New phenomena due to Kitaev interactions

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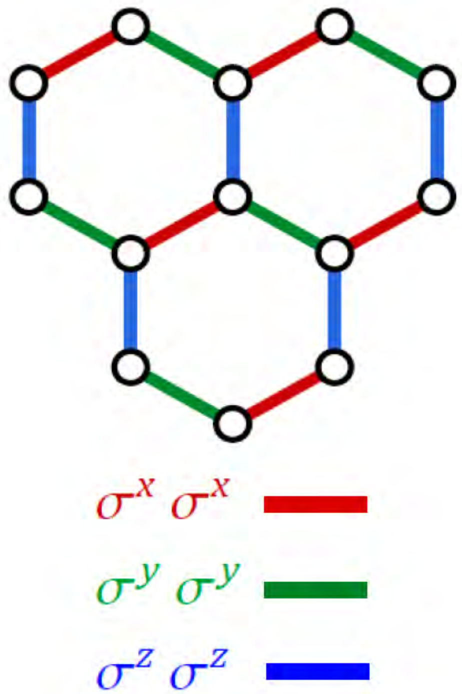
Outline

- Kitaev and Kitaev-Heisenberg model
- Relevance of the Kitaev-Heisenberg model to real materials.
- Possible extensions of the Kitaev-Heisenberg model.
- K_1-K_2 model. Classical and quantum phase diagrams

Kitaev model on the honeycomb lattice



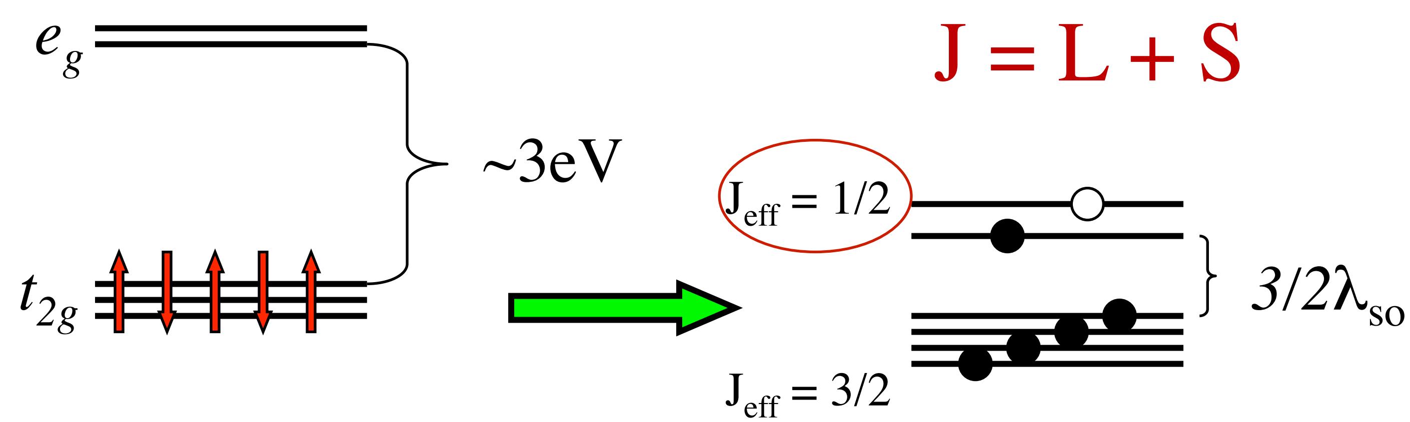
$$H = -\sum_{\langle jk \rangle} J_\alpha\, \sigma_j^\alpha \sigma_k^\alpha = -\sum_{\mathbf{r}\in A}\ \sum_{\alpha=x,y,z} J_\alpha \sigma_{\mathbf{r}}^\alpha \sigma_{\mathbf{r}+\mathbf{d}_\alpha}^\alpha$$

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

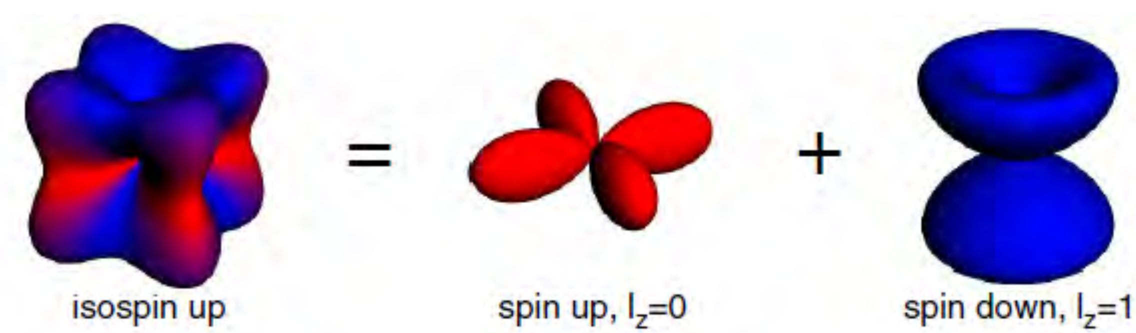
A. Kitaev, Annals of Physics **321**, 2 (2006)

$\lambda_{so} = 0.5\text{eV}$

$J = L + S$

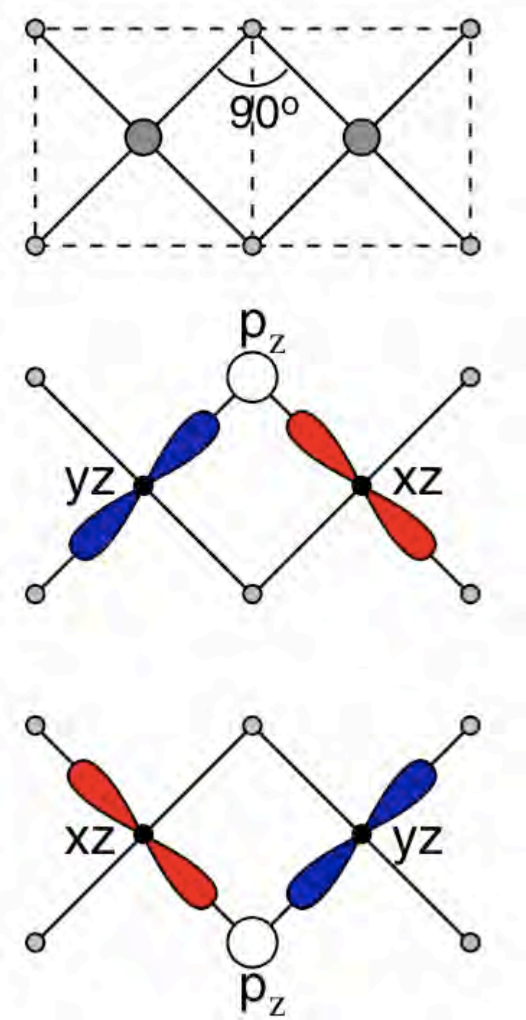


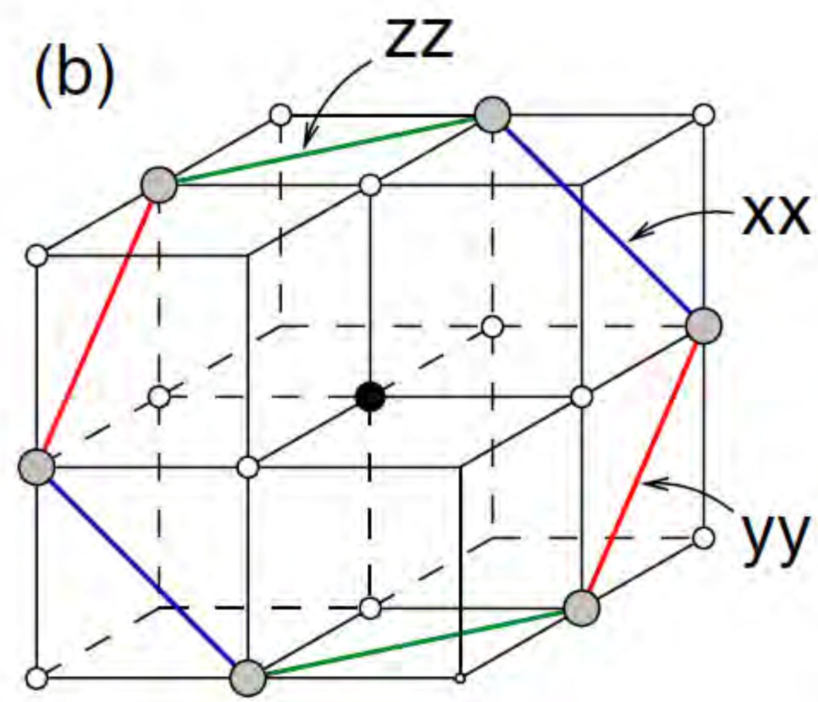
- Exactly solvable!
- Ground state is quantum spin liquid



Kitaev-Heisenberg (KH) model

Super-exchange in A_2IrO_3



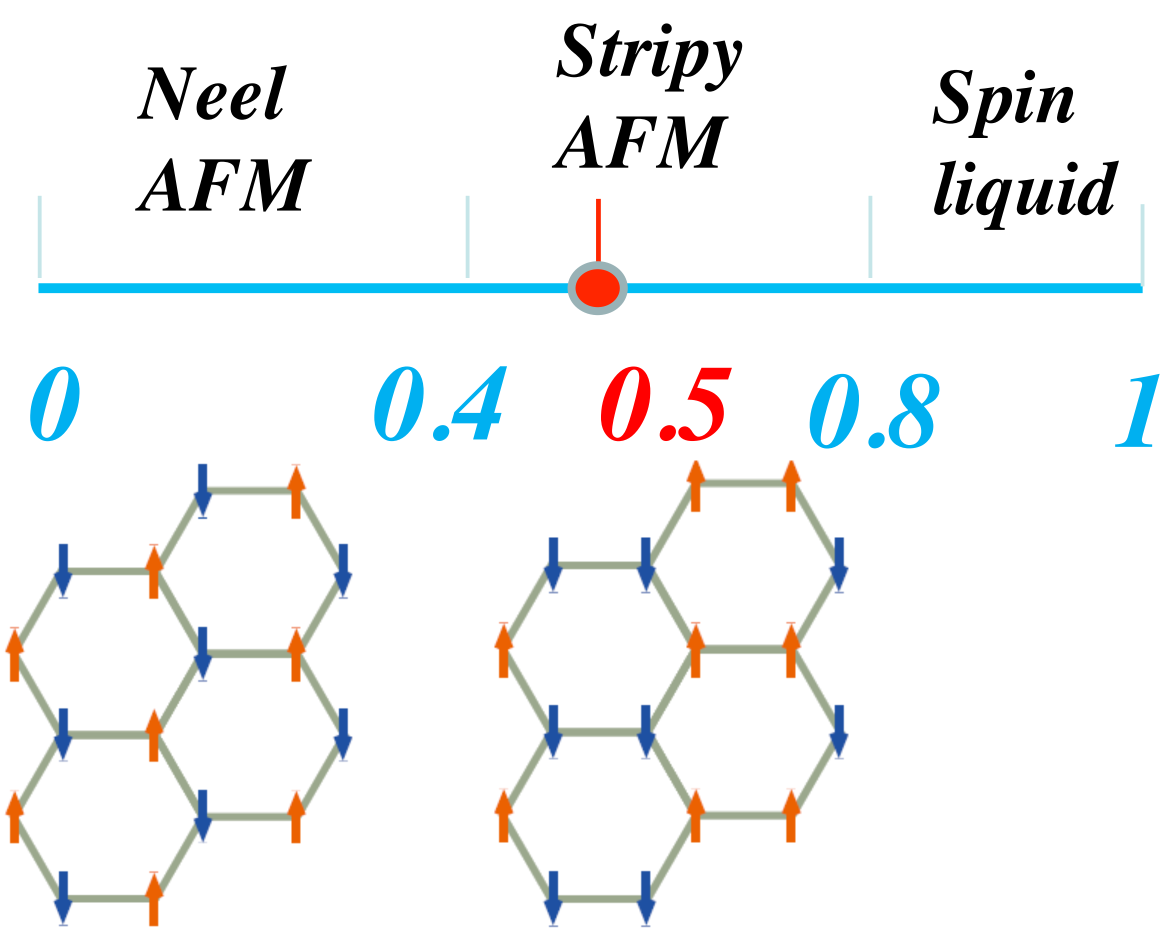


$$\mathcal{H} = -J_K \sum_{\langle ij \rangle_a} \hat{\sigma}_i^a \hat{\sigma}_j^a + J_H \sum_{\langle ij \rangle} \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j$$

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

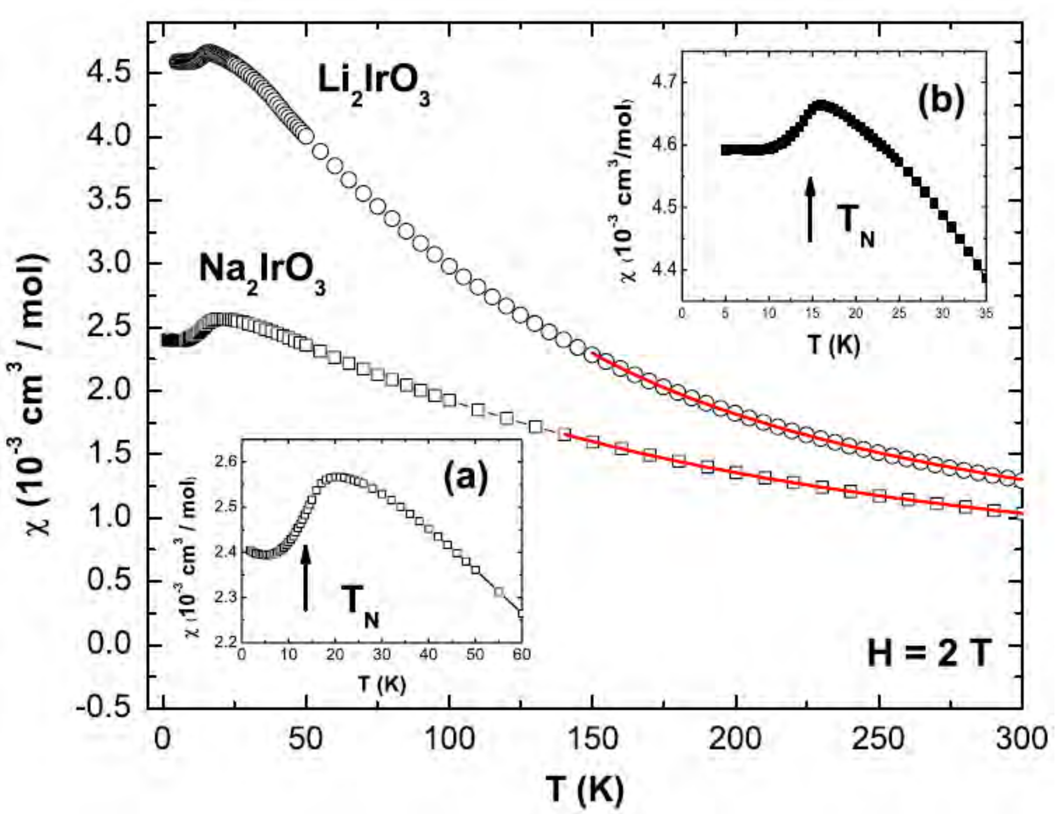
Phase diagram of the KH model

$$\mathcal{H}_{ij}^{(\gamma)} = (1-\alpha)\ \text{Heisenberg} - 2\alpha\ \text{Kitaev}$$

