From correlated topological insulators to iridates and spin liquids

Stephan Rachel

TECHNISCHE UNIVERSITÄT DRESDEN

DFG SPP 1666

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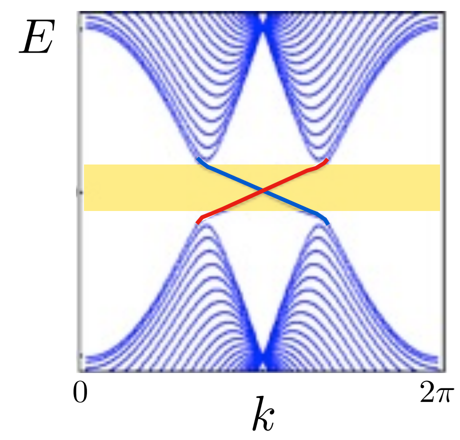
Thanks to...

Ronny Thomale
(Würzburg, Germany)

Johannes Reuther
(Caltech / Berlin)

Manuel Laubach
(Würzburg, Germany)



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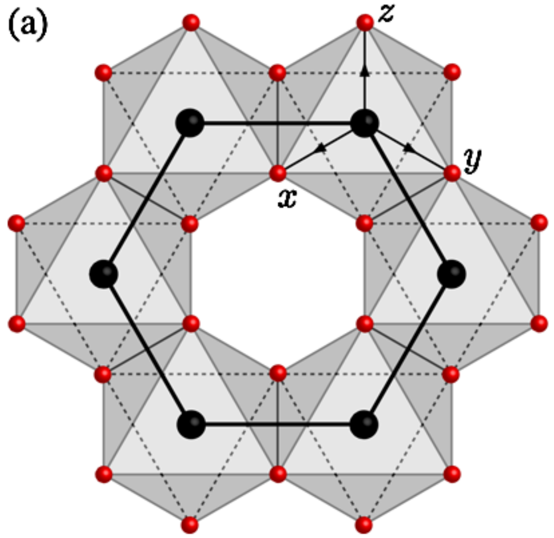
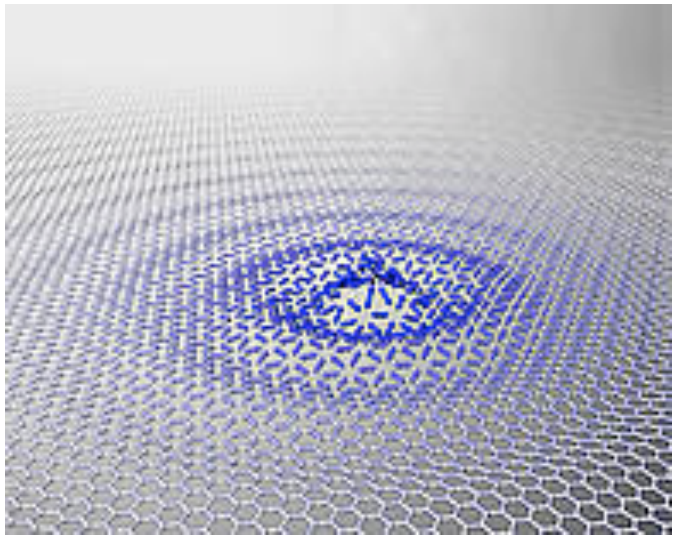
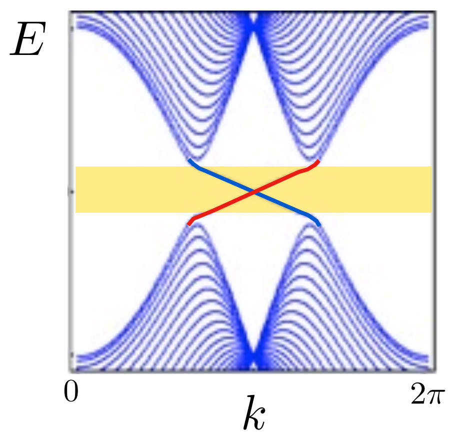
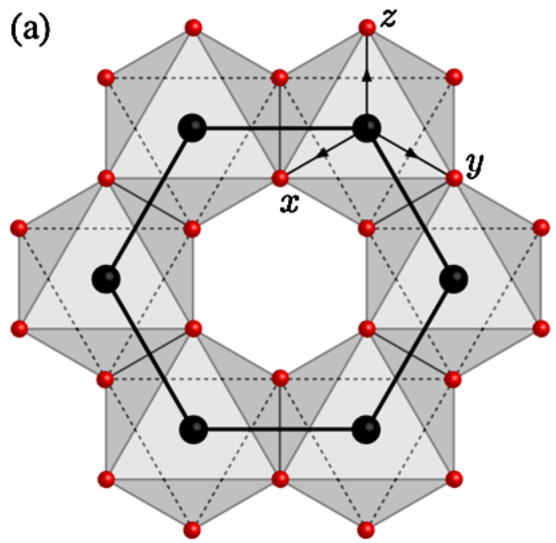


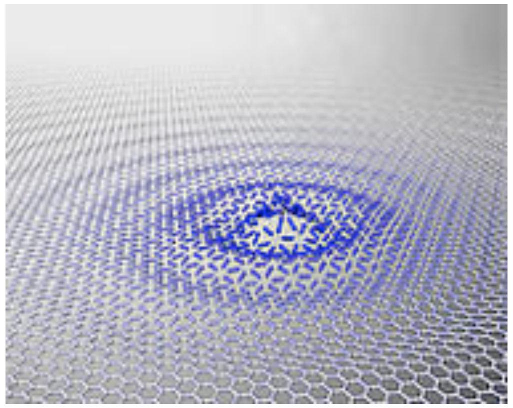


Outline:

- ❖ From correlated topological insulators to the honeycomb iridates
- ❖ Minimal model for Li_2IrO_3
- ❖ Spin liquid phase in the "Hubbard-Kitaev model" on the Δ-lattice







One of the first A_2IrO_3 papers:

PRL **102,** 256403 (2009) PHYSICAL REVIEW LETTERS week ending 26 JUNE 2009

Quantum Spin Hall Effect in a Transition Metal Oxide Na_2IrO_3

Atsuo Shitade,[1,*] Hosho Katsura,[2] Jan Kuneš,[3,4] Xiao-Liang Qi,[5] Shou-Cheng Zhang,[5] and Naoto Nagaosa[1,2]

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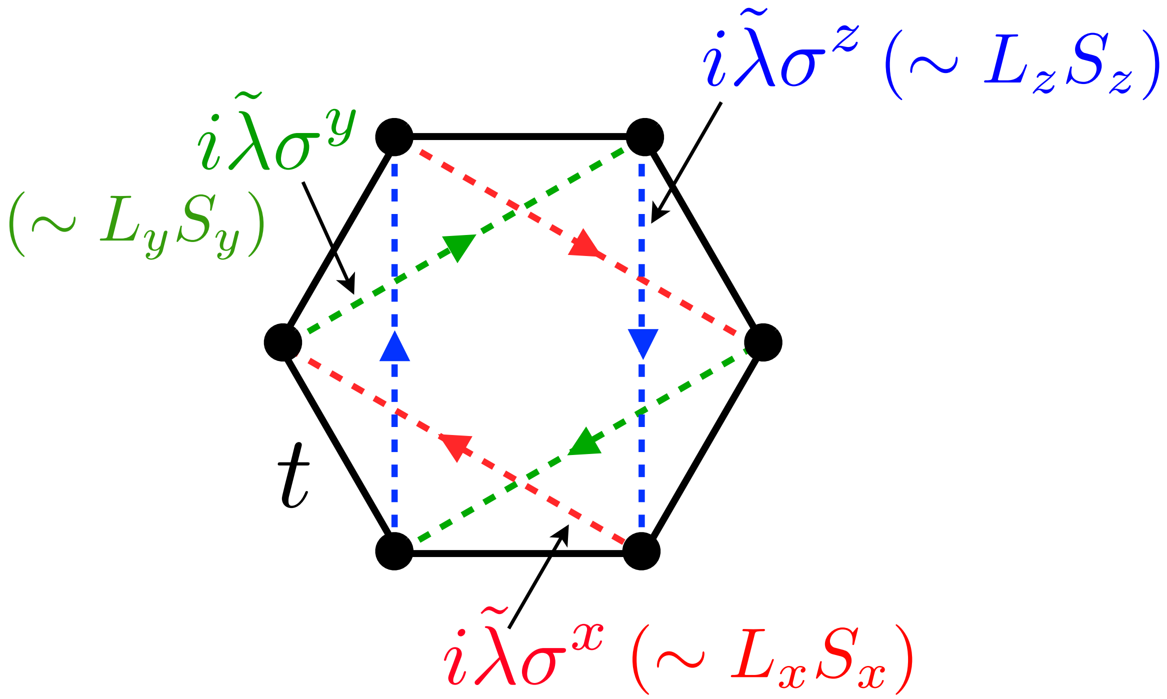

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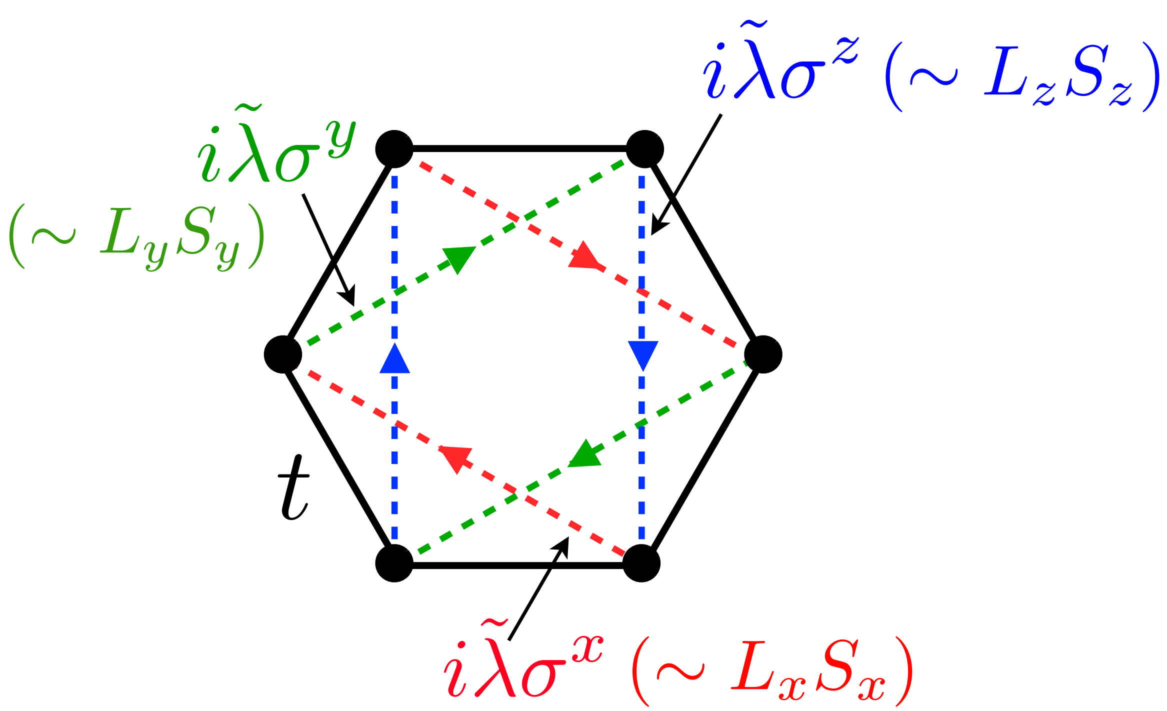
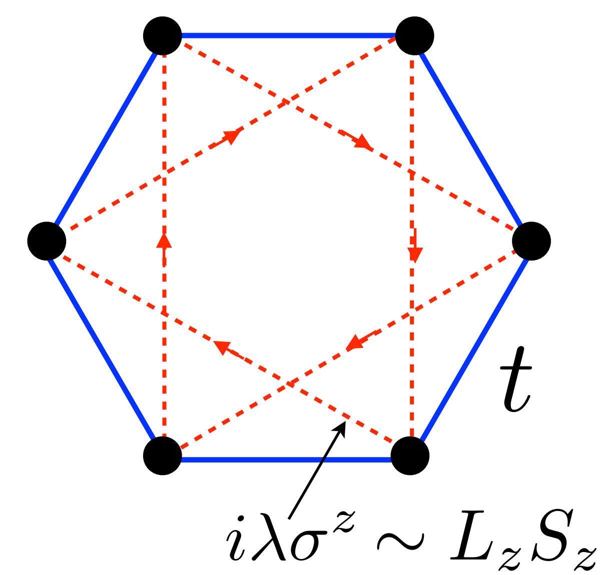




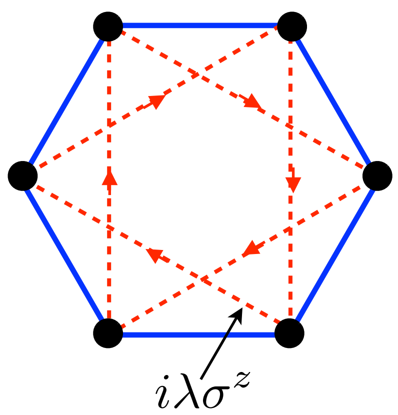
Kane & Mele, Phys. Rev. Lett. 2005

Graphene as a topological insulator (TI) ?

Idea: Dirac semi-metal + spin orbit coupling (SOC) = TI

tight-binding model for honeycomb lattice + spin orbit coupling

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + i\lambda \sum_{\langle\langle ij \rangle\rangle} \sum_{\sigma\sigma'} \nu_{ij}\, c_{i\sigma}^{\dagger}\, \sigma_{\sigma\sigma'}^{z}\, c_{j\sigma'}$$



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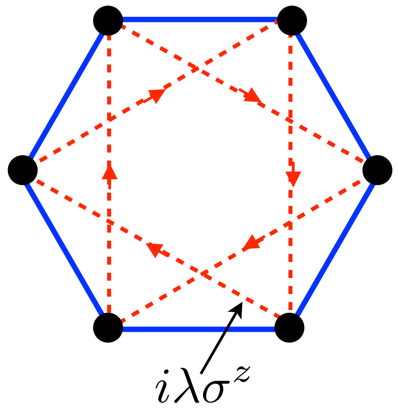

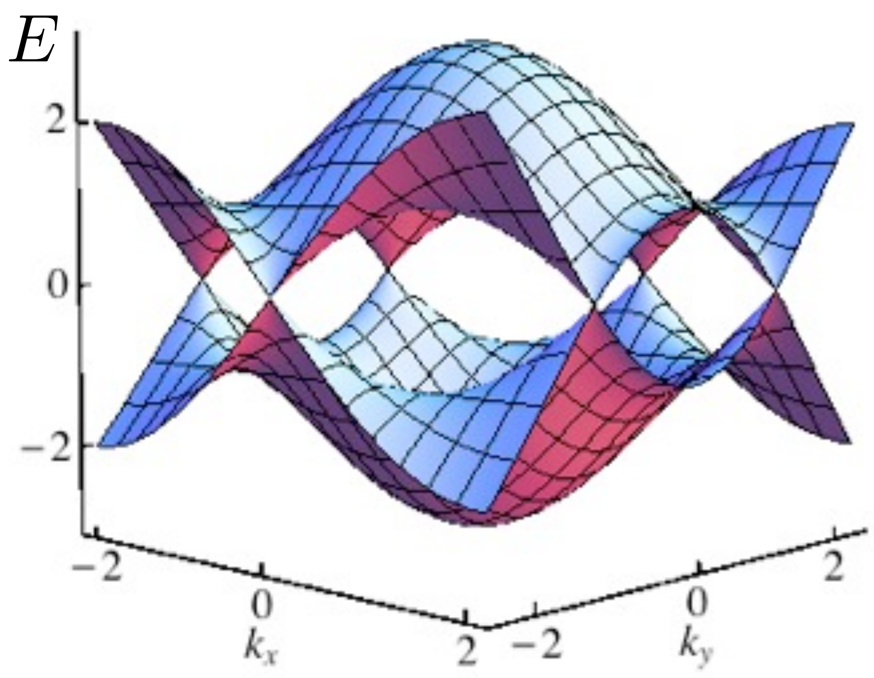

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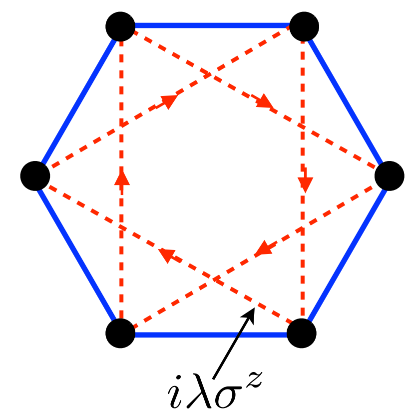
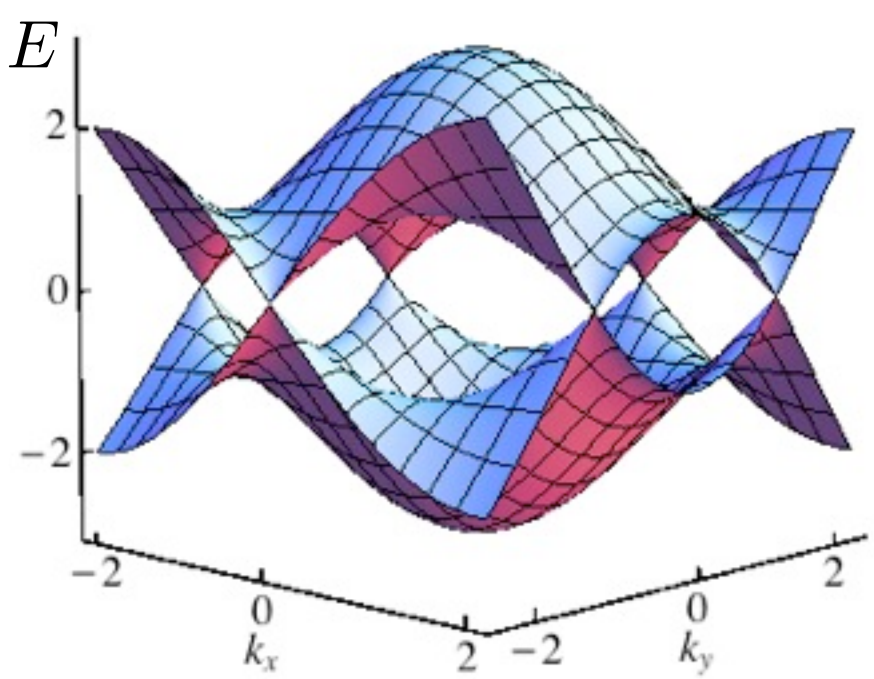
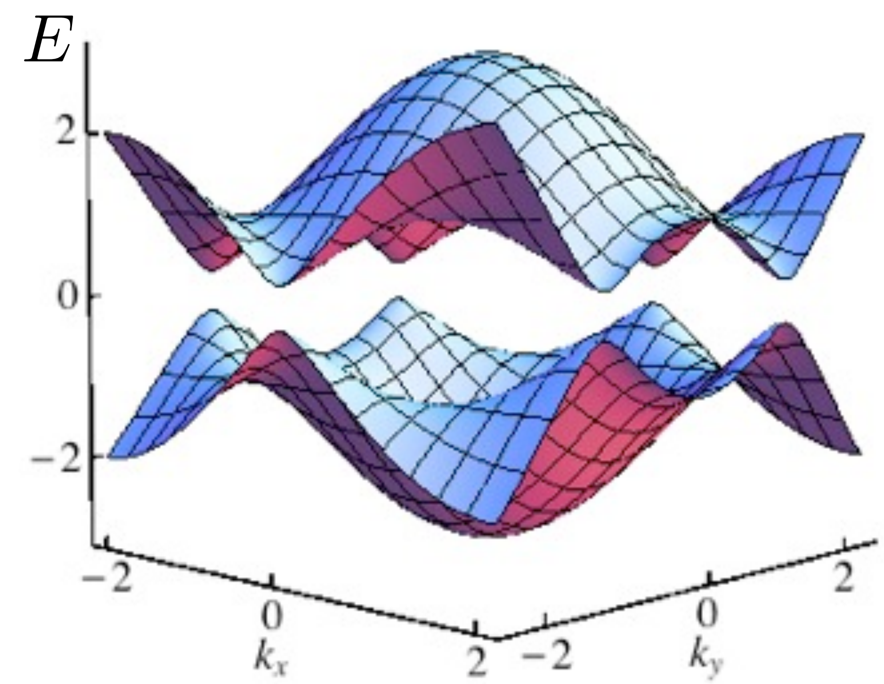




spin orbit



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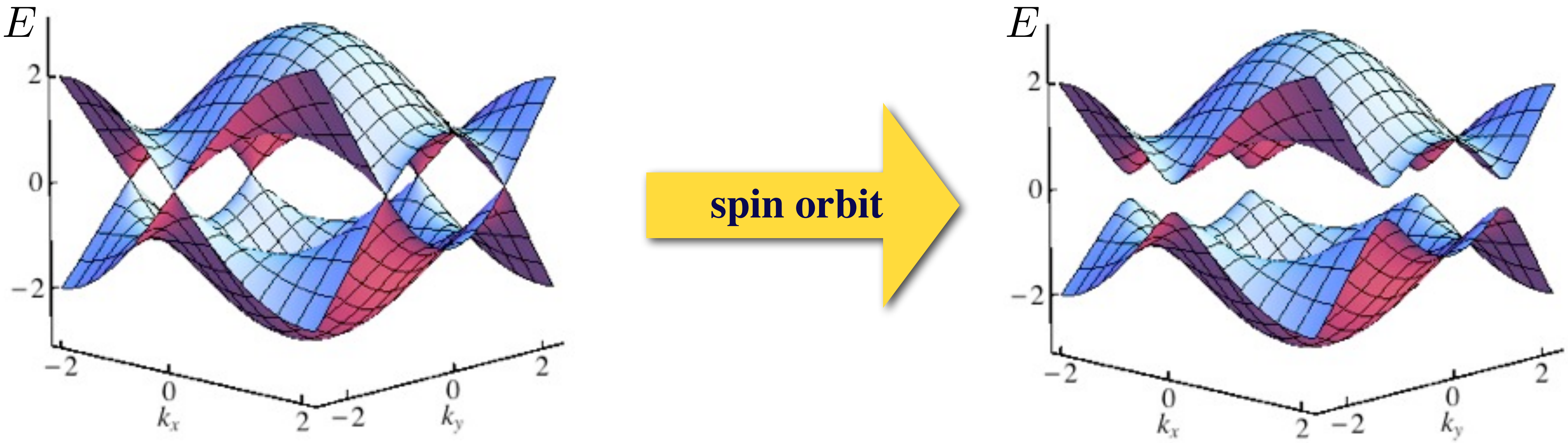

