Topological and Magnetic Phases in Hyperhoneycomb Iridates

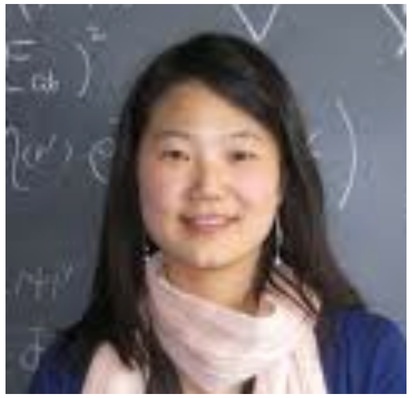
Yong Baek Kim
University of Toronto

Correlated Oxides and Oxide Interfaces
University of Minnesota, Minneapolis
May 2, 2014

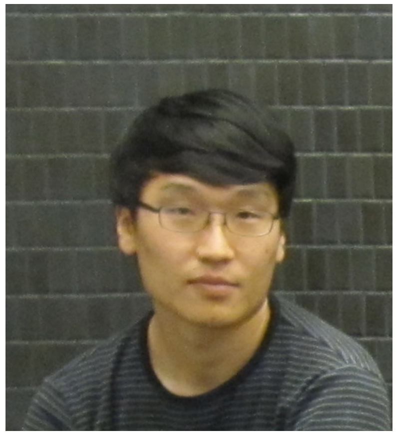
Eric K.-H. Lee
Toronto

Robert Schaffer
Toronto

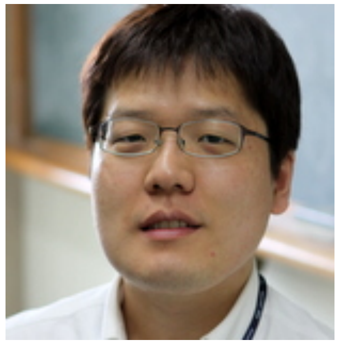
Subhro Bhattacharjee
Toronto



Sungbin Lee
Toronto



Kyusung Hwang
Toronto



Jae-Seung Jeong
KIAS

H. Jin
SNU

H.-S. Kim
KAIST

Discovery of Hyper-Honeycomb lattice material (H. Takagi)

