Phase diagram of $K_1 - K_2$ model on the honeycomb lattice

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Novel States in Spin-Orbit Coupled Quantum Matter:
from Models to Materials

July 28, KITP

Collaborators

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- **Peter Woelfle (KTM)**
- Stephan Rachel (TU Dresden)
- Johannes Reuter (TU Berlin)
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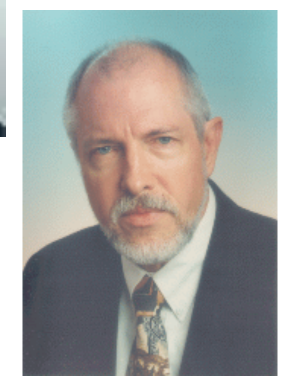
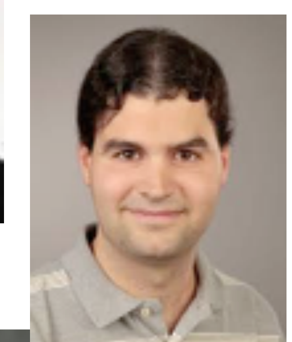
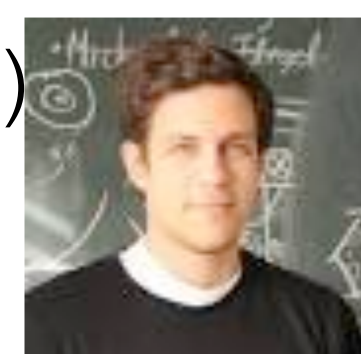


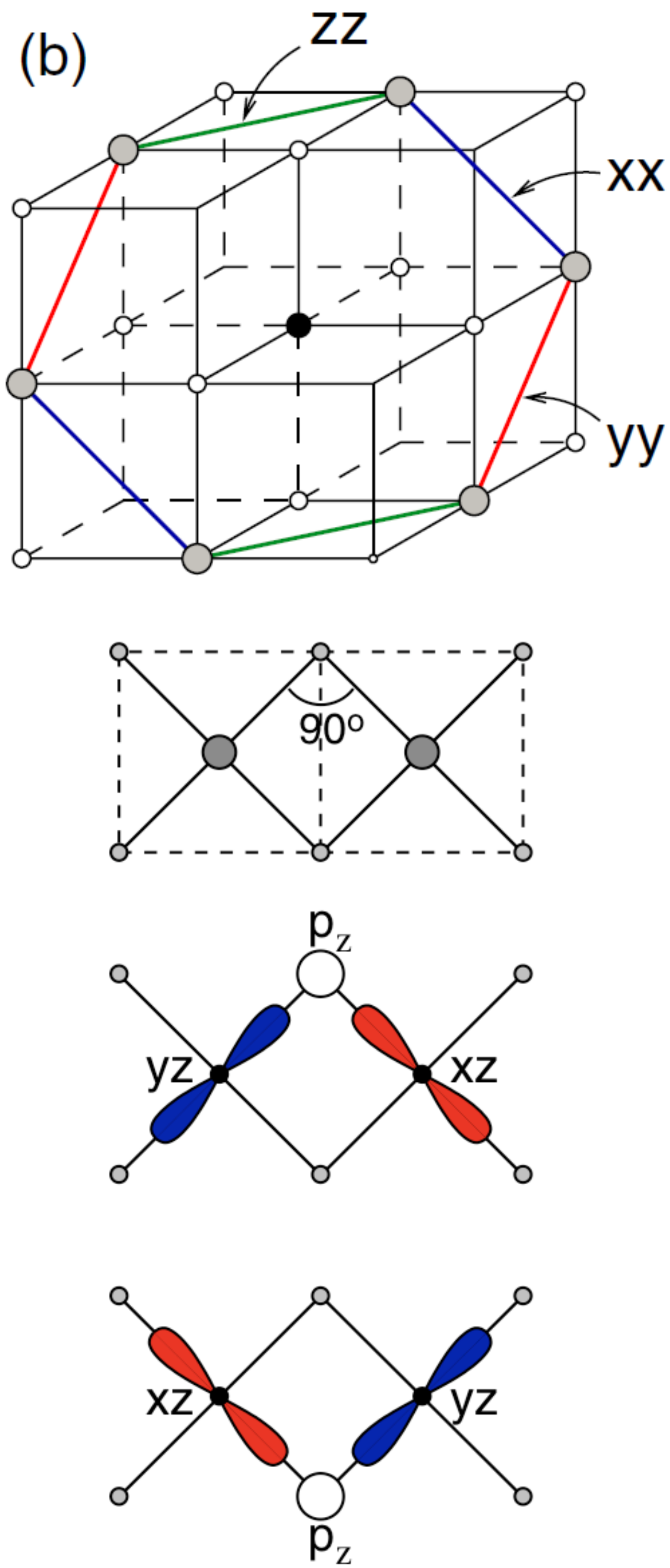
Outline

- Motivations
- Importance of K_2 interaction to resolve the puzzles related to Na_2IrO_3
- K_1-K_2 model
- Classical and quantum phase diagrams.
- Conclusions

I.Rousochatzakis, J. Reuther, R. Thomale, S. Rachel, N. B. Perkins, arXiv: 1506.09185

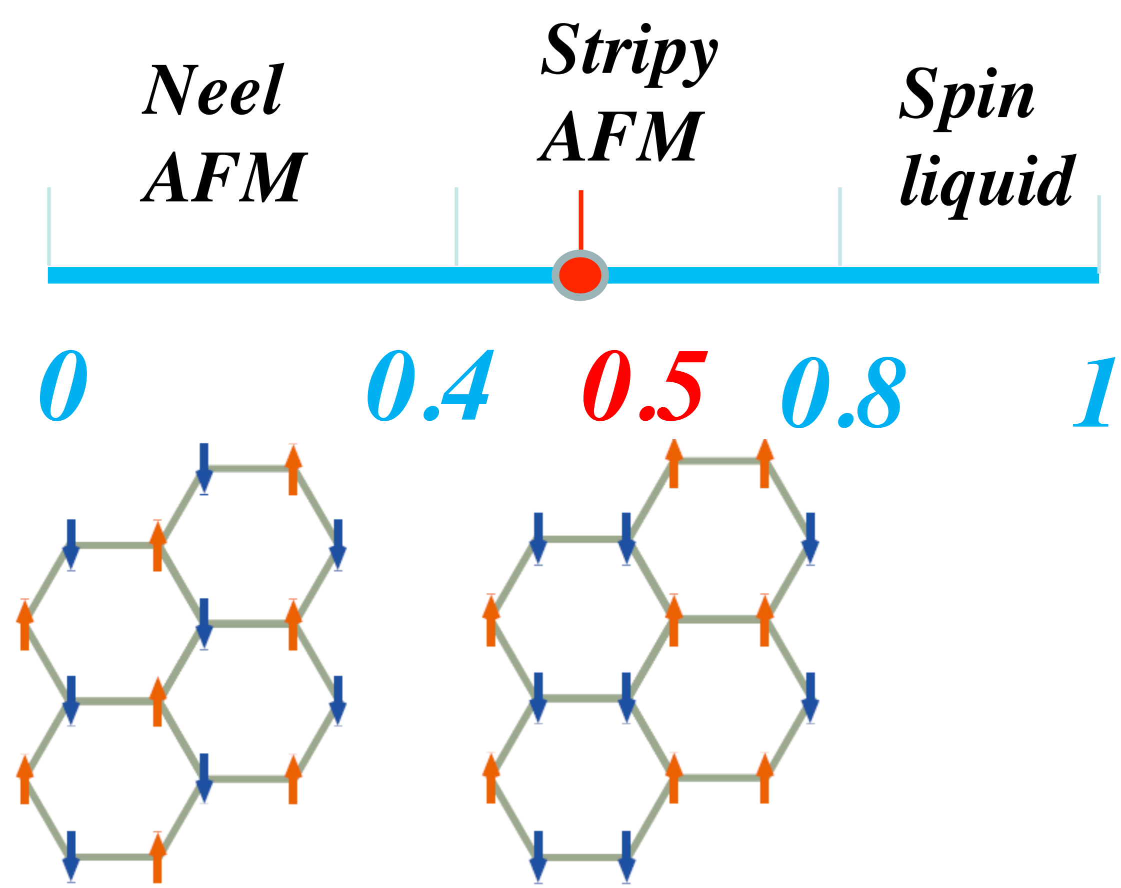
C. Price, I.Rousochatzakis, N. B. Perkins, in preparation

Motivations: Super-exchange in A_2IrO_3



G. Jackeli and G. Khaliullin,
PRL 102, 017205 (2009)

$$\mathcal{H} = -J_K \sum_{\langle ij \rangle_a} \hat{\sigma}_i^a \hat{\sigma}_j^a + J_H \sum_{\langle ij \rangle} \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j$$

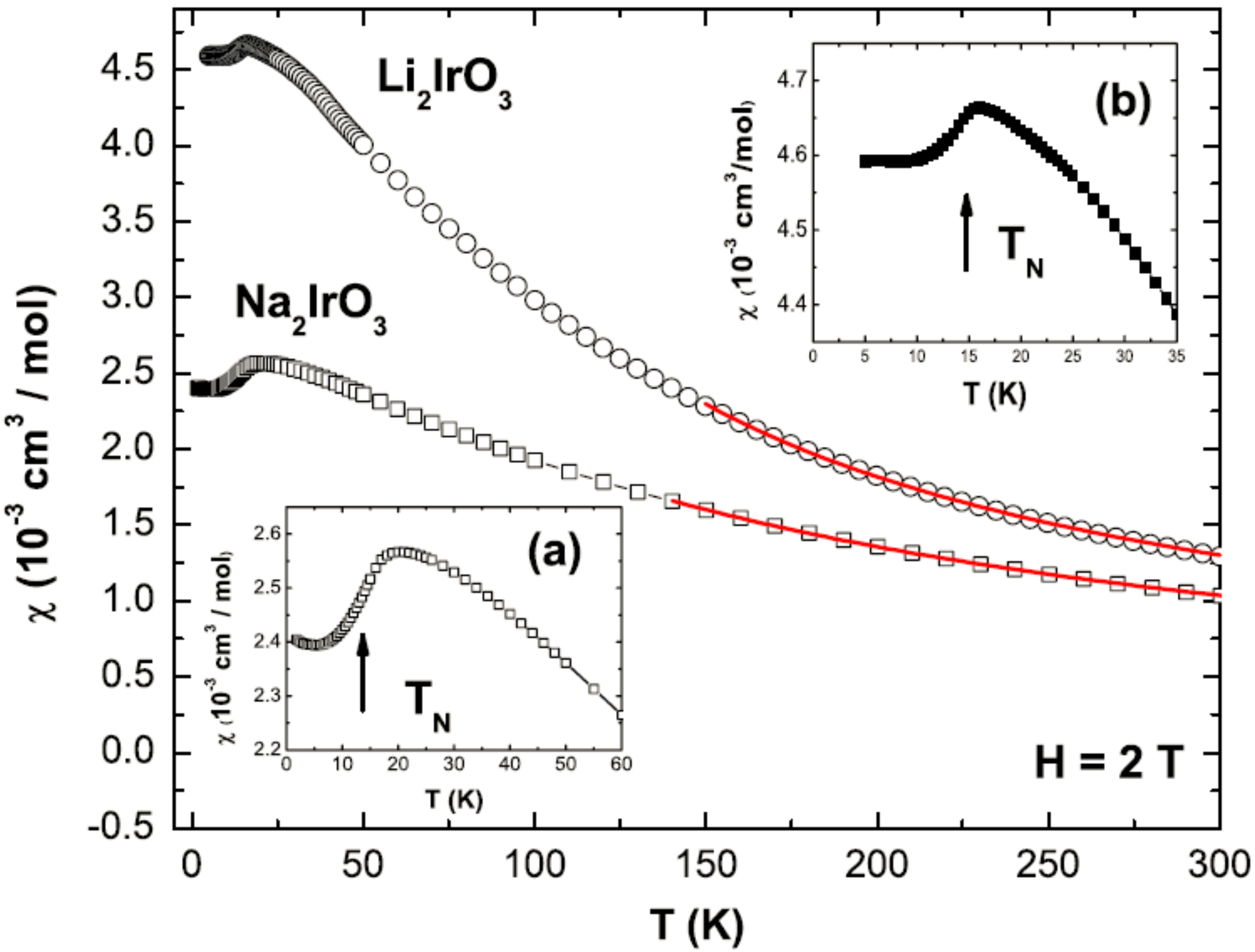


Kitaev spin liquid is stable
against Heisenberg perturbations!

Q1: why Na_2IrO_3 orders?