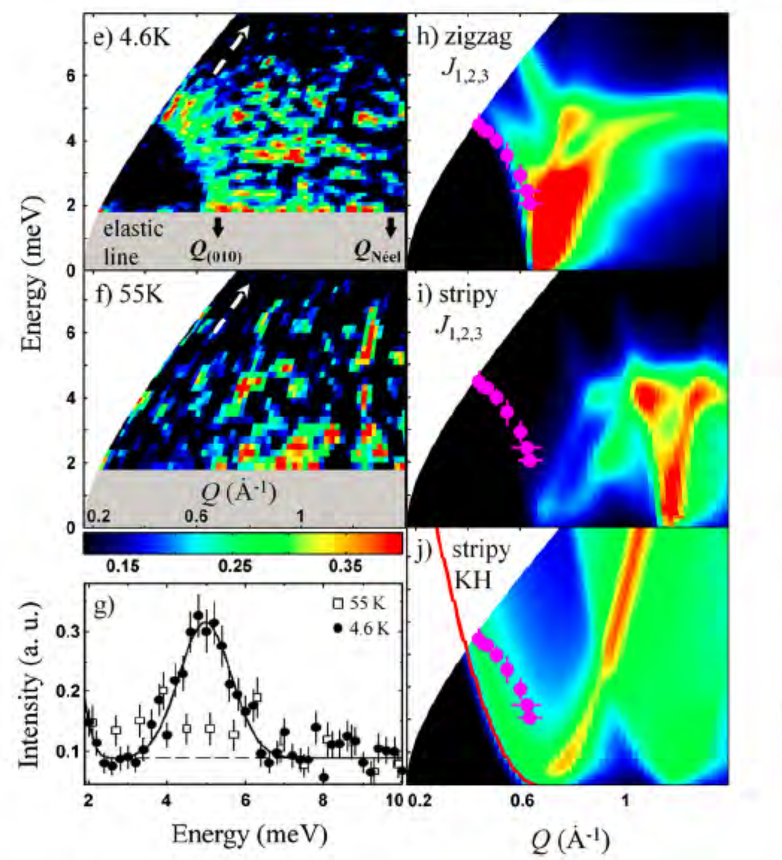


- *Neel* AF order at $\alpha<0.4$
- *Stripy* AF order at $0.4<\alpha<0.8$
  exact at $\alpha=1/2$
- Spin liquid at $0.8<\alpha<1$
  exact at $\alpha=1$

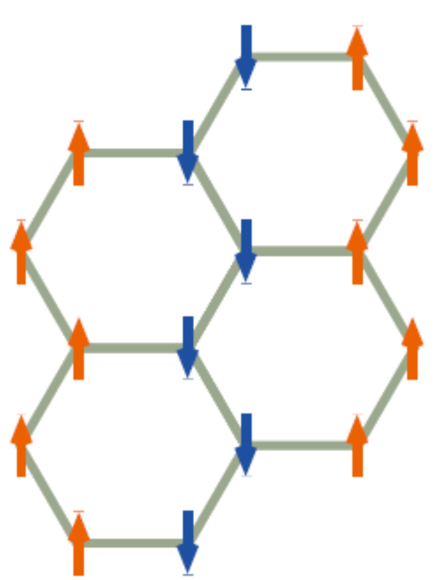
Na_2IrO_3: zigzag order



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

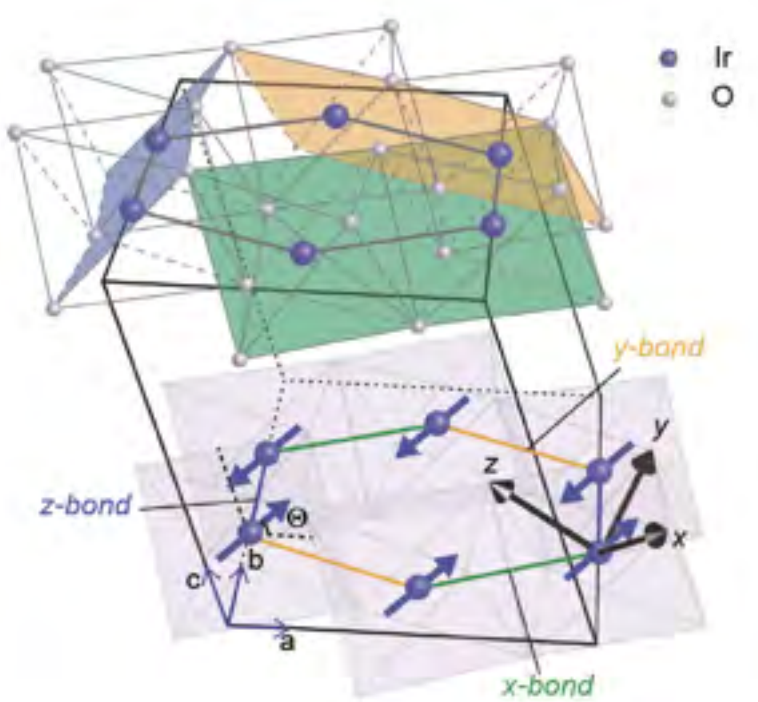


S. K. Choi et al PRL 2012



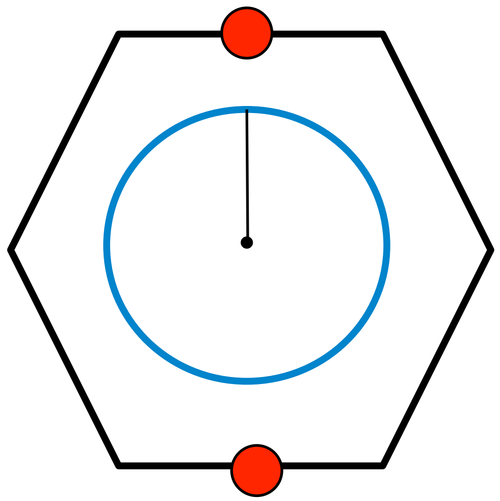
X. Liu et al, PRB 2011

Feng Ye et al, PRB 2012



S.H.Chun et al, Nature Physics 2015

Li_2IrO_3: spiral order

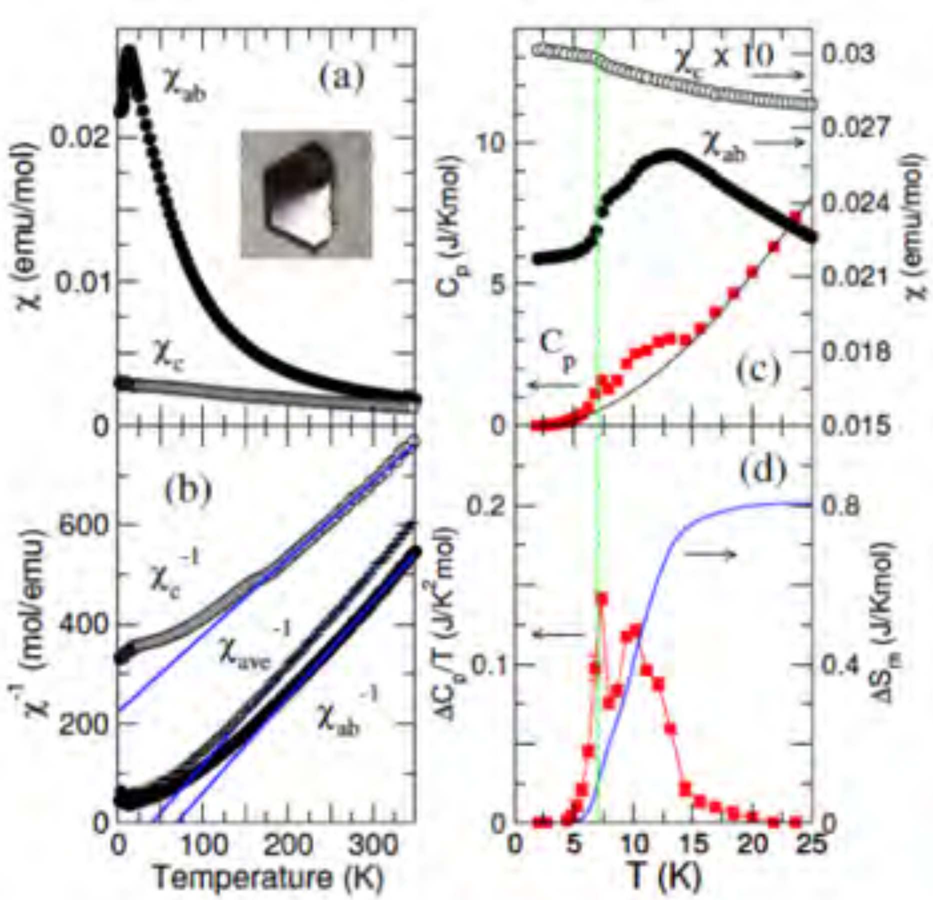


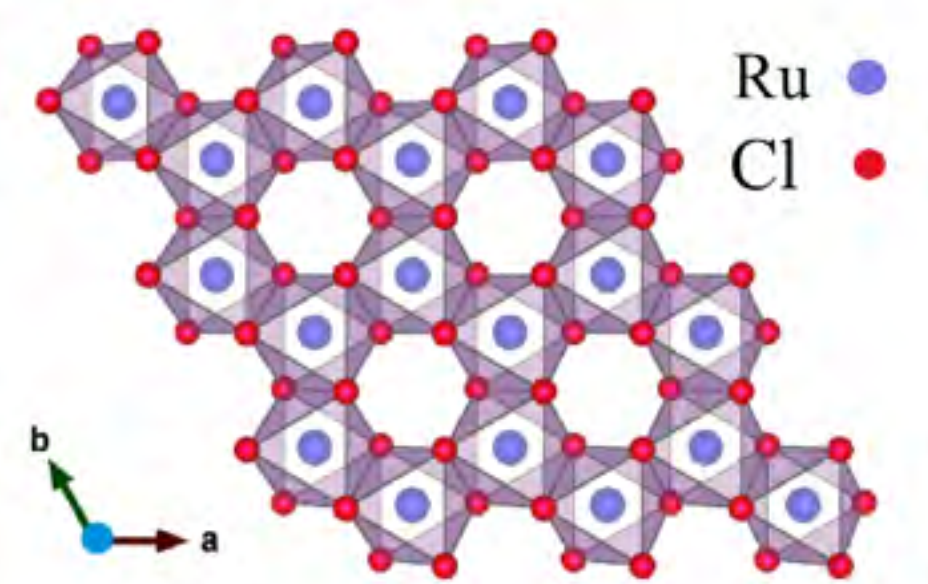
zigzag with $Q=(0,2\pi/\sqrt{3})$

spiral with $Q=(x,q)$

Radu Coldea, *SPORE13*,unpublished

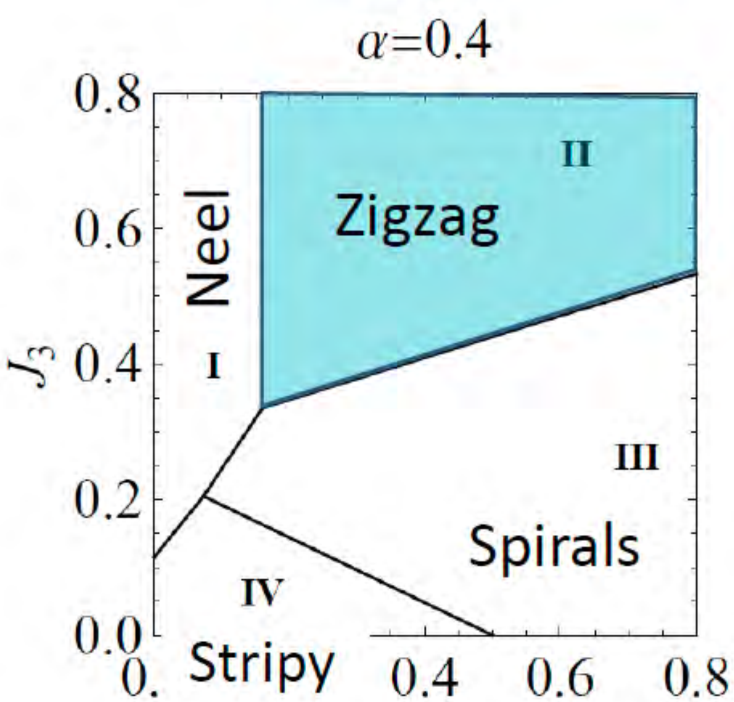
α-$RuCl_3$: zigzag order





K. W. Plumb, *et al* PRB 2014
J. A. Sears, *et al* PRB 2015

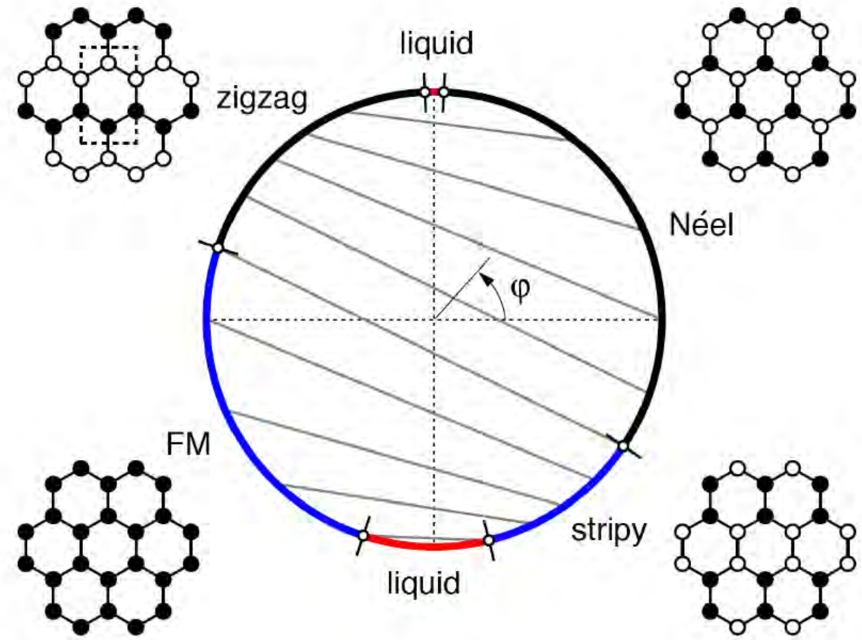
Extensions of KH model for Na_2IrO_3



J_1-K_1-J_2-J_3

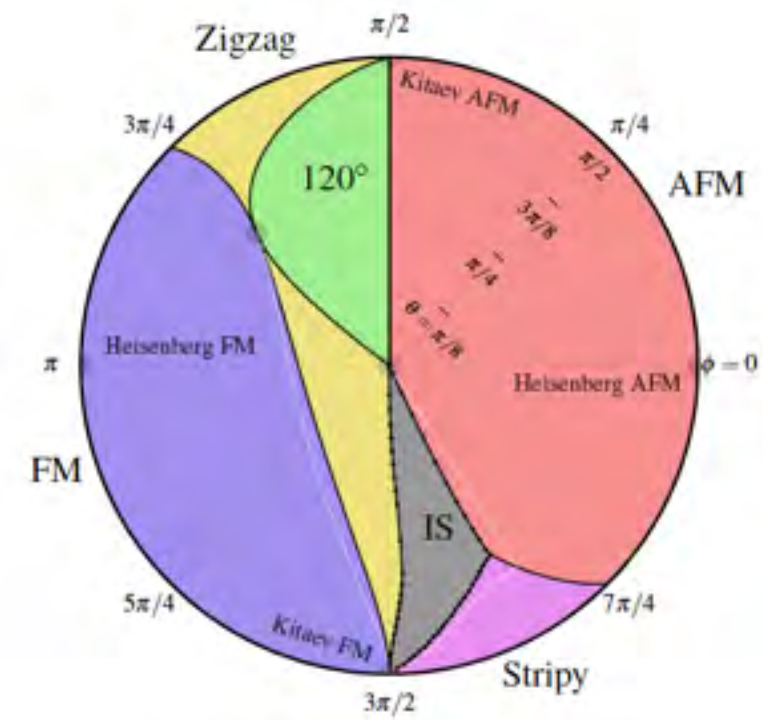
I.Kimchi & Y.Z. You, PRB 2011

S. K. Choi et al PRL 2012



$$\mathcal{H}_{ij}^{(\gamma)} = A\,(2\sin\varphi\; S_i^\gamma S_j^\gamma + \cos\varphi\; \boldsymbol{S}_i\cdot\boldsymbol{S}_j)$$