β - Li_2IrO_3 arXiv:1403.3296

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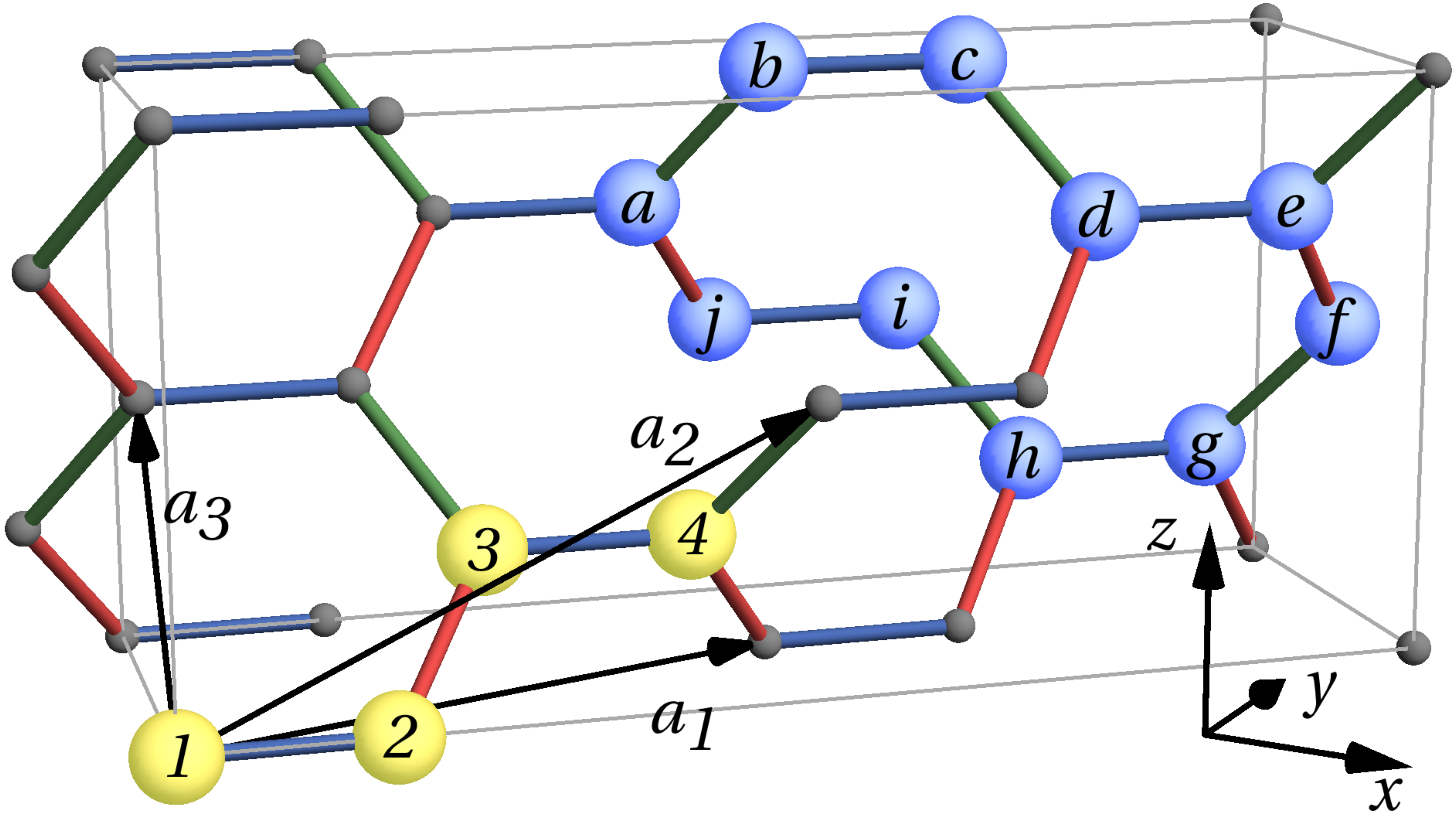

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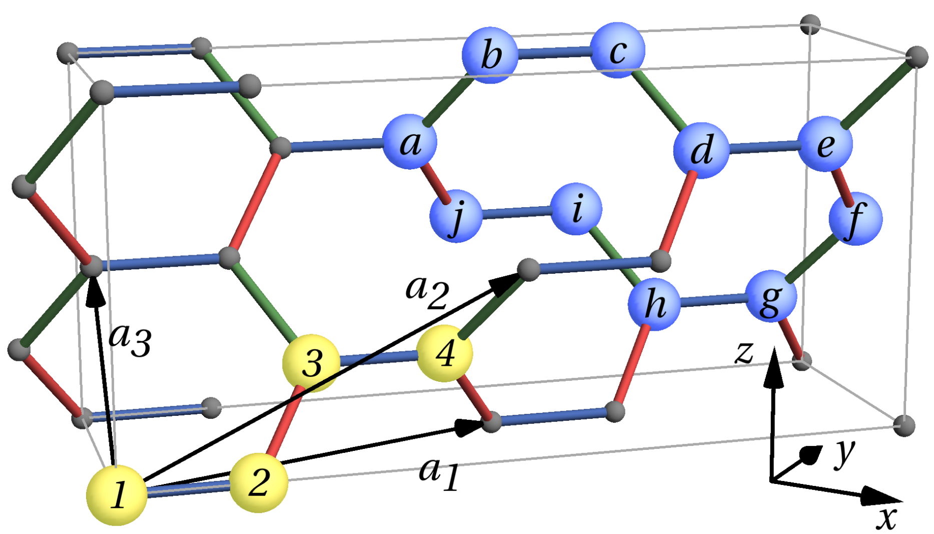