Quantum chemistry results: $J_1 = 3\ \mathrm{meV}$ $K_1 = -17\ \mathrm{meV}$

V.M.Katukuri et al, New J. Phys. 2014

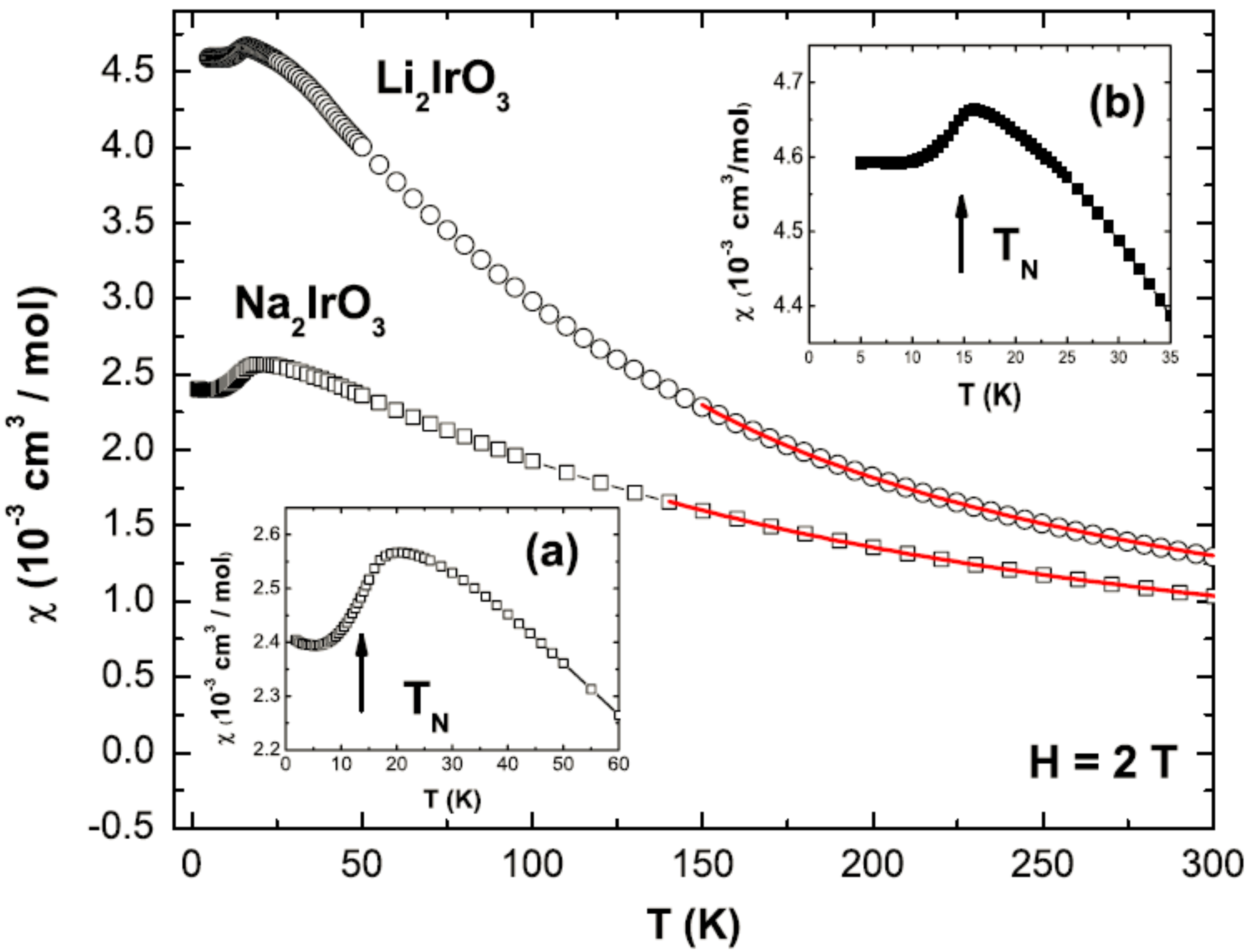


Singh and Gegenwart, PRB 82, 064412 (2010);
Singh et al, PRL 108, 127203 (2012)

Q2: why CW temperature in Na_2IrO_3 is large and AFM?

$$J_1 = 3\ \mathrm{meV} \quad K_1 = -17\ \mathrm{meV}$$

V.M.Katukuri et al, New J. Phys. 2014



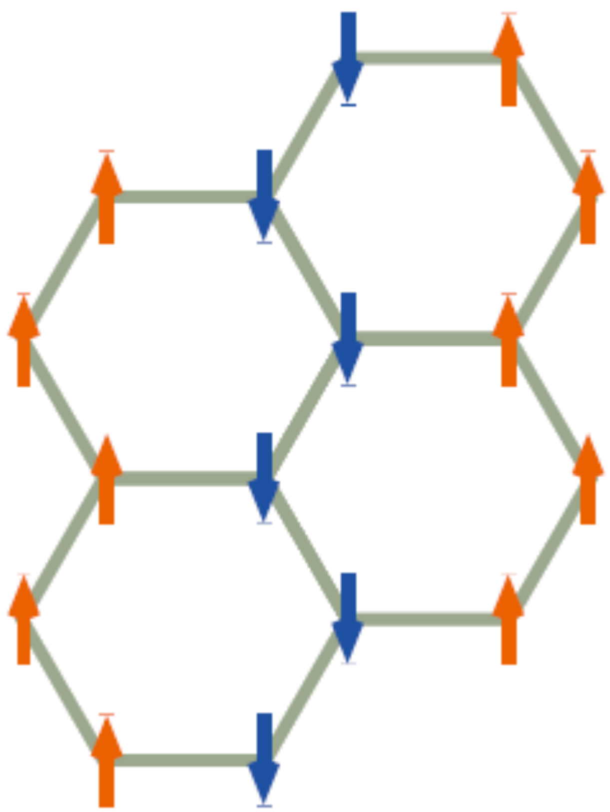
θ_{CW}=-125 K

Singh and Gegenwart, PRB 82, 064412 (2010);
Singh et al, PRL 108, 127203 (2012)

Q3: why Na_2IrO_3 orders to zigzag?

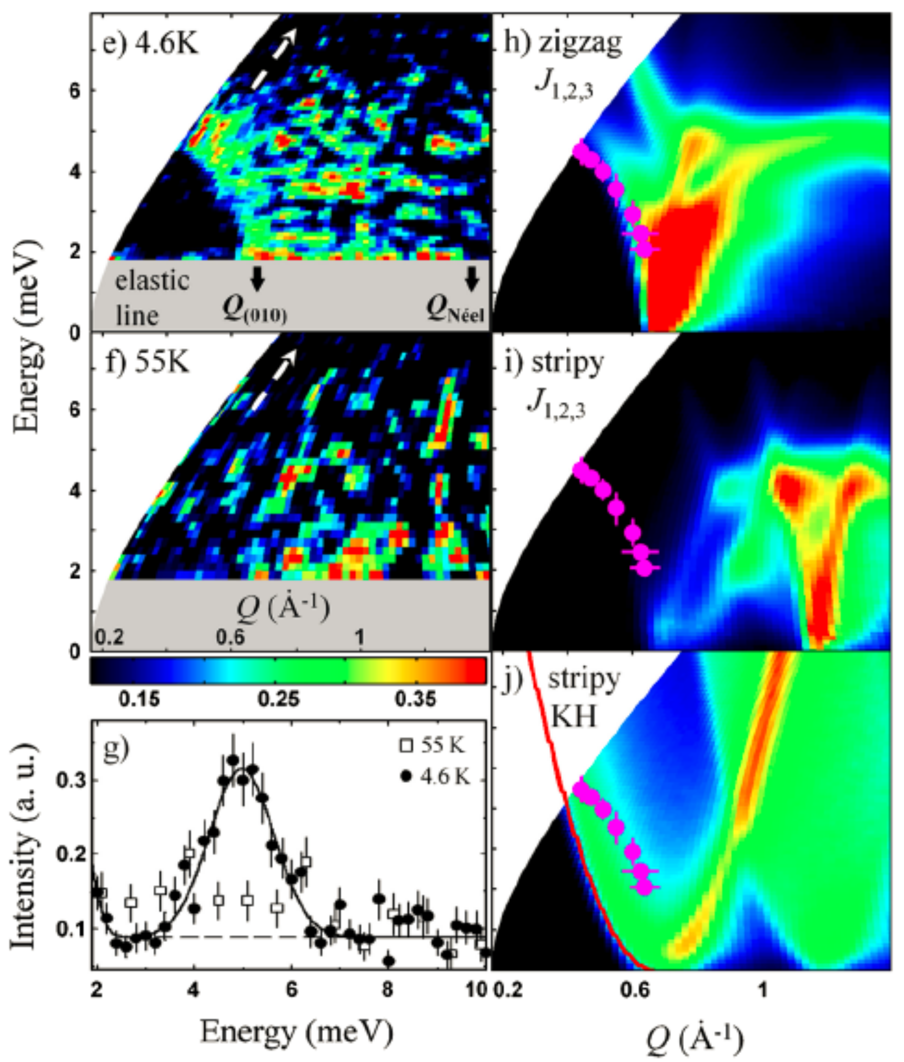
$$J_1 = 3 \text{ meV} \quad K_1 = -17 \text{ meV}$$

V.M.Katukuri et al, New J. Phys. 2014



X. Liu et al, PRB 2011

Feng Ye et al, PRB 2012

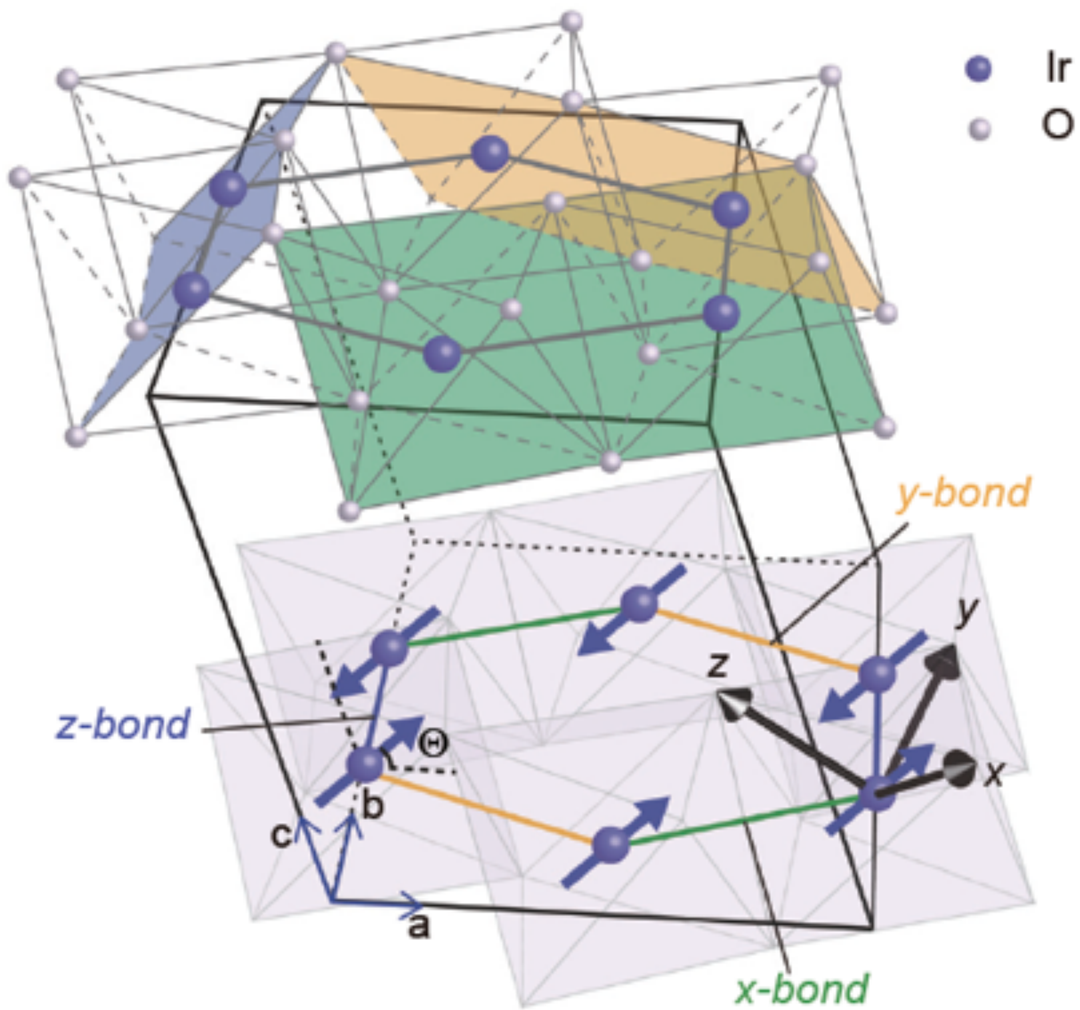


S. K. Choi et al PRL 2012

further neighbors interactions

I.Kimchi & Y.Z. You, PRB 2011

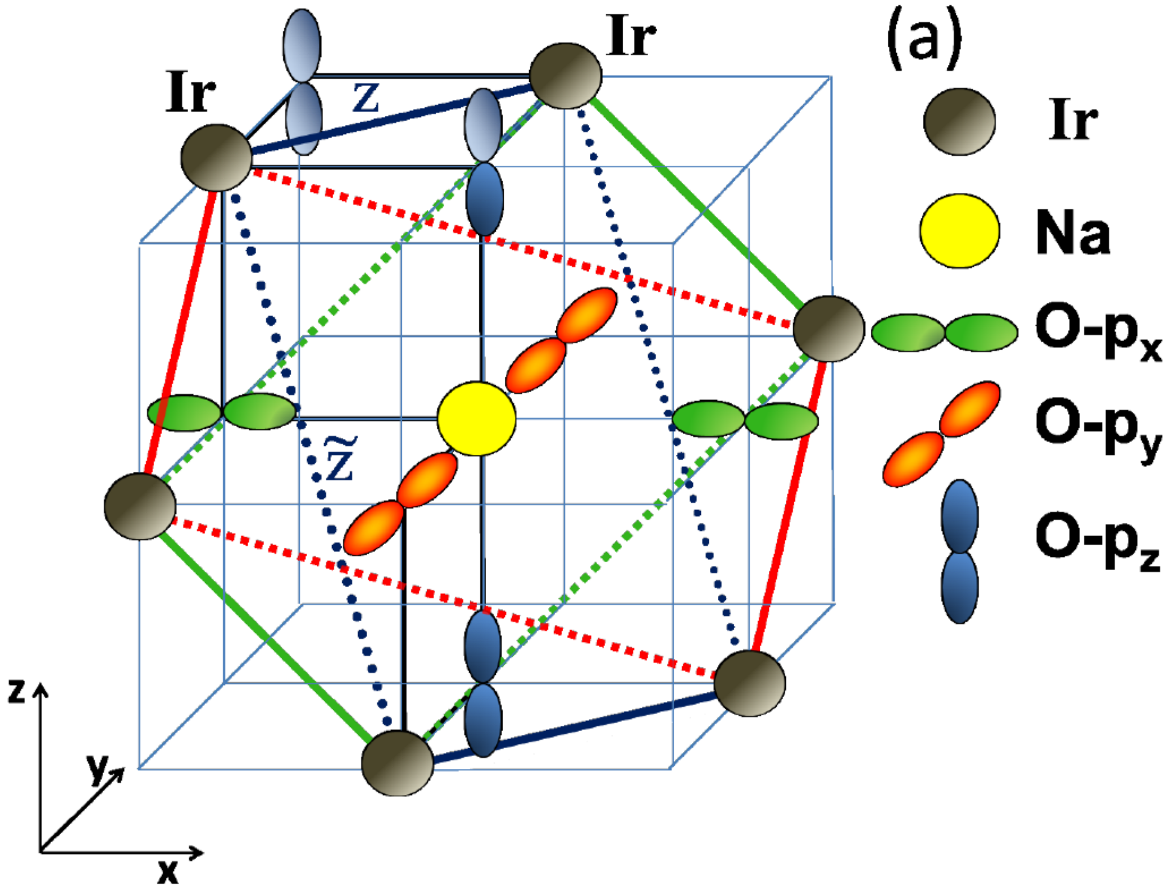
Q4: why spins in Na_2IrO_3 point along face diagonal directions?