J. Chaloupka, G. Jackeli, G. Khaliullin PRL 2013



(a) Classical phase diagram with Γ > 0

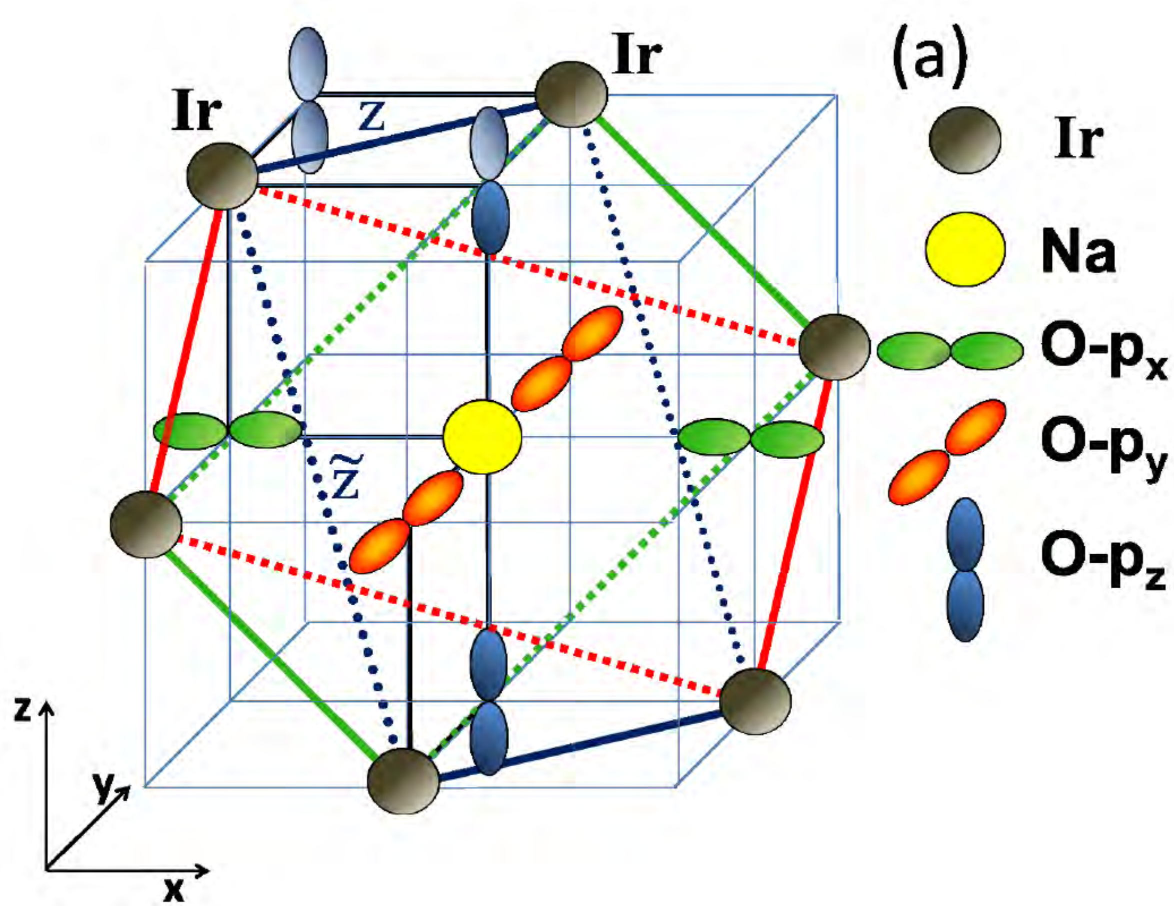
NN KH model +

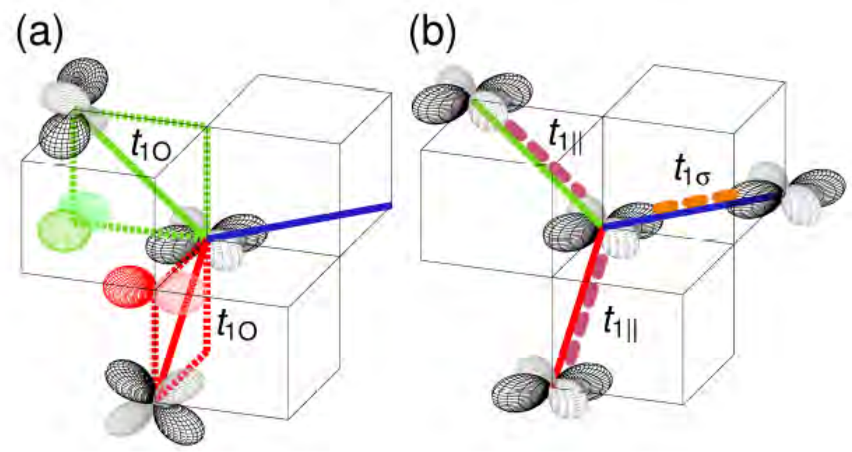
$$+\Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)$$

J.G. Rau, E. K.-H. Lee, H.-Y. Kee, PRL 2014

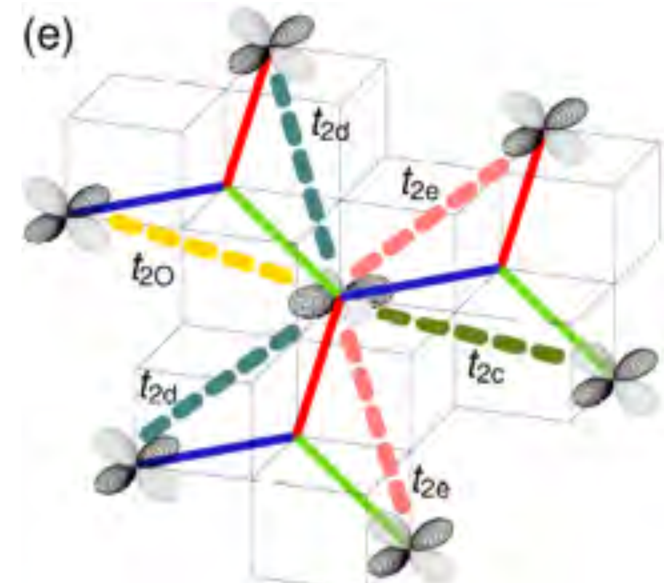
J. Chaloupka, G. Khaliullin, arXiv:1502.02587

Revision of the super-exchange model for Na_2IrO_3





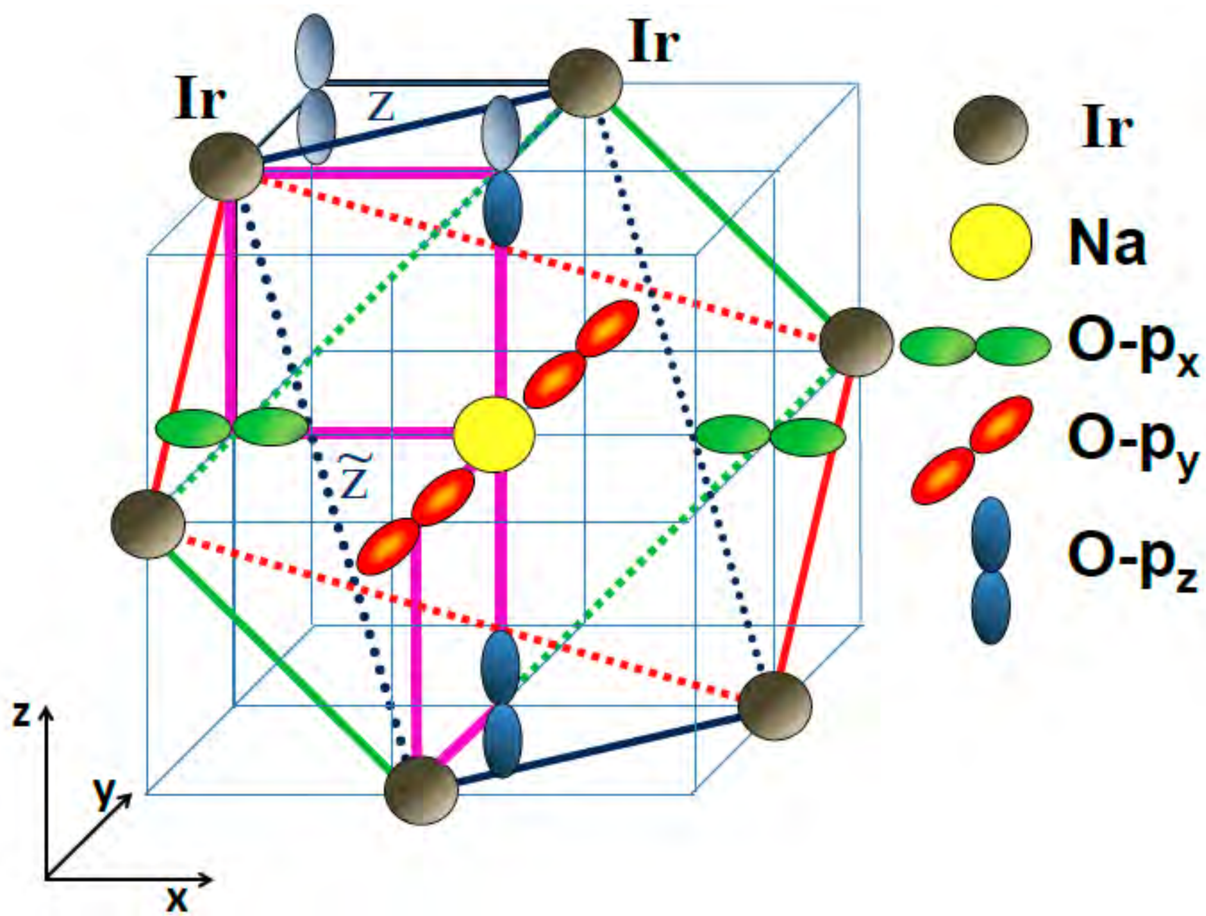
$$t_{1o} = 230 \text{ meV}$$
$$t_{1\sigma} = 67 \text{ meV}$$

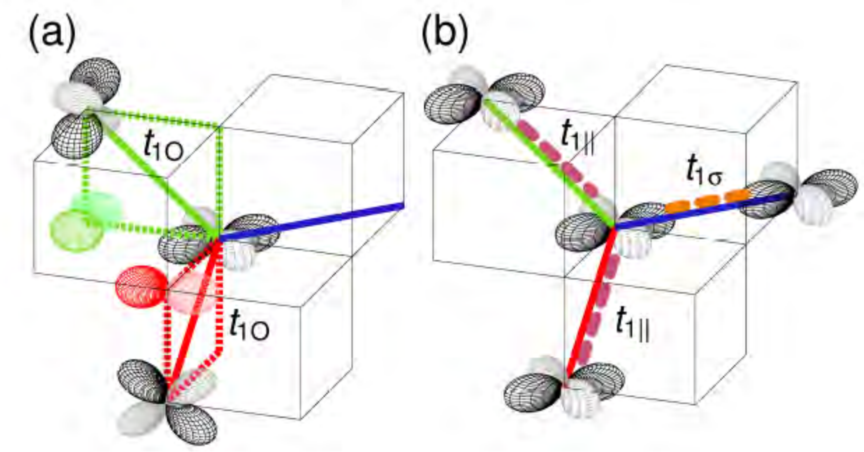


$$t_{2o} = 94.7 \text{ meV}$$

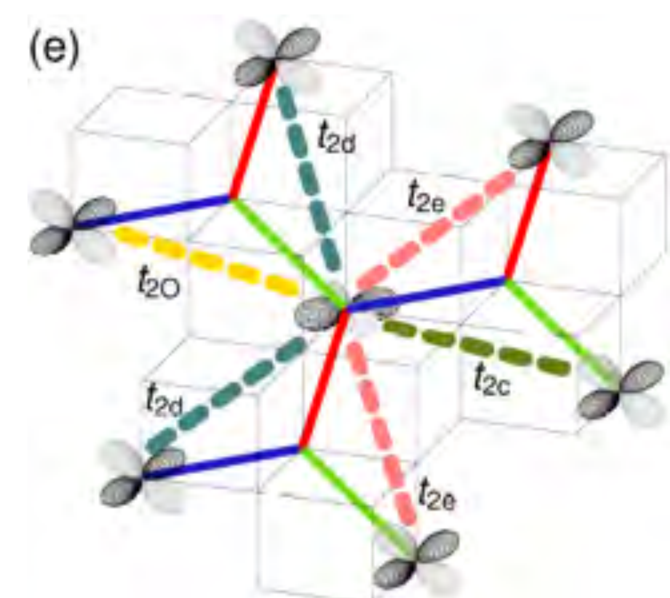
Kateryna Foyevtsova *et al*, PRB 2013

Revision of the super-exchange model for Na_2IrO_3





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



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

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 : $\mathrm{Ir}\,(Y) \to \mathrm{O}\,(p_x) \to$ I