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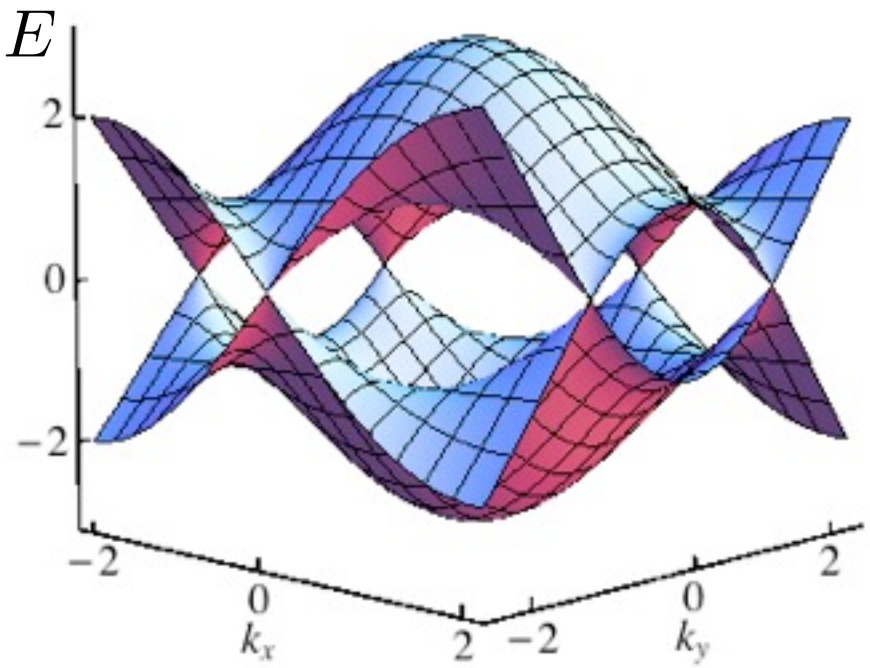

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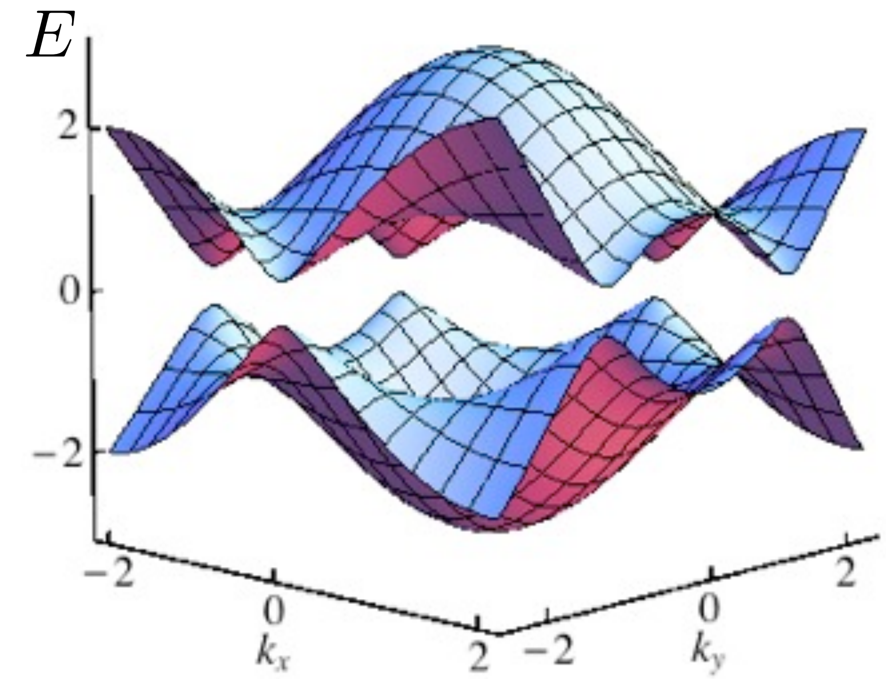
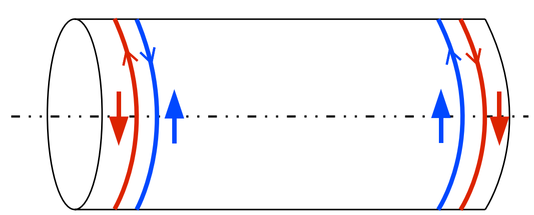
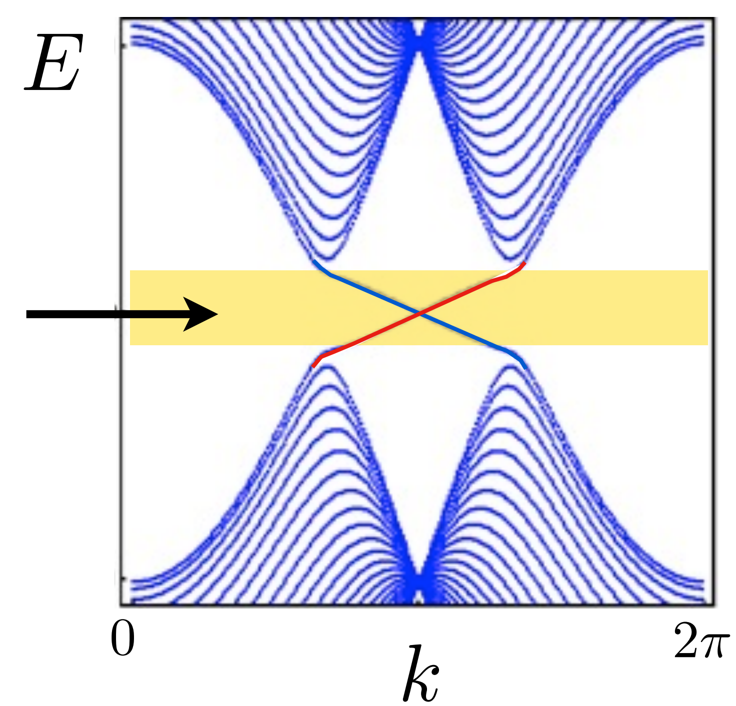


Consider cylinder geometry:



bands on a cylinder:

band-gap



edge states appear in the band-gap

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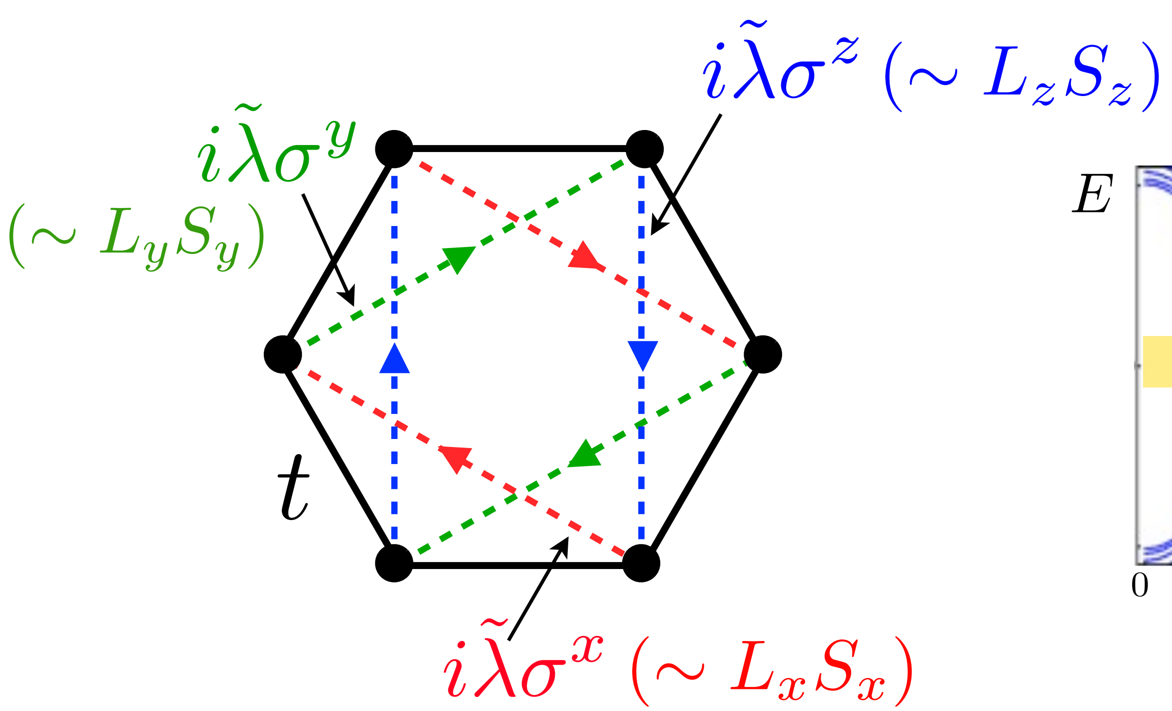

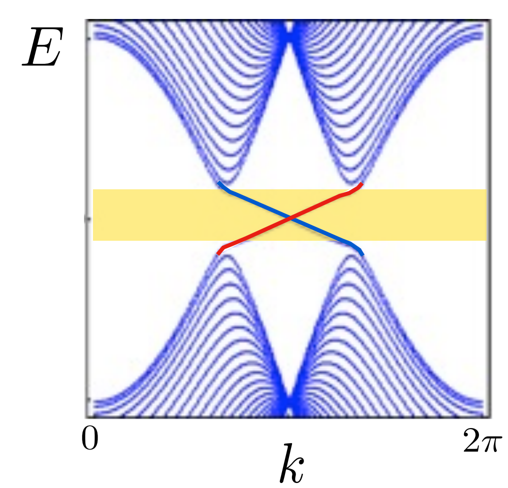

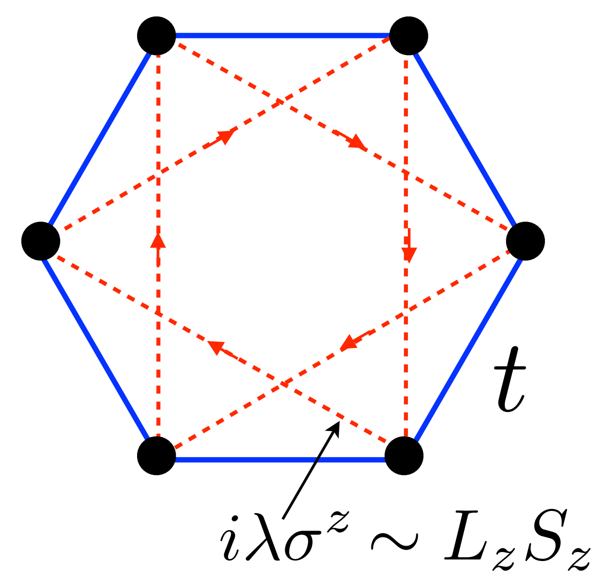

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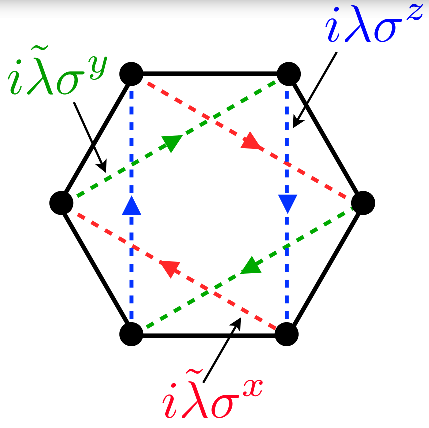
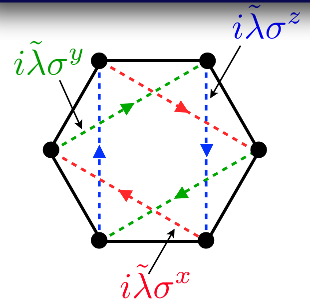


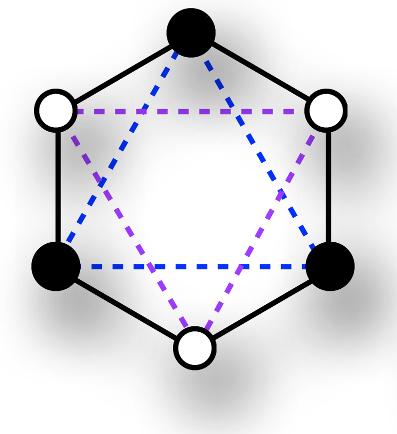
+ *strong* local Coulomb interactions

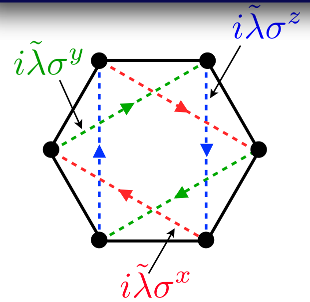
Can we describe the physics (e.g. magnetism) of the honeycomb iridates?



$U = \infty$: spin model

$$H = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j - J_{\mathrm{SO}} \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + 2J_{\mathrm{SO}} \sum_{\substack{\mathrm{NNN} \\ \gamma-\mathrm{links}}} S_i^\gamma S_j^\gamma$$





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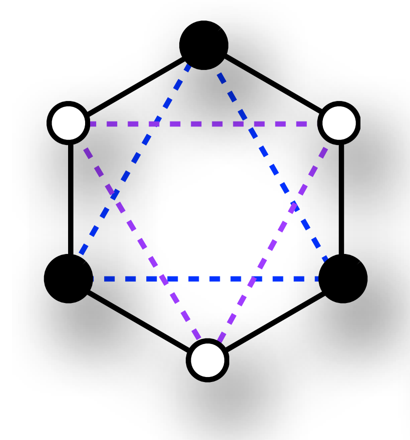
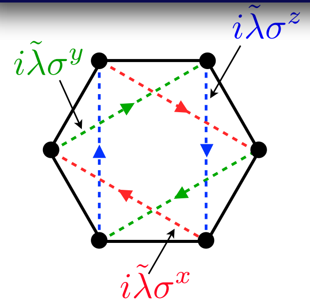
NN-Heisenberg NNN-Heisenberg-Kitaev





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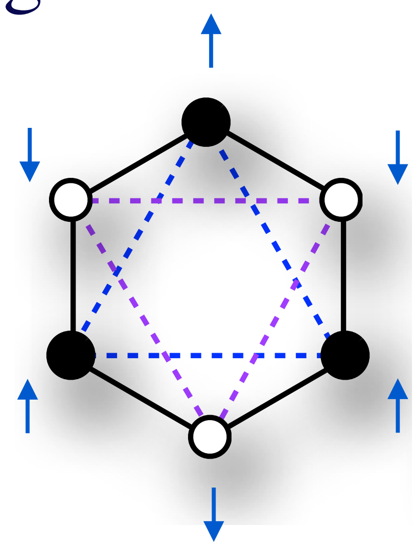
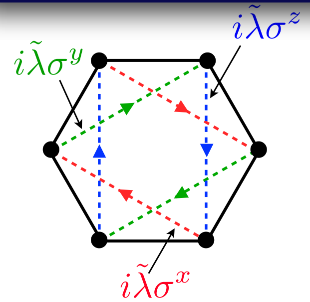


favors Neel order

+ Kitaev model
on triangular lattice



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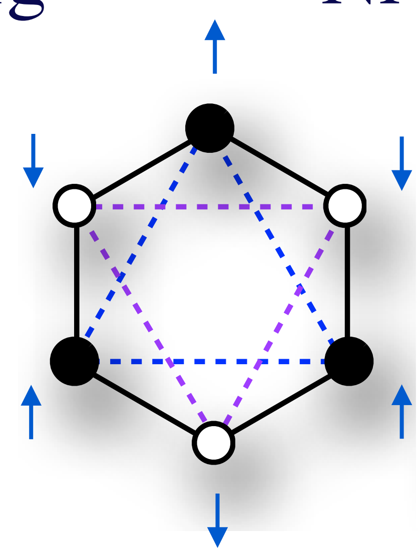

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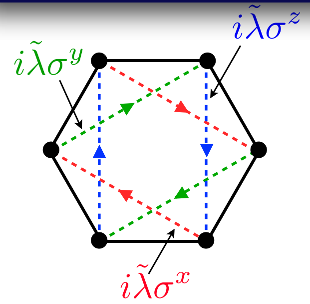
+ Kitaev model
on triangular lattice

for small SOC: Neel order will win

for larger SOC: ?



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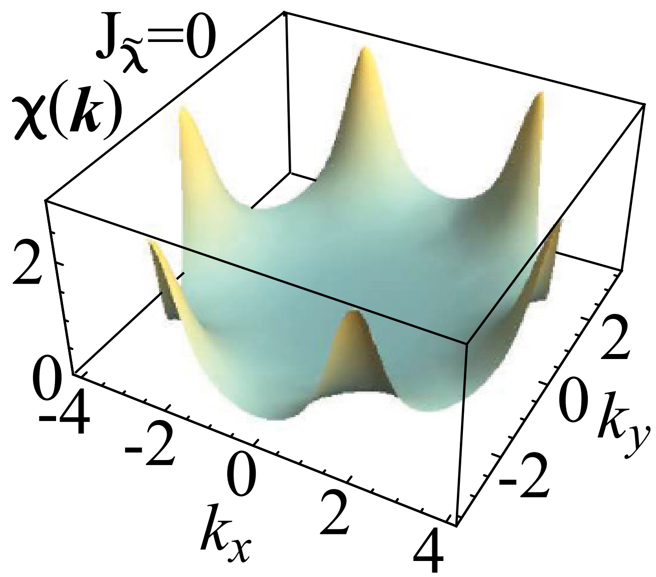