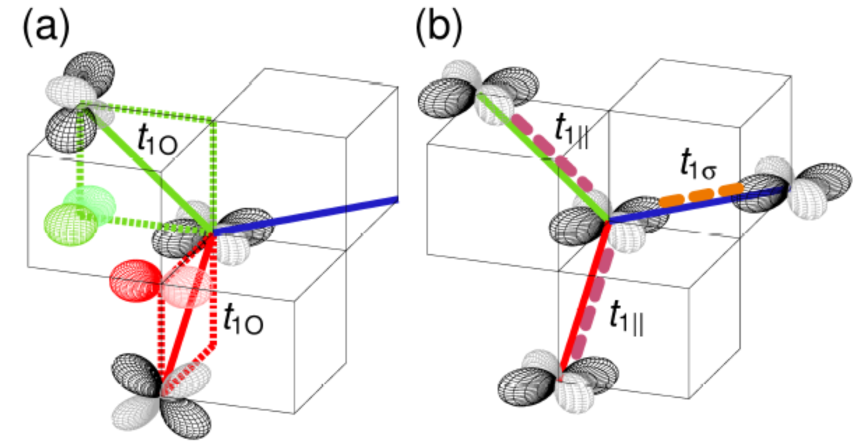


S.H.Chun et al, Nature Physics 2015

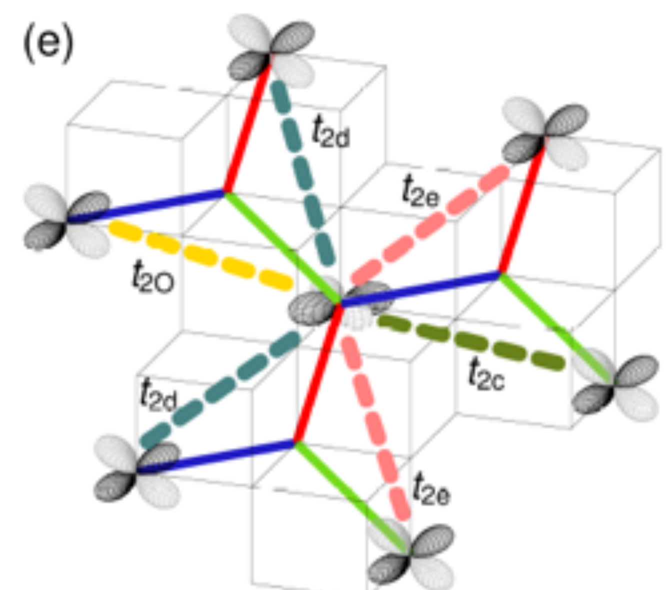
But in KH model both quantum and thermal fluctuations choose cubic directions.

Revision of the super-exchange model for Na_2IrO_3





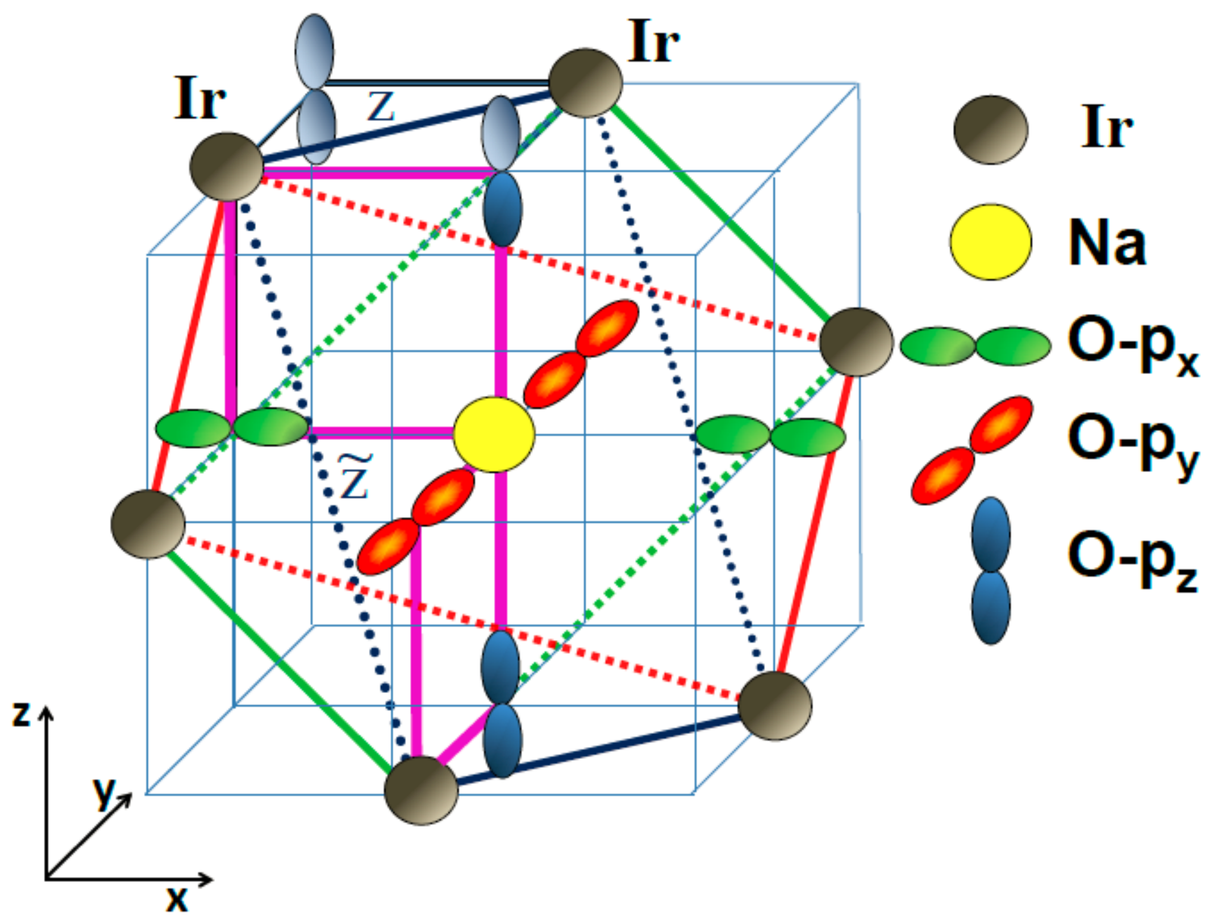
$$t_{1o} = 230 \text{ meV}$$
$$t_{1\sigma} = 67 \text{ meV}$$

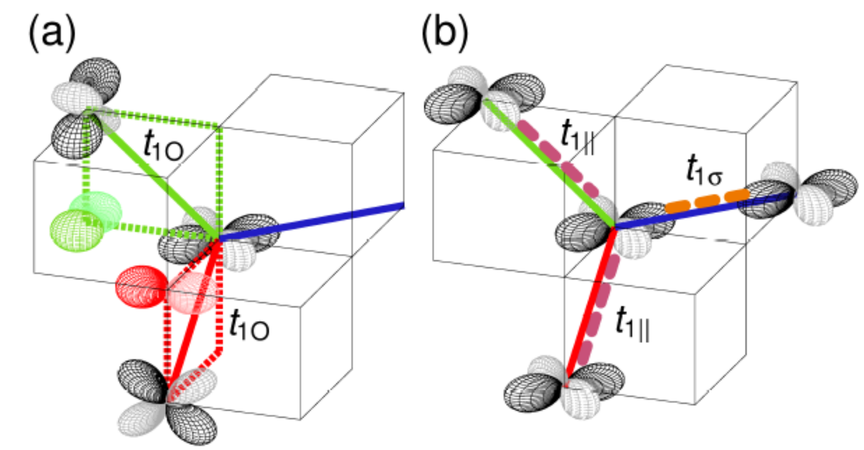


$$t_{2o} = 94.7 \text{ meV}$$

Kateryna Foyevtsova *et al*, PRB 2013

Revision of the super-exchange model for Na_2IrO_3





$$t_{1o} = 230 \text{ meV}$$
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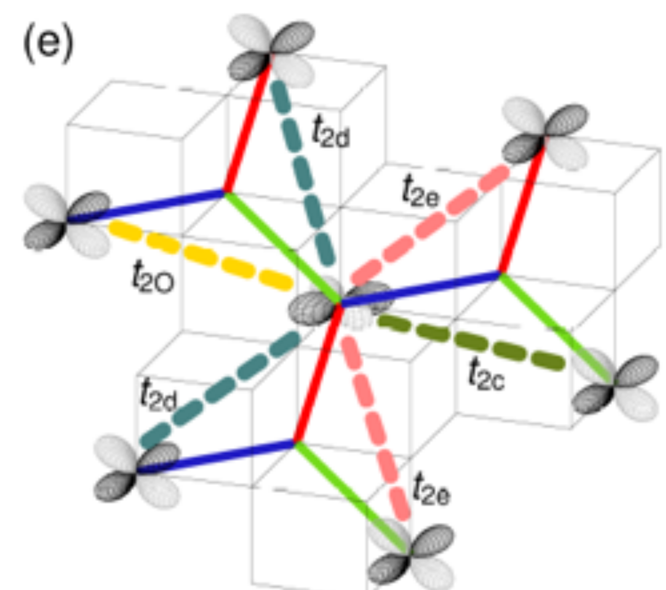


$$t_{2o} = 94.7 \text{ meV}$$

Kateryna Foyevtsova *et al*, PRB 2013

Second neighbors hopping

Path 1 : $\mathrm{Ir}(Y) \to \mathrm{O}(p_z) \to \mathrm{Na}(s) \to \mathrm{O}(p_z) \to \mathrm{Ir}(X)$

Path 2 : $\mathrm{Ir}(Y) \to \mathrm{O}(p_z) \to \mathrm{Na}($ …

Path 3 : $\mathrm{Ir}(Y) \to \mathrm{O}(p_x) \to$ …

Path 4 : $\mathrm{Ir}(Y) \to \mathrm{O}(p_x) \to \mathrm{Na}(s)$ …

Kitaev interaction

$|X\rangle = |yz\rangle,\ |Y\rangle = |zx\rangle$, and $|Z\rangle = |xy\rangle$

J_1-K_1-J_2-K_2 model

$$\mathcal{H} = J_1 \sum_{\langle n,n' \rangle_\gamma} \mathbf{S}_n \mathbf{S}_{n'} + K_1 \sum_{\langle n,n' \rangle_\gamma} S_n^\gamma S_{n'}^\gamma$$

$$+ J_2 \sum_{\langle\langle n,n' \rangle\rangle_{\tilde{\gamma}}} \mathbf{S}_n \mathbf{S}_{n'} + K_2 \sum_{\langle\langle n,n' \rangle\rangle_{\tilde{\gamma}}} S_n^\gamma S_{n'}^{\tilde{\gamma}}$$

$J_1 \boldsymbol{SS} + K_1 S^x S^x$

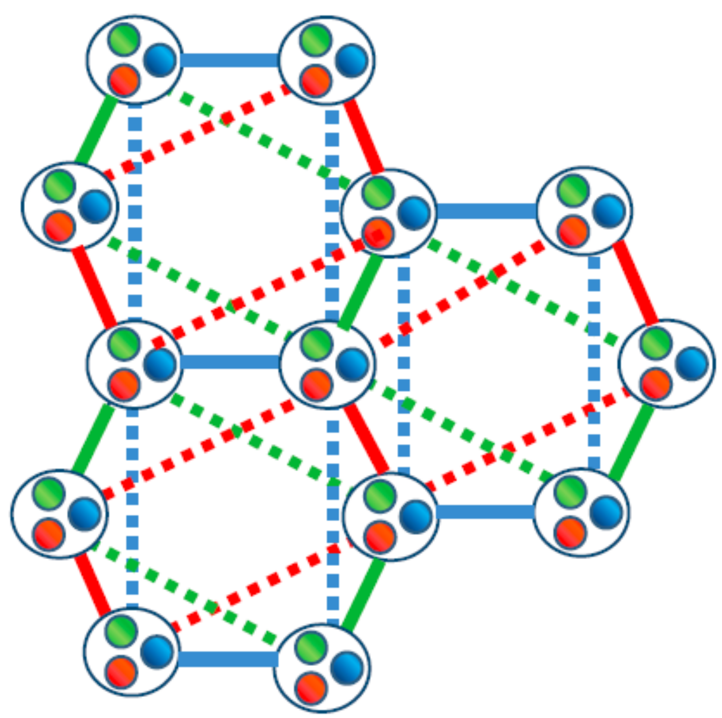
$J_1 \boldsymbol{SS} + K_1 S^y S^y$

$J_1 \boldsymbol{SS} + K_1 S^z S^z$

$J_2 \boldsymbol{SS} + K_2 S^x S^x$

$J_2 \boldsymbol{SS} + K_2 S^y S^y$

$J_2 \boldsymbol{SS} + K_2 S^z S^z$



Na_2IrO_3

$$\Delta = 0.1 \text{ eV}, \; \lambda = 0.4 \text{ eV}$$
$$J_H = 0.3 \text{ eV}, \; U_2 = 1.8 \text{ eV}$$
$$t_{1o} = 230 \text{ meV}, \; t_d = 67 \text{ meV}$$
$$t_{2o} = 95 \text{ meV}$$

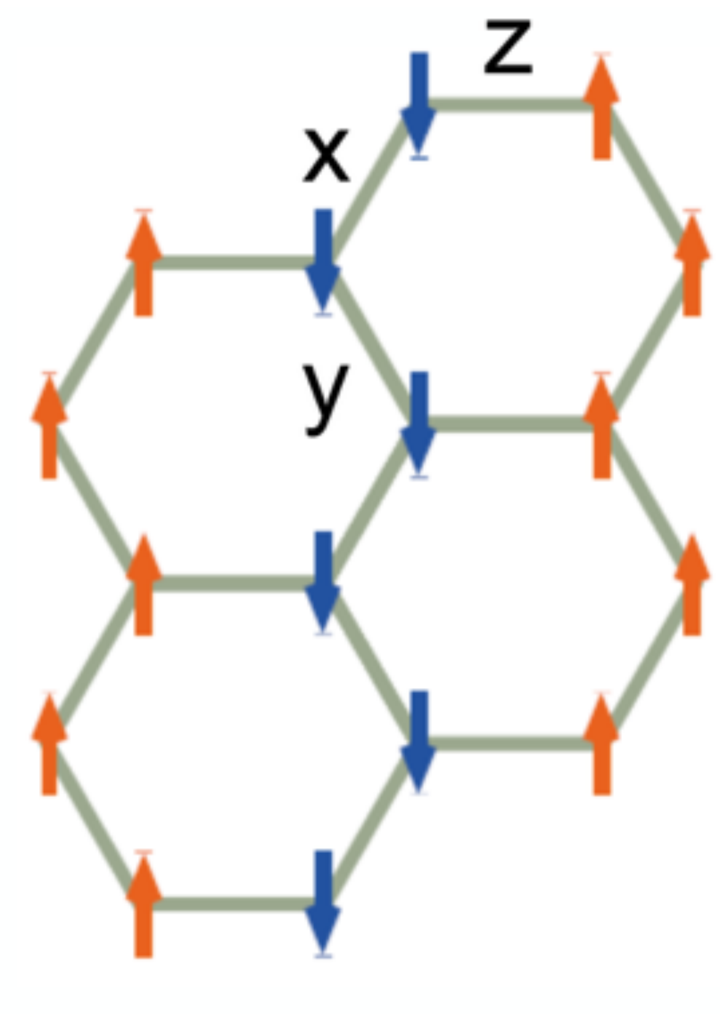
$$J_1 = 5.1\,\text{meV}, \; K_1 = -14.8\,\text{meV}$$
$$J_2 = -4.5\,\text{meV}, \; K_2 = 9\,\text{meV}$$

zigzag

$\theta_{CW} \approx$ -98 K

Y.Sizyuk, C.Price, P. Wölfle, **N.B.P.**, PRB 2014

Locking of the spin direction to the spatial orientation of the zigzag in Na_2IrO_3