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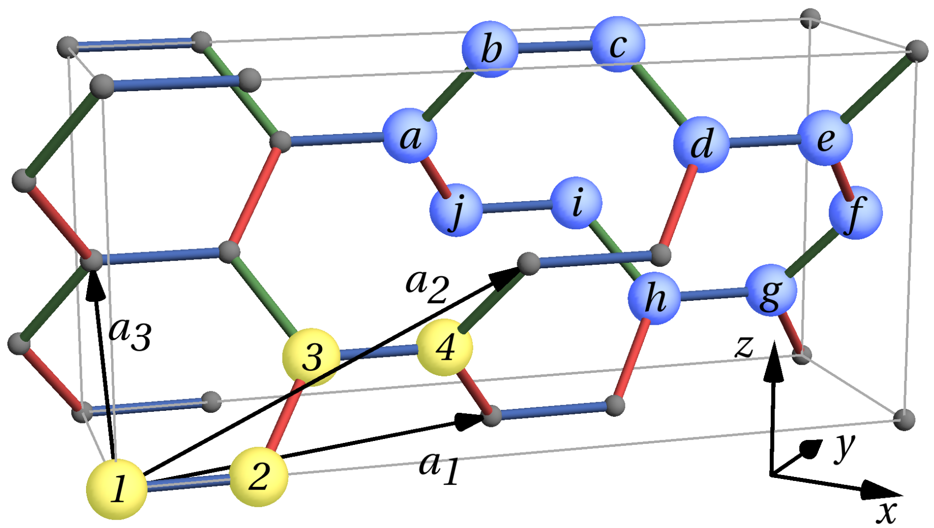

AF ordering (no net magnetization) in zero magnetic field

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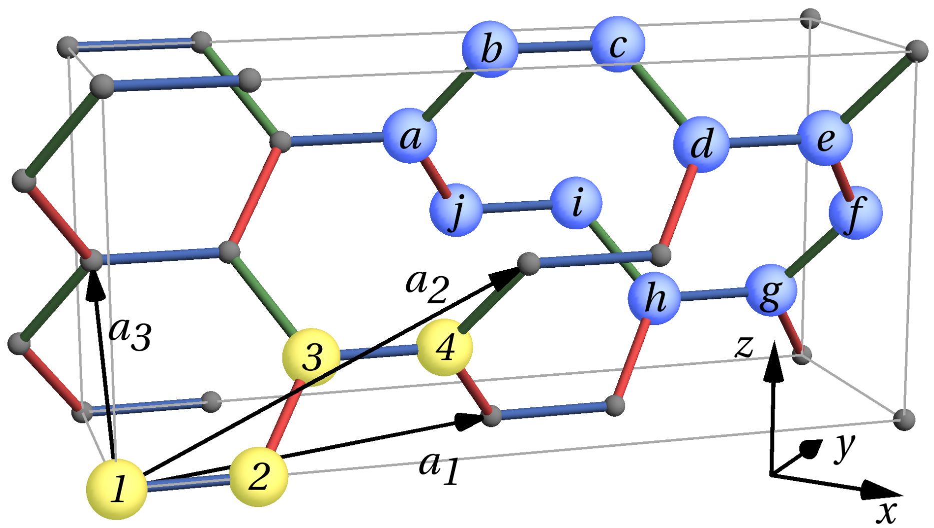

AF ordering (no net magnetization) in zero magnetic field

But with positive (ferro-like) Curie-Weiss temperature

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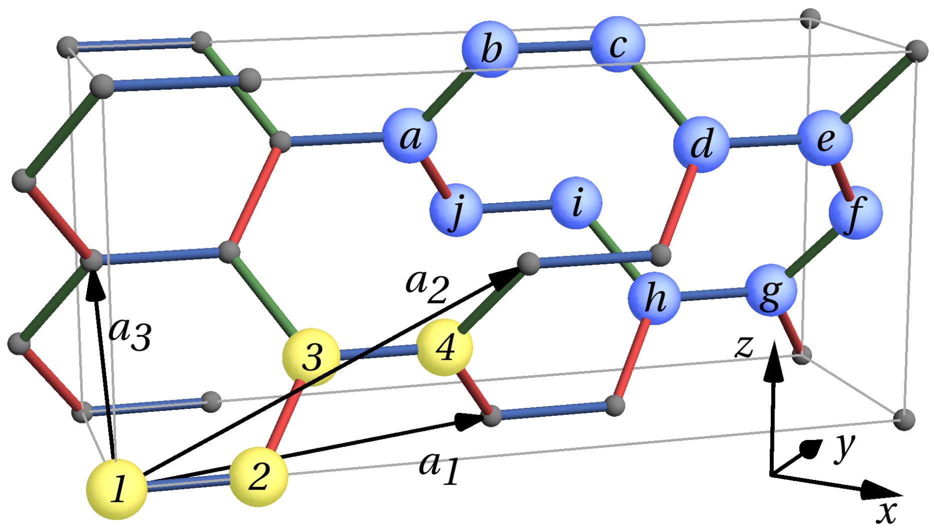