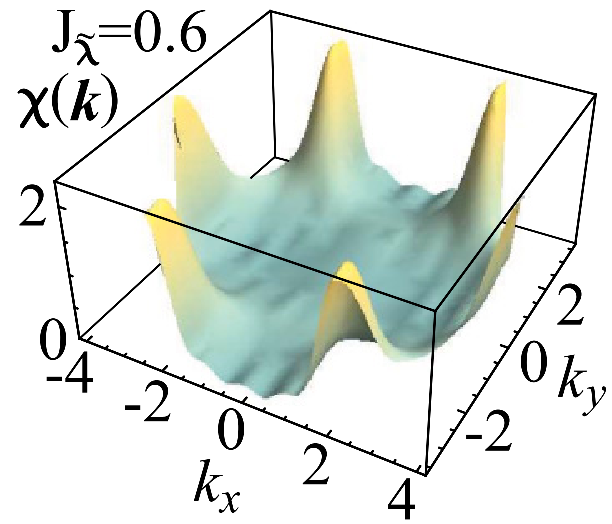

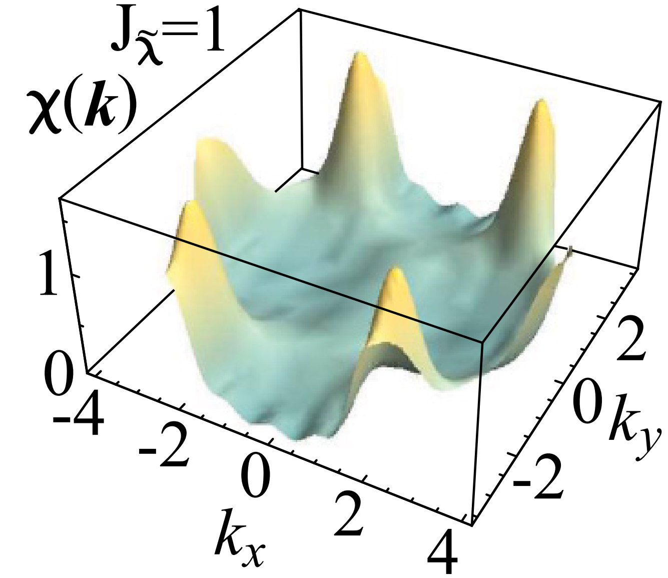

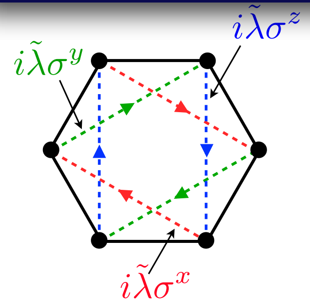

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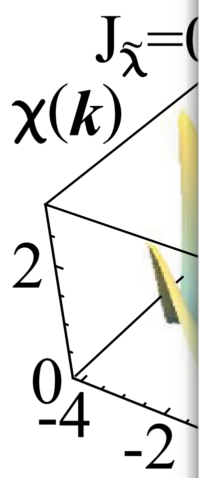
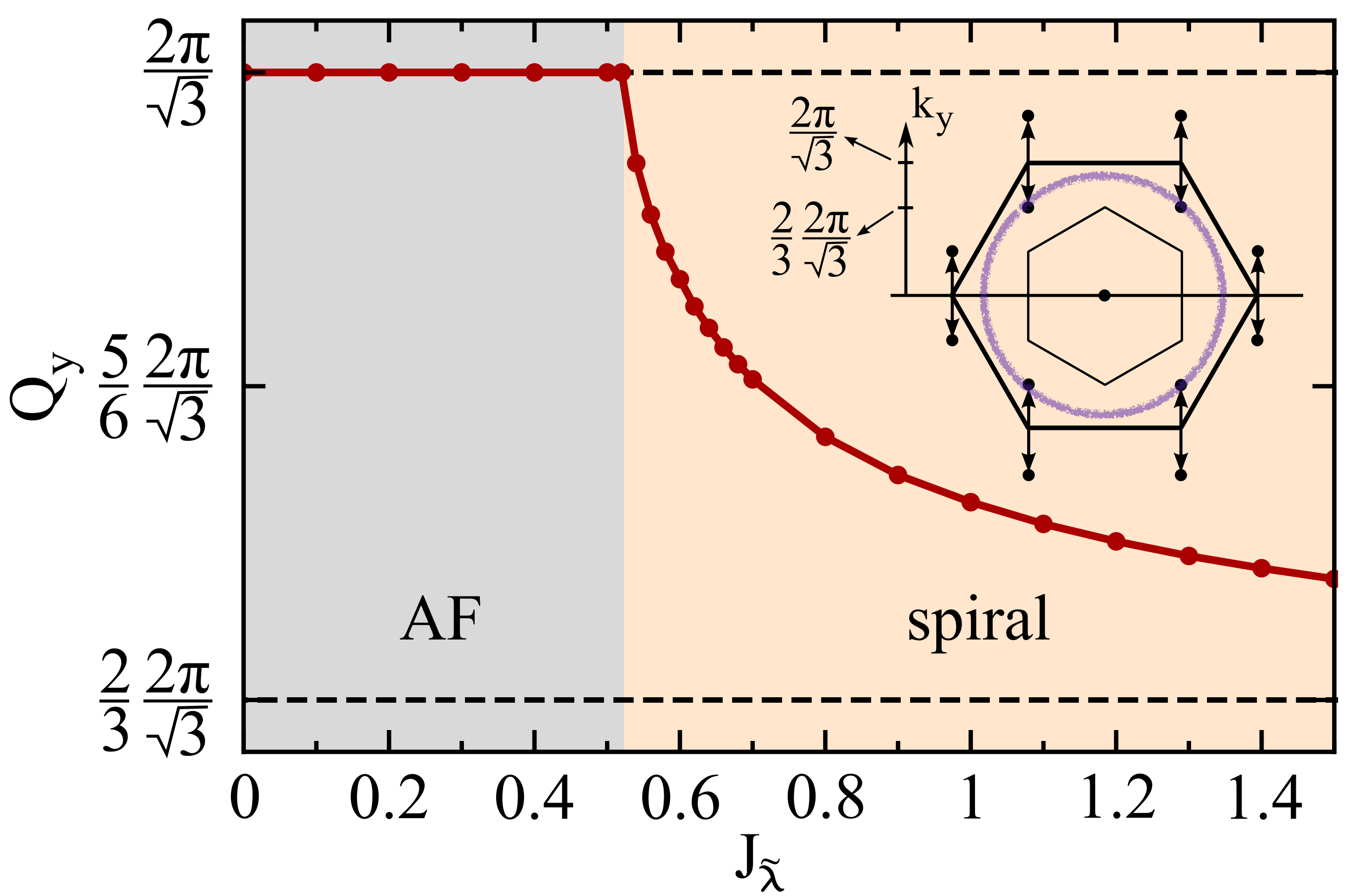
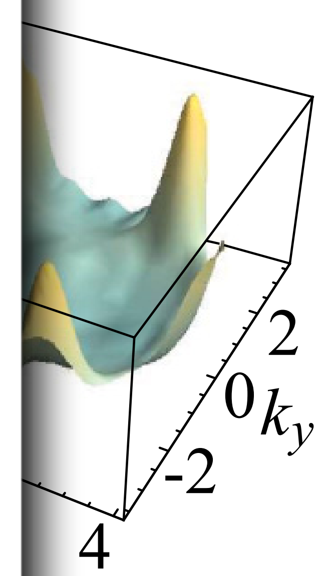
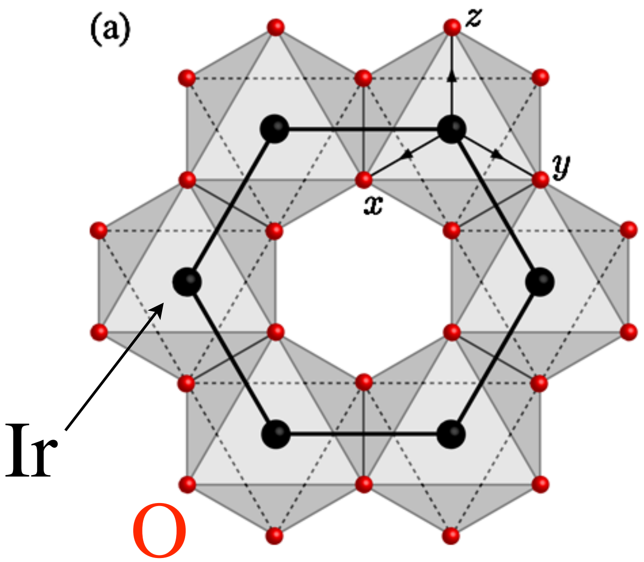


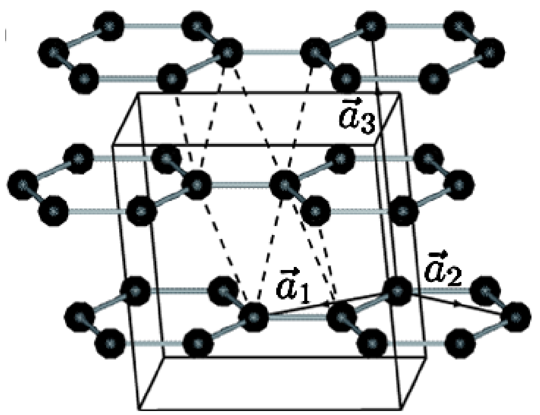




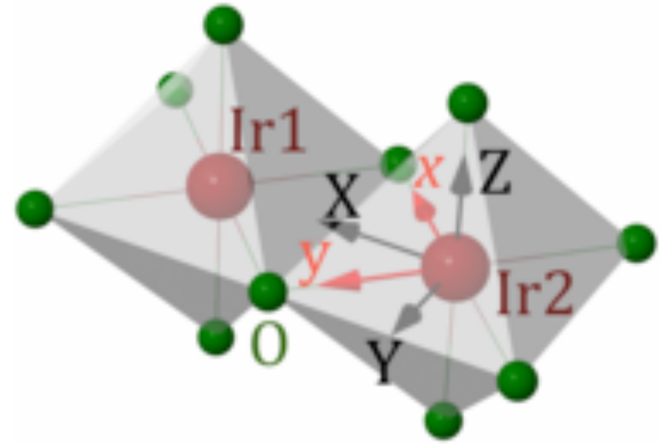
Reuther, Thomale, SR, Phys. Rev. B (2012)

Layered honeycomb compound Na_2IrO_3





AB-stacking



Theoretical results:

Heisenberg-Kitaev model

G. Jackeli and G. Khaliullin, Phys. Rev. Lett. (2009)

2D topological insulator

A. Shitade *et al.*, Phys. Rev. Lett. (2009)

3D strong topological insulator

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J. Rau, E. Lee, H.-Y. Kee, Phys. Rev. Lett. (2014)
Yamaji *et al.*, Phys. Rev. Lett. (2014)

Molecular Orbital Crystal

I. Mazin *et al.*, Phys. Rev. Lett. (2012)

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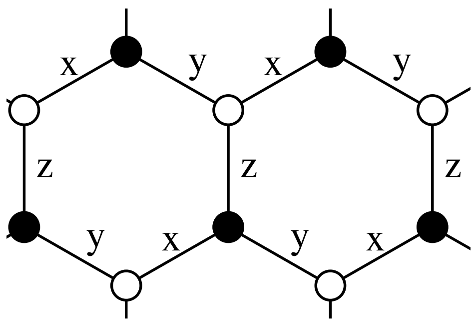
Anyons in an exactly solved model and beyond

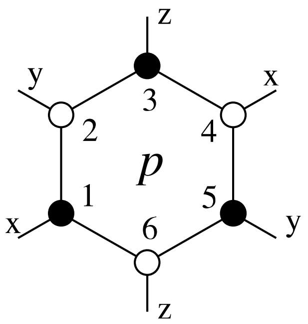
Alexei Kitaev *

California Institute of Technology, Pasadena, CA 91125, USA

Received 21 October 2005; accepted 25 October 2005

$$H = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z$$



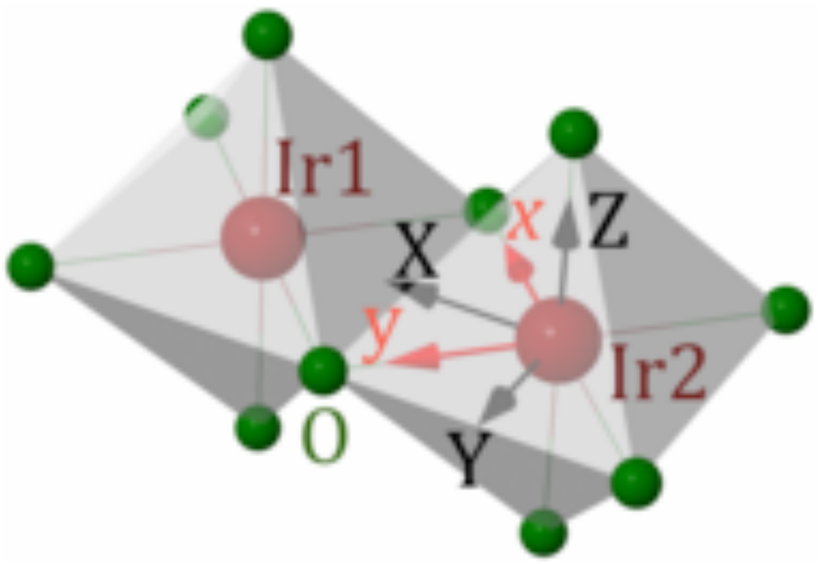


$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z = K_{12} K_{23} K_{34} K_{45} K_{56} K_{61}$$

for J_x=J_y=J_z gapless spin liquid !

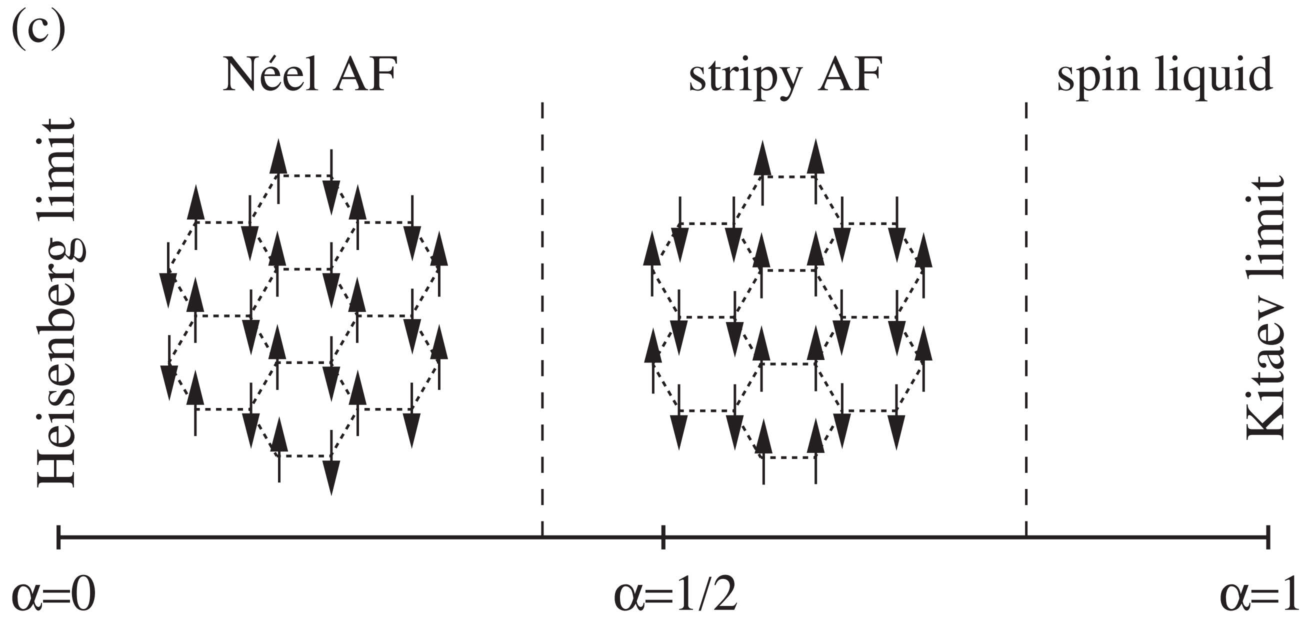
Heisenberg-Kitaev model

Jackeli, Khaliullin (2009)



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

destructive interference of
the two Ir-O-Ir paths !



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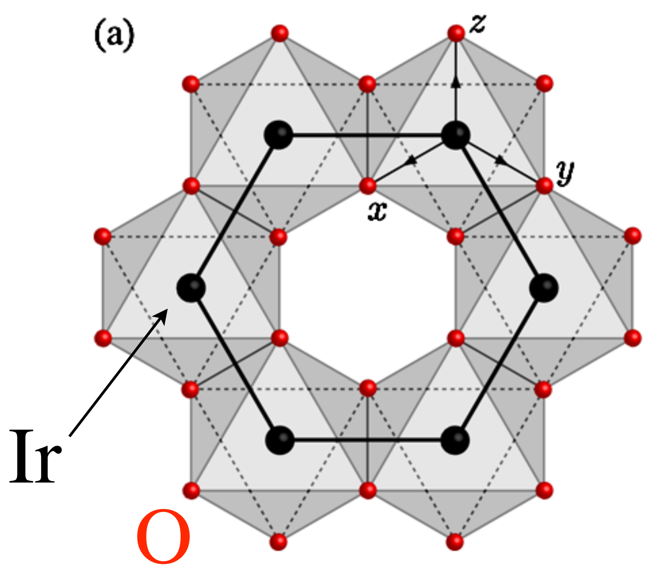

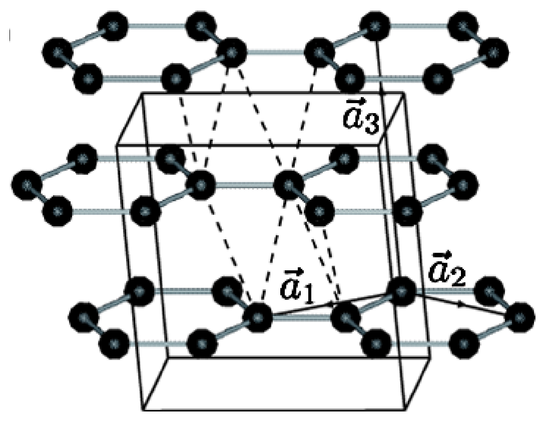

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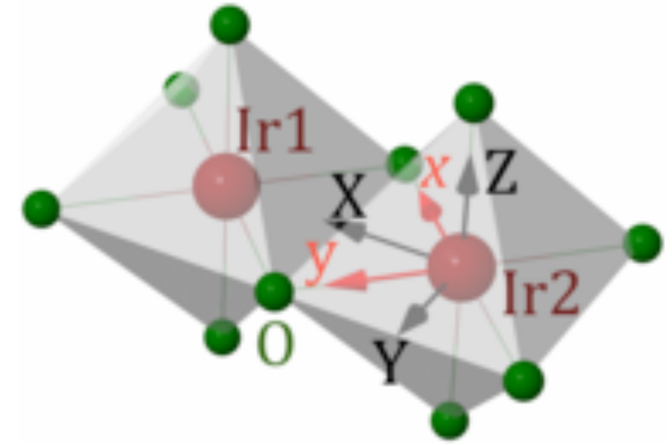

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I. Mazin *et al.*, Phys. Rev. Lett. (2012)

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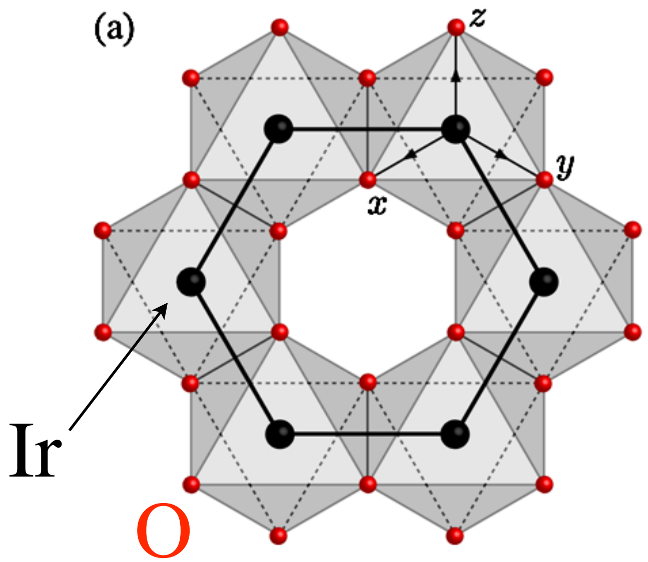
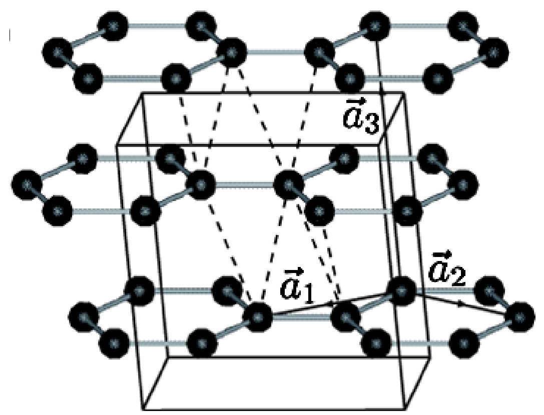




AB-stacking

Experimental results:

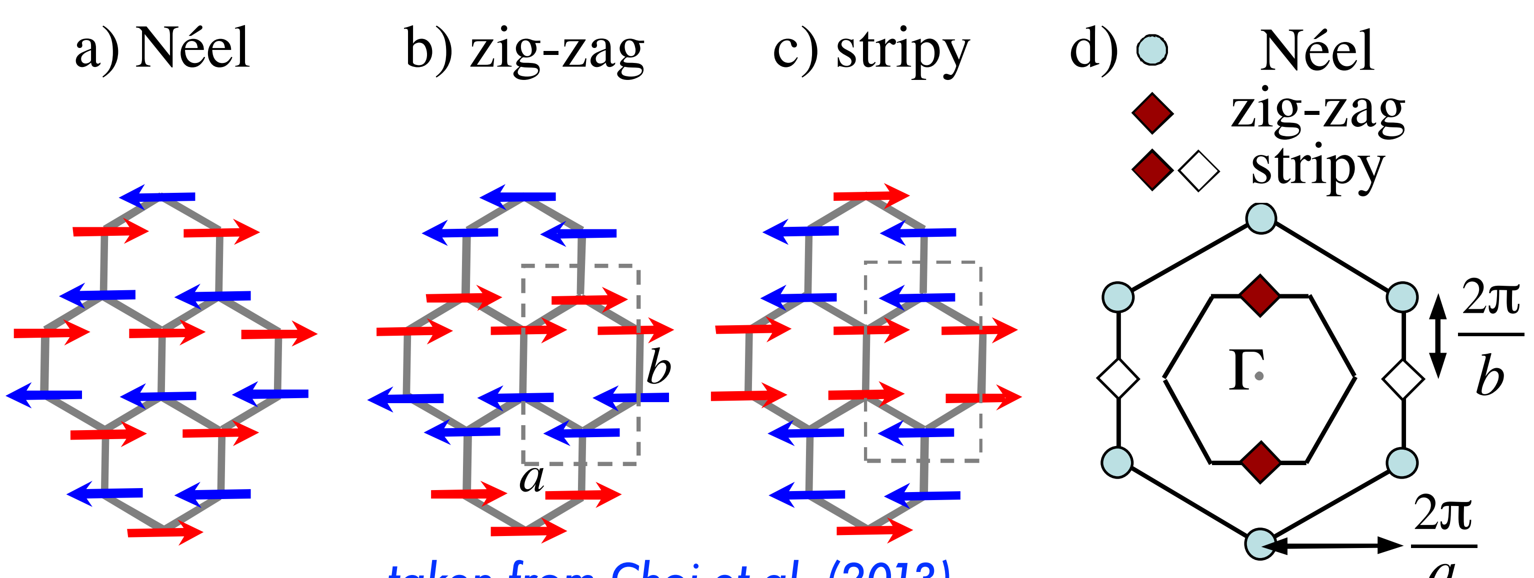
magnetic long-range order below T_N = 15 K
negative Curie-Weiss temperature Θ = -125 K

Y. Singh and P. Gegenwart, Phys. Rev. B (2010)

magnetic order of zig-zag type

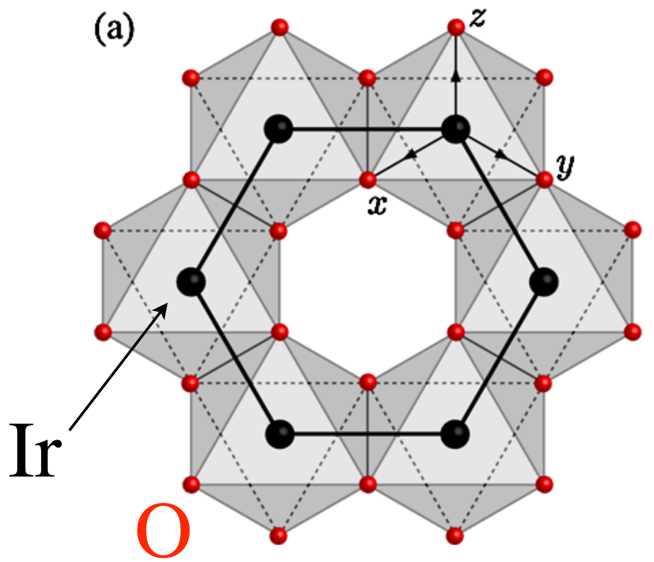
X. Liu *et al.*, Phys. Rev. B (2011)
F. Ye *et al.*, Phys. Rev. B (2012)
S.K. Choi *et al.*, Phys. Rev. Lett. (2012)