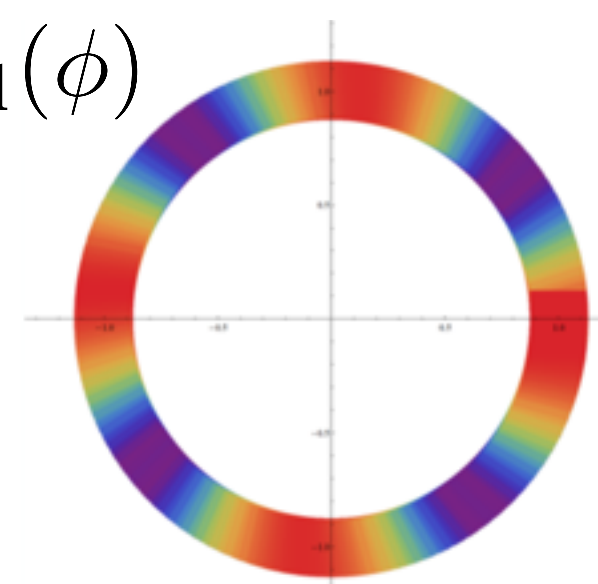


$$S = S_0 + S_{\text{fl}}(\theta, \phi)$$

$$S_{\text{fl}} = -\sum_{\boldsymbol{q}} \sum_{\kappa,\kappa'=A,B} \sum_{\mu,\mu'=0}^{2} \tilde{A}_{\boldsymbol{q}}^{\kappa\mu;\kappa'\mu'} \delta\phi_{-\boldsymbol{q}}^{\kappa\mu} \delta\phi_{\boldsymbol{q}}^{\kappa'\mu'}$$

$$\tilde{A}_{\boldsymbol{q}} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 1/(J_{\boldsymbol{q}}^x)^* & 0 & 0 \\ c_{12} & c_{22} & c_{23} & 0 & 1/(J_{\boldsymbol{q}}^y)^* & 0 \\ c_{13} & c_{23} & c_{33} & 0 & 0 & 1/(J_{\boldsymbol{q}}^z)^* \\ 1/J_{\boldsymbol{q}}^x & 0 & 0 & c_{11} & c_{12} & c_{13} \\ 0 & 1/J_{\boldsymbol{q}}^y & 0 & c_{12} & c_{22} & c_{23} \\ 0 & 0 & 1/J_{\boldsymbol{q}}^z & c_{13} & c_{23} & c_{33} \end{pmatrix}$$

$S_{\text{fl}}(\phi)$

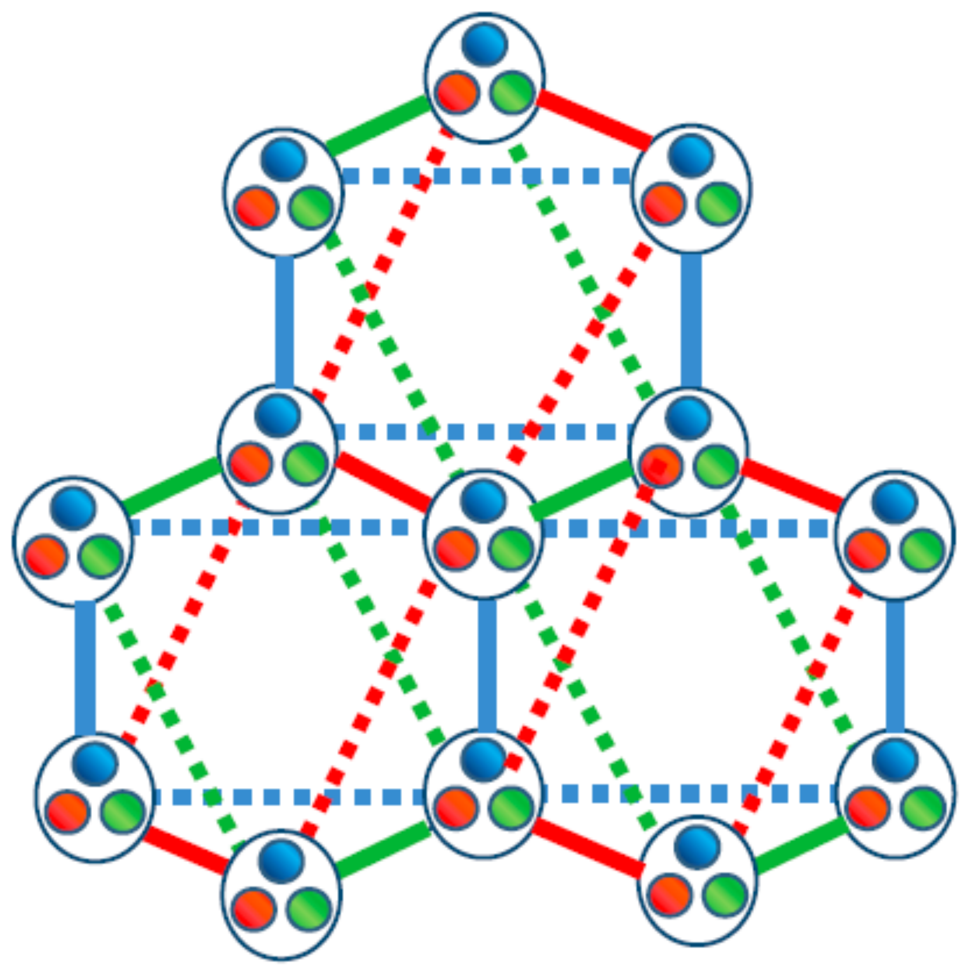


spin fluctuations select one of the diagonals in xy-plane

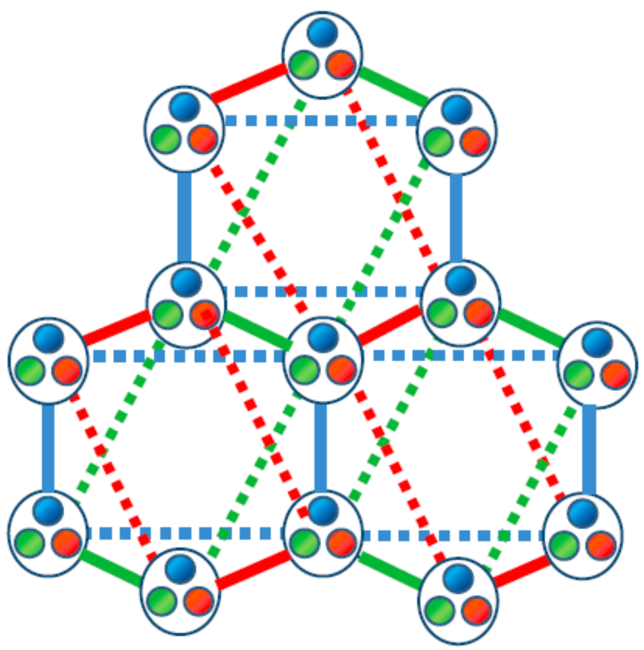
Y.Sizyuk, N.B.P, P. Wölfle 2015

K_1-K_2 model

$$\mathcal{H} = = K_1 \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + K_2 \sum_{\langle\langle ij \rangle\rangle_\lambda} S_i^\lambda S_j^\lambda$$



Classical K_1-K_2 model



$$\mathcal{H} = = K_1 \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + K_2 \sum_{\langle\langle ij \rangle\rangle_\lambda} S_i^\lambda S_j^\lambda$$

$$H = \sum_{\vec{k},\alpha,ij} S^\alpha_{-\vec{k},i} \Lambda^\alpha_{ij}(-\vec{k}) S^\alpha_{\vec{k},j}$$

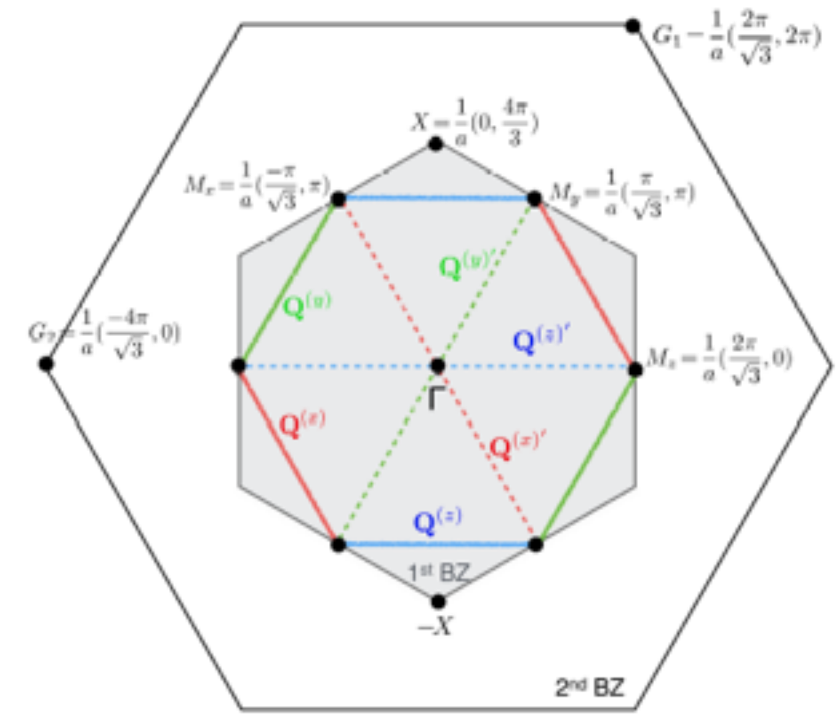
$$\mathbf{t}_1 = \mathbf{x}, \ \mathbf{t}_2 = \frac{1}{2}\mathbf{x} + \frac{\sqrt{3}}{2}\mathbf{y}$$

$$\mathbf{t}_3 = \mathbf{t}_1 + \mathbf{t}_2$$

$$\lambda^x_\pm = K_2 \cos(\vec{k}\cdot\vec{t}_2) \pm \frac{1}{2} K_1$$

$$\lambda^y_\pm = K_2 \cos(\vec{k}\cdot\vec{t}_3) \pm \frac{1}{2} K_1$$

$$\lambda^z_\pm = K_2 \cos(\vec{k}\cdot\vec{t}_1) \pm \frac{1}{2} K_1$$



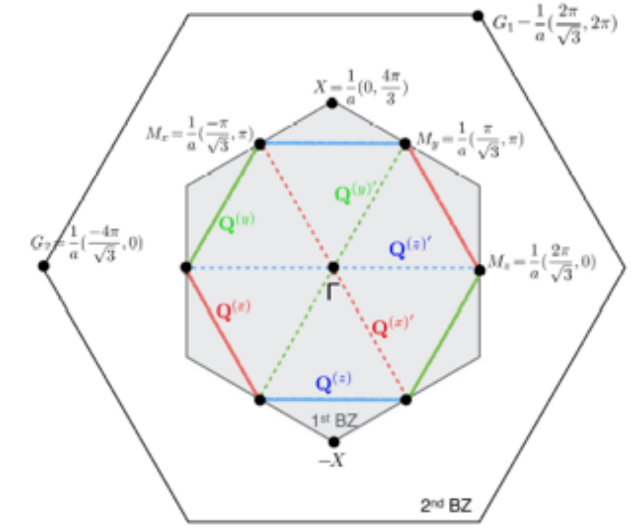
Degeneracy of the ground state: 3×2^L

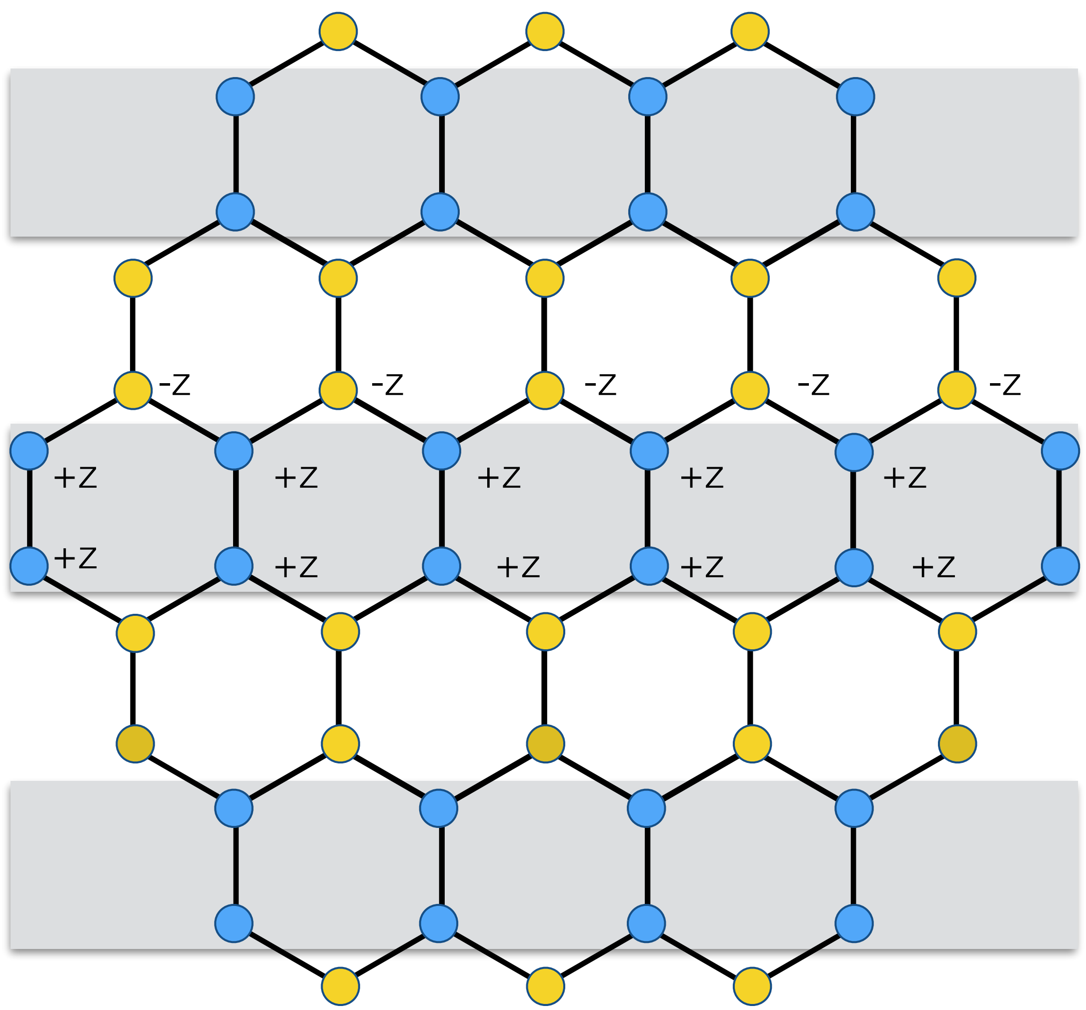
This degeneracy is not accidental but it is related to the sliding gauge-like symmetries in the Hamiltonian.