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Inversion Center for Red and Green Bonds (x- and y-bonds)

Inversion Broken for Blue Bonds (z-bonds)

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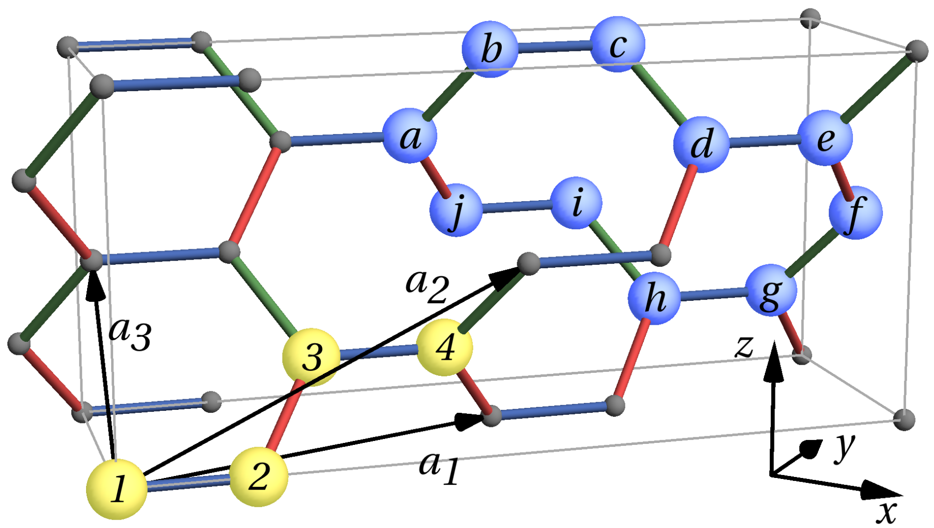

AF ordering (no net magnetization) in zero magnetic field

But with positive (ferro-like) Curie-Weiss temperature

Inversion Center for Red and Green Bonds (x- and y-bonds)

Inversion Broken for Blue Bonds (z-bonds)