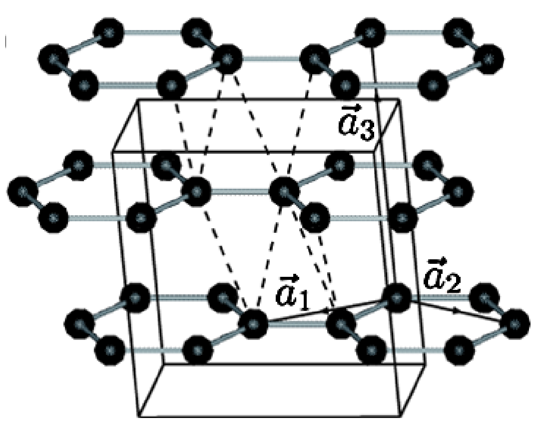
see also Gretarsson *et al.*, Phys. Rev. Lett. + Phys. Rev. B (2013)



taken from Choi et al. (2013)

Layered honeycomb compound Na_2IrO_3





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Y. Singh and P. Gegenwart, Phys. Rev. B (2010)

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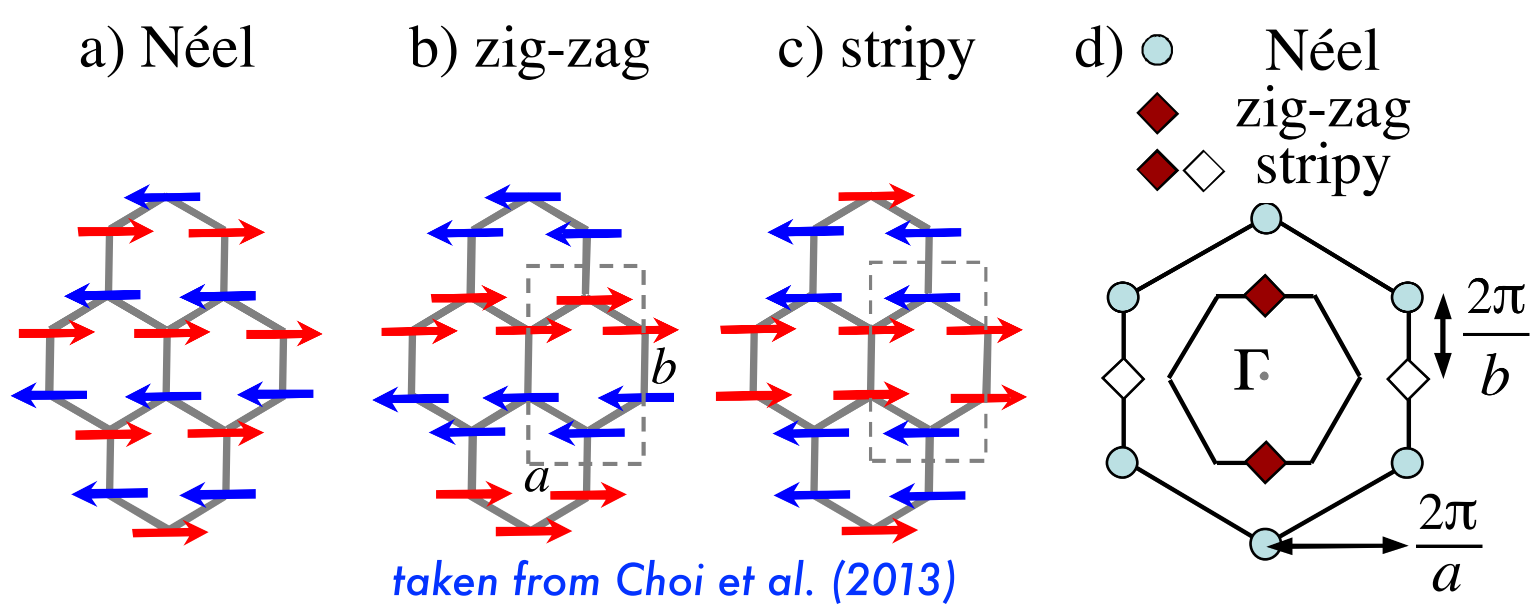
X. Liu *et al.*, Phys. Rev. B (2011)
F. Ye *et al.*, Phys. Rev. B (2012)
S.K. Choi

no spiral phase :(

see also C (2013)



taken from Choi et al. (2013)

Layered honeycomb compound Li_2IrO_3

magnetic long-range order below T_N = 15 K
negative Curie-Weiss temperature Θ = -33K

Y. Singh *et al.*,
Phys. Rev. Lett. (2012)

Layered honeycomb compound Li_2IrO_3

magnetic long-range order below $T_N = 15$ K
negative Curie-Weiss temperature $\Theta = -33$K

Y. Singh *et al.*,
Phys. Rev. Lett. (2012)

magnetic orders are **different** in Na- and Li-compound

G. Cao,..., R.Kaul,
Phys. Rev. B (2013)

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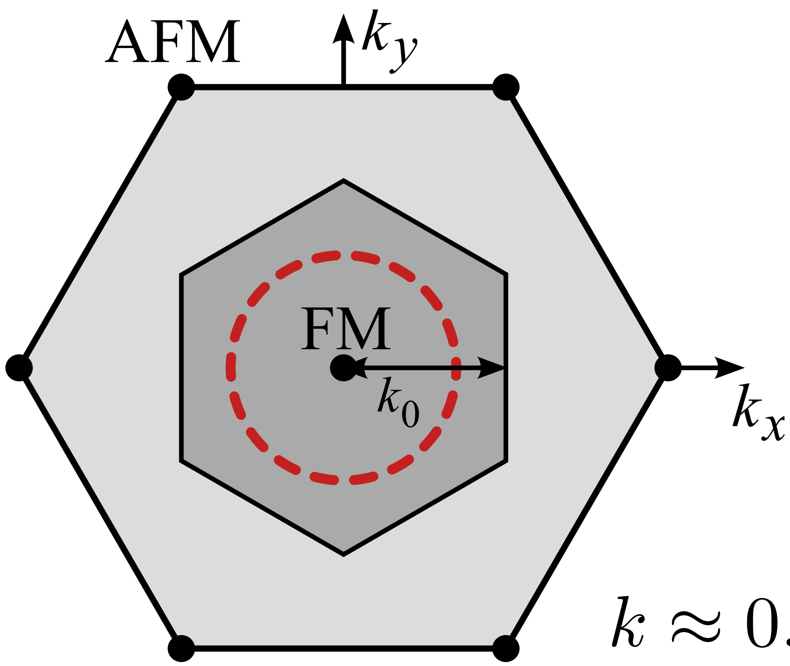
G. Cao,..., R.Kaul, Phys. Rev. B (2013)

Recent neutron powder diffraction experiments:

Incommensurate spiral order

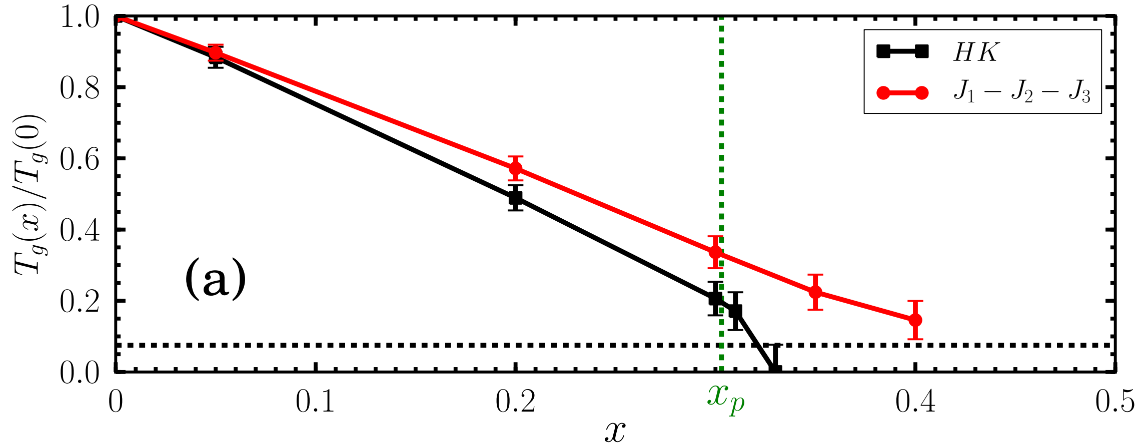
R. Coldea, *unpublished*.



$k \approx 0.41\ \text{Å}^{-1}$

Further input

short- vs. longer-ranged spin exchange:
Talks by **Matthias Vojta** and **Philipp Gegenwart**



Andrade & Vojta, arXiv:1309.2951

PHYSICAL REVIEW B **89**, 241102(R) (2014)

Effect of nonmagnetic dilution in the honeycomb-lattice iridates Na_2IrO_3 and Li_2IrO_3

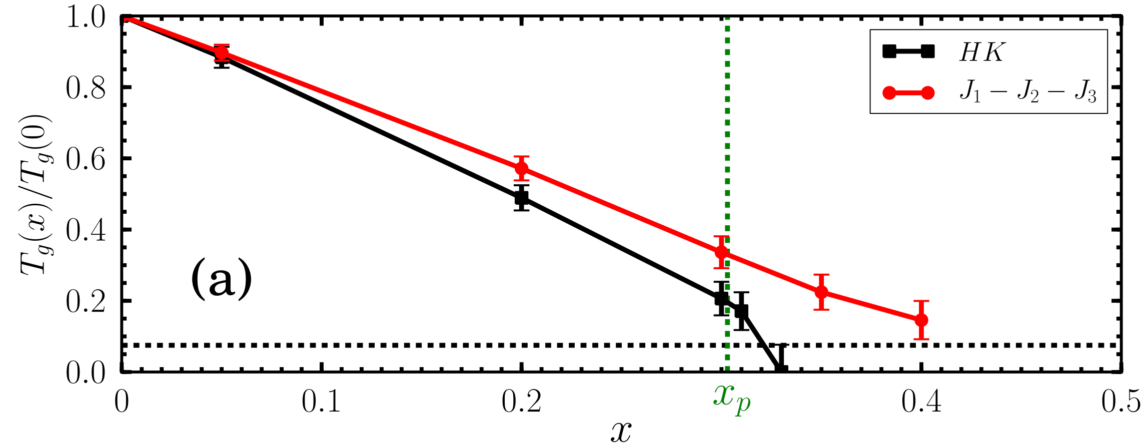
S. Manni,[1] Y. Tokiwa,[1,*] and P. Gegenwart[1,2]
[1] *I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany*
[2] *Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany*
(Received 23 April 2014; revised manuscript received 23 May 2014; published 12 June 2014)

We have synthesized single crystals of $Na_2(Ir_{1-x}Ti_x)O_3$ and polycrystals of $Li_2(Ir_{1-x}Ti_x)O_3$ and studied the effect of magnetic depletion on the magnetic properties by measurements of the magnetic susceptibility, specific heat, and magnetocaloric effect at temperatures down to 0.1 K. In both systems, the nonmagnetic substitution rapidly changes the magnetically ordered ground state into a spin glass, indicating strong frustration. While for the Li system the Weiss temperature Θ_W remains unchanged up to $x = 0.55$, a strong decrease $|\Theta_W|$ is found for the Na system. This suggests that only for the former system magnetic exchange beyond nearest neighbors is dominating. This is also corroborated by the observation of a smeared quantum phase transition in $Li_2(Ir_{1-x}Ti_x)O_3$ near $x = 0.5$, i.e., much beyond the site percolation threshold of the honeycomb lattice.

DOI: 10.1103/PhysRevB.89.241102 PACS number(s): 75.40.Cx, 75.10.Jm, 75.40.Gb, 75.50.Lk

Further input

short- vs. longer-ranged spin exchange:
Talks by **Matthias Vojta** and **Philipp Gegenwart**



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for the Na system. This suggests that only for the former system magnetic exchange beyond nearest neighbors is dominating. This is also corroborated by the observation of a smeared quantum phase transition in $Li_2(Ir_{1-x}Ti_x)O_3$

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DOI: 10.1103/PhysRevB.89.241102 PACS number(s): 75.40.Cx, 75.10.Jm, 75.40.Gb, 75.50.Lk

α-Li_2IrO_3

Tentative experimental evidence

1) incommensurate spiral order, Bragg peak(s) inside the 1st BZ
2) negative Curie-Weiss temperature
3) dominant exchange beyond nearest neighbors

Goal:

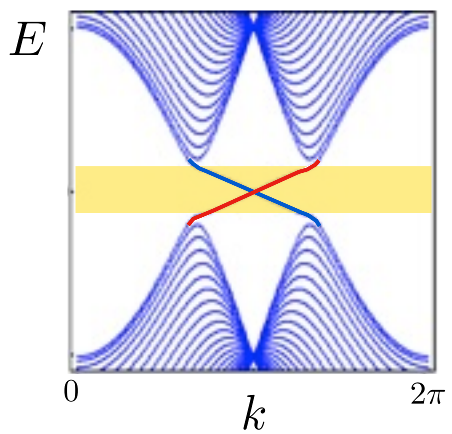
find a *minimal* spin Hamiltonian fulfilling 1) - 3)

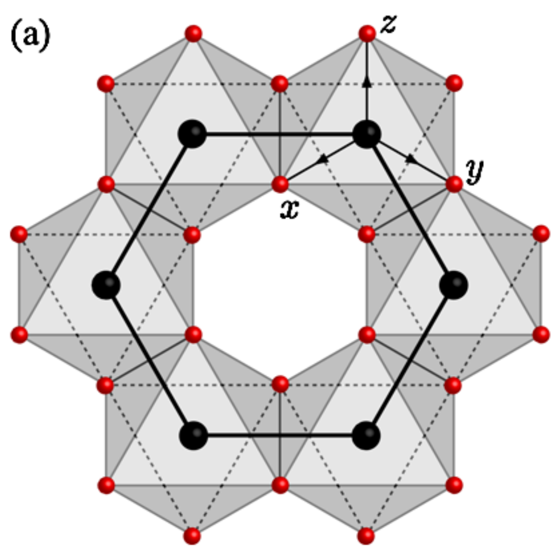
Outline:

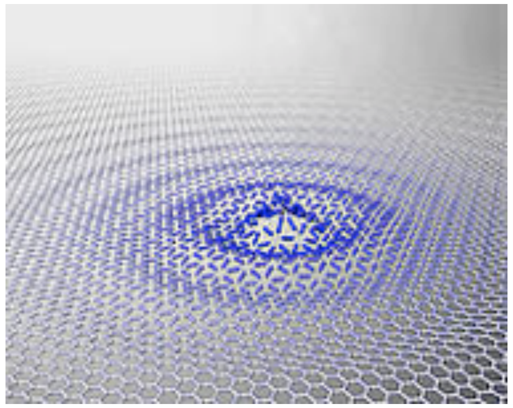
❖ From correlated topological insulators to the honeycomb iridates

❖ Minimal model for Li_2IrO_3

❖ Spin liquid phase in the "Hubbard-Kitaev model" on the Δ-lattice

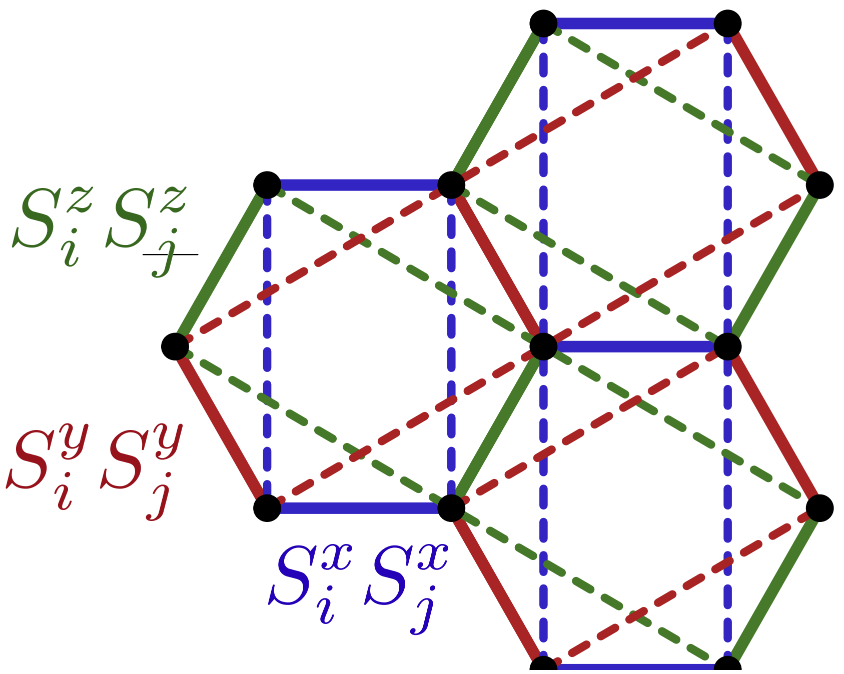






Extended Heisenberg-Kitaev model

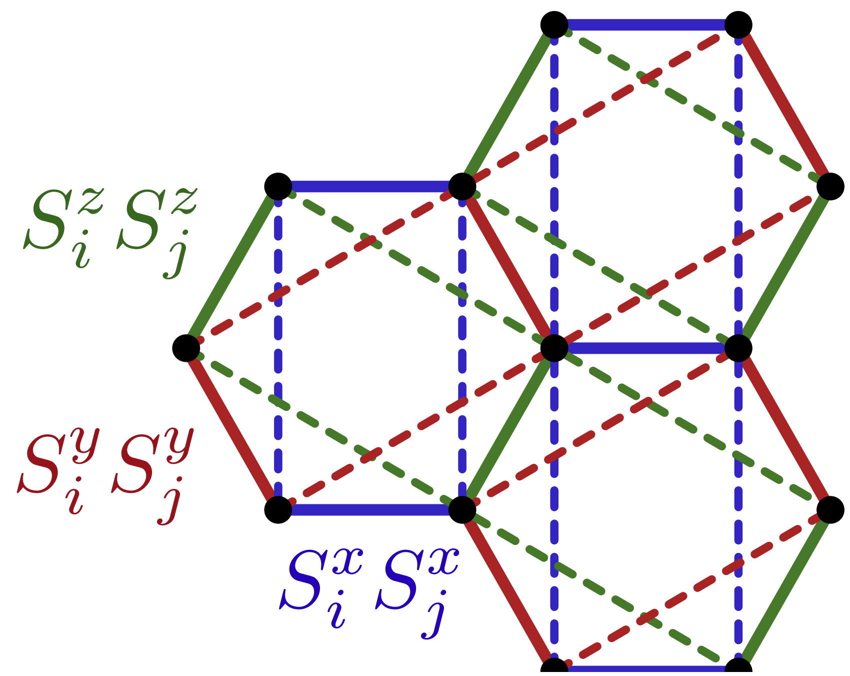
(1st + 2nd neighbor Kitaev *and* Heisenberg exchange)



$$H = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_{1\mathrm{K}} \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + J_2 \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_{2\mathrm{K}} \sum_{\langle\langle ij \rangle\rangle_\gamma} S_i^\gamma S_j^\gamma$$

J.Reuther, R.Thomale, SR, PRB 90, 100405(R) (2014)

Extended Heisenberg-Kitaev model

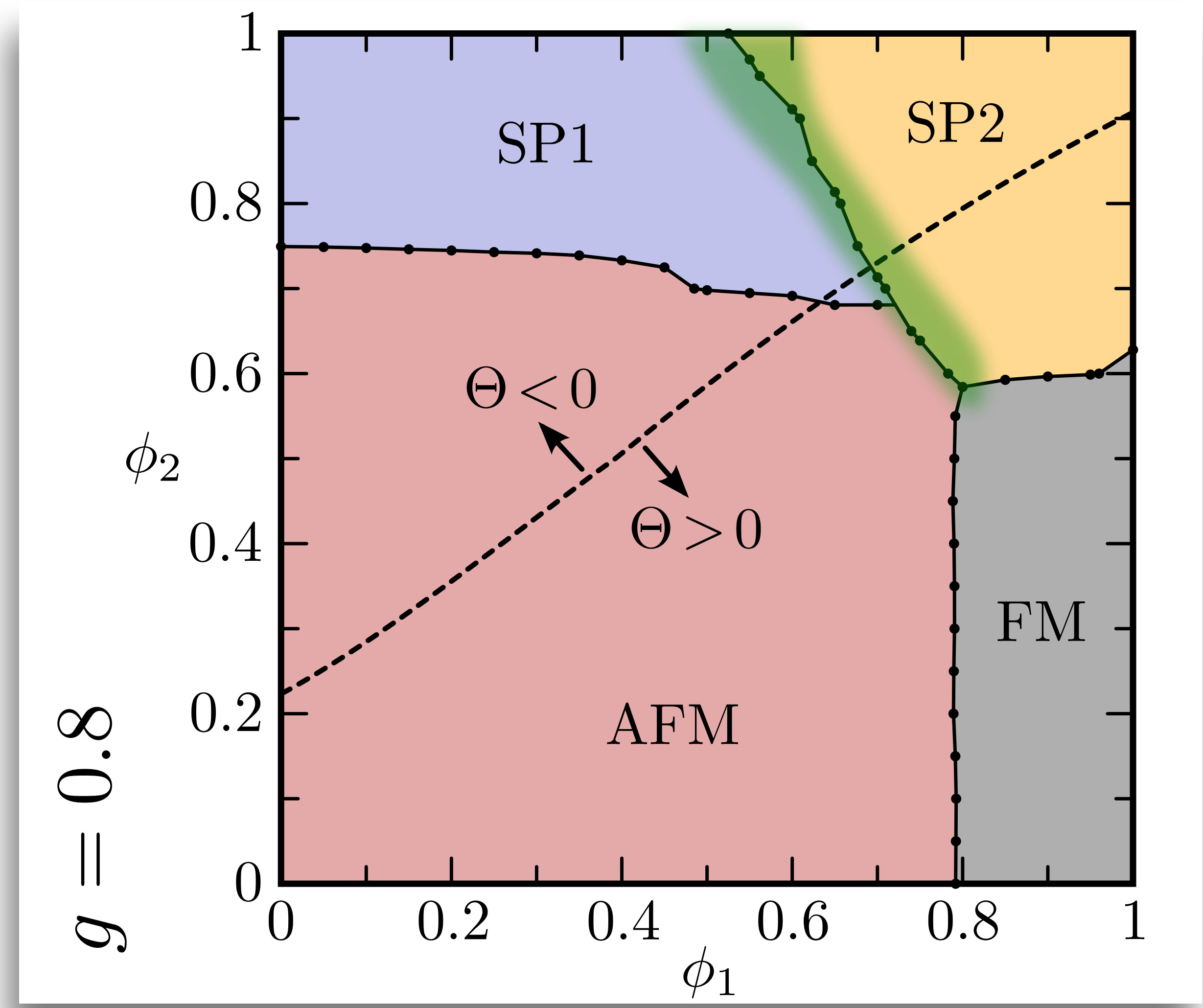


$$H = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_{1\mathrm{K}} \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + J_2 \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_{2\mathrm{K}} \sum_{\langle\langle ij \rangle\rangle_\gamma} S_i^\gamma S_j^\gamma$$