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

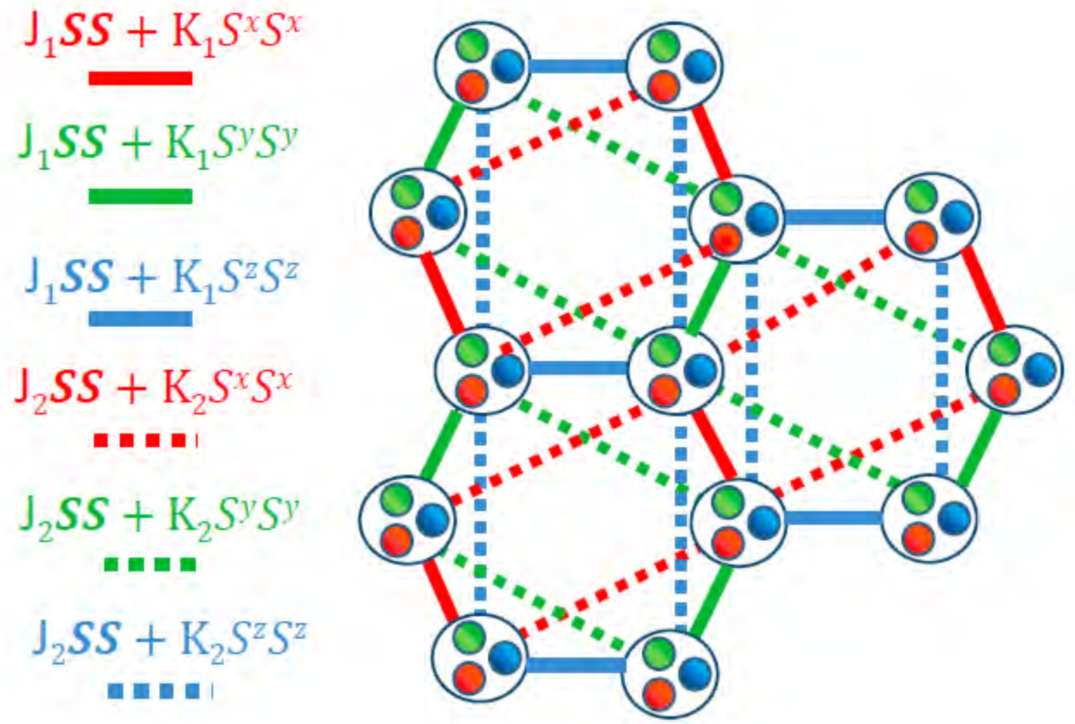
Kitaev interaction

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

J_1-K_1-J_2-K_2 model

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

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



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

Na_2IrO_3

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

$J_1 = 5.8$ meV, $K_1 = -14.8$ meV
$J_2 = -4.4$ meV, $K_2 = -2J_2$

zigzag

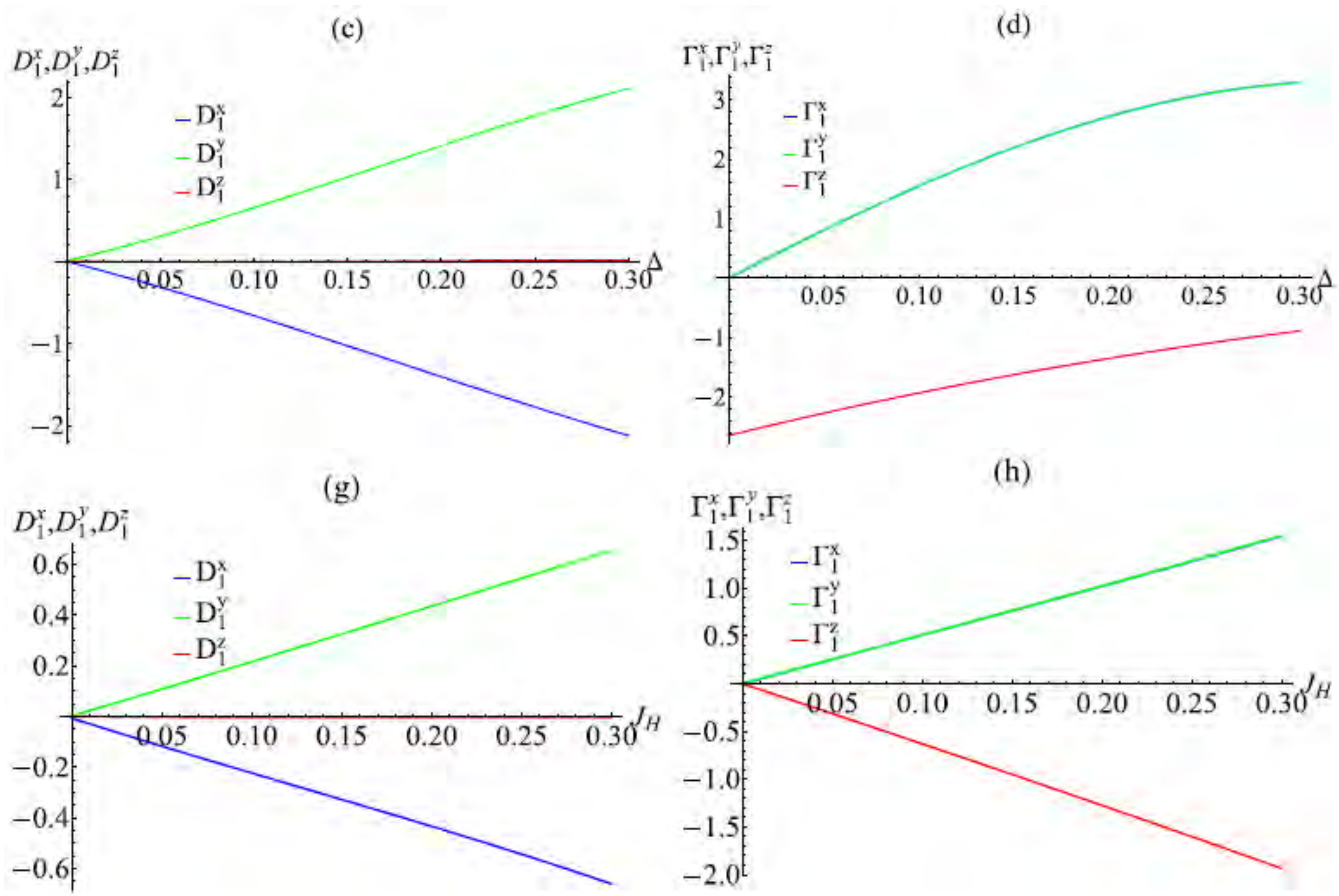
$J_1 = 3$ meV $\quad K_1 = -17$ meV

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

Curie-Weiss temperature:
θcw = -125K (Na)

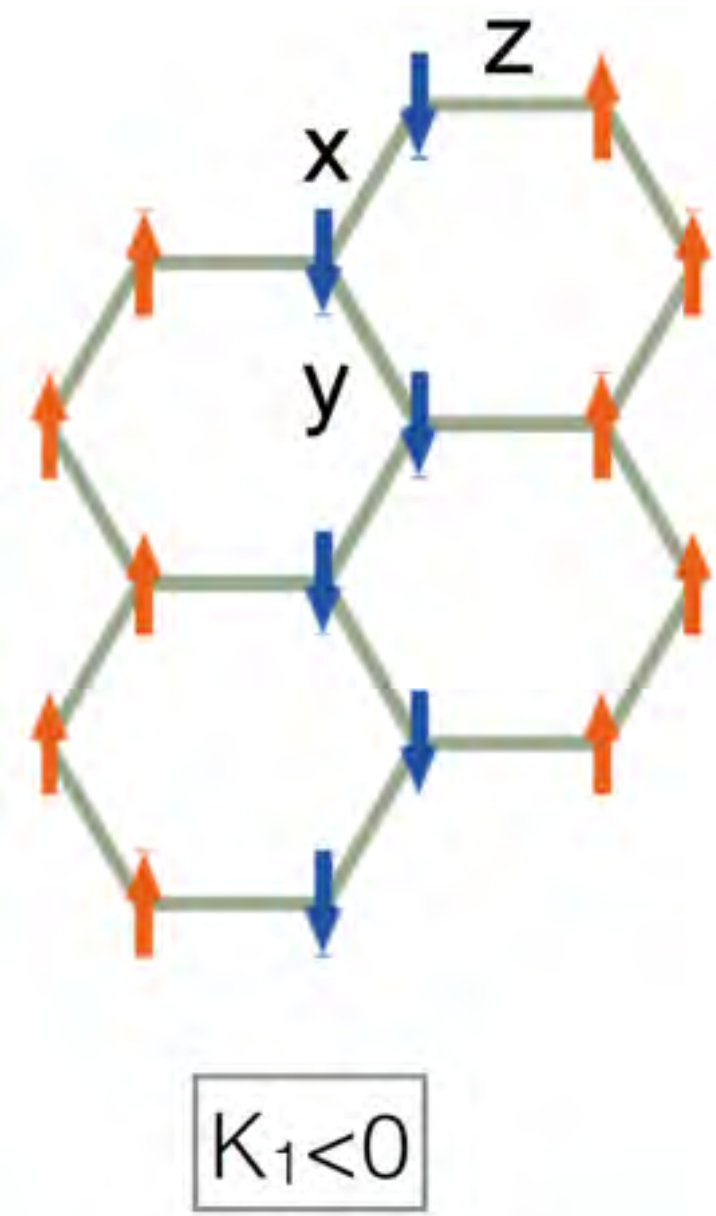
Off-diagonal interactions In Na_2IrO_3

$$H_{ex,n,n'} = \sum_{\alpha\beta} \Theta^{\alpha\beta}_{n,n'} S^{\alpha}_{n} S^{\beta}_{n'}$$



$$D_1^x = \frac{1}{2}\left(J_1^{yz} - J_1^{zy}\right)$$
$$D_1^y = \frac{1}{2}\left(J_1^{zx} - J_1^{xz}\right)$$
$$D_1^z = \frac{1}{2}\left(J_1^{xy} - J_1^{yx}\right)$$
$$\Gamma_1^x = \frac{1}{2}\left(J_1^{yz} + J_1^{zy}\right)$$
$$\Gamma_1^y = \frac{1}{2}\left(J_1^{zx} + J_1^{xz}\right)$$
$$\Gamma_1^z = \frac{1}{2}\left(J_1^{xy} + J_1^{yx}\right)$$