x-, y-, and z-bonds not strictly equivalent

Is J_{eff}=1/2 picture valid ?
Weak Coupling Limit

E. K.-H. Lee, S. Bhattacharjee, K. Hwang, H.-S. Kim, H. Jin, Y. B. Kim,
arXiv:1402.2654 (2014)

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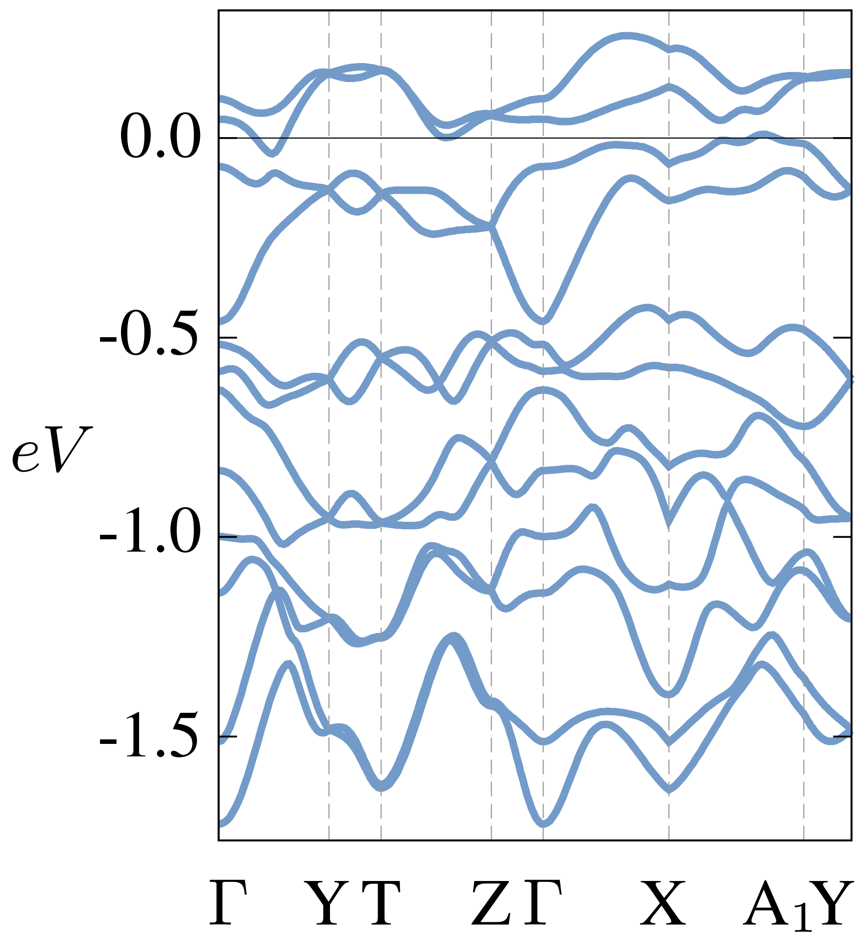
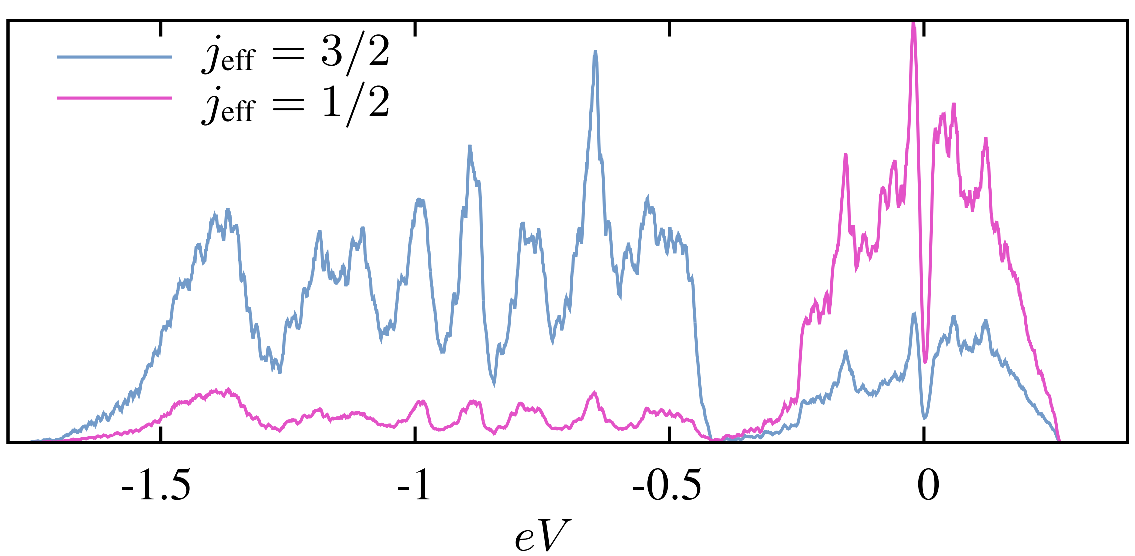
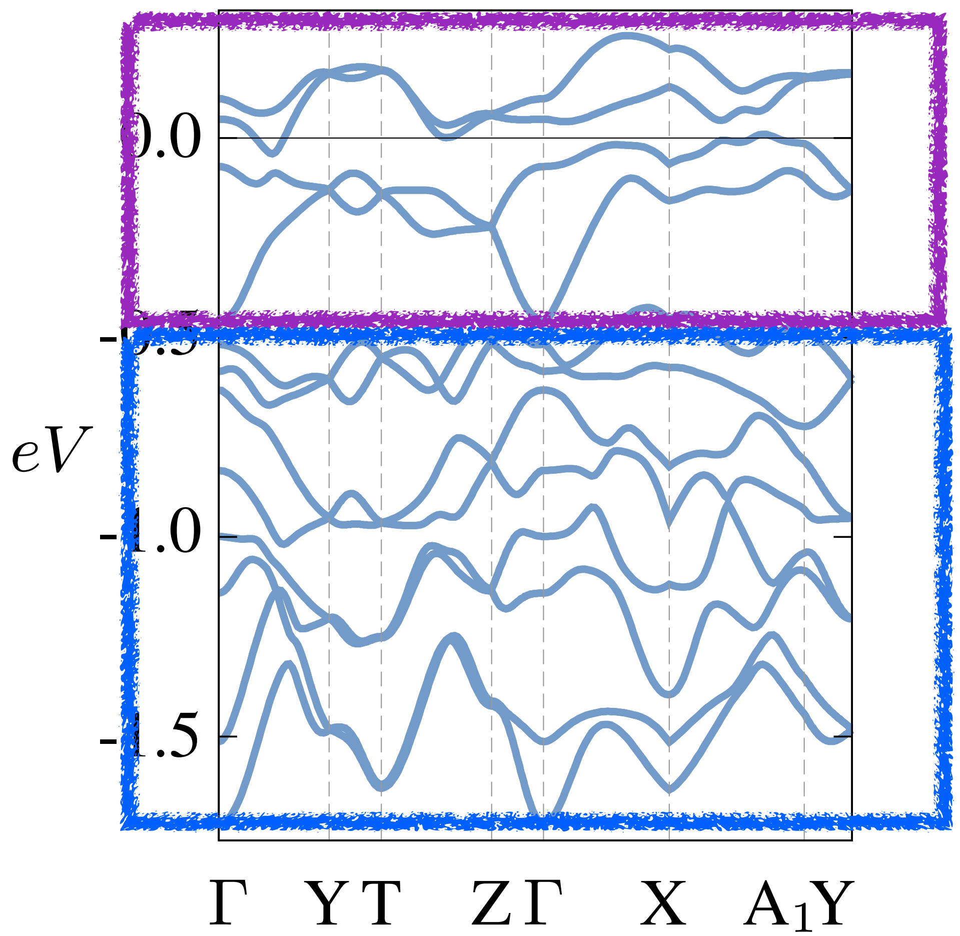