AFM FM FM AFM

$J_1 = \cos(\pi\Phi_1/2)$ $J_{1\mathrm{K}} = -\sin(\pi\Phi_1/2)$ $J_2 = -g\cos(\pi\Phi_2/2)$ $J_{2\mathrm{K}} = g\sin(\pi\Phi_2/2)$

Extended Heisenberg-Kitaev model



$$H = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_{1\mathrm{K}} \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + J_2 \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_{2\mathrm{K}} \sum_{\langle\langle ij \rangle\rangle_\gamma} S_i^\gamma S_j^\gamma$$

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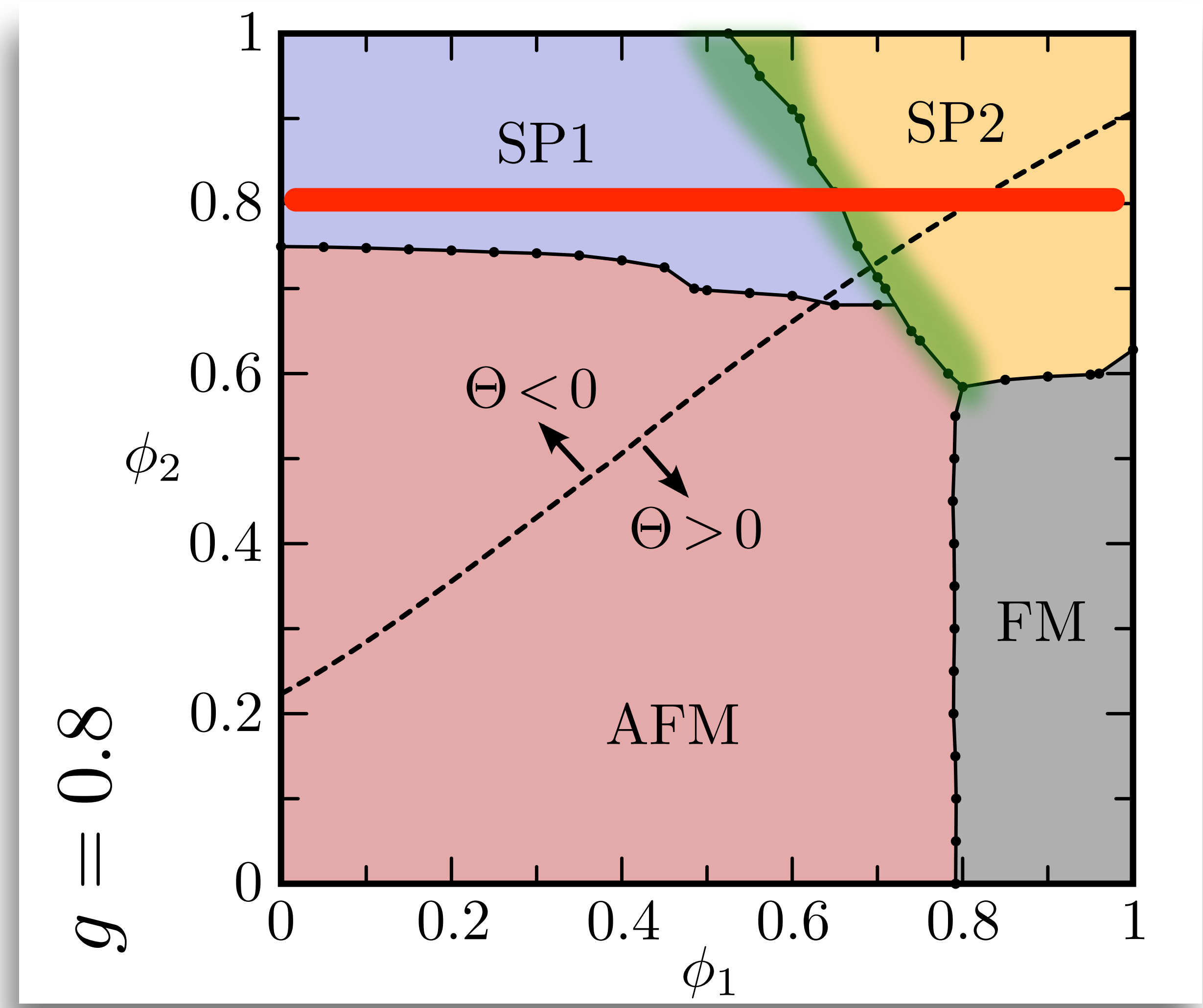

$$H = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_{1\mathrm{K}} \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + J_2 \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_{2\mathrm{K}} \sum_{\langle\langle ij \rangle\rangle_\gamma} S_i^\gamma S_j^\gamma$$

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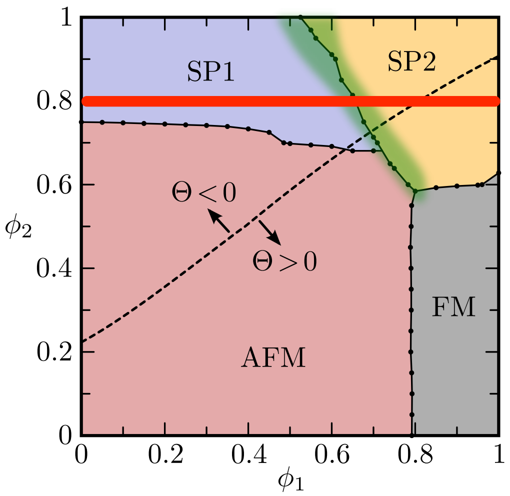
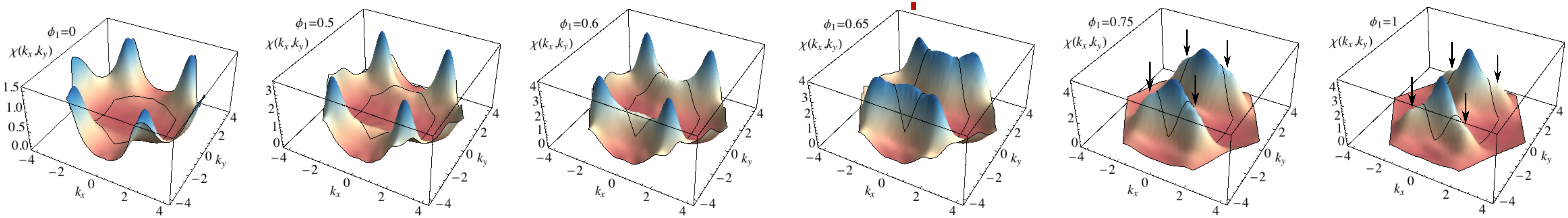


Spiral phases of the ext. Heisenberg-Kitaev model

$\Phi_2 = 0.8$

$\Phi_1 = 0$ $\Phi_1 = 0.5$ $\Phi_1 = 0.6$ $\Phi_1 = 0.65$ $\Phi_1 = 0.75$ $\Phi_1 = 1$



SP1-phase

Bragg peaks outside the 1st BZ

SP2-phase

Bragg peaks inside the 1st BZ

Curie-Weiss temperature < 0

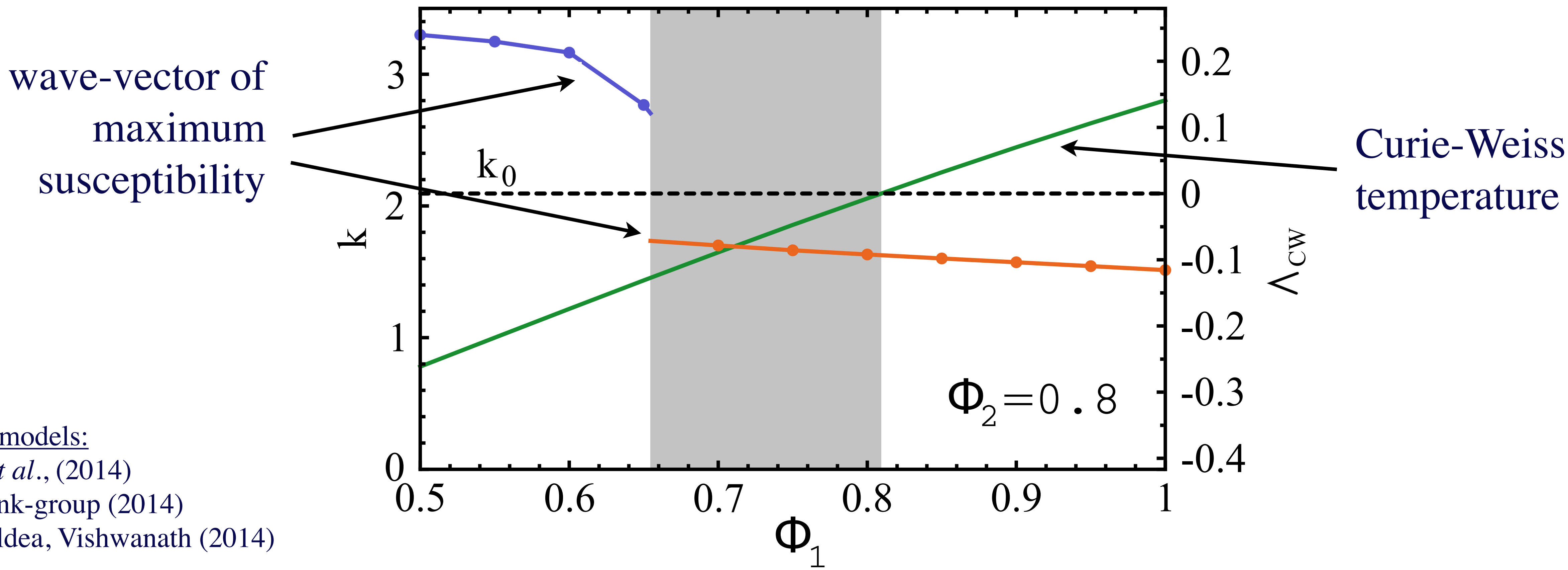
α-Li_2IrO_3

Tentative experimental evidence

1) incommensurate spiral order, Bragg peak(s) inside the 1st BZ

2) negative Curie-Weiss temperature

3) dominant exchange beyond nearest neighbors



Alternative models:
H.-Y. Kee *et al.*, (2014)
van den Brink-group (2014)
Kimchi, Coldea, Vishwanath (2014)

α-Li_2IrO_3

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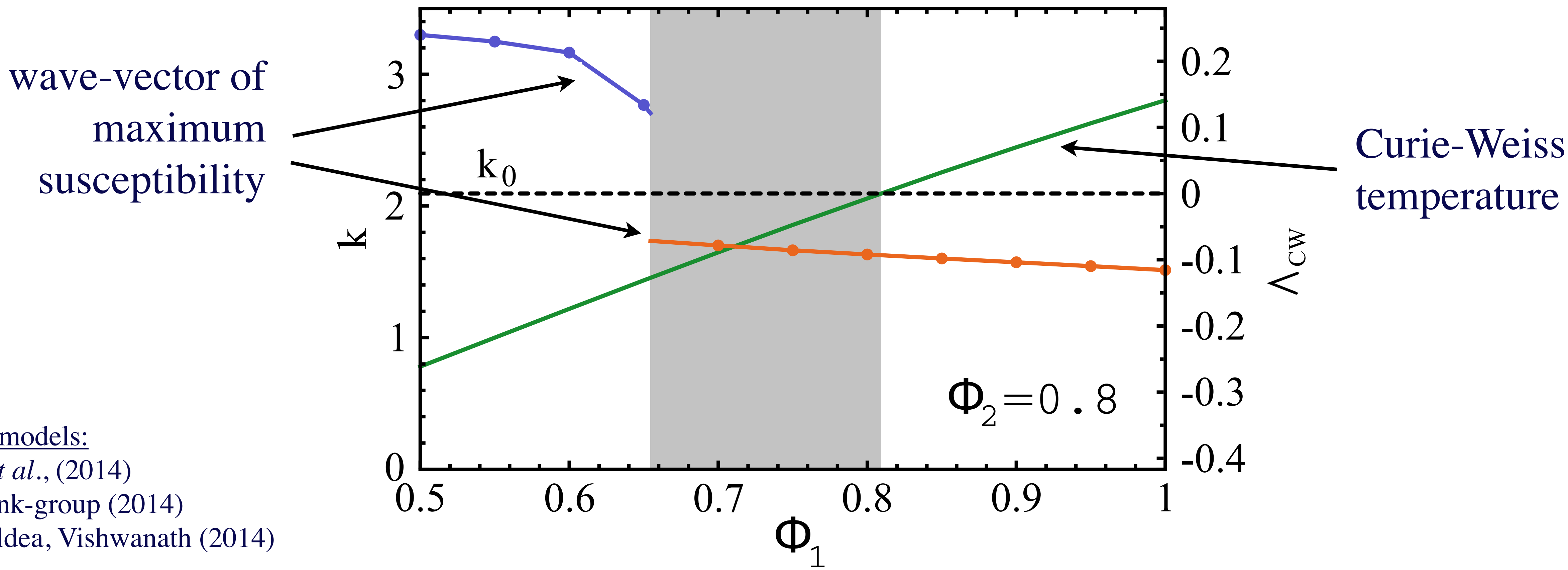

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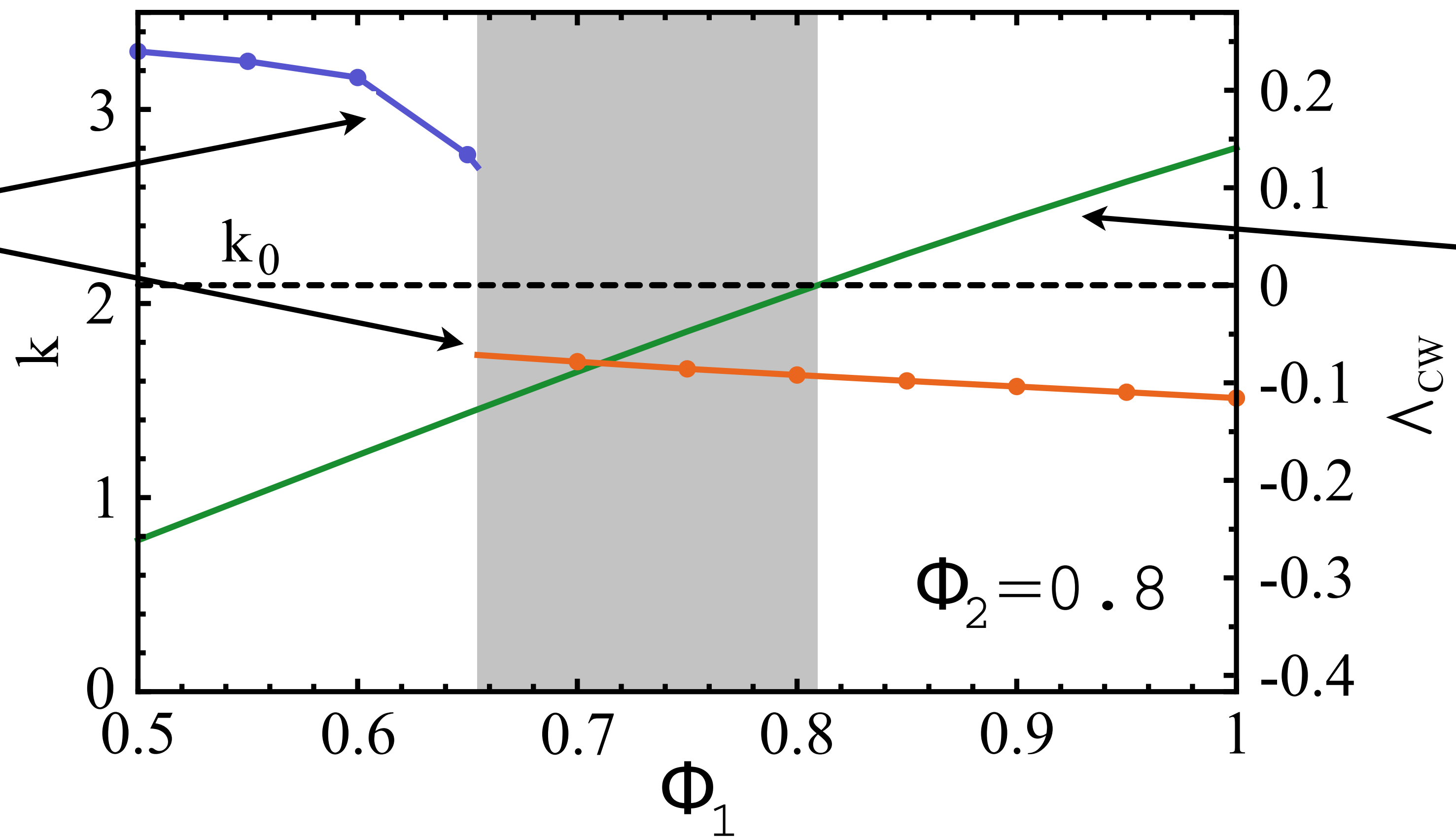

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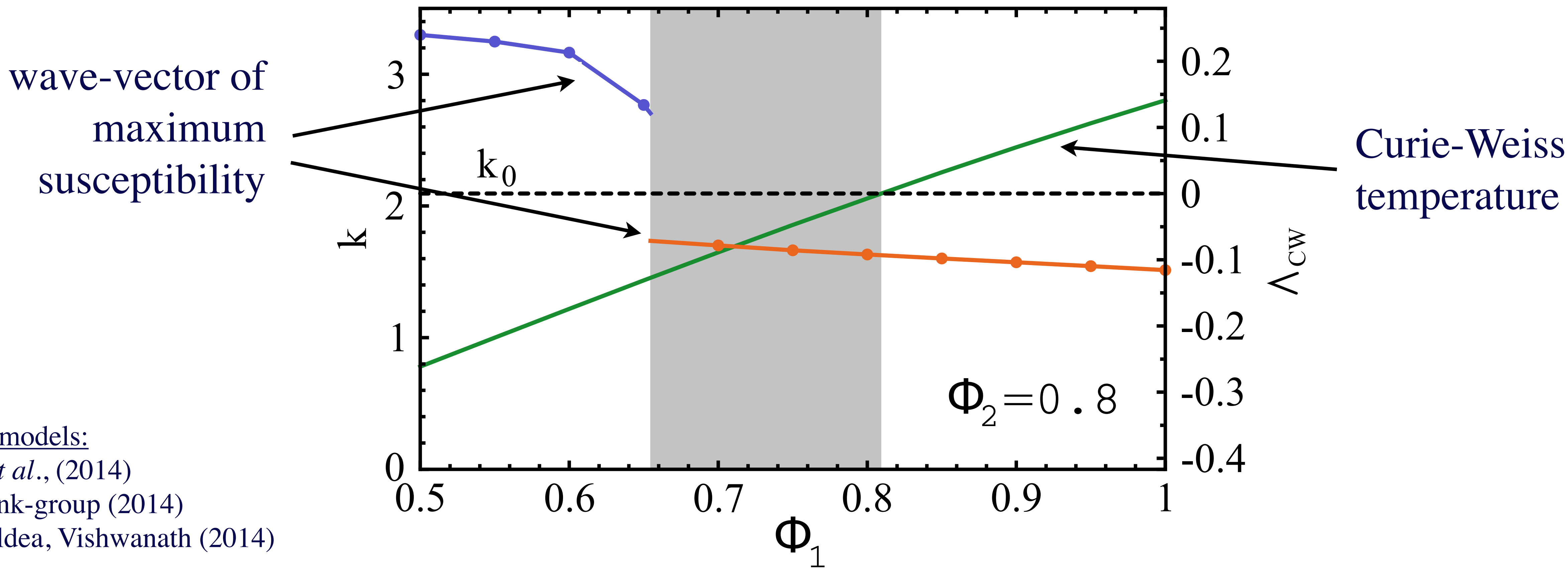

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Kimchi, Coldea, Vishwanath (2014)

