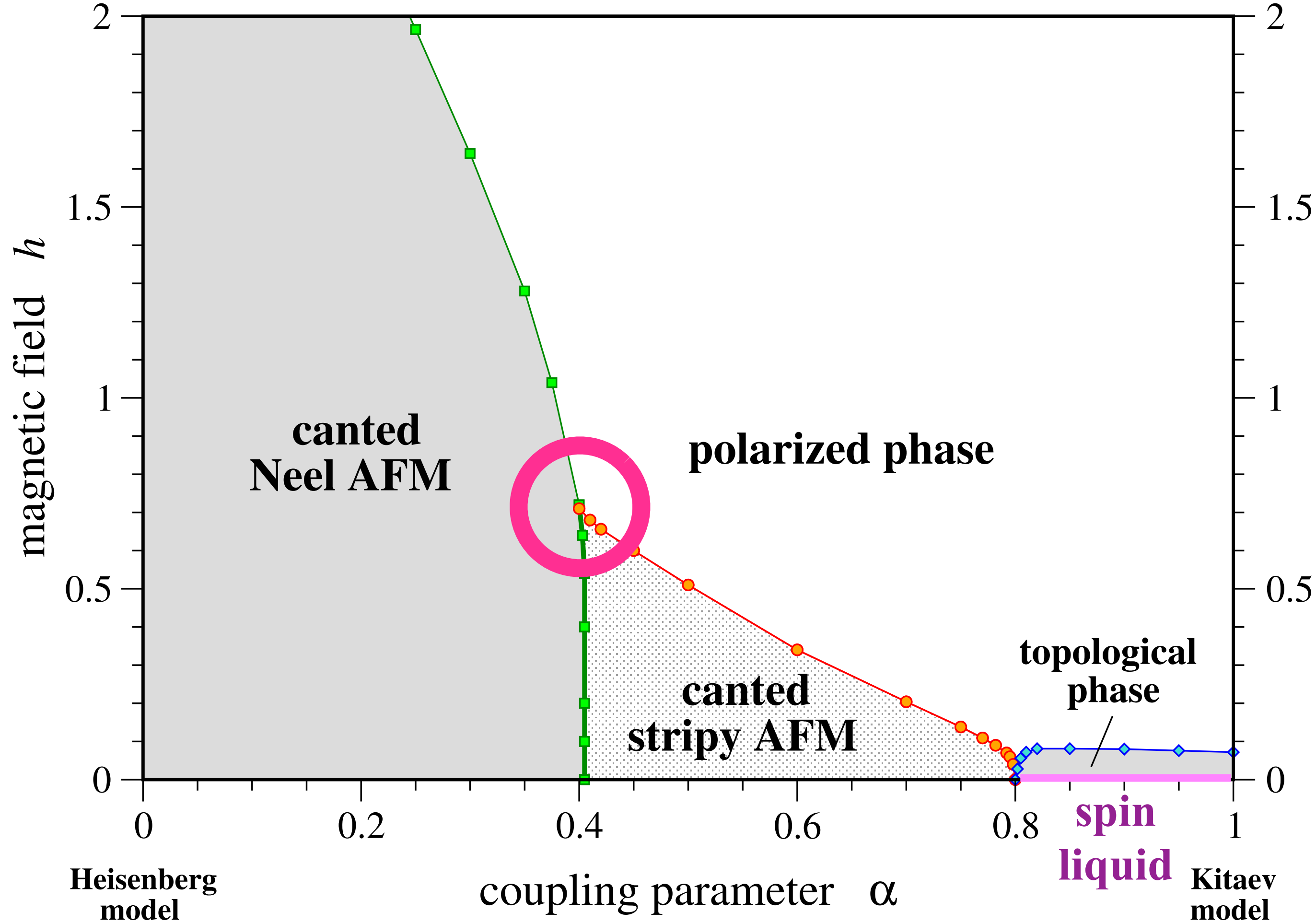


vortices are **Ising anyons** with **Majorana fermion** zero modes

Heisenberg-Kitaev model + field

H.-C. Jiang, Z.-C. Gu, X.-L. Qi,, ST, PRB **83**, 245104 (2011).

$$H_{\mathrm{HK}} = (1-\alpha)\sum_{\langle i,j\rangle}\vec{\sigma}_i\cdot\vec{\sigma}_j - 2\alpha\sum_{\gamma-\mathrm{links}}\sigma_i^\gamma\sigma_j^\gamma - \sum_i \vec{h}\cdot\vec{\sigma}_i$$