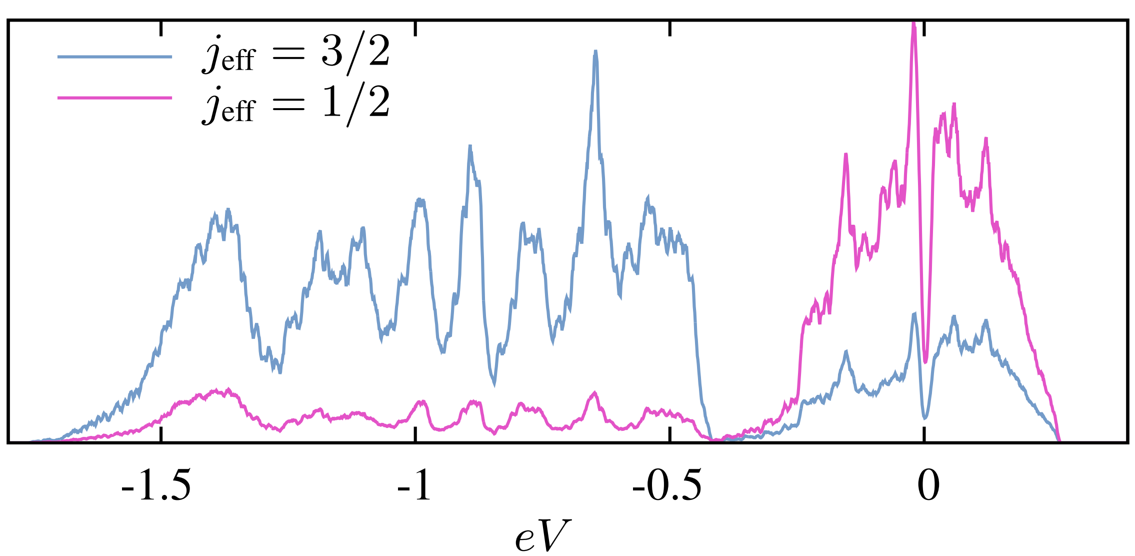
Ab Initio
(OpenMx, PBE-GGA)

Is J_{eff}=1/2 picture valid ?