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

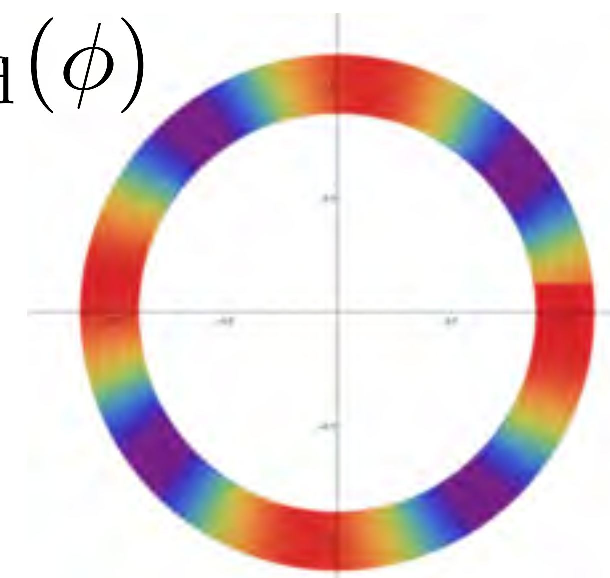


$$S = S_0 + S_{\mathrm{fl}}(\theta, \phi)$$

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

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

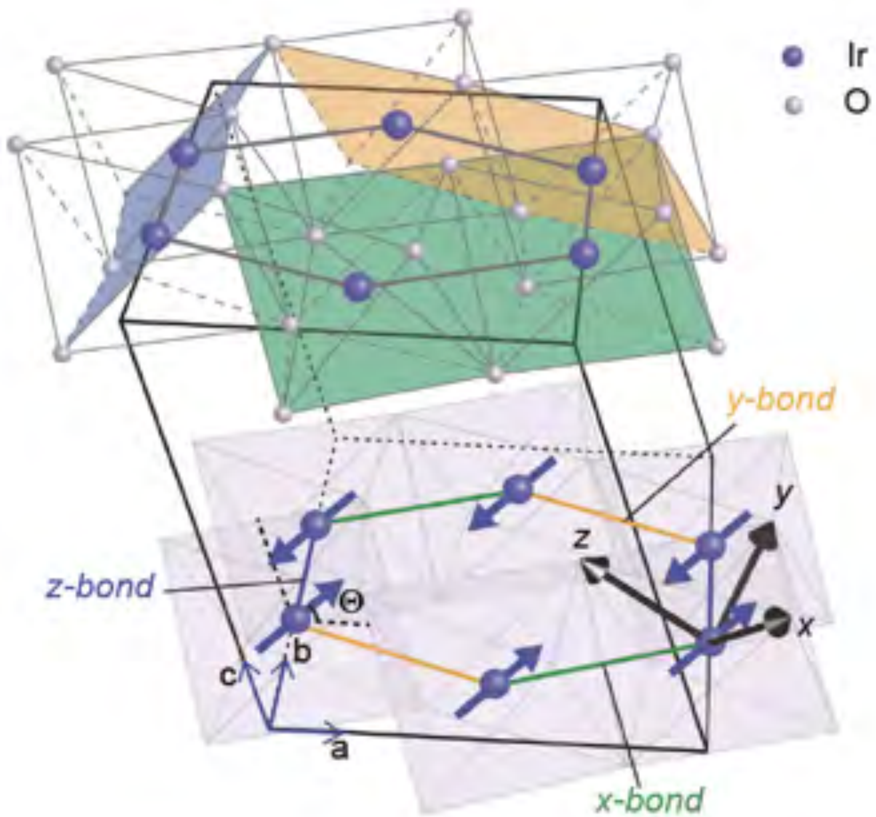
$S_{\mathrm{fl}}(\phi)$



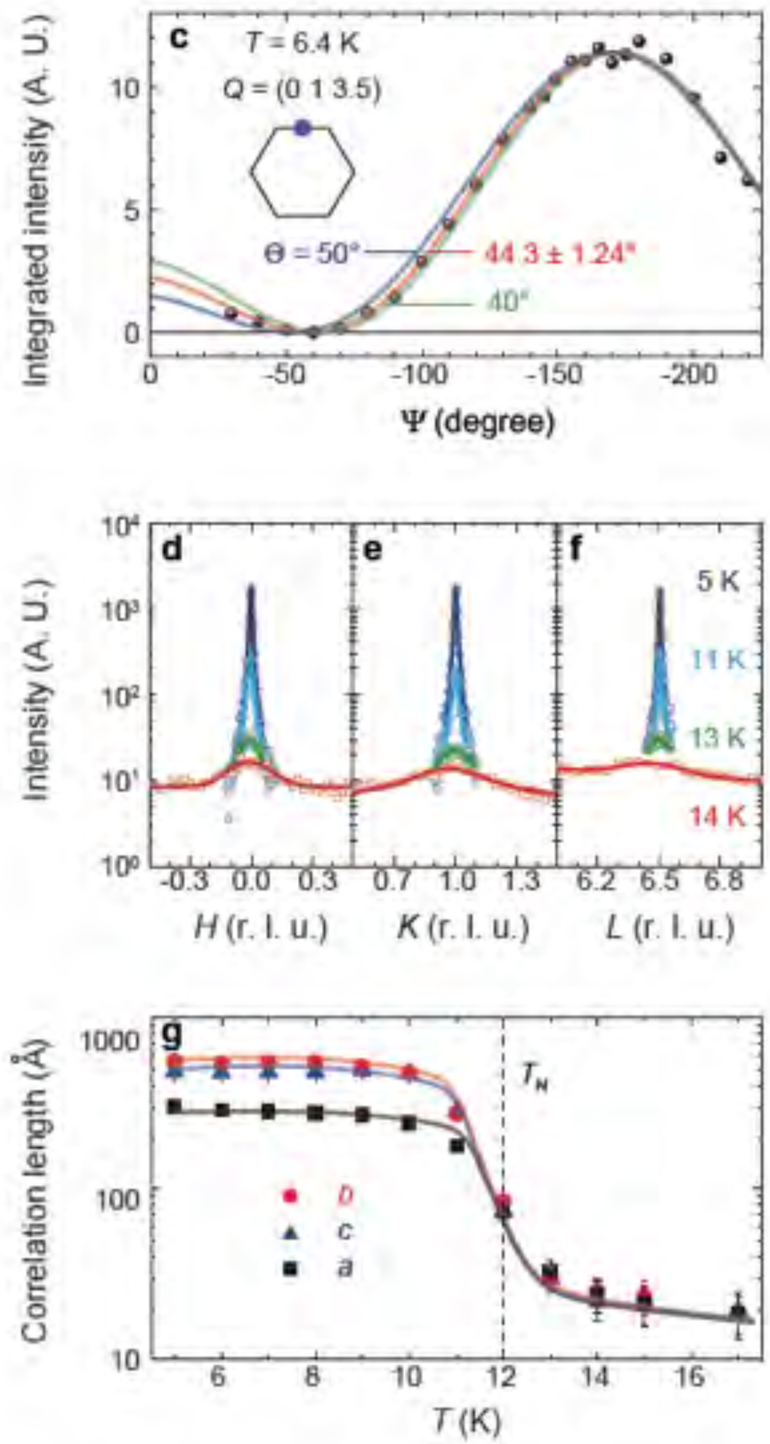
spin fluctuations select one of the diagonals in xy-plane