α-Li_2IrO_3

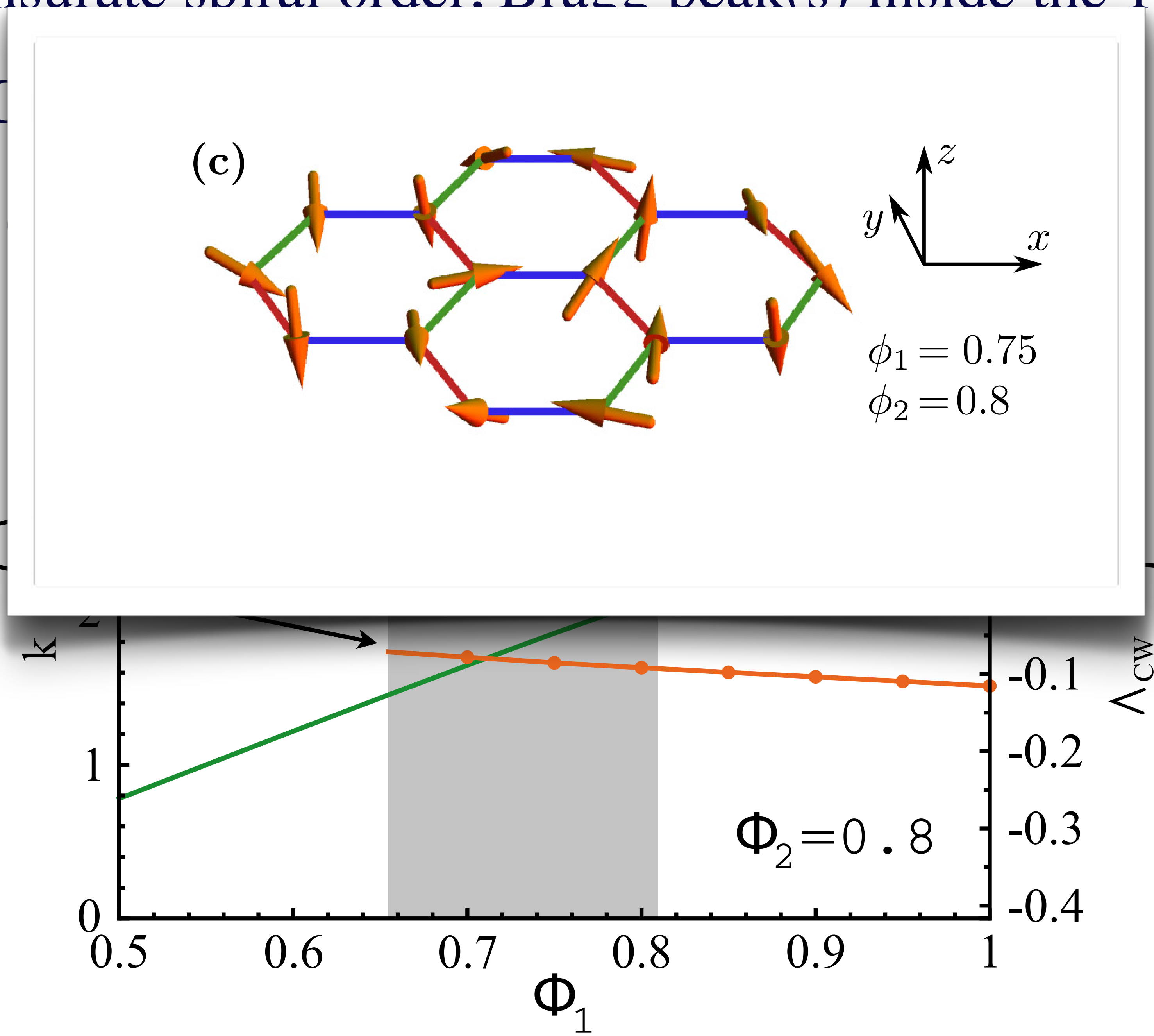
Tentative experimental evidence

1) incommensurate spiral order. Bragg peak(s) inside the 1st BZ

2) negative C

3) dominant

wave-vector of maximum susceptibility



Curie-Weiss temperature

Alternative models:
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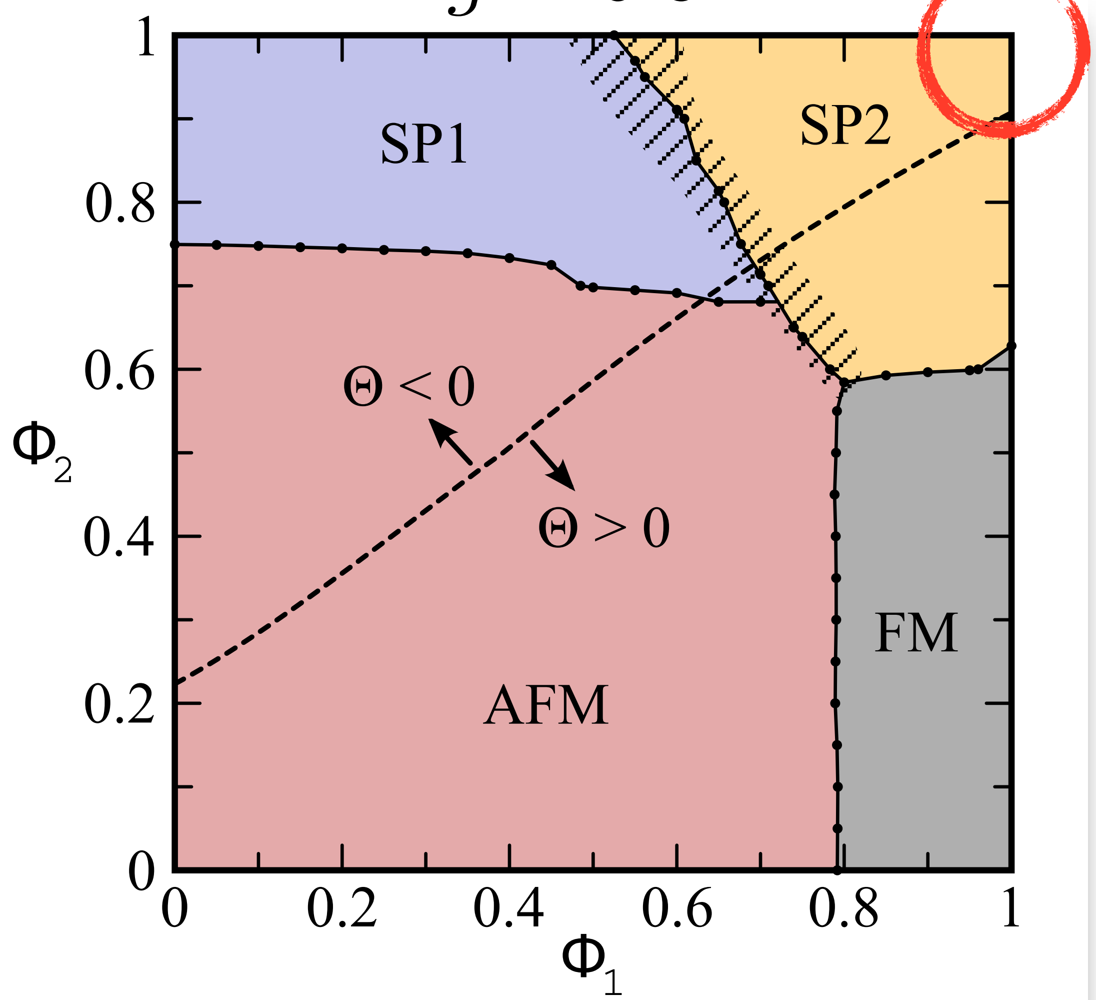
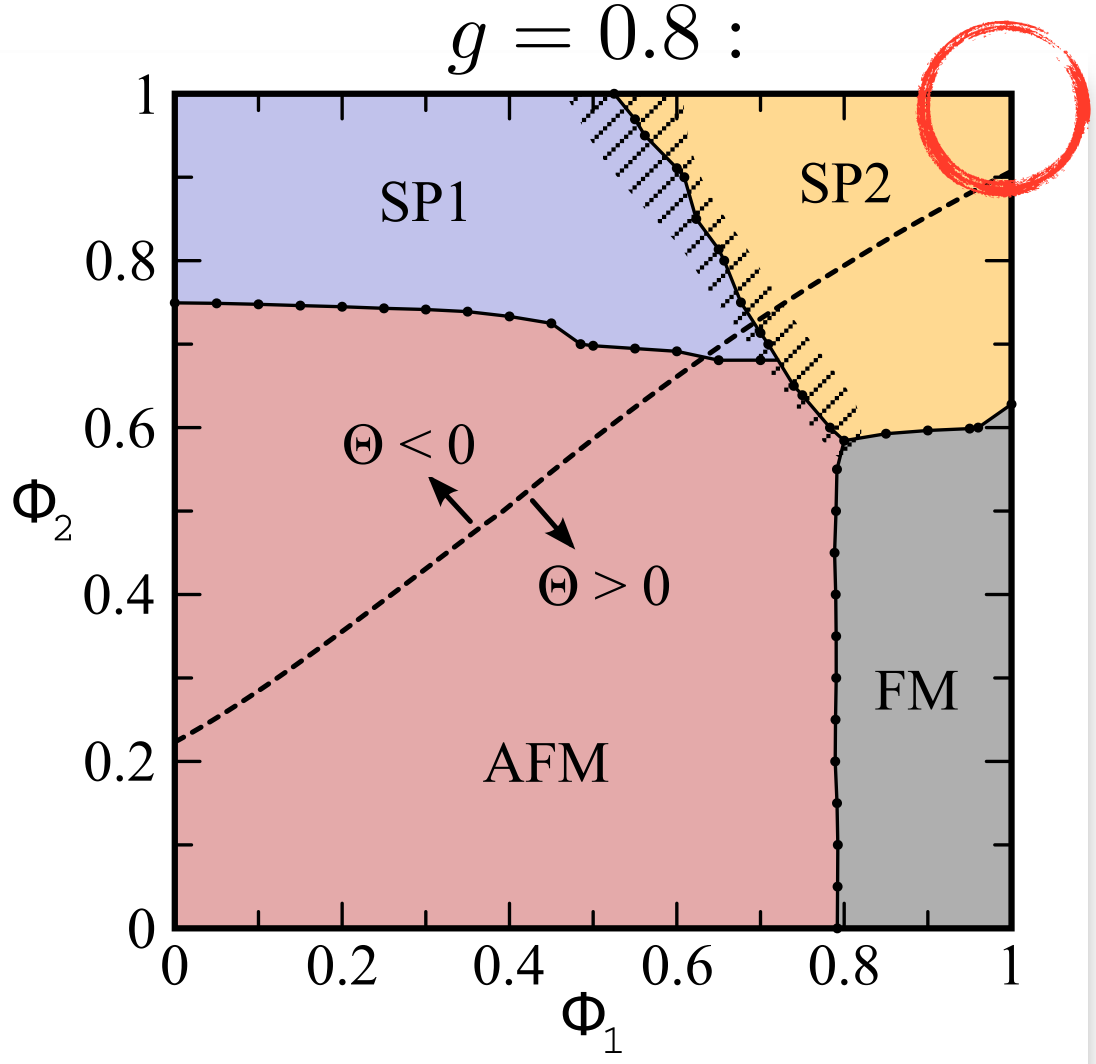
van den Brink-group (2014)
Kimchi, Coldea, Vishwanath (2014)

Vicinity to the Kitaev spin liquid ?

$g = 0.8:$



Vicinity to the Kitaev spin liquid ?



$$H_{K_1-K_2} = -\sum_{\langle ij\rangle_\gamma} S_i^\gamma S_j^\gamma + g \sum_{\langle\langle ij\rangle\rangle_\gamma} S_i^\gamma S_j^\gamma$$

cf. N.Perkins, P.Wölfle, arXiv:1408.3647

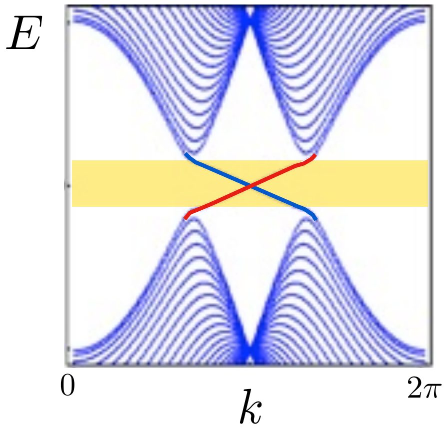
$g \to \infty$ decoupled Ising chains (Daghofer *et al*. 2012)

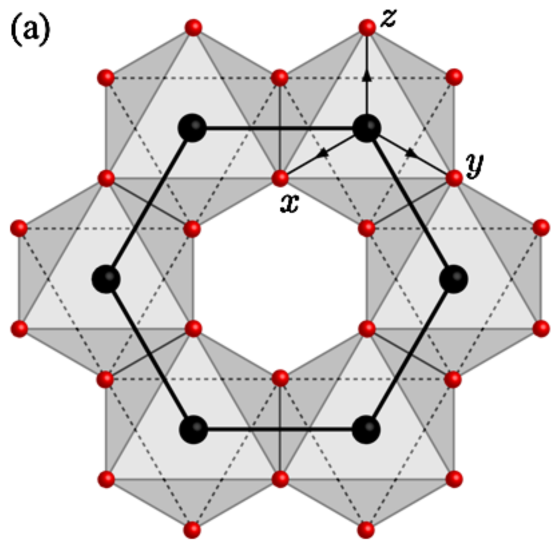
Outline:

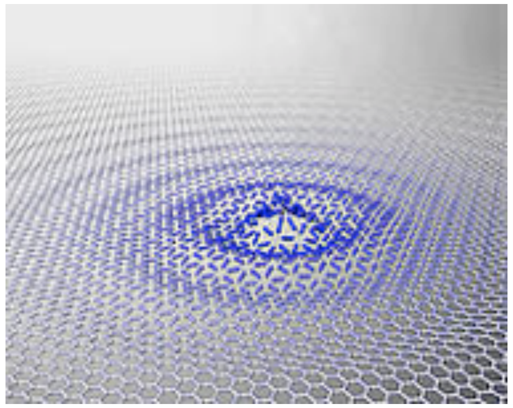
❖ From correlated topological insulators to the honeycomb iridates

❖ Minimal model for Li_2IrO_3

❖ Spin liquid phase in the "Hubbard-Kitaev model" on the Δ-lattice







“Kitaev-Hubbard model” on the Δ-lattice

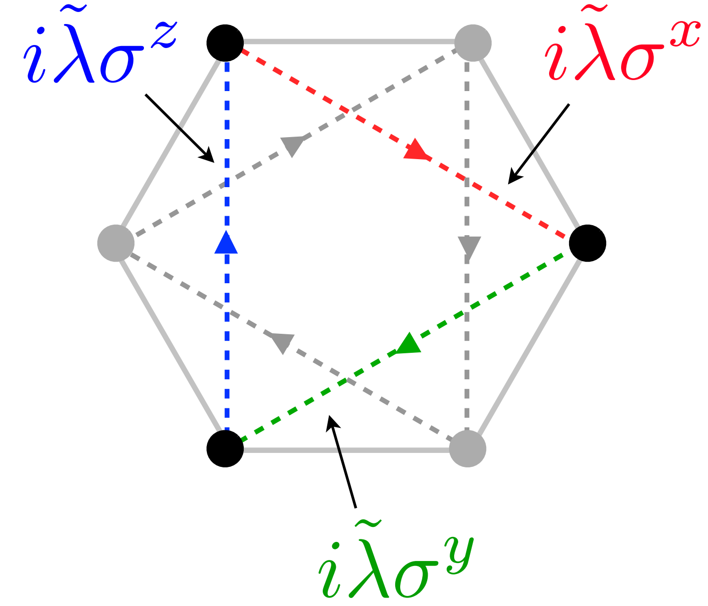
- various people speculated that the physics of $Ba_3IrTi_2O_9$ might be described by Heisenberg-Kitaev model on the Δ-lattice

  T.Dey *et al*., PRB 2012;

  I.Rousochatzakis, ..., M.Daghofer, arXiv:1209.5895

  M.Becker, ..., S.Trebst, arXiv:1409.6972

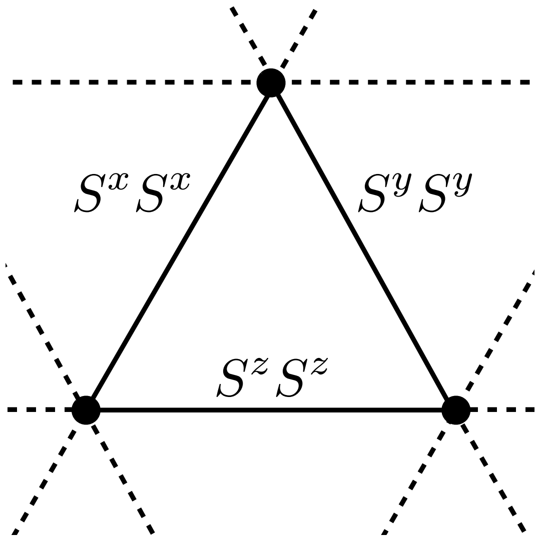
considering decoupled triangular lattice



$$H_0 = \sum_{\langle ij \rangle_\gamma} i\,\lambda\, c^\dagger_{i\alpha}\, \sigma^\gamma_{\alpha\beta}\, c_{j\beta}$$

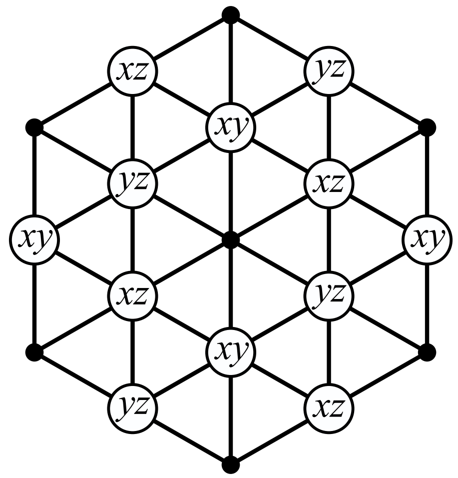
Kitaev-Heisenberg model on the triangular lattice

$$\mathcal{H}_\triangle = -\sum_{\langle ij\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + 2\sum_{\langle ij\rangle}\sum_{\gamma-\mathrm{links}} S_i^\gamma S_j^\gamma$$



- coordinate transformation:

(see also Kimchi, Vishvanath)



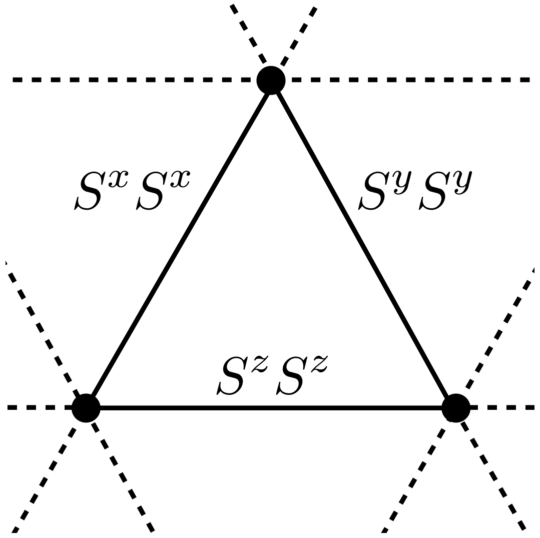
$$\begin{aligned}
i \in \bullet: &\quad \tilde{\mathbf{S}}_i = (S_i^x, S_i^y, S_i^z),\\
i \in xy: &\quad \tilde{\mathbf{S}}_i = (-S_i^x, -S_i^y, S_i^z),\\
i \in xz: &\quad \tilde{\mathbf{S}}_i = (-S_i^x, S_i^y, -S_i^z),\\
i \in yz: &\quad \tilde{\mathbf{S}}_i = (S_i^x, -S_i^y, -S_i^z);
\end{aligned}$$

cf. Khaliullin (2005)

Reuther, Thomale, SR (2012)

Kitaev-Heisenberg model on the triangular lattice

$$\mathcal{H}_\triangle = -\sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + 2 \sum_{\langle ij \rangle} \sum_{\gamma-\text{links}} S_i^\gamma S_j^\gamma$$



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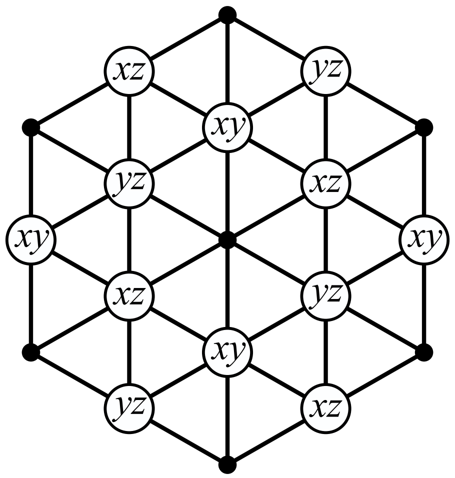