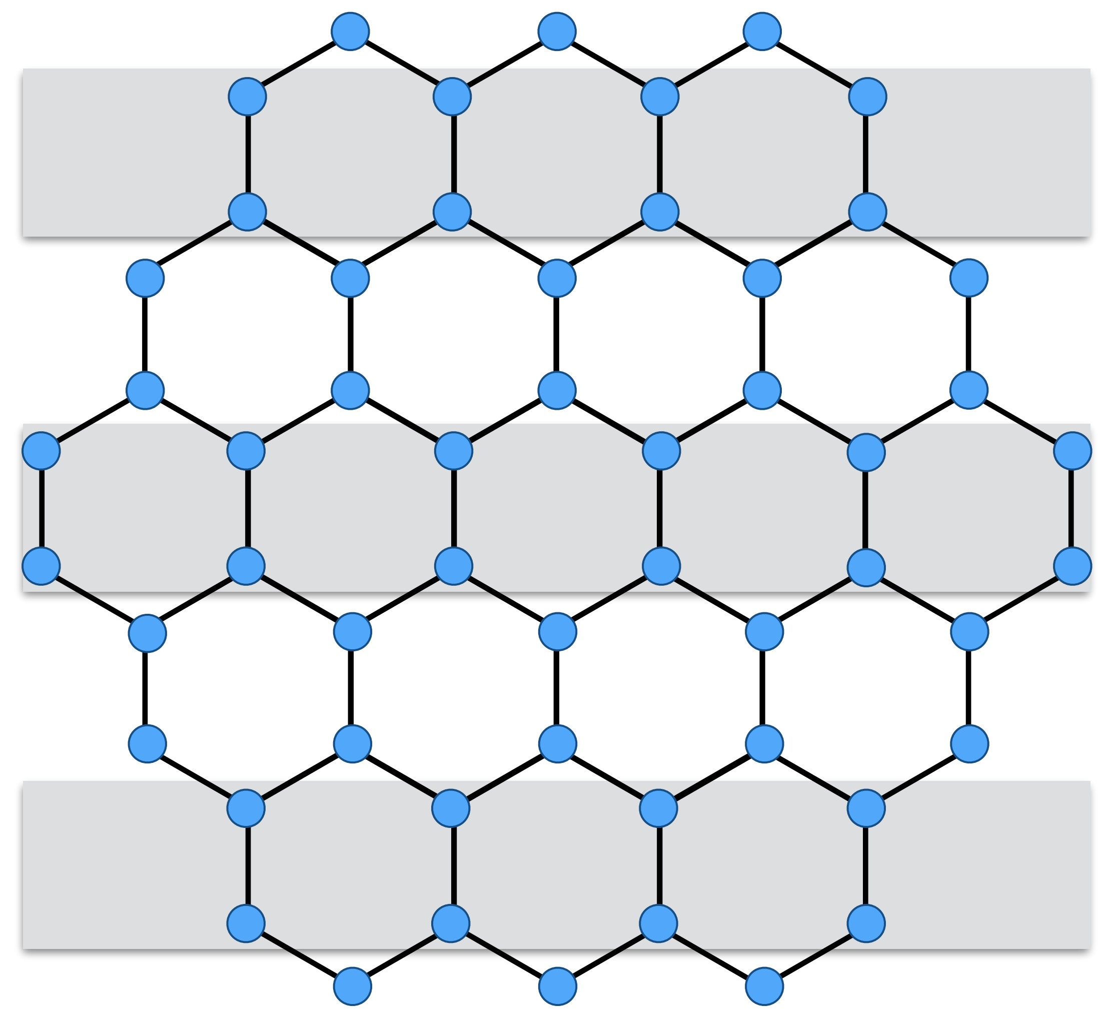
$$K_1 < 0$$
$$K_2 < 0$$

$$\lambda^z = K_2 \cos(\vec{k} \cdot \vec{t}_1) + \frac{1}{2} K_1$$

$$\min(\lambda^z) \text{ is for } \cos(\vec{k} \cdot \vec{t}_1) = -1$$







I.Kimchi & Y.Z. You, PRB 2011

Classical order is Nematic-like

n.n. z-bond

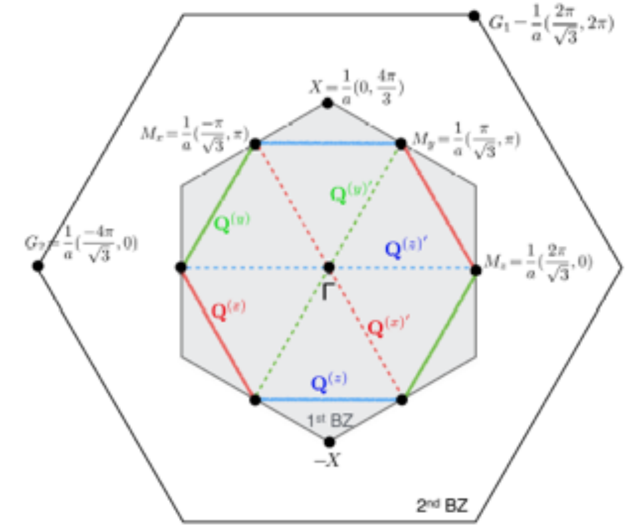
n.n.n. z-bond

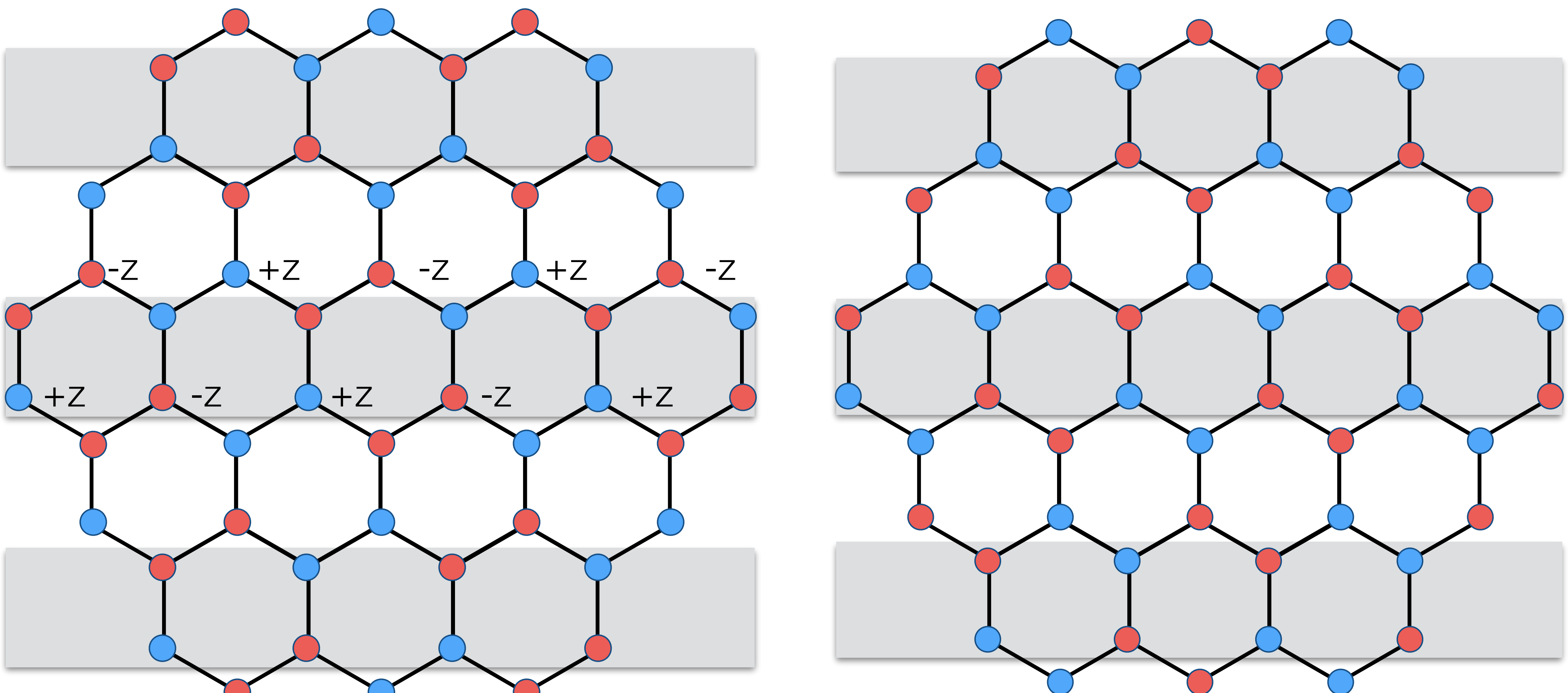
$K_1 > 0$

$K_2 > 0$

$$\lambda^z = K_2 \cos(\vec{k} \cdot \vec{t}_1) - \frac{1}{2} K_1$$

$$\min(\lambda^z) \text{ is for } \cos(\vec{k} \cdot \vec{t}_1) = 1$$





Classical order is Nematic-like

n.n. z-bond

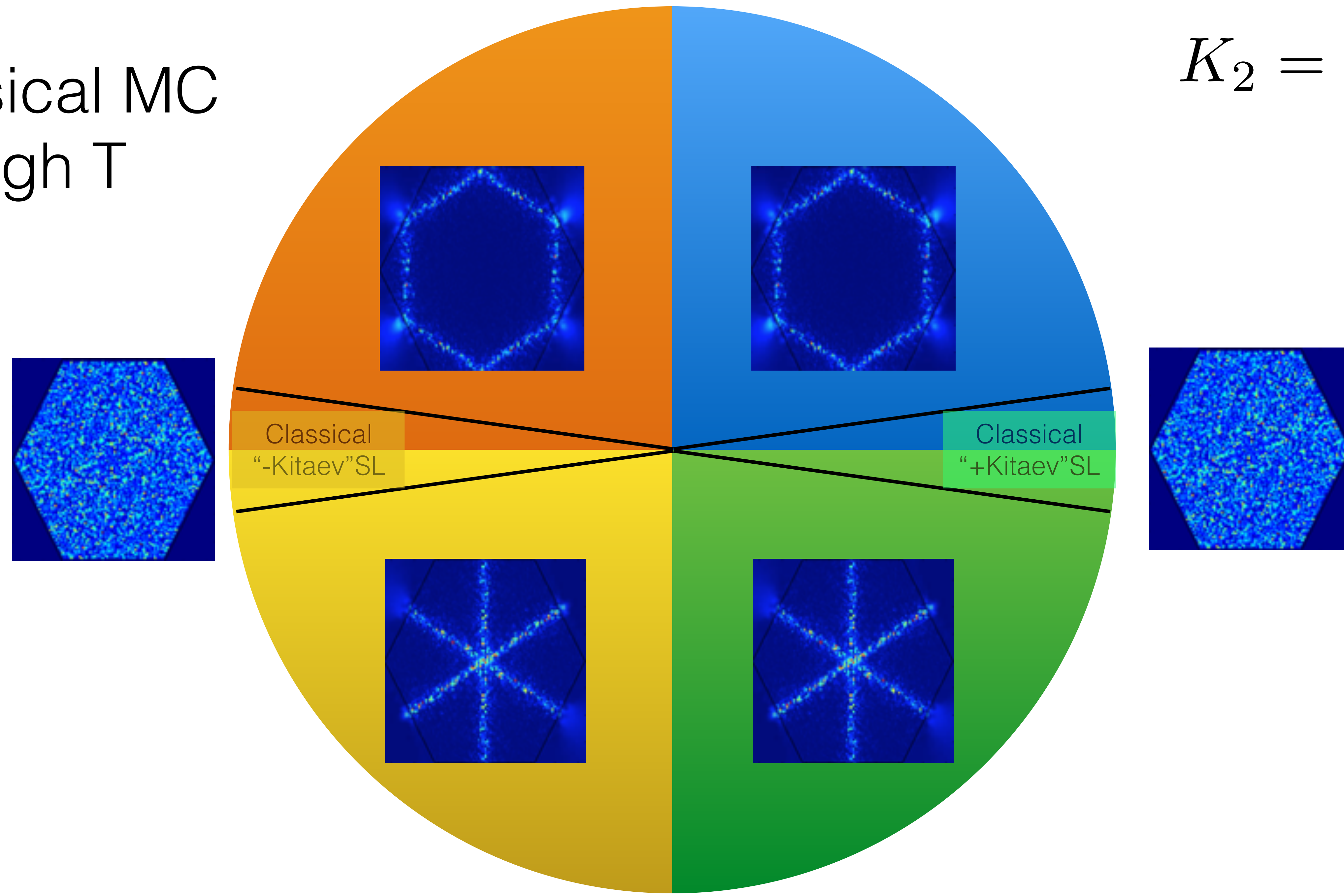
n.n.n. z-bond

$$H(\varphi) = \cos(\varphi) \sum_{\langle ij\rangle_\gamma} S_i^\gamma S_j^\gamma + \sin(\varphi) \sum_{\langle\langle ij\rangle\rangle_\lambda} S_i^\lambda S_j^\lambda$$

$$K_1 = \cos\phi$$

$$K_2 = \sin\phi$$

Classical MC
High T



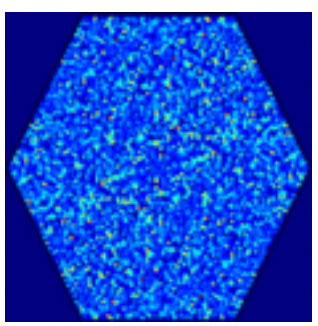
$$H(\varphi) = \cos(\varphi) \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + \sin(\varphi) \sum_{\langle\langle ij \rangle\rangle_\lambda} S_i^\lambda S_j^\lambda$$