Mostly J_{eff}=1/2

Mostly J_{eff}=3/2

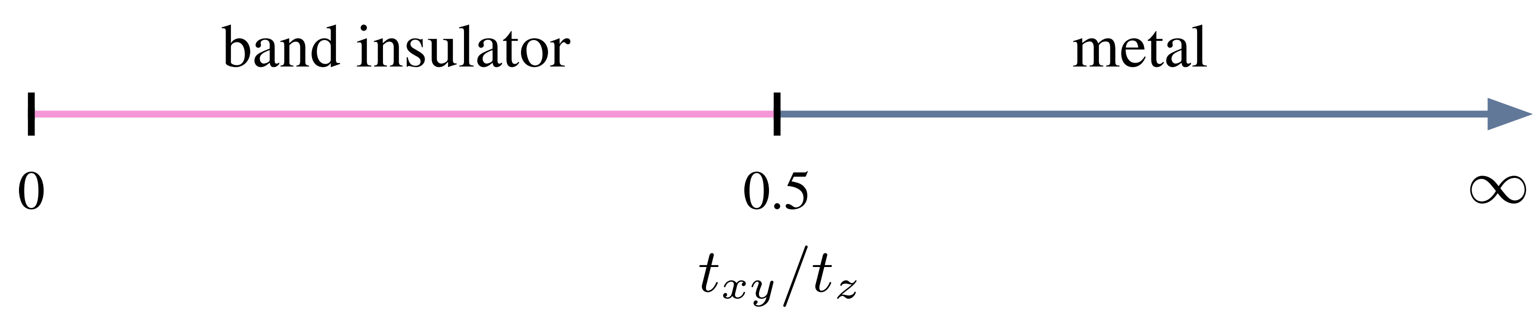


Ab Initio
(OpenMx, PBE-GGA)

Effective Tight-Binding Model

$$H_{\text{tb}} = \sum_{ij} c_i^\dagger h_{ij} c_j \qquad c_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger) \qquad h_{ij} = t_{ij}\mathbb{I} + i\mathbf{v}_{ij}\cdot\sigma$$

❑ 1 NN terms: $h_{x/y}^{1\text{NN}} = t_{xy}\mathbb{I} \qquad h_z^{1\text{NN}} = t_z^{1\text{NN}}\mathbb{I}$