Y.Sizyuk, N.B.P, P. Wölfle 2015

Diffuse magnetic x-ray scattering

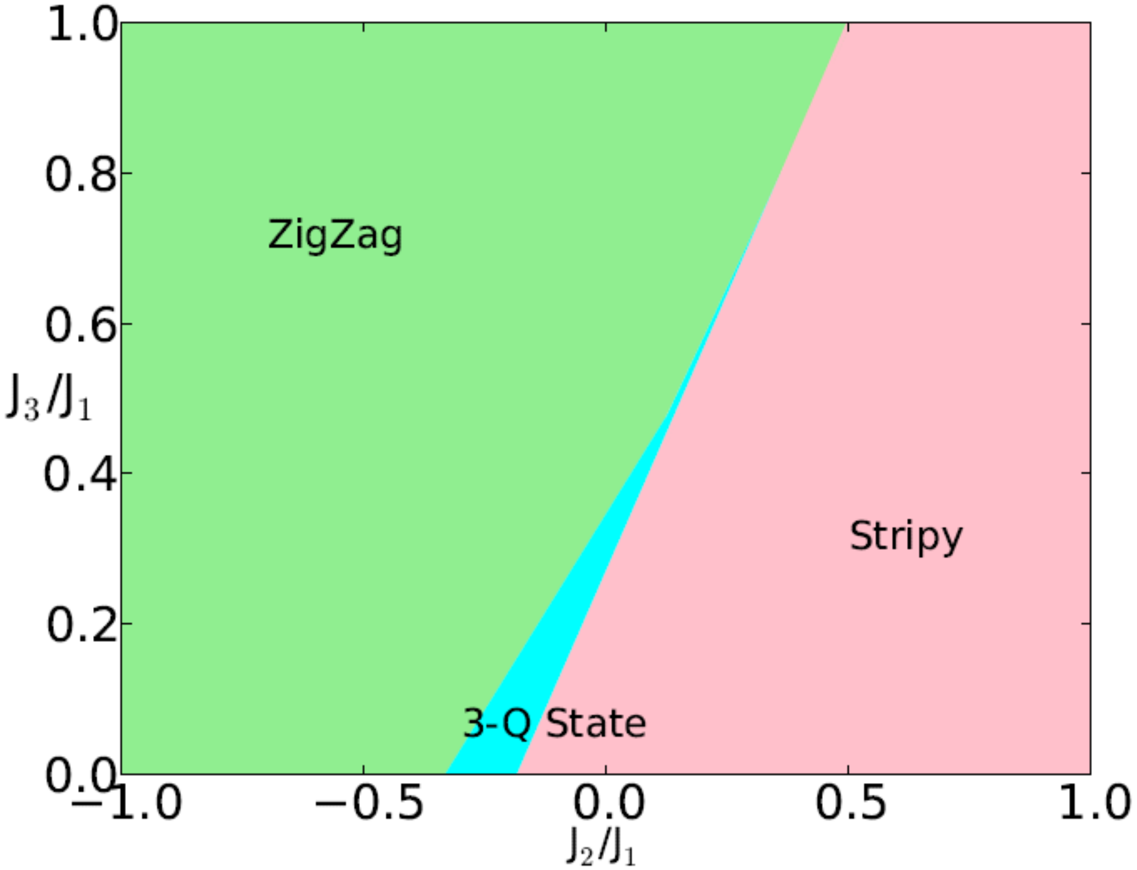


S.H.Chun et al, Nature Physics 2015



Phase diagram

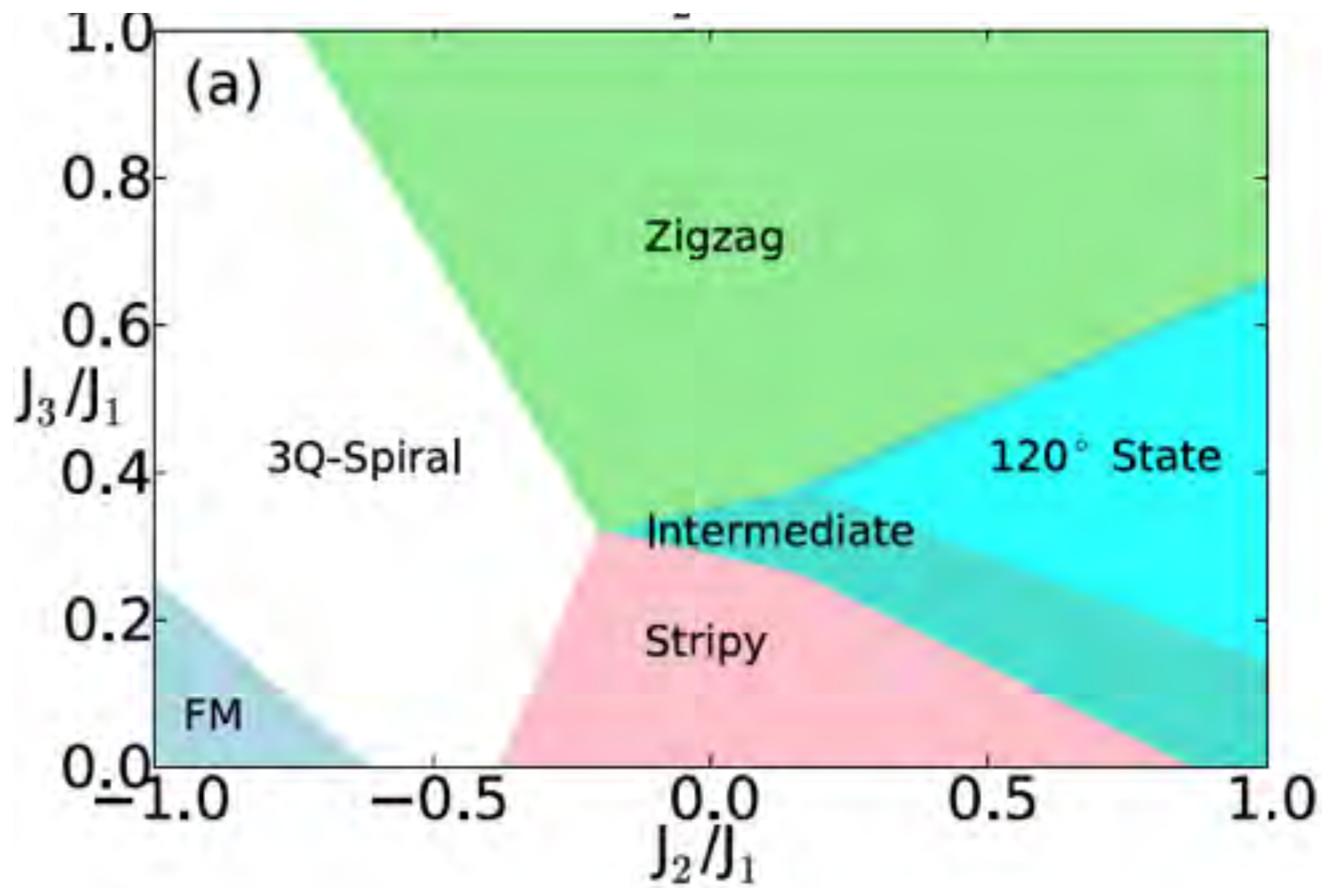
$K_2 = -2J_2$

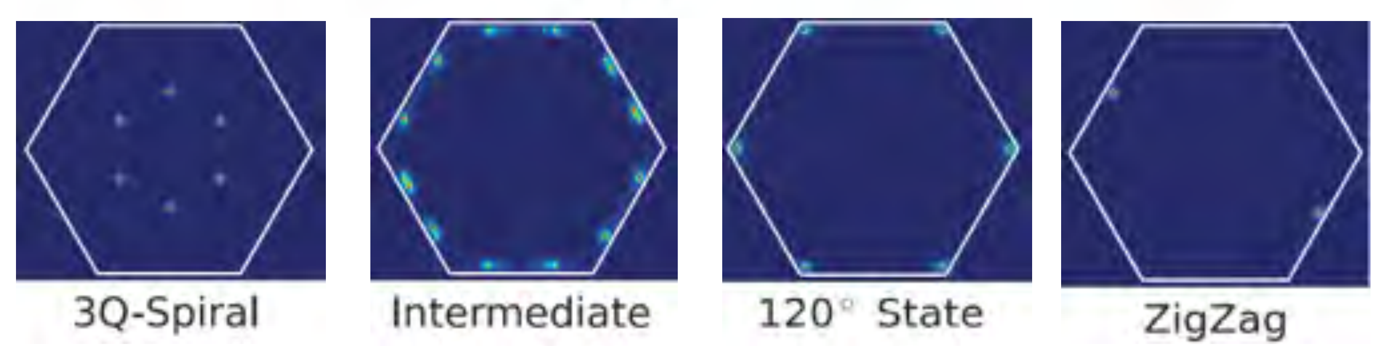


$J_1 = 3$ meV

$K_1 = -17$ meV

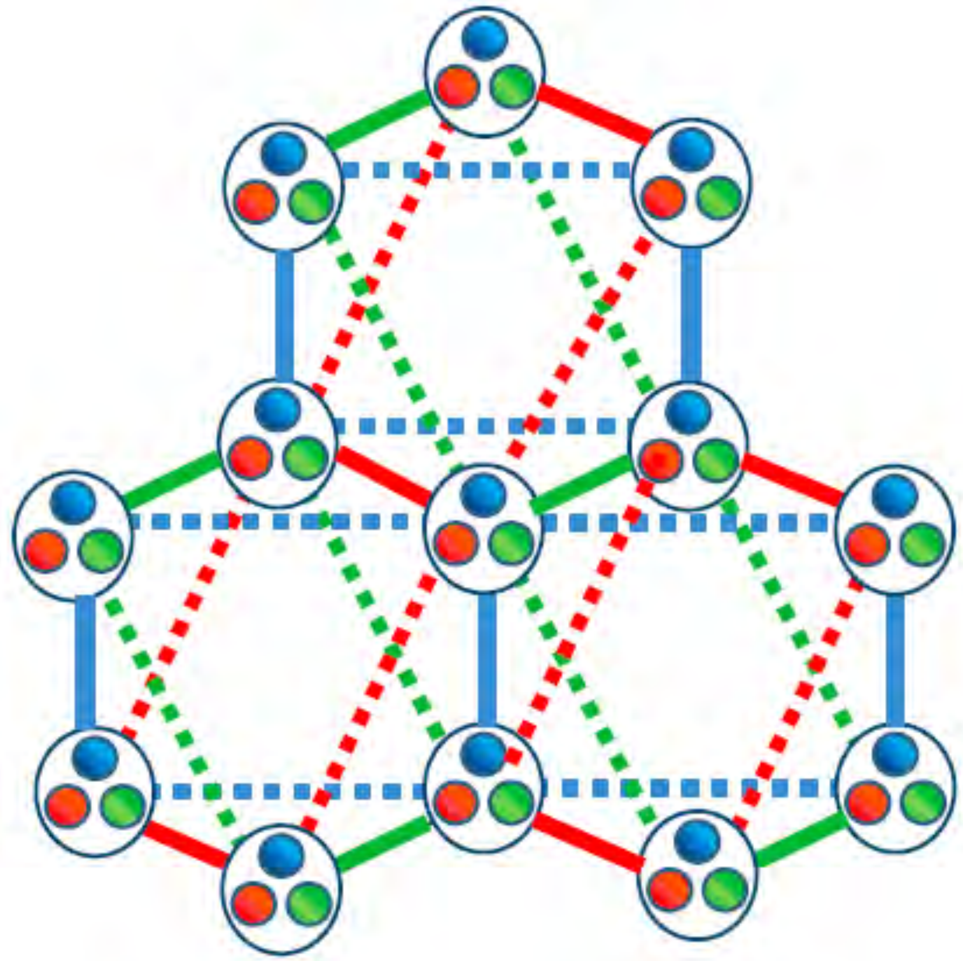
$K_2 < -2J_2$



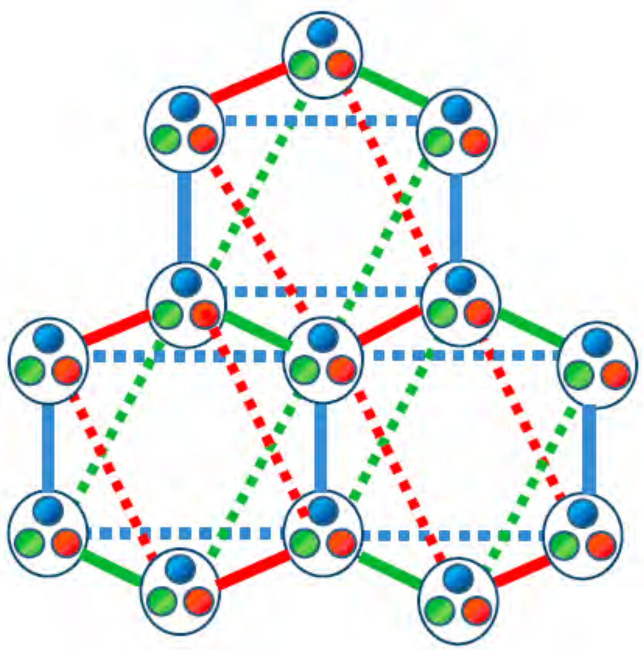


K_1-K_2 model

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



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

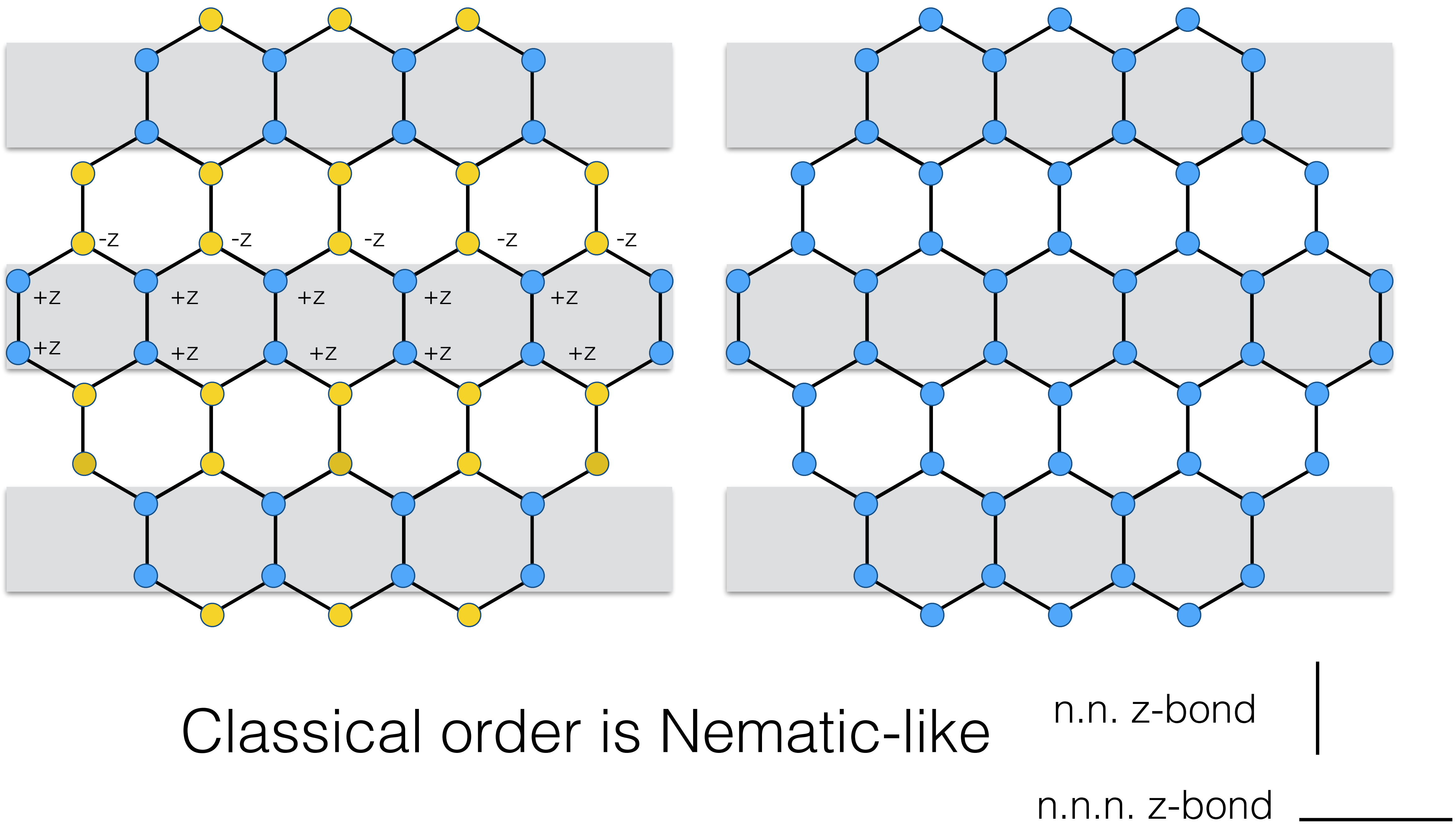
This degeneracy is not accidental but it is related to the presence of gauge-like symmetries in the Hamiltonian.

$K_1 < 0$

$K_2 < 0$

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