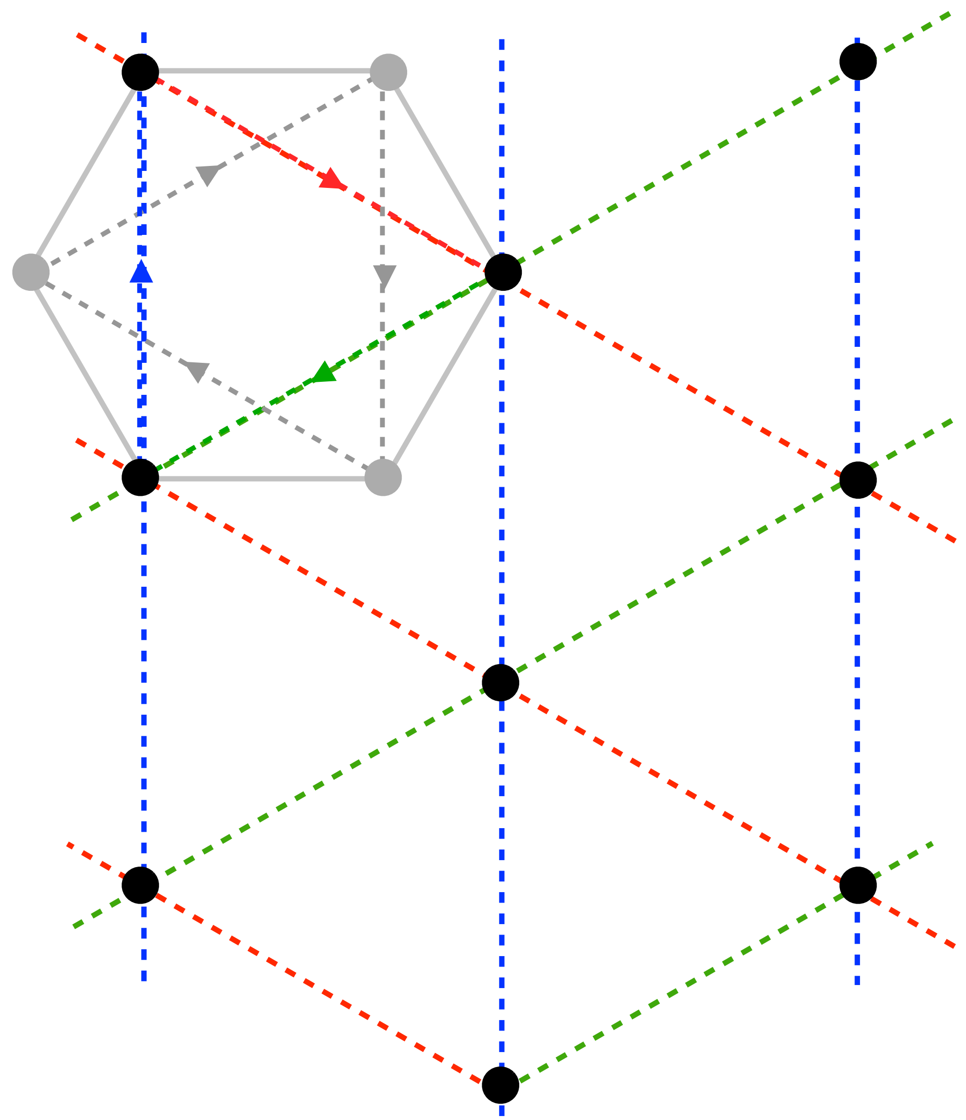
$$\begin{aligned}
i \in \bullet: \quad & \tilde{\mathbf{S}}_i = (S_i^x, S_i^y, S_i^z), \\
i \in xy: \quad & \tilde{\mathbf{S}}_i = (-S_i^x, -S_i^y, S_i^z), \\
i \in xz: \quad & \tilde{\mathbf{S}}_i = (-S_i^x, S_i^y, -S_i^z), \\
i \in yz: \quad & \tilde{\mathbf{S}}_i = (S_i^x, -S_i^y, -S_i^z);
\end{aligned}$$

cf. Khaliullin (2005)

- transformed spin Hamiltonian: $\mathcal{H} = \sum_{\langle ij \rangle} \tilde{\boldsymbol{S}}_i \tilde{\boldsymbol{S}}_j$
- transforming 120-degree Neel order back = spiral order

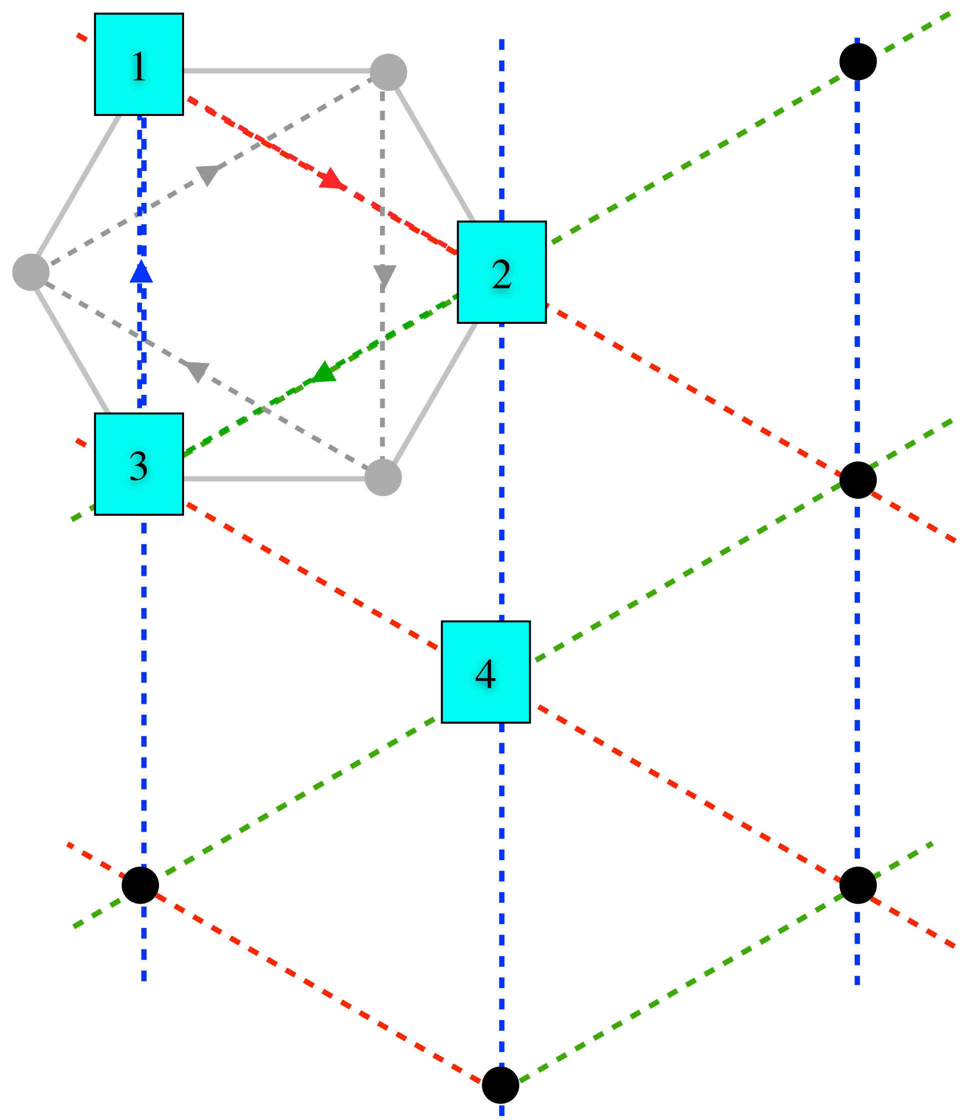
Reuther, Thomale, SR (2012)

considering decoupled triangular lattice



$$H_0 = \sum_{\langle ij \rangle_\gamma} i\,\lambda\, c^\dagger_{i\alpha}\, \sigma^\gamma_{\alpha\beta}\, c_{j\beta}$$

considering decoupled triangular lattice

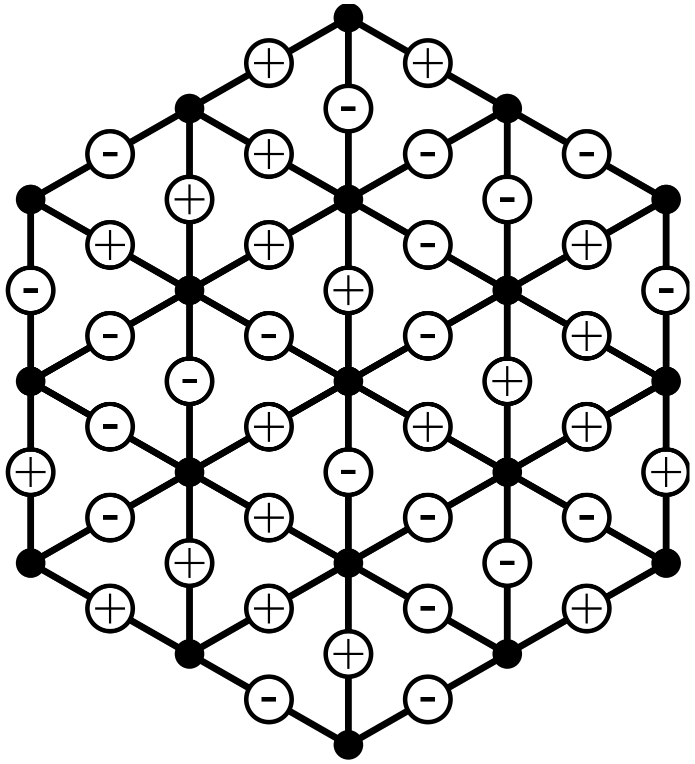


$$H_0 = \sum_{\langle ij \rangle_\gamma} i\,\lambda\, c^\dagger_{i\alpha}\, \sigma^\gamma_{\alpha\beta}\, c_{j\beta}$$

"Kitaev-Hubbard model"

Let's apply Klein-mapping for $U = 0$

after coordinate transformation: all hoppings are real $\pm t$



"Kitaev-Hubbard model"

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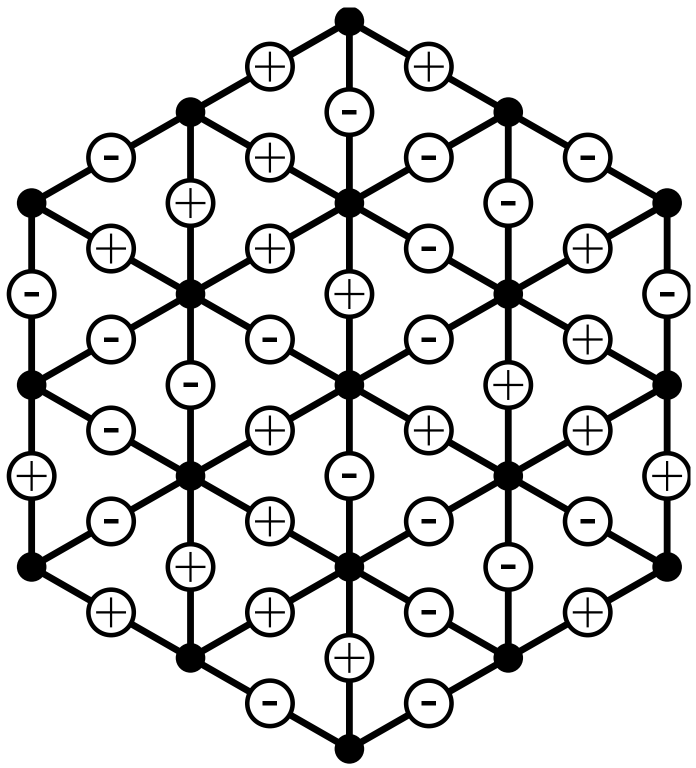

$-1 = e^{i\pi}$

"Kitaev-Hubbard model"

Let's apply Klein-mapping for U = 0

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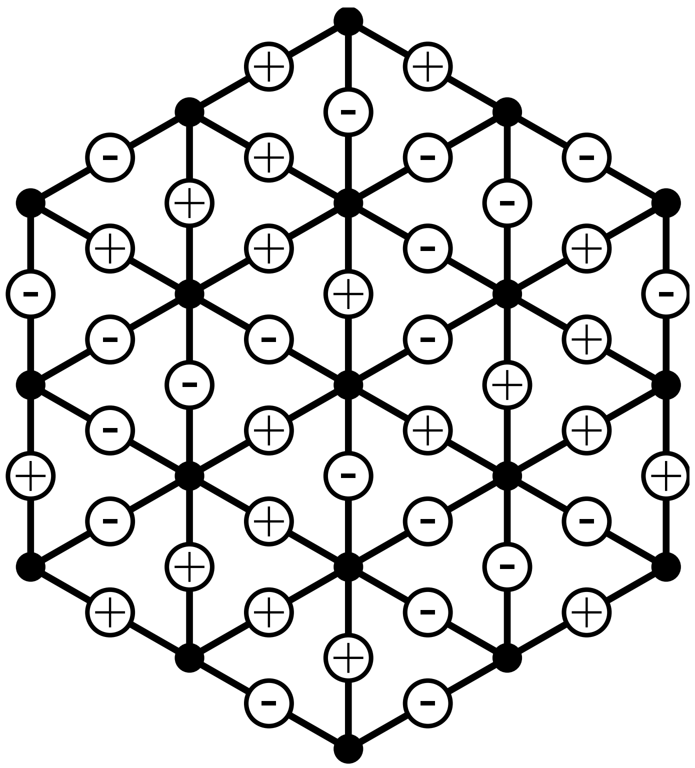
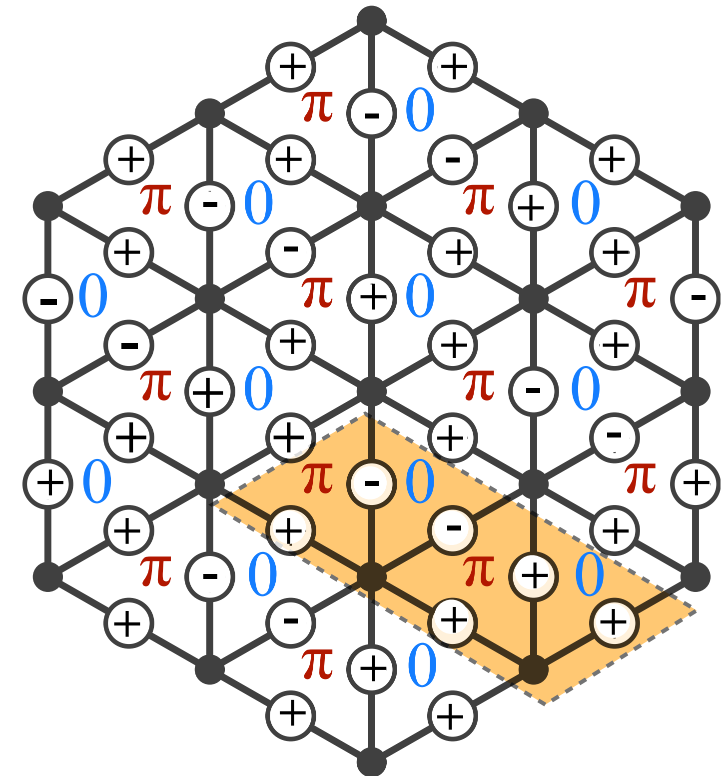


$$-1 = e^{i\pi}$$

alternating "0-π" flux lattice



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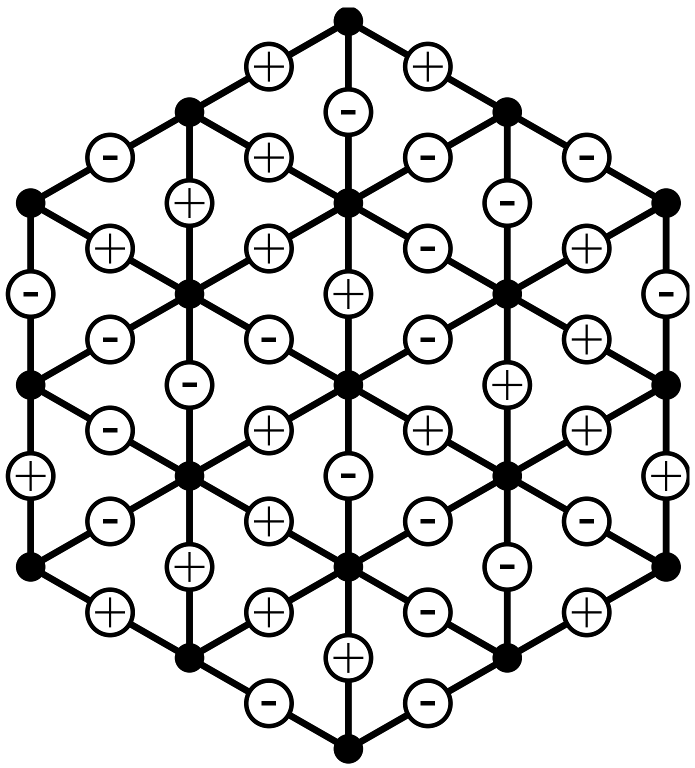

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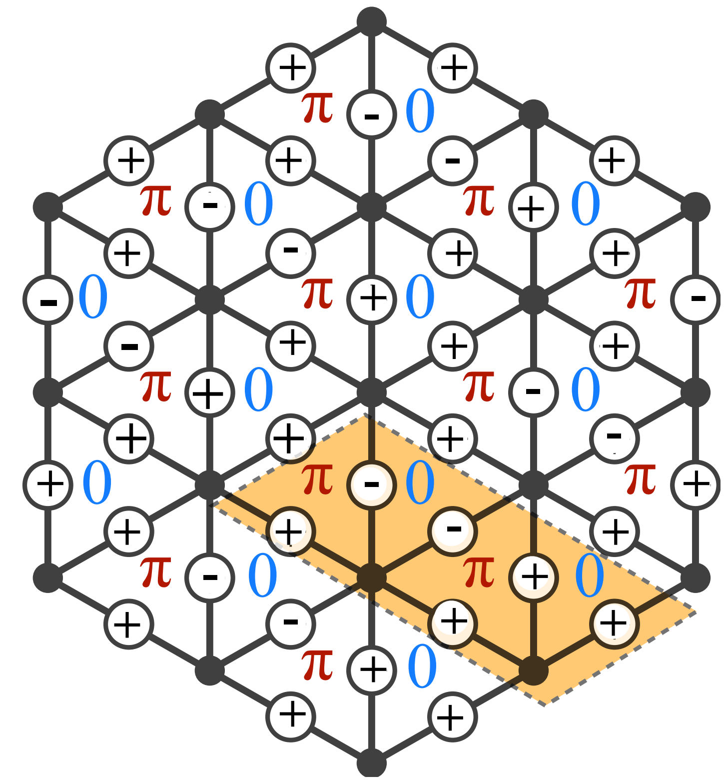
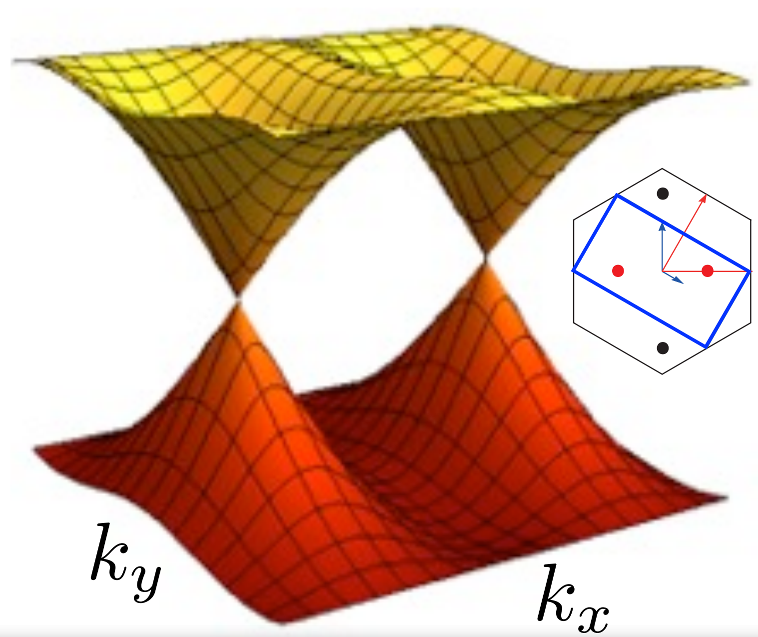
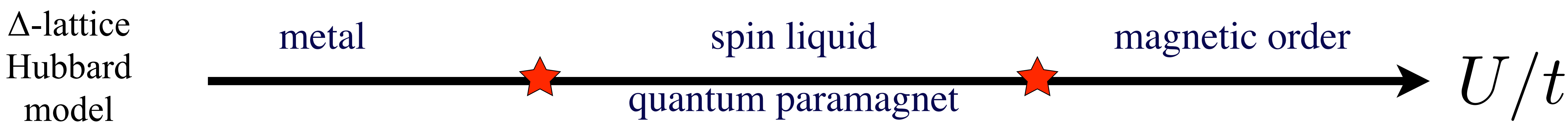


flux pattern corresponds to a Dirac semi-metal at U=0



let's speculate...



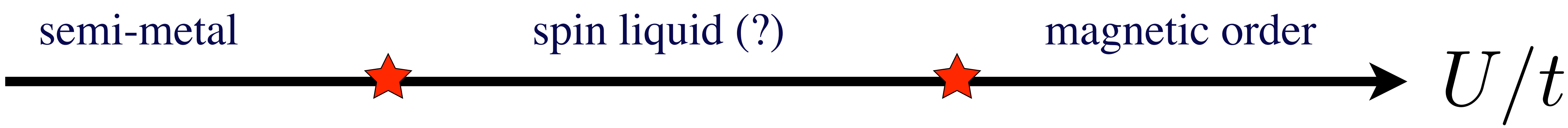
P.Lee, Motrunich, Senthil, *and many other people...*

let’s speculate…

Δ-lattice Hubbard model

P.Lee, Motrunich, Senthil, *and many other people*…

HC-lattice Hubbard model



Meng *et al.*, Nature (2010); Sorella *et al.*, Sci. Rep. (2012); Assaad & Herbut, PRX (2013);

let's speculate...

Δ-lattice Hubbard model

metal — spin liquid / quantum paramagnet — magnetic order U/t

P.Lee, Motrunich, Senthil, *and many other people...*

HC-lattice Hubbard model

semi-metal — spin liquid (?) — magnetic order U/t

Meng *et al.*, Nature (2010); Sorella *et al.*, Sci. Rep. (2012); Assaad & Herbut, PRX (2013);

Δ-lattice π-flux Hubbard model

semi-metal — magnetic order U/t

let's speculate...