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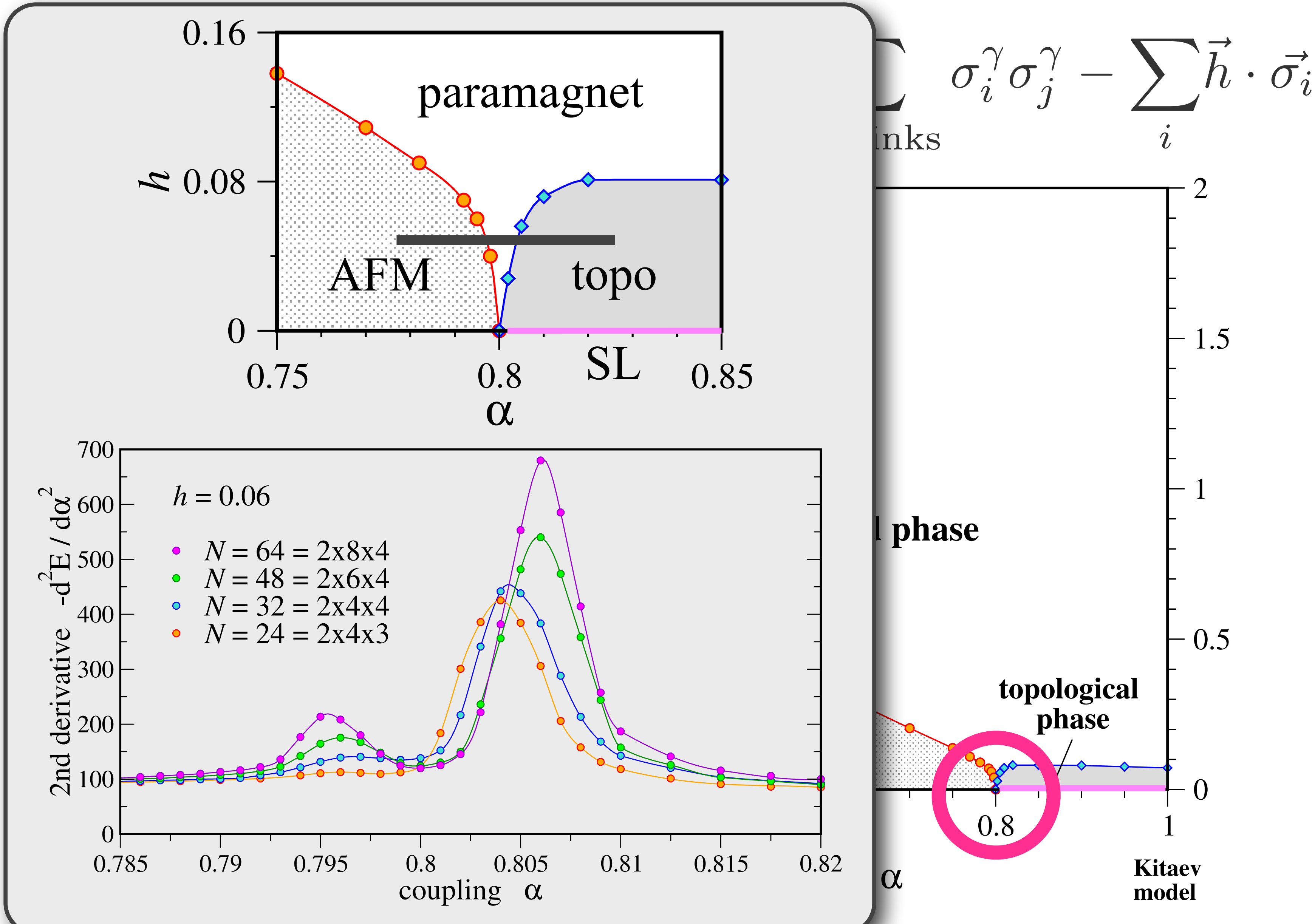
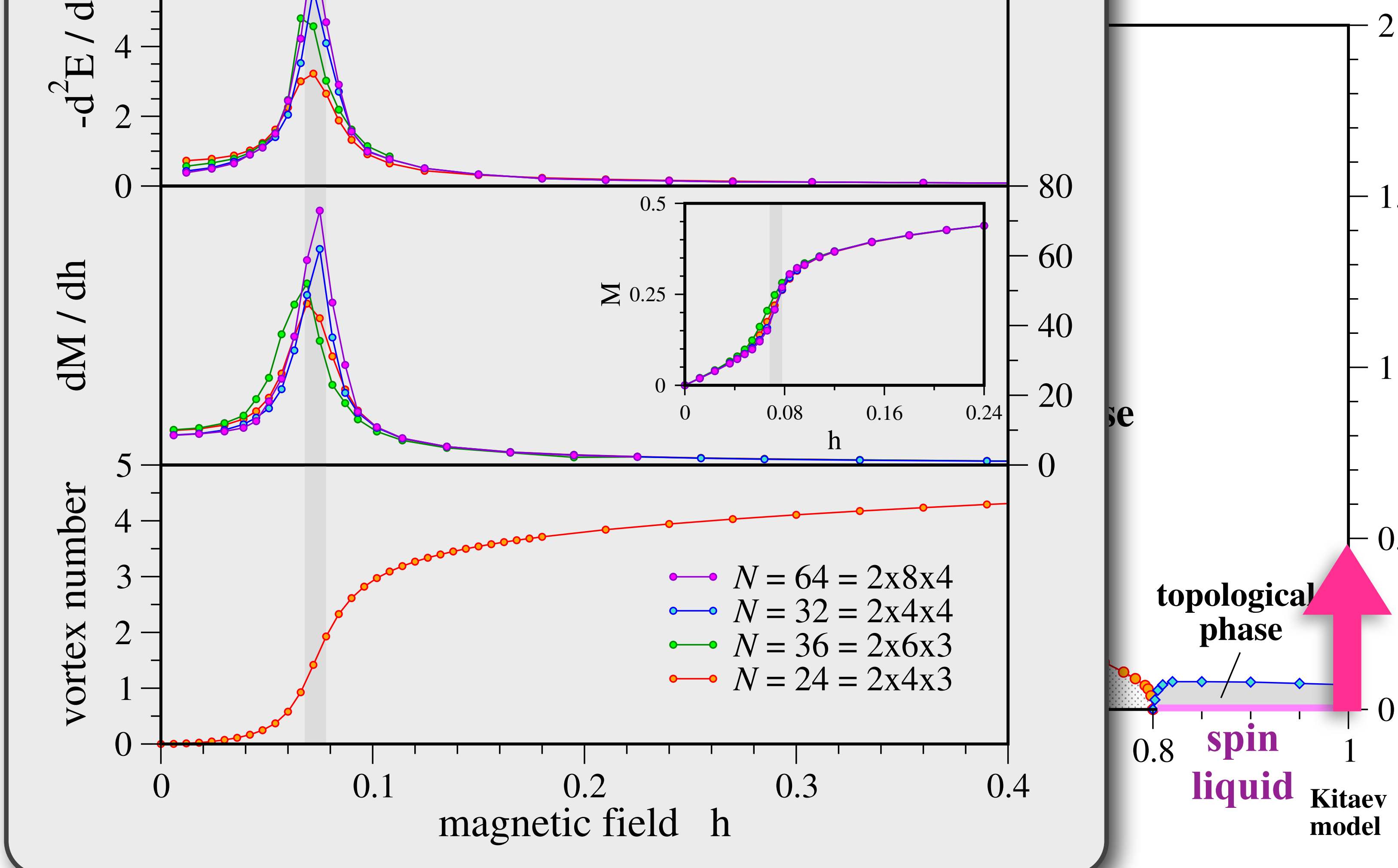