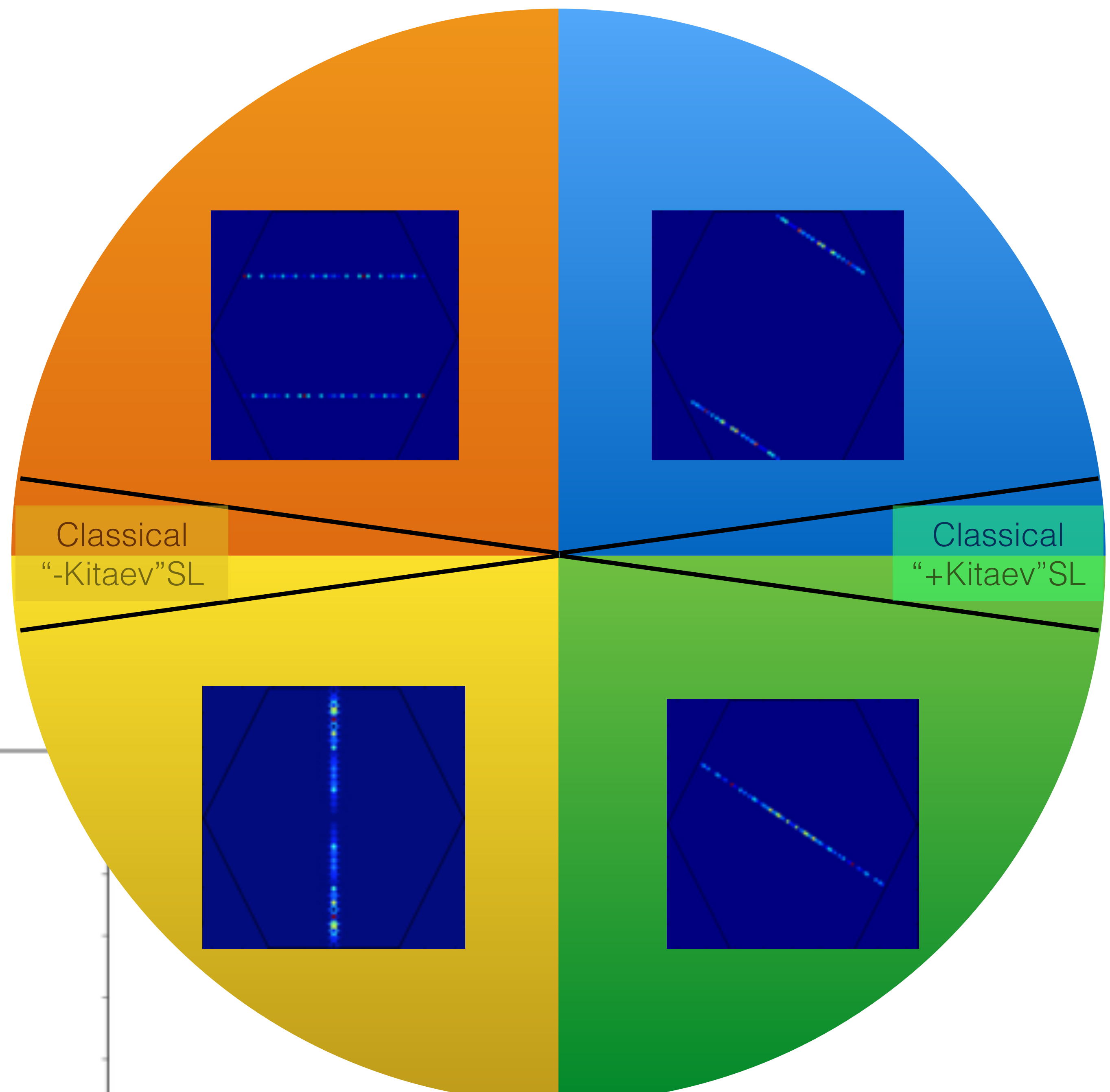
$$K_1 = \cos\phi$$

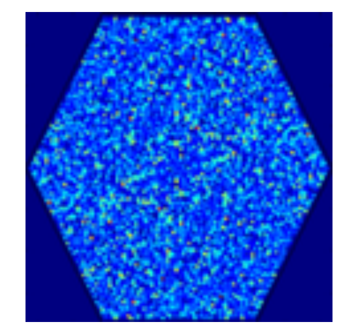
$$K_2 = \sin\phi$$

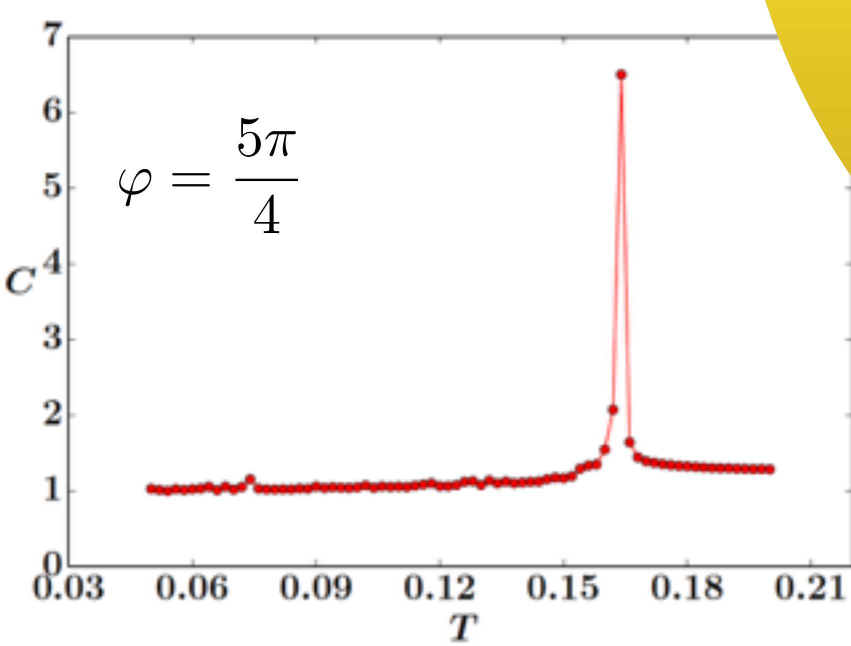
Classical MC

$T<T_C$



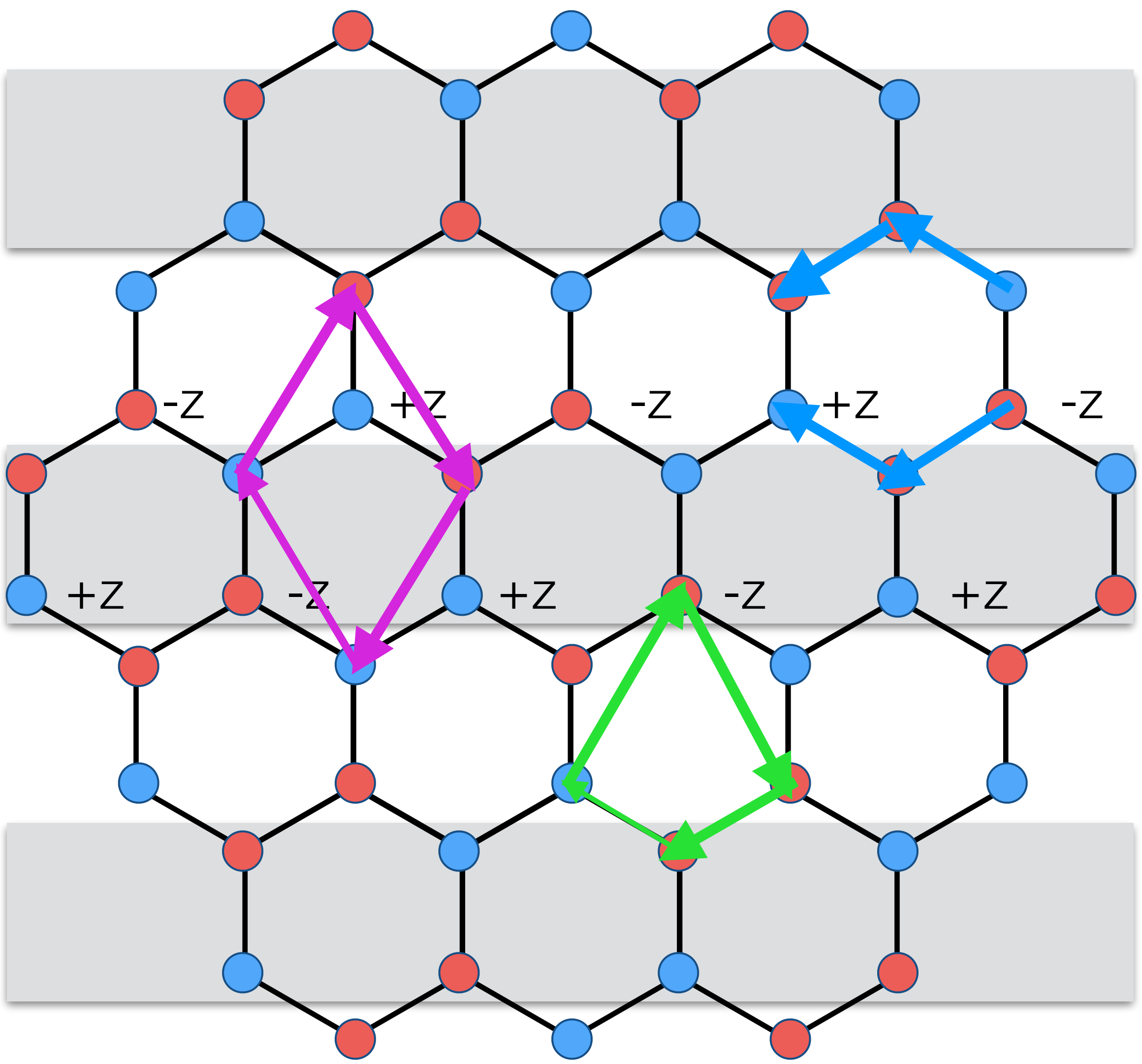


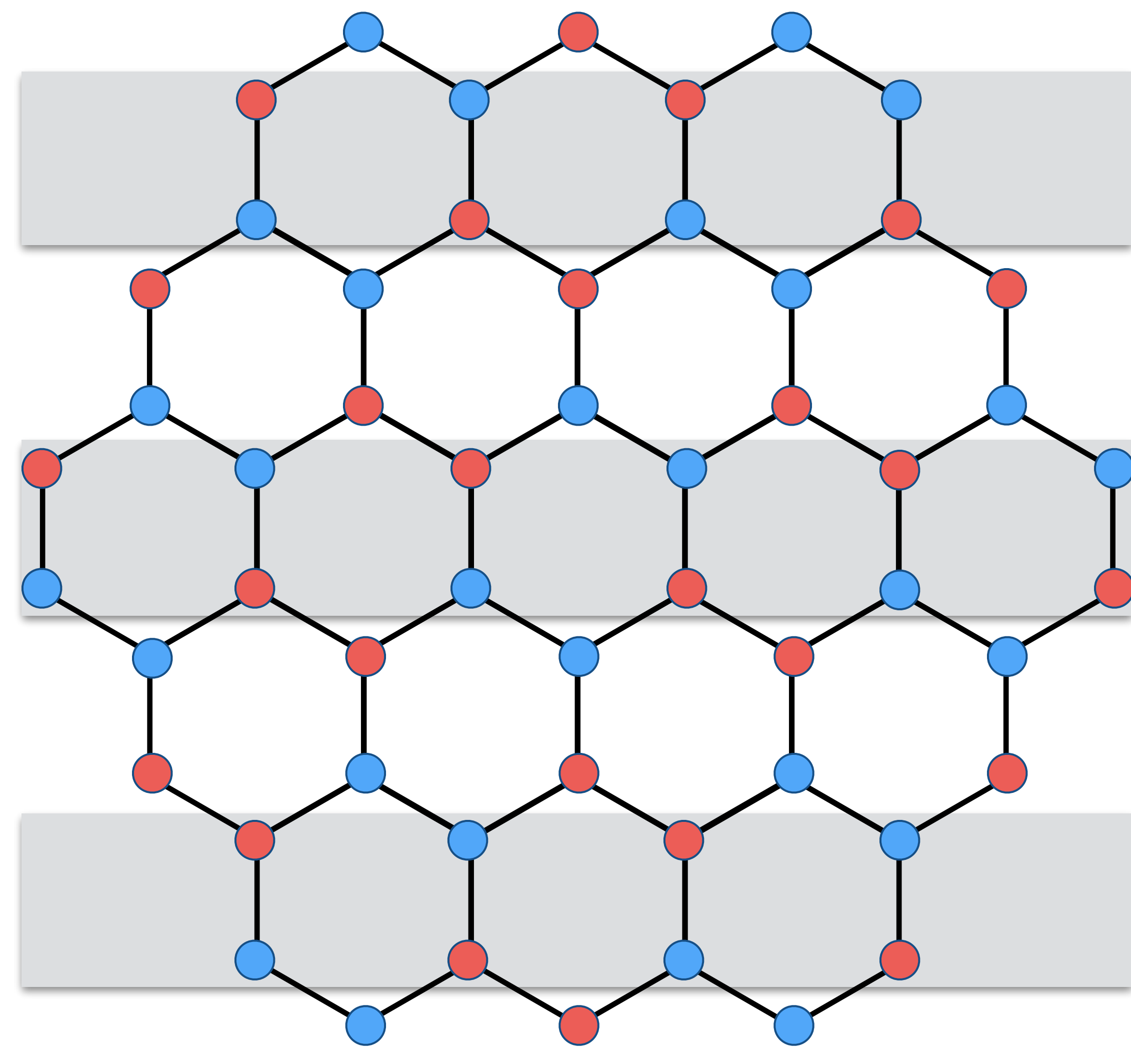




Quantum K_1-K_2 model

LR magnetic order is possible



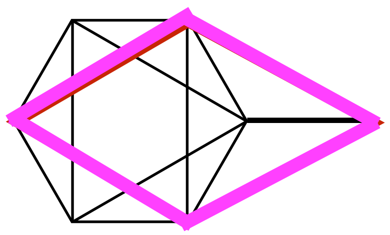


$K_1 > 0$

$K_2 > 0$

Perturbation theory: $K_{1x} = K_{1y} = xK_{1z}$, $K_{2x} = K_{2y} = xK_{2z}$, $x < 1$