Δ-lattice
Hubbard
model

P.Lee, Motrunich, Senthil, *and many other people...*

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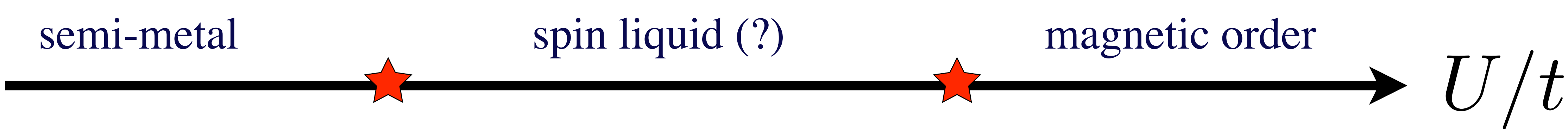

Meng *et al.*, Nature (2010); Sorella *et al.*, Sci. Rep. (2012); Assaad & Herbut, PRX (2013);

Δ-lattice
π-flux
Hubbard
model

Let’s go beyond Heisenberg exchange

$$
\begin{aligned}
\mathcal{H} = &\left(\frac{4t^2}{U} + \frac{12t^4}{U^3}\right) \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + \frac{12t^4}{U^3} \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j \\
&+ \frac{4t^4}{U^3} \sum_{\langle\langle\langle ij \rangle\rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j - \frac{80t^3}{U^4} \sum_{p} \Big[(\boldsymbol{S}_1 \boldsymbol{S}_2)(\boldsymbol{S}_3 \boldsymbol{S}_4) \\
&+ (\boldsymbol{S}_2 \boldsymbol{S}_3)(\boldsymbol{S}_1 \boldsymbol{S}_4) - (\boldsymbol{S}_1 \boldsymbol{S}_3)(\boldsymbol{S}_2 \boldsymbol{S}_4) \Big] .
\end{aligned}
$$

compare to ordinary Δ-lattice Hubbard model:

resonating valence bond loops

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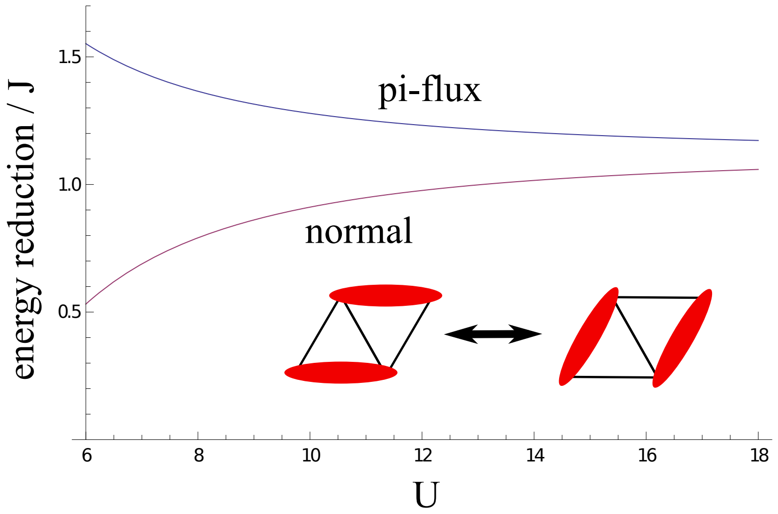
resonating valence bond loops



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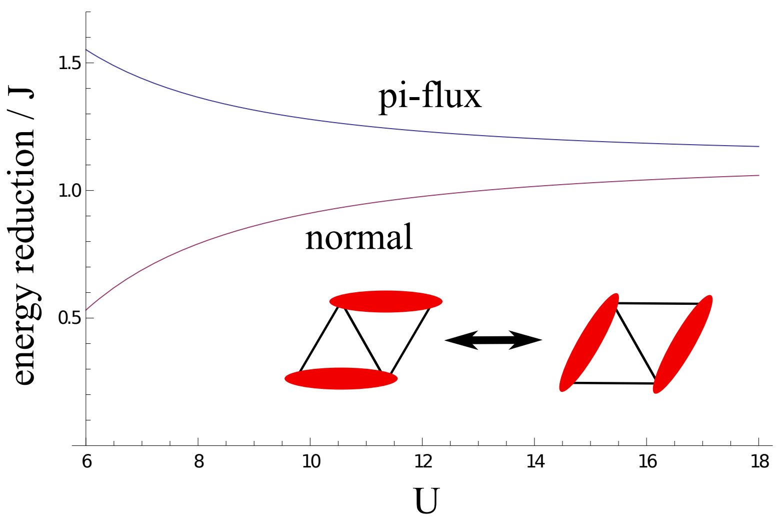

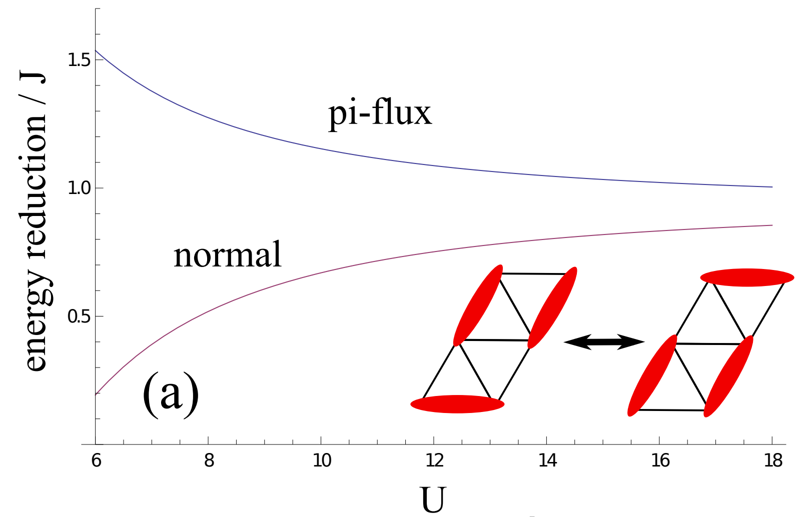

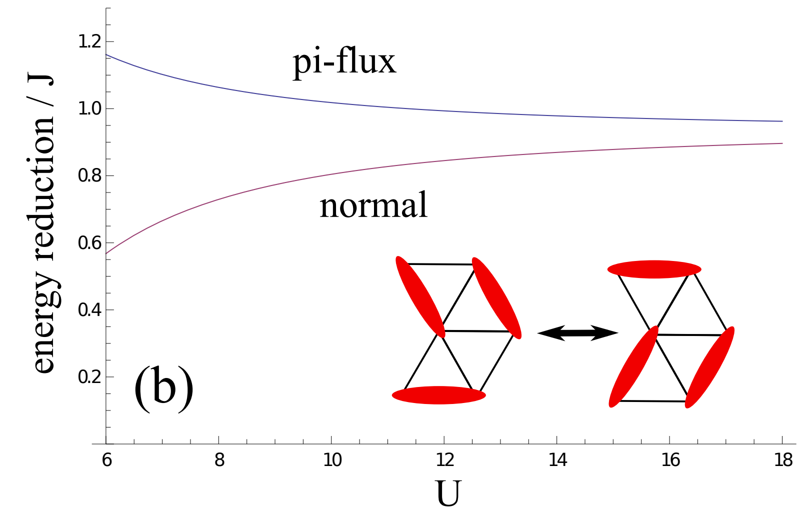

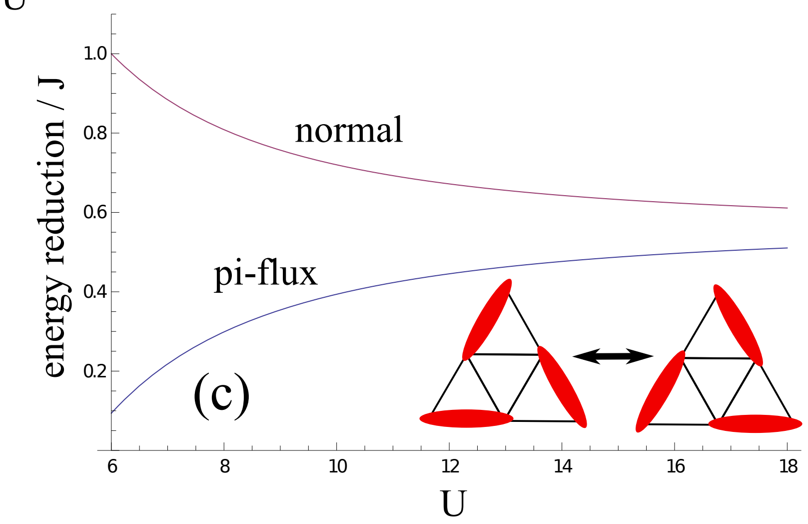

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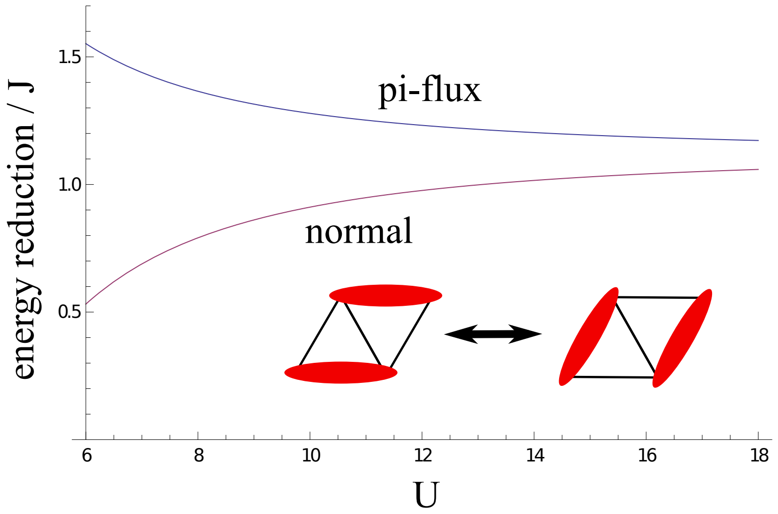
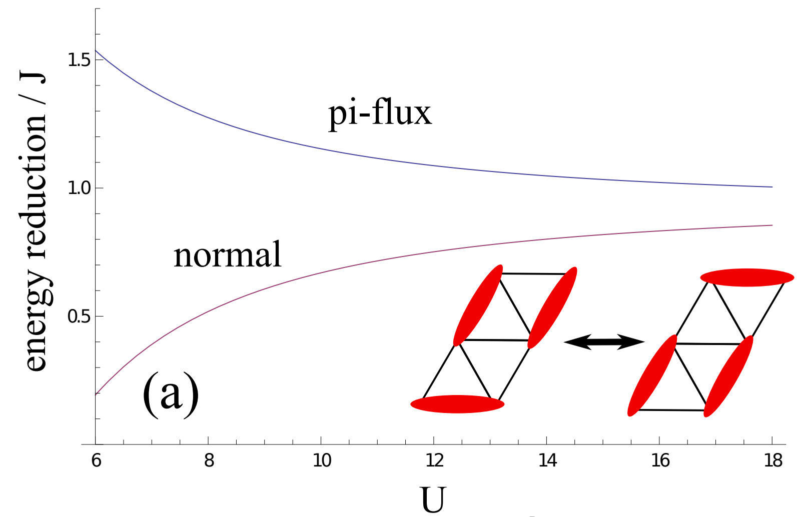
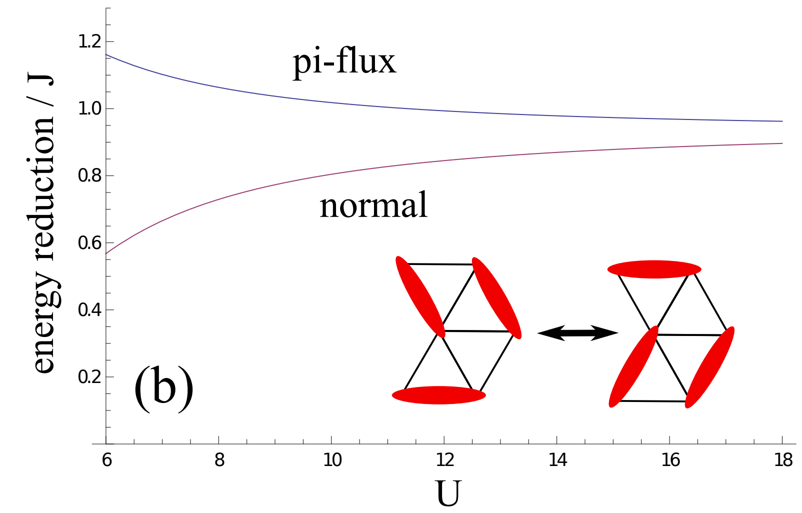
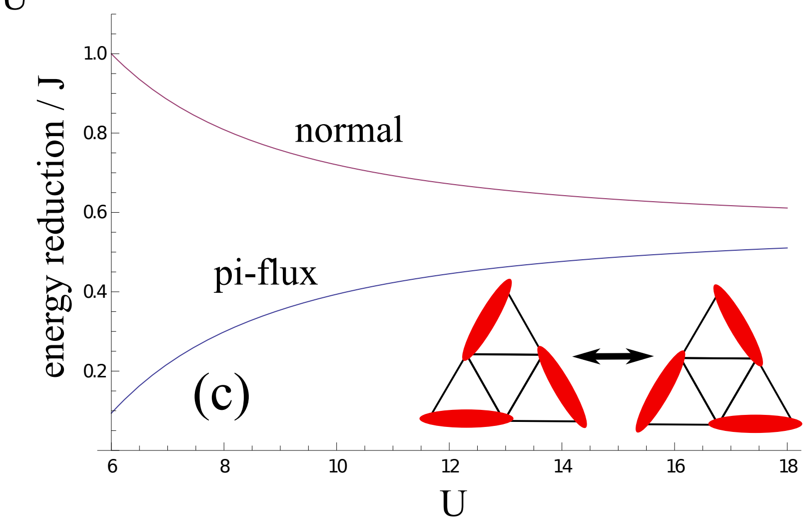




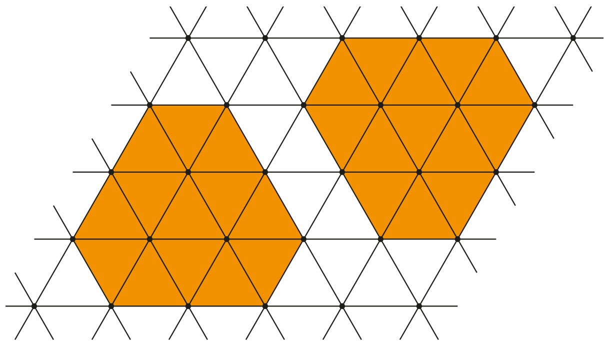




π-flux Δ-lattice wins !!!

Δ-lattice π-flux Hubbard model

- apply Variational Cluster Approach (VCA)
- use 12-site cluster



opening of single-particle gap vs. onset of magnetization:

Δ-lattice π-flux Hubbard model

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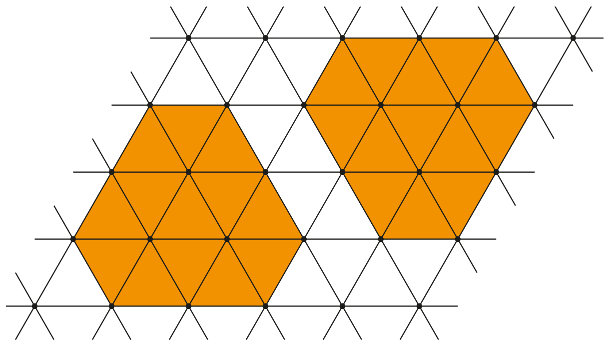

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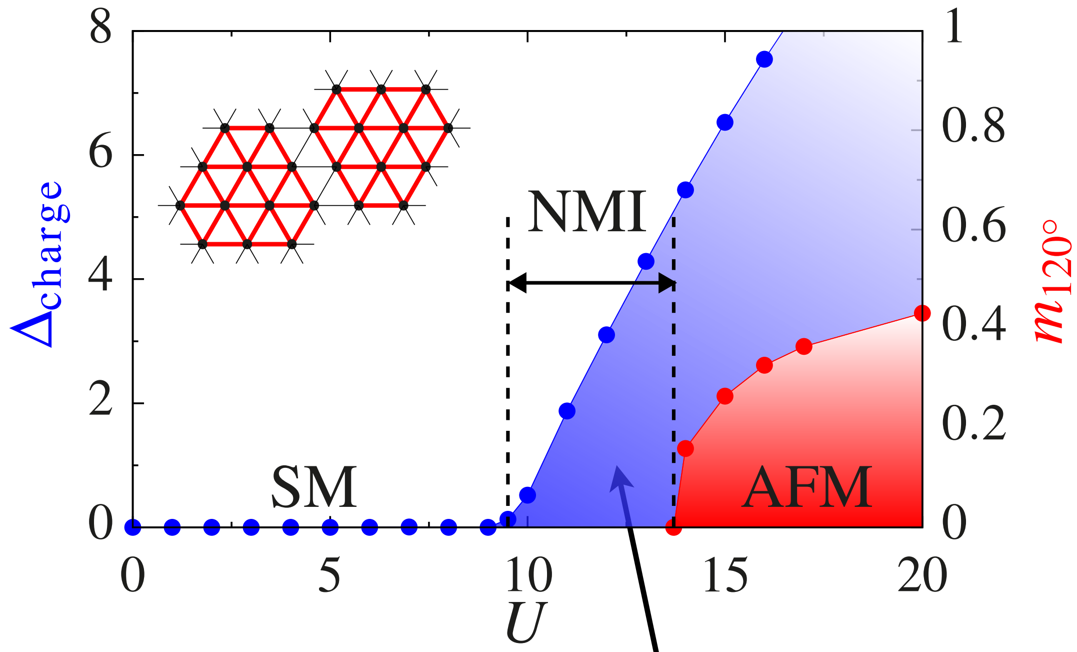
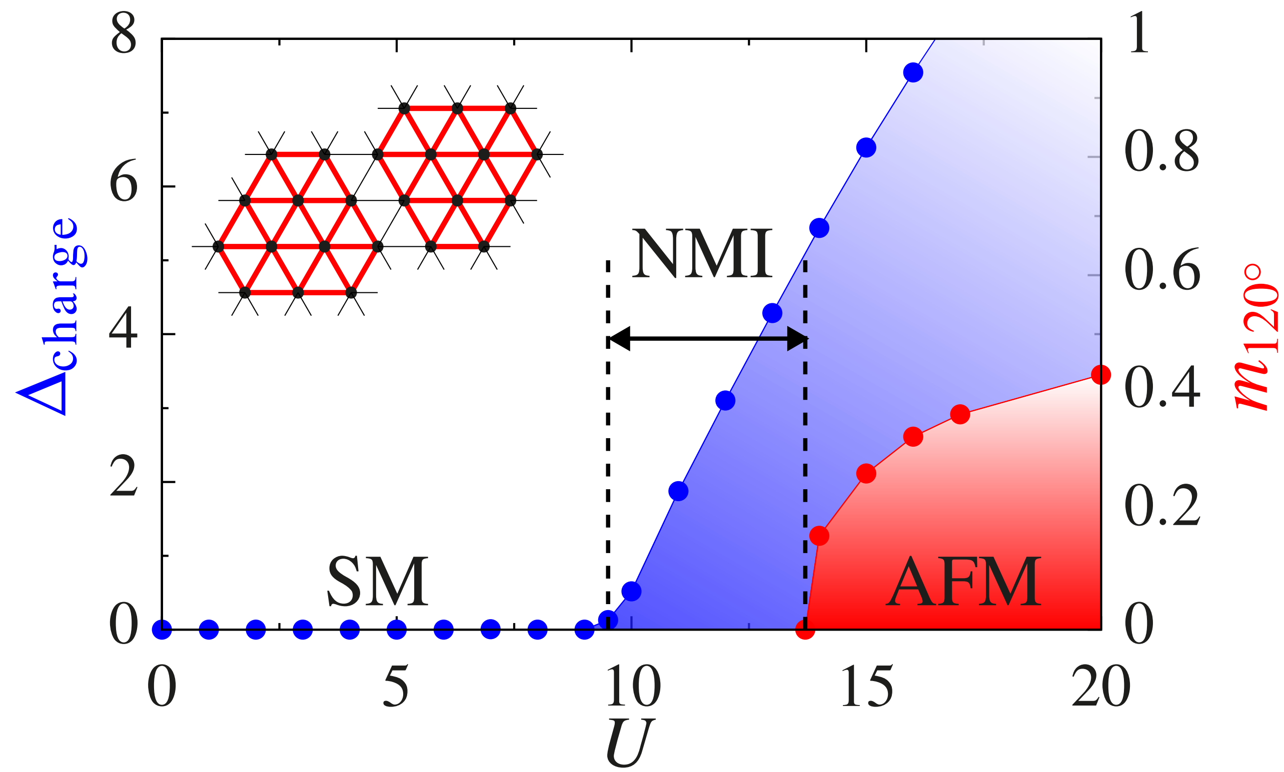


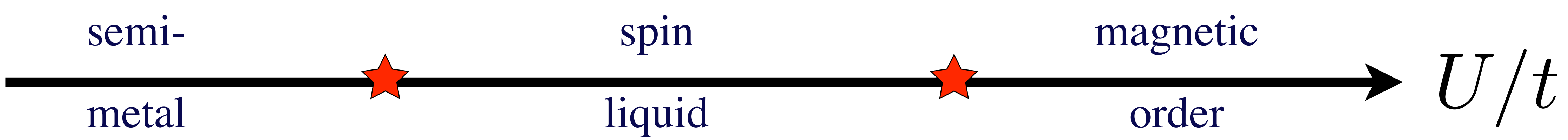
compare to ordinary Δ-lattice Hubbard model: $U_{c,2} = 8.5$

Non-magnetic insulator within VCA

- Must be a quantum paramagnet !
- Strong hint for a spin-liquid phase (not a metal, not a magnet)

Δ-lattice π-flux Hubbard model





SR, M.Laubach, J.Reuther, R.Thomale, arXiv:1410.soon

Conclusion

- Spiral order in the honeycomb iridate Li_2IrO_3:
  extended HK model explains all the tentative experimental evidence

- Vicinity of the spiral phase to the Kitaev phase

- Spin-liquid phase of the Δ-lattice π-flux Hubbard model

J.Reuther, R.Thomale, SR, PRB 86, 155127 (2012)

J.Reuther, R.Thomale, SR, PRB 90, 100405(R) (2014)

SR, M.Laubach, J.Reuther, R.Thomale, arXiv:1410.soon