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



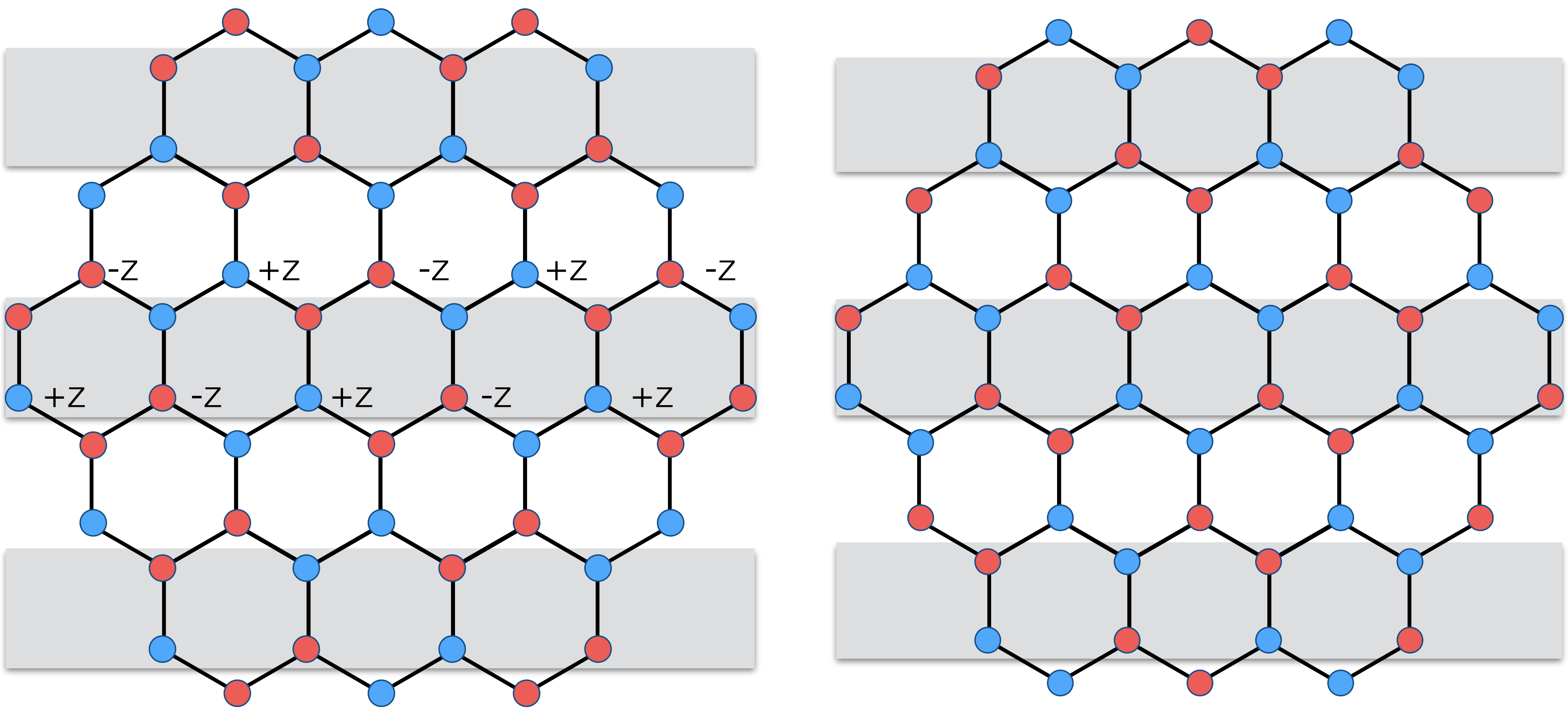
Classical order is Nematic-like

$K_1 > 0$

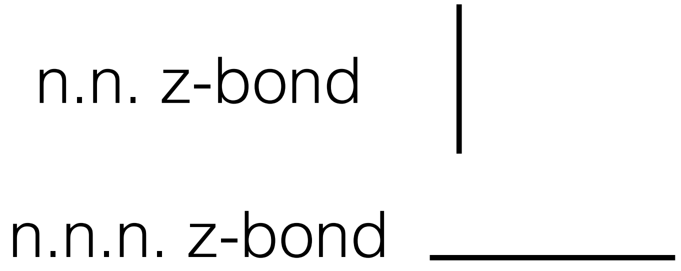
$K_2 > 0$

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

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



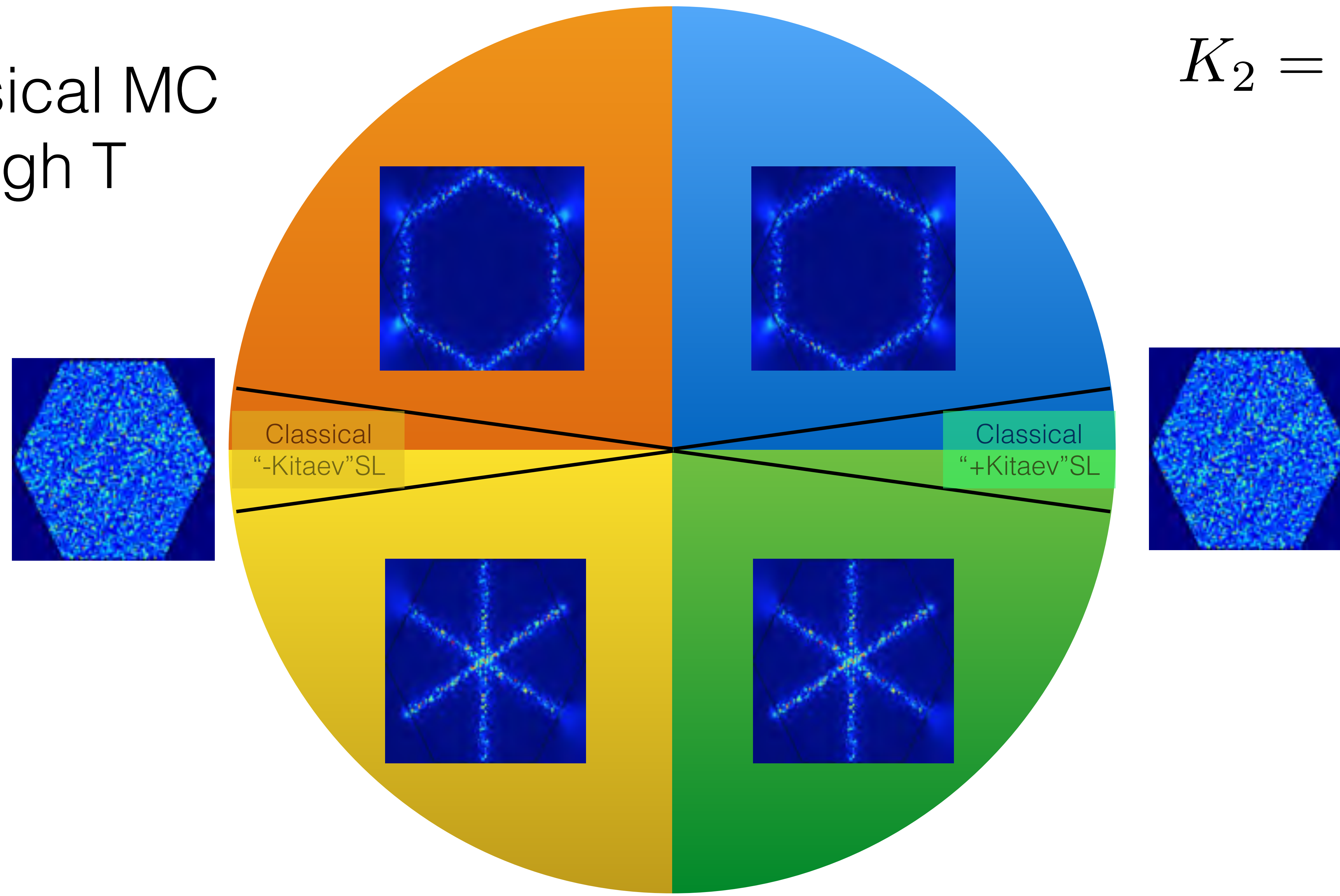
Classical order is Nematic-like



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

$$K_1 = \cos\phi$$
$$K_2 = \sin\phi$$

Classical MC
High T



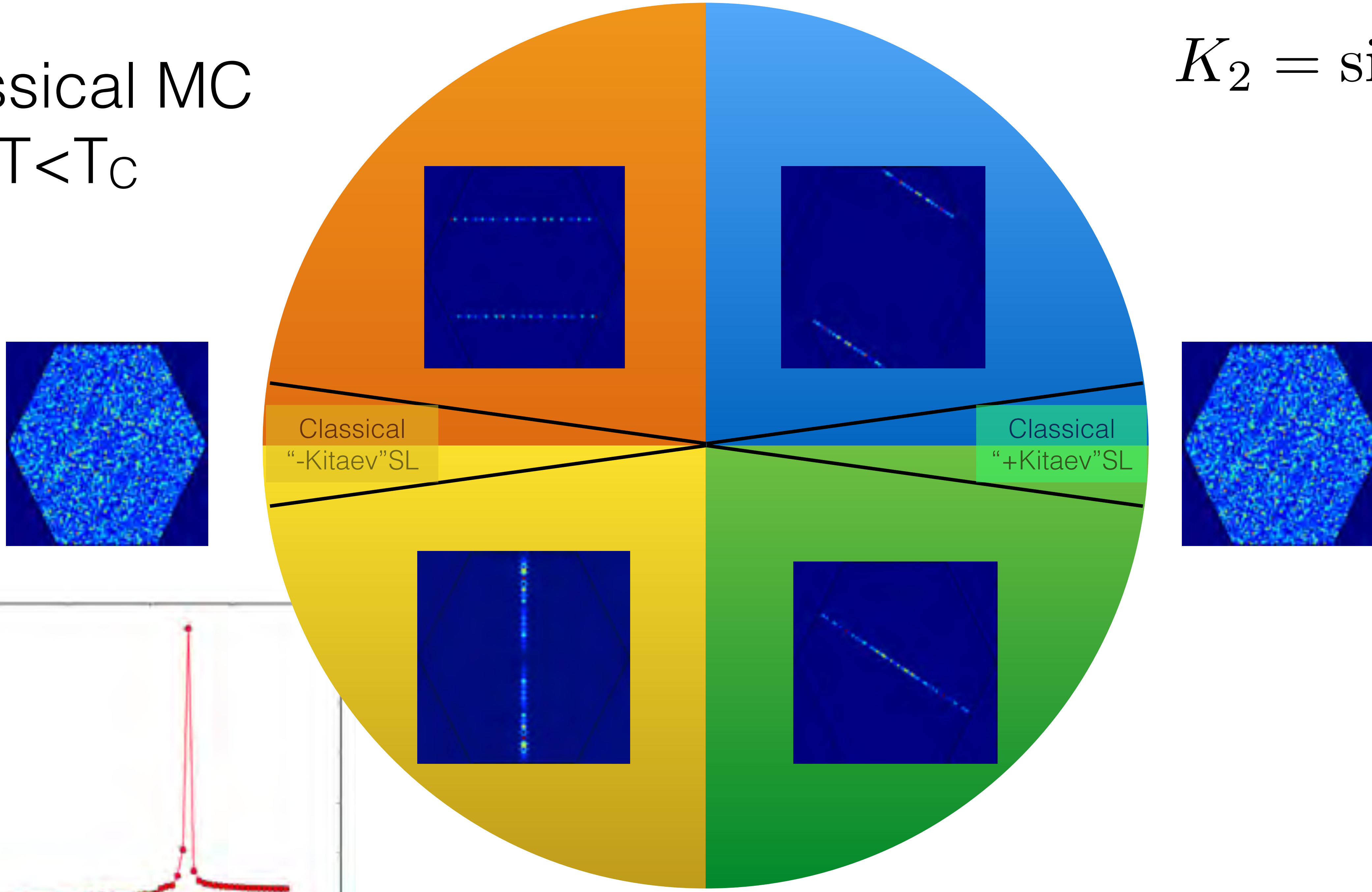
$$H(\varphi) = \cos(\varphi) \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma + \sin(\varphi) \sum_{\langle\langle ij \rangle\rangle_\lambda} S_i^\lambda S_j^\lambda$$