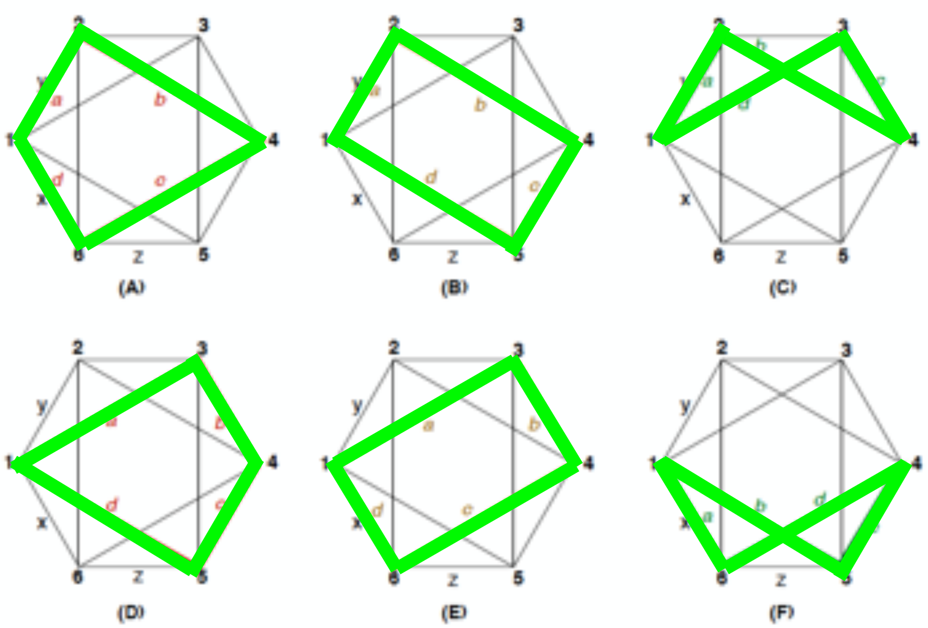
I



$$J_{\text{eff},1} = +\frac{K_{2x}^2 K_{2y}^2}{8(|K_{1z}|+2|K_{2z}|)^2(2|K_{1z}|+3|K_{2z}|)}\text{sgn}(K_{2z})$$

Jackeli & Avella, arXiv:1504.03618

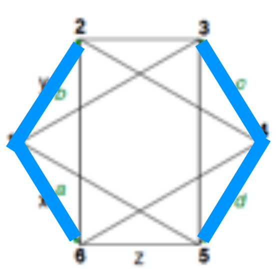
II



$$J_{\text{eff},2} = -\frac{\kappa}{4\Delta_{12}^3}\left[\frac{|K_{1z}|+|K_{2z}|}{2|K_{1z}|+3|K_{2z}|} + \frac{2|K_{2z}|}{|K_{1z}|+4|K_{2z}|}\right] > 0$$

$$\kappa = K_{1x}K_{1y}K_{2x}K_{2y}$$

III



$$J_{\text{eff},3} = \frac{\mu|K_{1z}|}{(|K_{1z}|+2|K_{2z}|)^2(|K_{1z}|+3|K_{2z}|)(|K_{1z}|+4|K_{2z}|)}$$

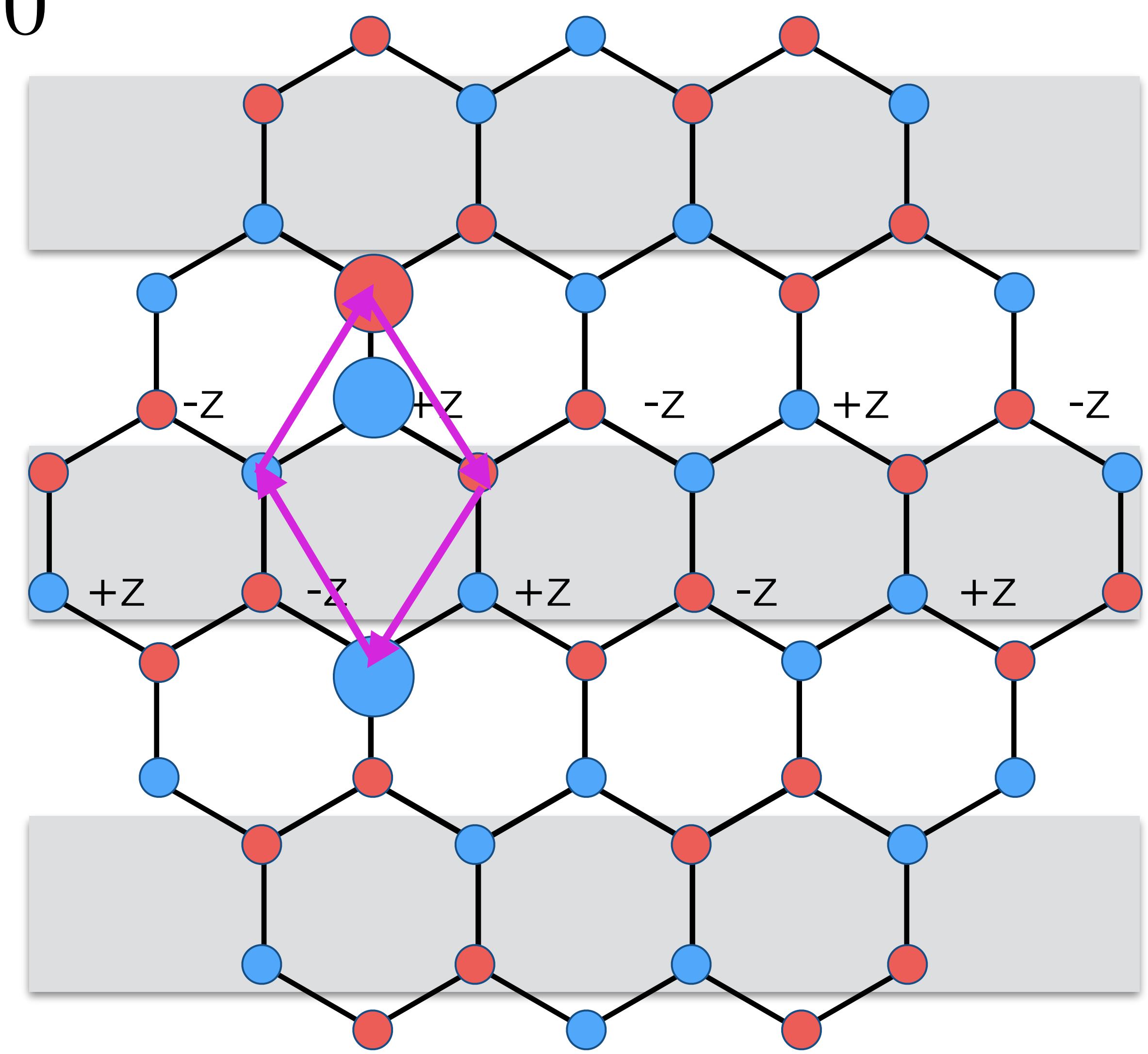
A. Kitaev, Annals of Physics **321**, 2 (2006)