Heisenberg-Kitaev model + field

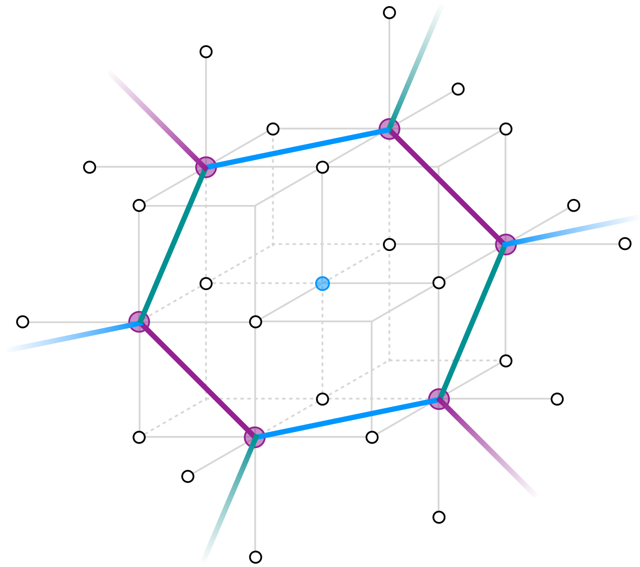
H.-C. Jiang, Z.-C. Gu, X.-L. Qi,, ST, PRB **83**, 245104 (2011).

$$\sigma_i^\gamma \sigma_j^\gamma - \sum_i \vec{h} \cdot \vec{\sigma_i}$$



Summary

- Spin-orbit coupling in correlated electron materials can lead to a plethora of novel electronic states
  - spin-orbital ordered states
  - spin liquids
  - topological order
  - ...



- 5d transition metal oxides, particularly Iridates (Osmates?), offer a first glimpse of such spin-orbit entangled collective states.
- $(Na,Li)_2IrO_3$ show signs of spin-orbital order, but the Li-system might be close to even more exotic states.

J. Reuther, R. Thomale, ST, PRB **84**, 100406(R) (2011).
H.-C. Jiang, Z.-C. Gu, X.-L. Qi,, ST, PRB **83**, 245104 (2011).
Y. Singh *et al.,* arXiv:1106.0429