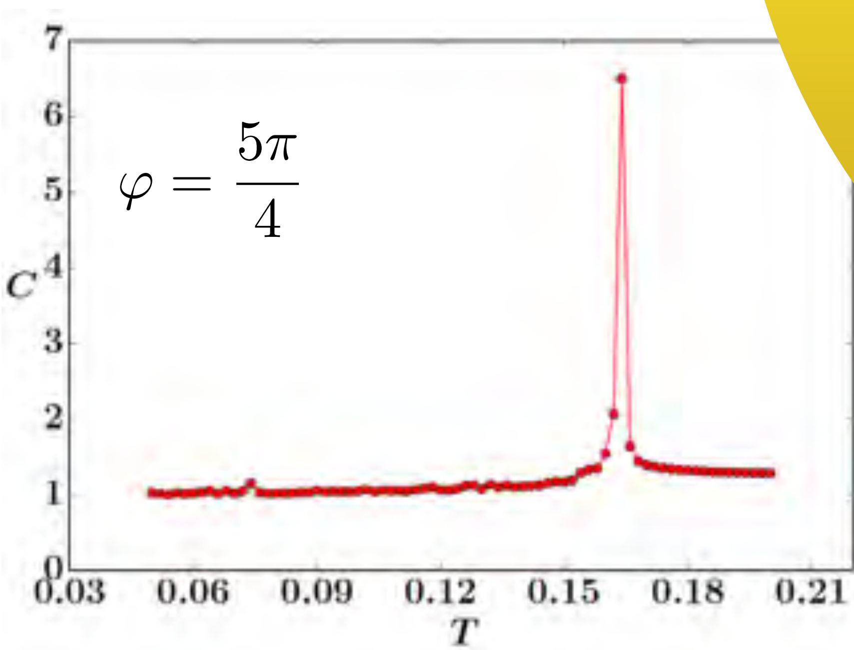
$K_1 = \cos\phi$

$K_2 = \sin\phi$

Classical MC

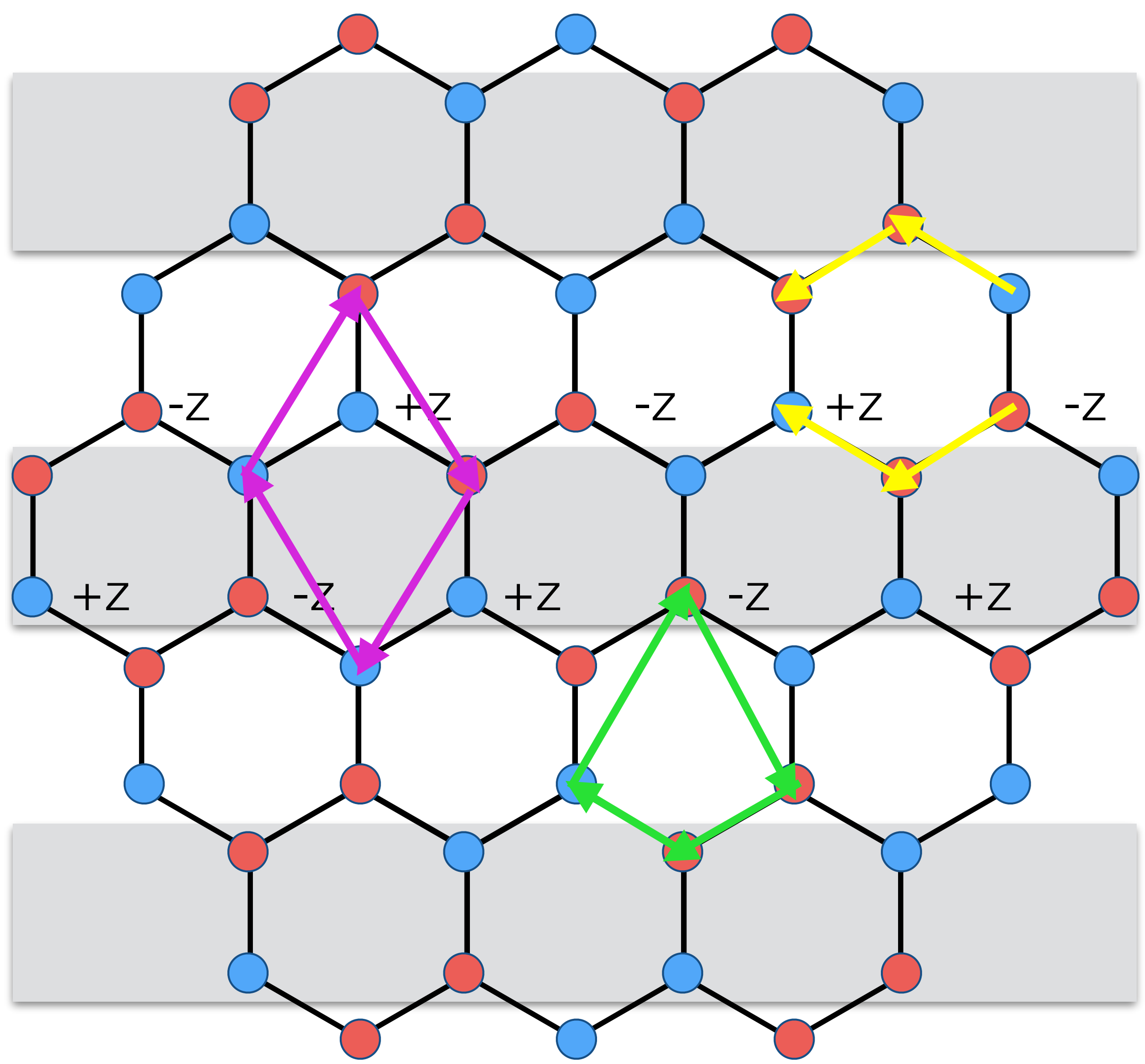
T<Tc

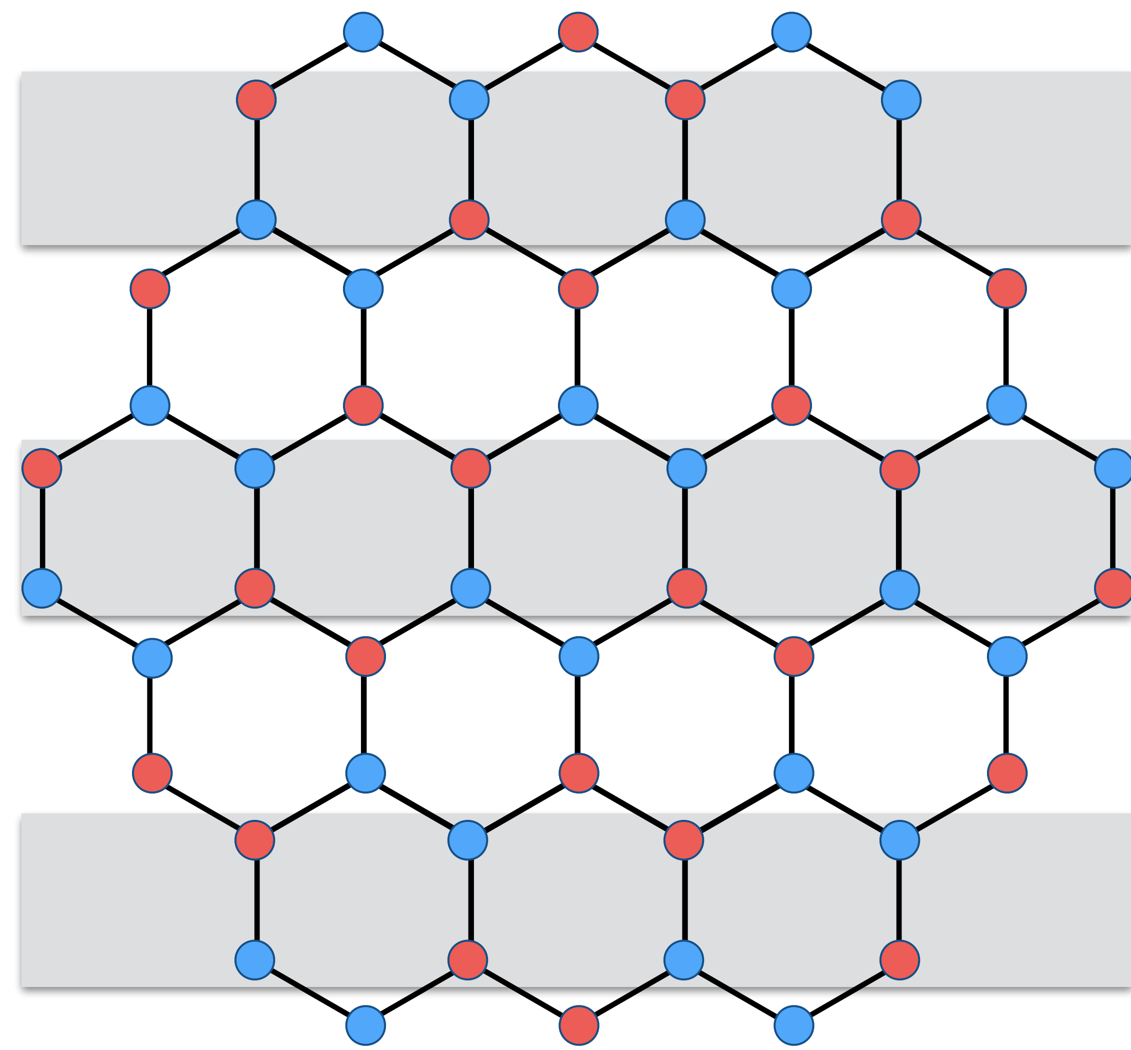




Quantum K_1-K_2 model

LR magnetic order is possible





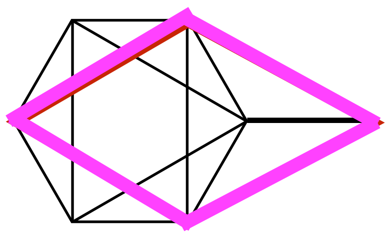
$$K_1 > 0$$

$$K_2 > 0$$

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

$K_{2x} = K_{2y} = xK_{2z}$ $\quad x < 1$

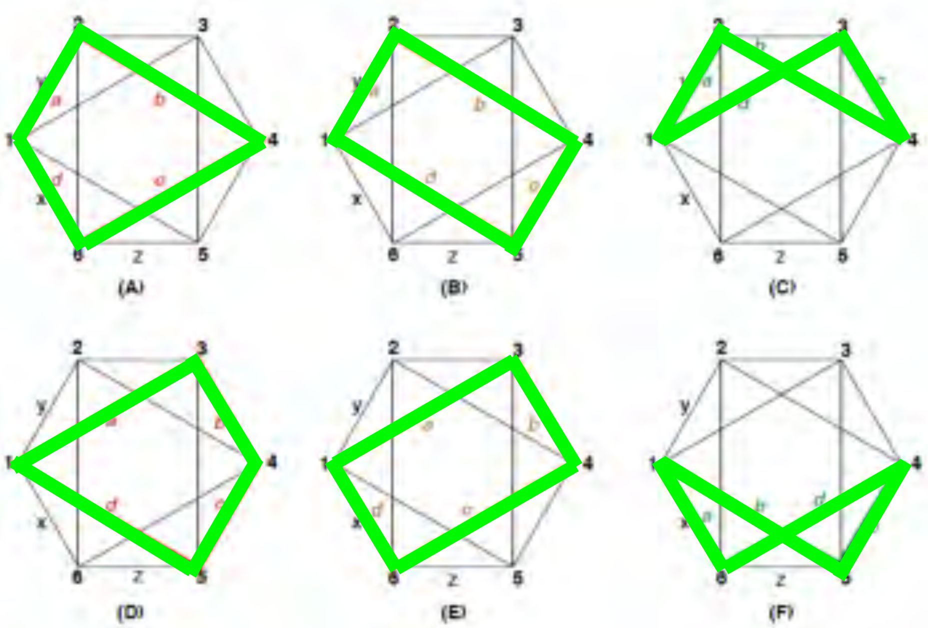
I



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

Jackeli & Avella, arXiv:1504.03618

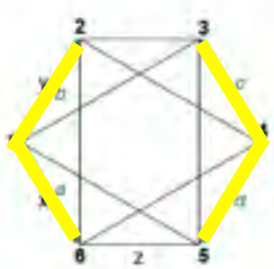
II



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

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

III



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

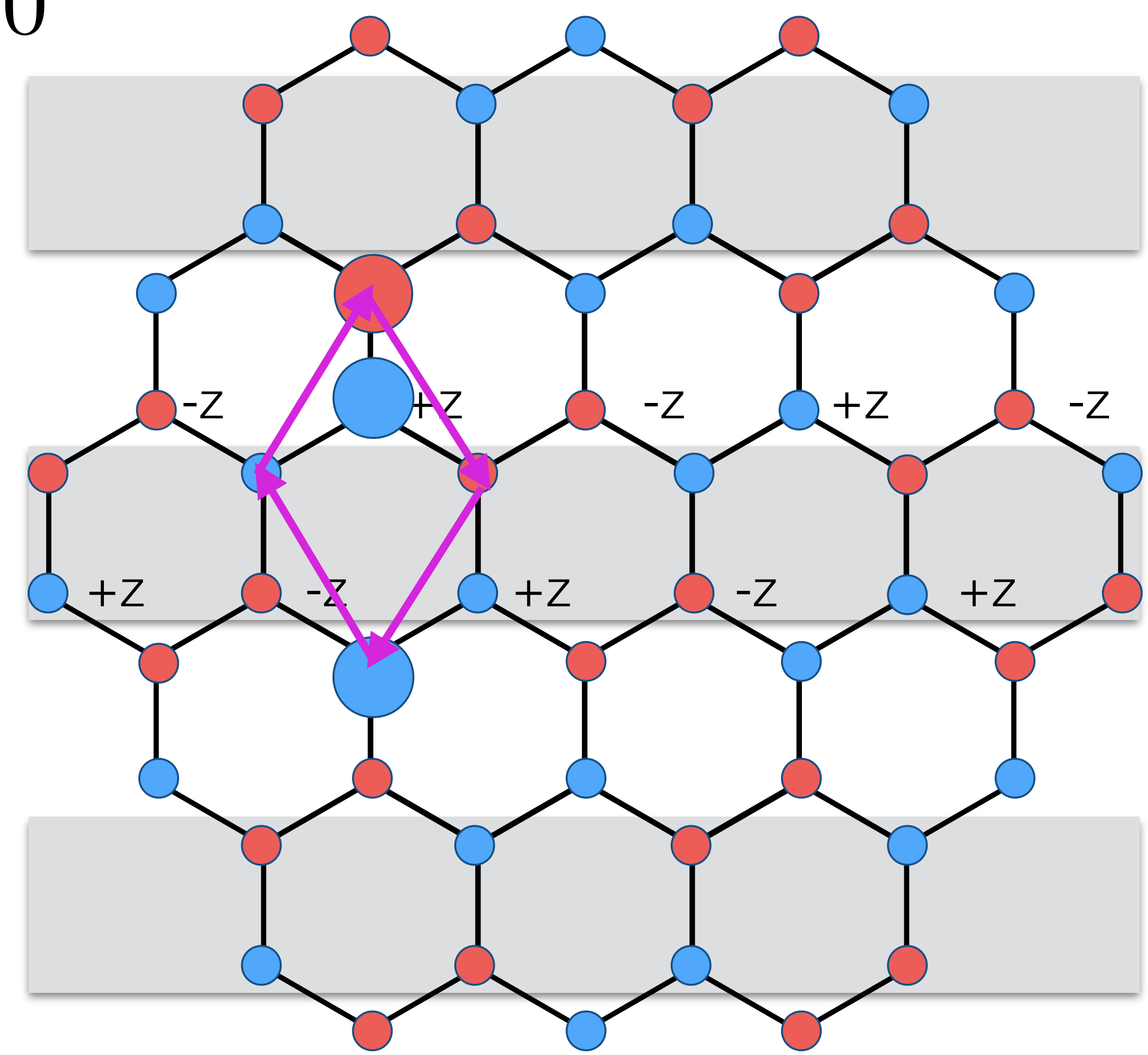
A. Kitaev, Annals of Physics **321**, 2 (2006)

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

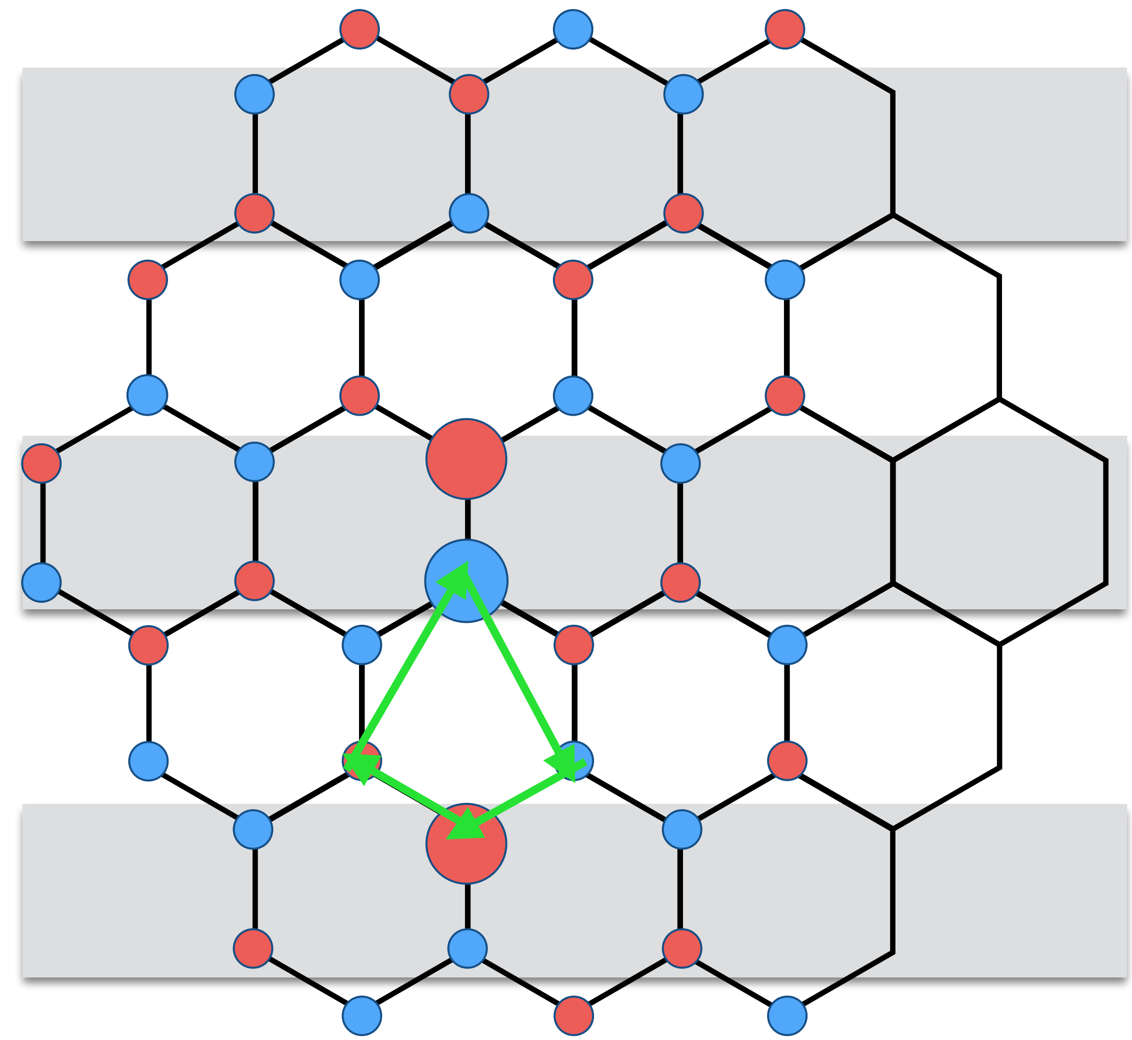
Competing phases

$K_1 > 0$

$K_2 > 0$

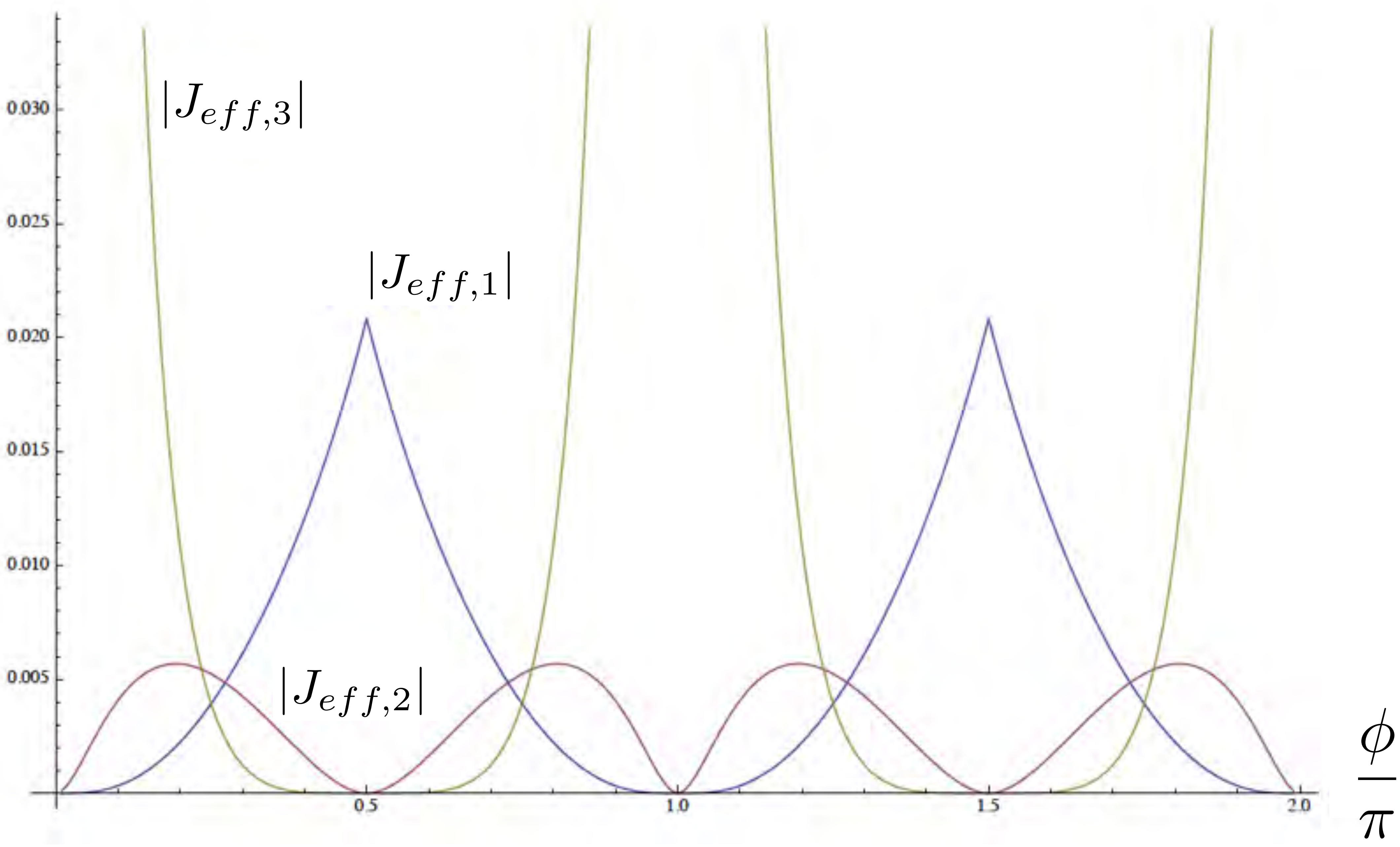


$|J_{eff,1}| > |J_{eff,2}|$

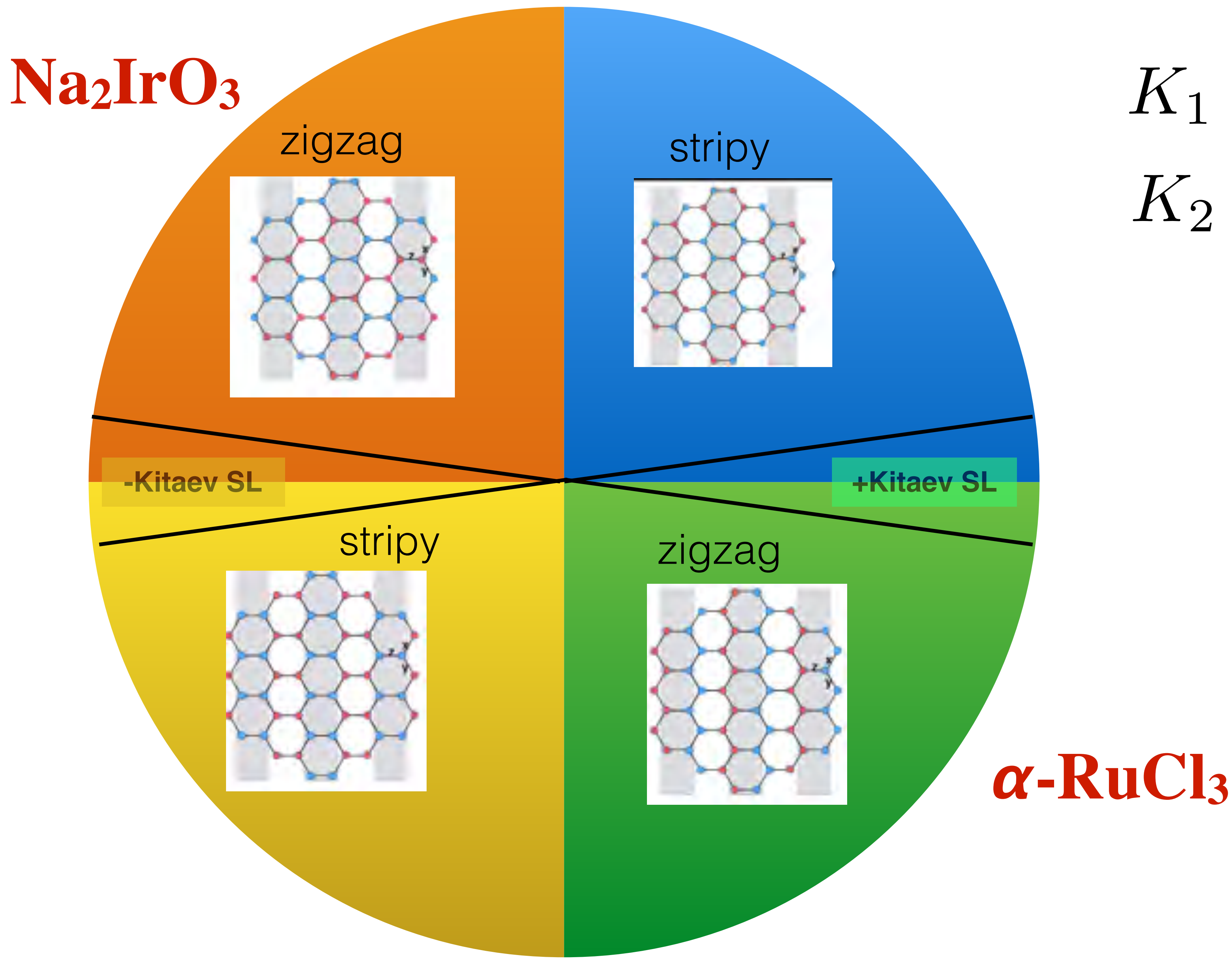


$|J_{eff,2}| > |J_{eff,1}|$

Effective couplings: x=0.1



Quantum phase diagram of K_1-K_2 model



$$K_1 = \cos\phi$$

$$K_2 = \sin\phi$$

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

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Thank you