$$\mu = K_{1x}^2 K_{1z}^2$$

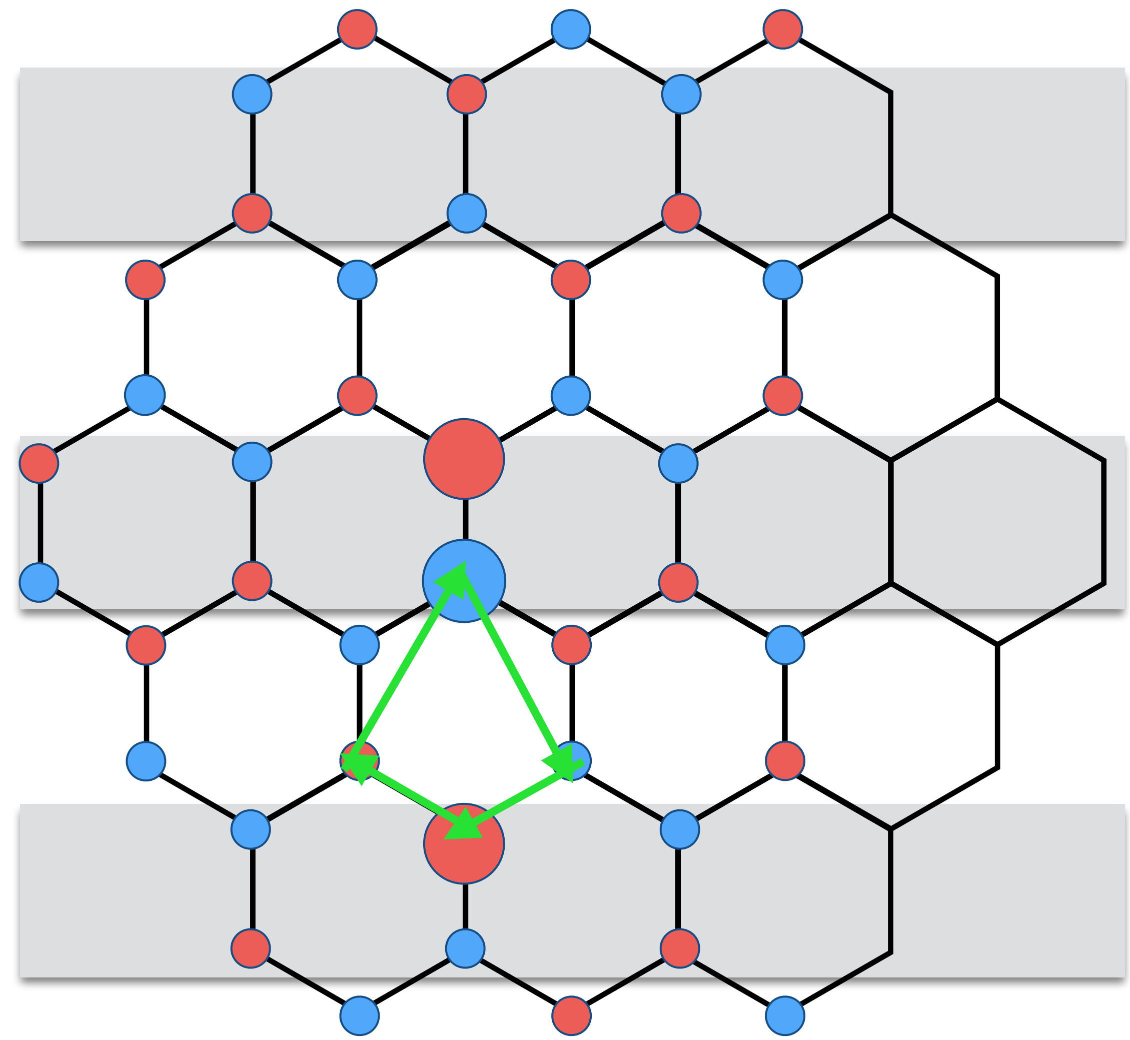
Competing phases

$K_1 > 0$

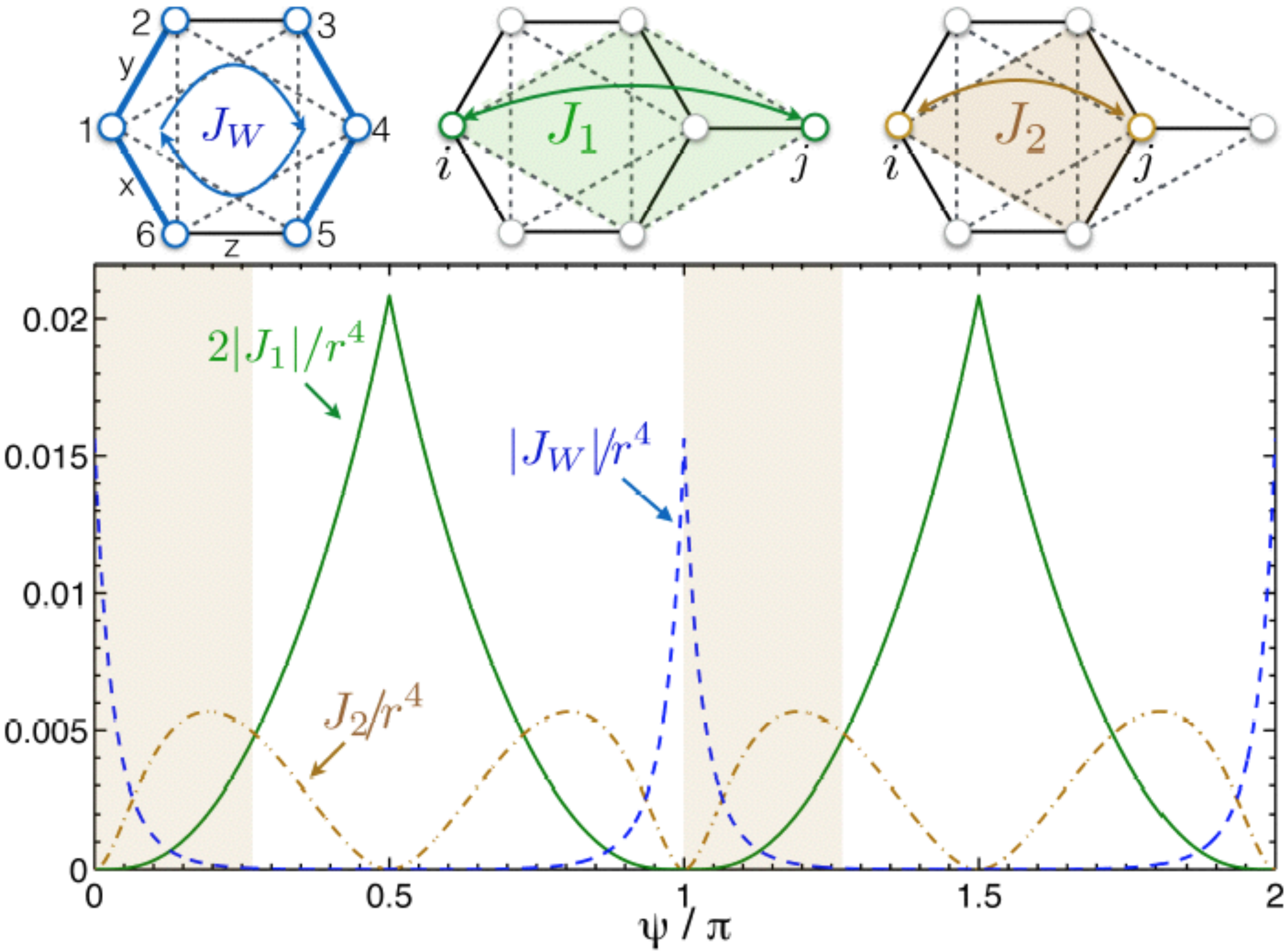
$K_2 > 0$



$$|J_{eff,1}| > |J_{eff,2}|$$

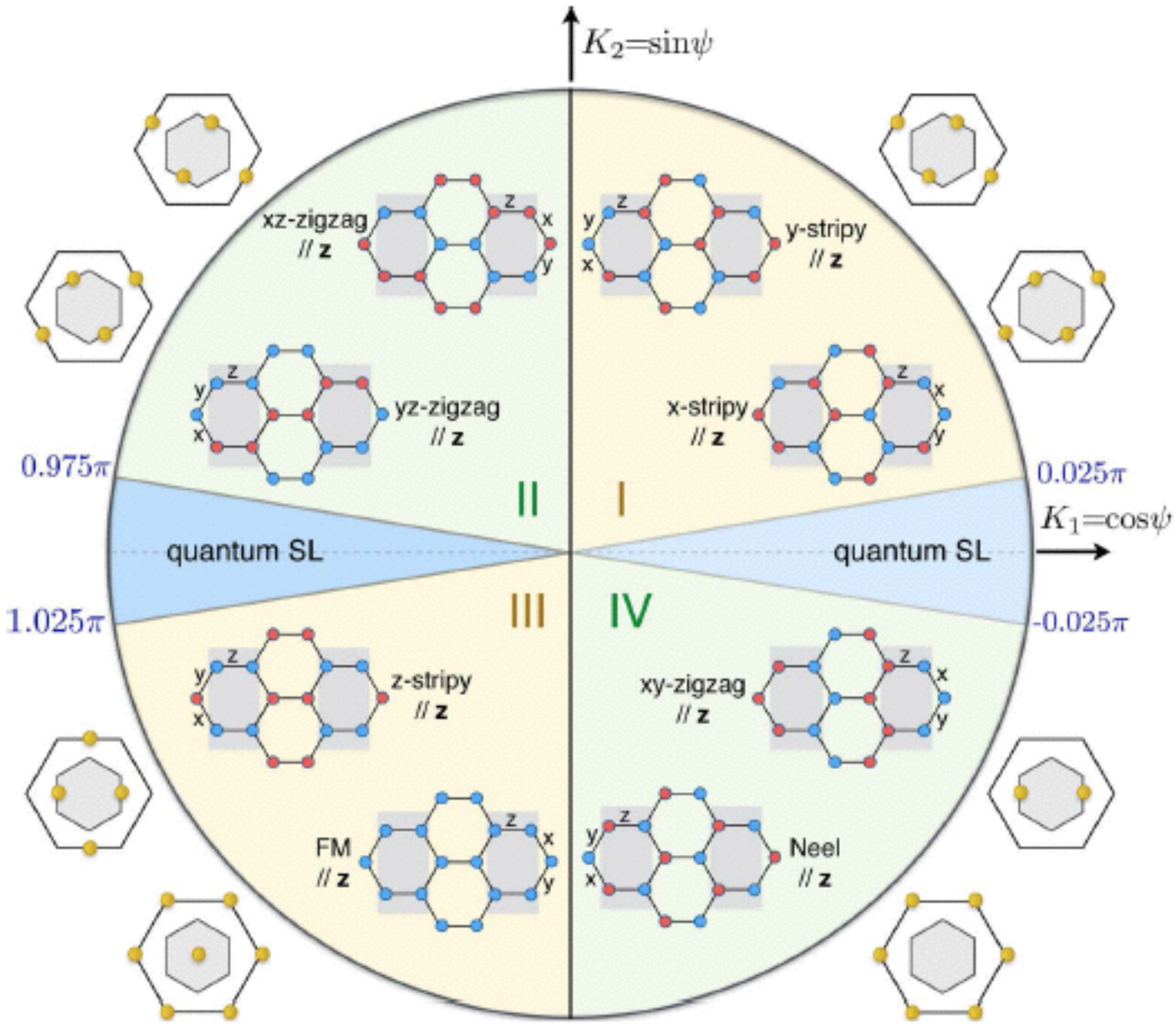


$$|J_{eff,2}| > |J_{eff,1}|$$



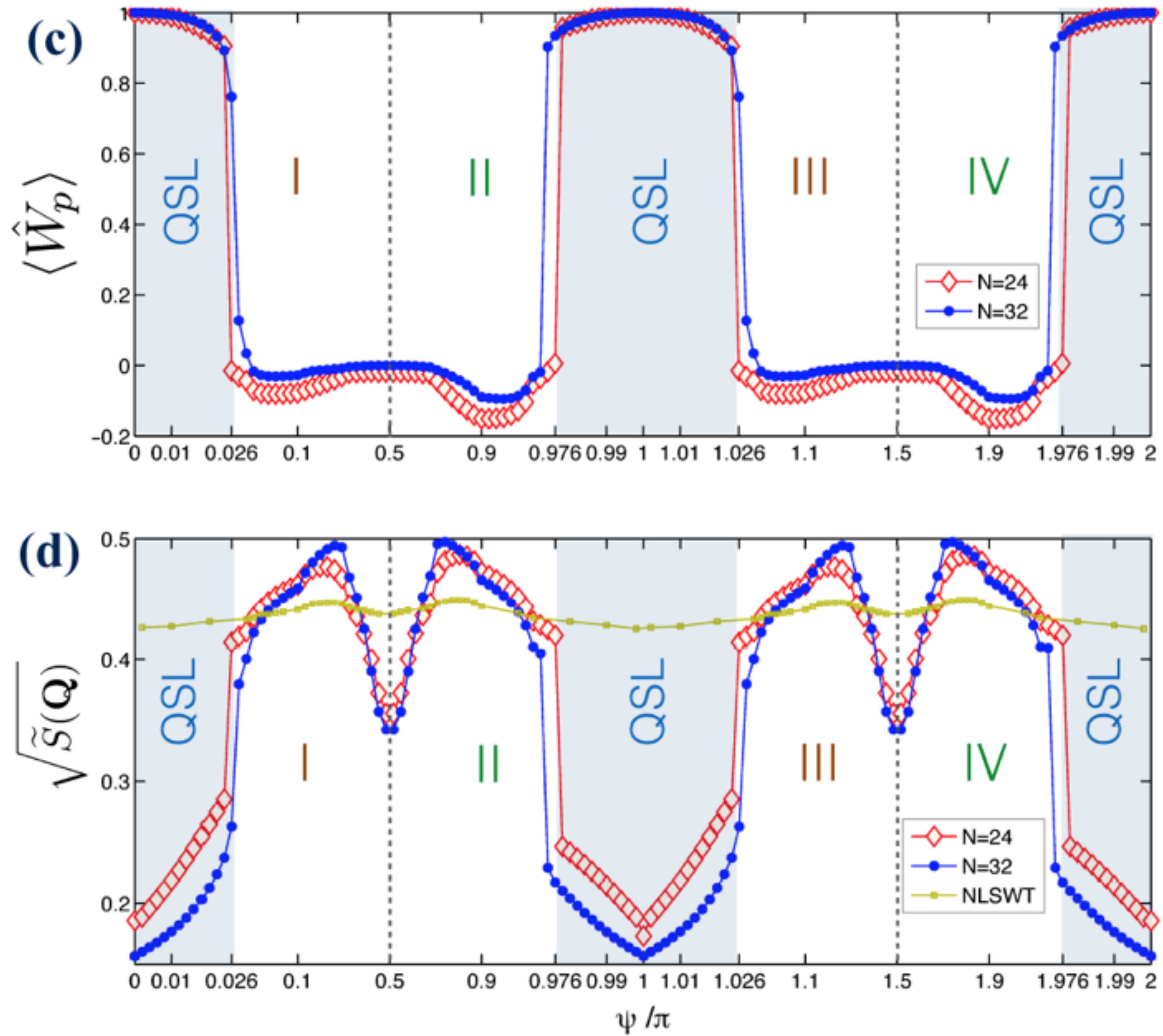
The shaded strips denote the regions where J_2 competes with J_1 and $J_2>2|J_1|$.

Quantum phase diagram of K_1-K_2 model



Each of the magnetic regions (I-IV) hosts twelve degenerate quantum states.

Flux operator and structure factor

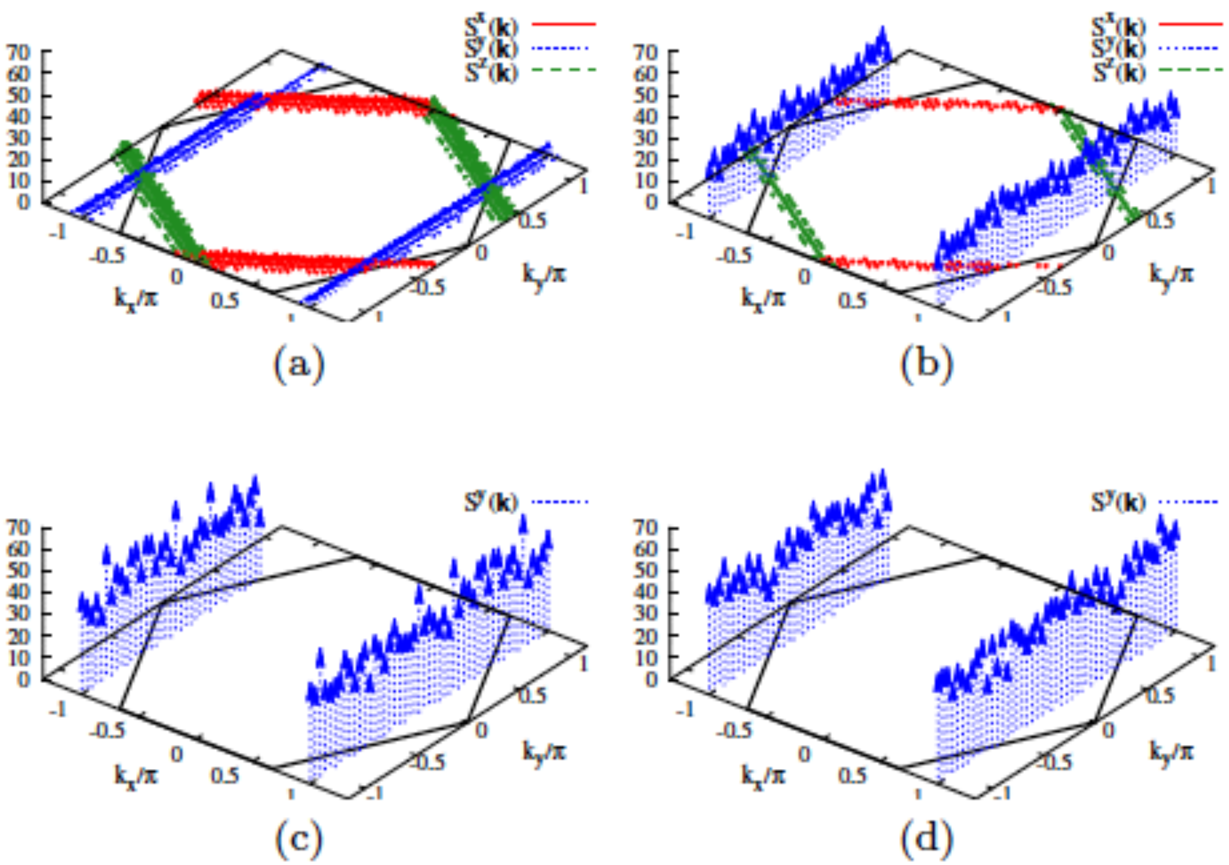


Triangular points: $K_1=0$

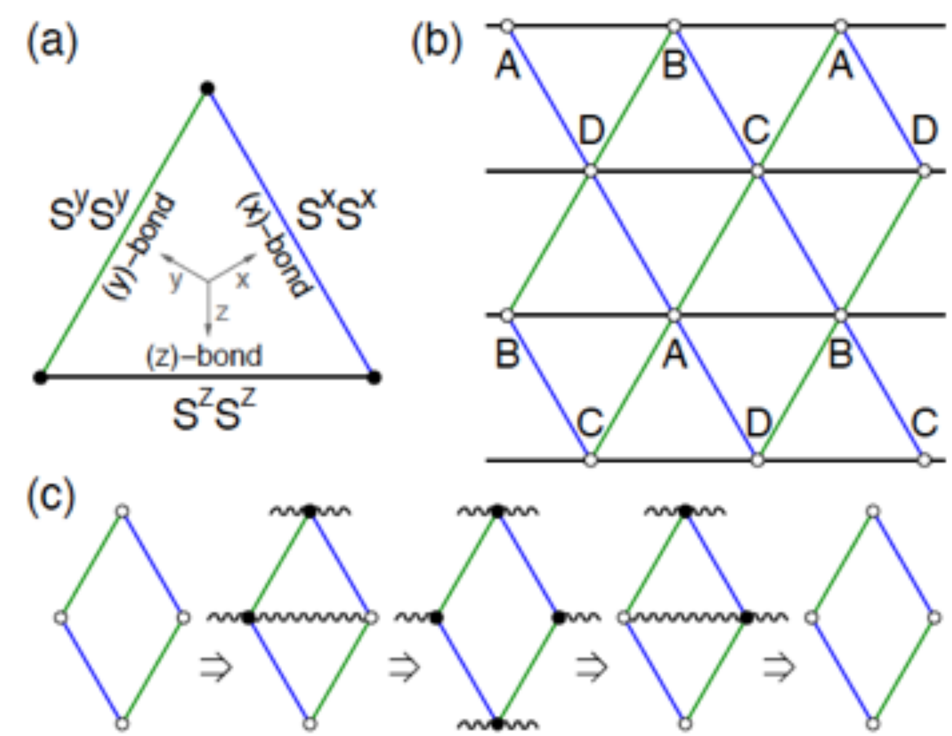
I.Rousochatzakis,U.K. Roessler,
J. van der Brink, M. Daghofer, arXiv:1209.5895

G.Jackeli and A. Avella,arXiv:1504.

Classical



Quantum



Also:
I.Kimchi and A. Vishwanath PRB 2014
M.Becker, M Hermanns, B.Bauer, M.Garst, S.Trebst PRB 2015

Conclusions

1. K_1-K_2 model hosts a number of unconventional aspects, such as the fundamentally different role of thermal and quantum fluctuations.

2. Magnetic phases of the K_1-K_2 model i are only stabilized for quantum spins and not for classical spins, despite having a strong classical character.

3.Classical spins have only nematic order at finite temperatures.

4. Relevance to Na_2IrO_3: the K_2 coupling is the largest energy scale after the NN coupling K_1. The Kitaev spin liquid is significantly more fragile against K_2 than against isotropic Heisenberg terms that shows that Na_2IrO_3 is deep inside the magnetically ordered phase.

Thank you