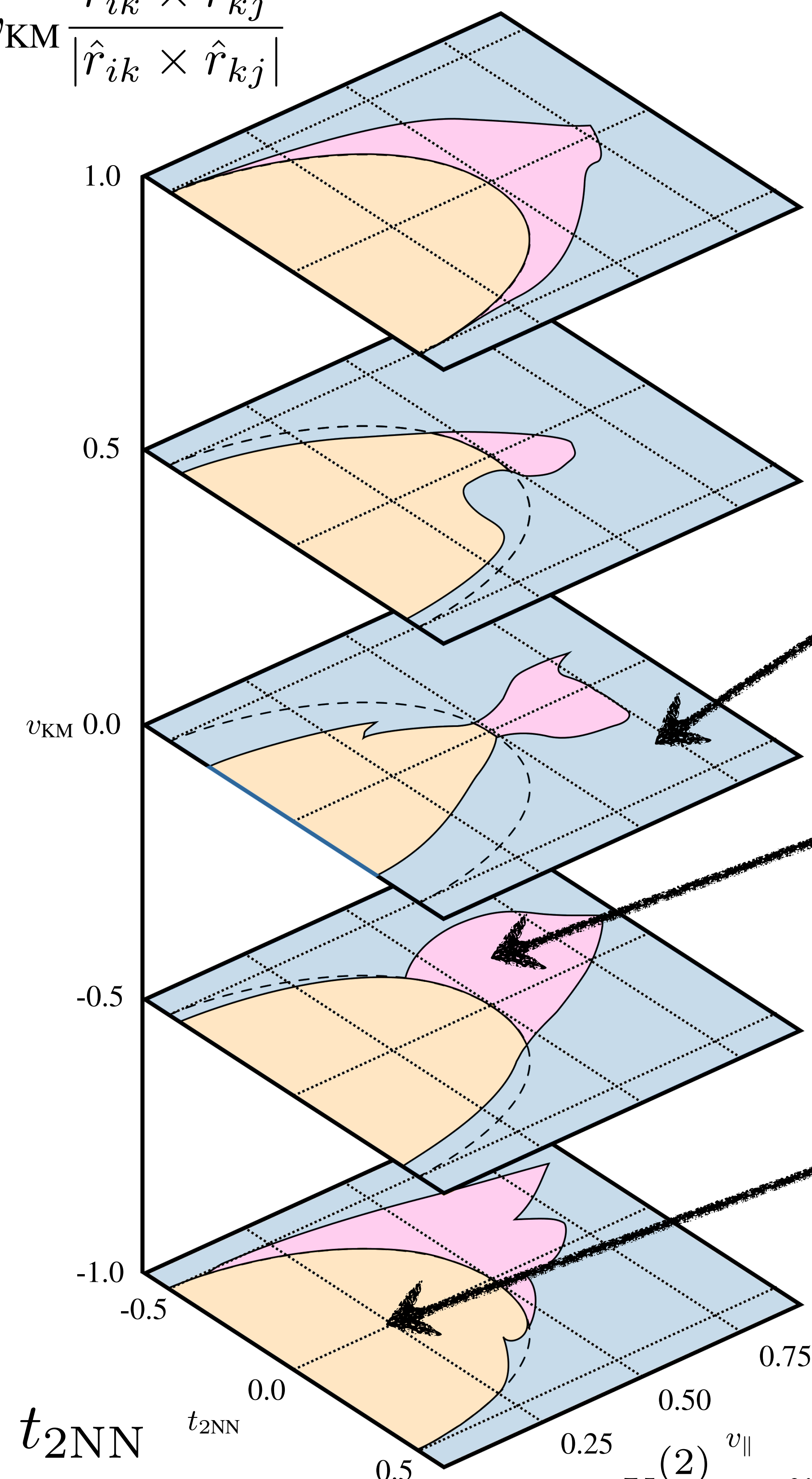
❑ 2 NN terms: $h_{ij}^{2\text{NN}} = t_{2\text{NN}}\mathbb{I} + i\left(\mathbf{v}_{ij}^{(1)} + \mathbf{v}_{ij}^{(2)}\right)\cdot\sigma$

$$\mathbf{v}_{ij}^{(1)} = v_{\text{KM}}\frac{\hat{r}_{ik}\times\hat{r}_{kj}}{|\hat{r}_{ik}\times\hat{r}_{kj}|} \qquad \mathbf{v}_{ij}^{(2)} = v_{\parallel}\epsilon_{ij}\hat{\mathbf{r}}_{ij} \qquad \epsilon_{ij} = \pm 1$$

$$\begin{aligned} t_{xy,z} &= 0.1744\, eV, & v_{\text{KM}} &= -0.1331\, eV, \\ t_{2\text{NN}} &= -0.1150\, eV, & v_{\parallel} &= -0.0222\, eV, \end{aligned}$$

Emergence of Topological Insulator !

$$\mathbf{v}_{ij}^{(1)} = v_{\mathrm{KM}} \frac{\hat{r}_{ik} \times \hat{r}_{kj}}{|\hat{r}_{ik} \times \hat{r}_{kj}|}$$



$t_{2\mathrm{NN}}$

$$\mathbf{v}_{ij}^{(2)} = v_{\parallel} \epsilon_{ij} \hat{\mathbf{r}}_{ij}$$

Set $t_{xy} = t_z = 1$

Metal

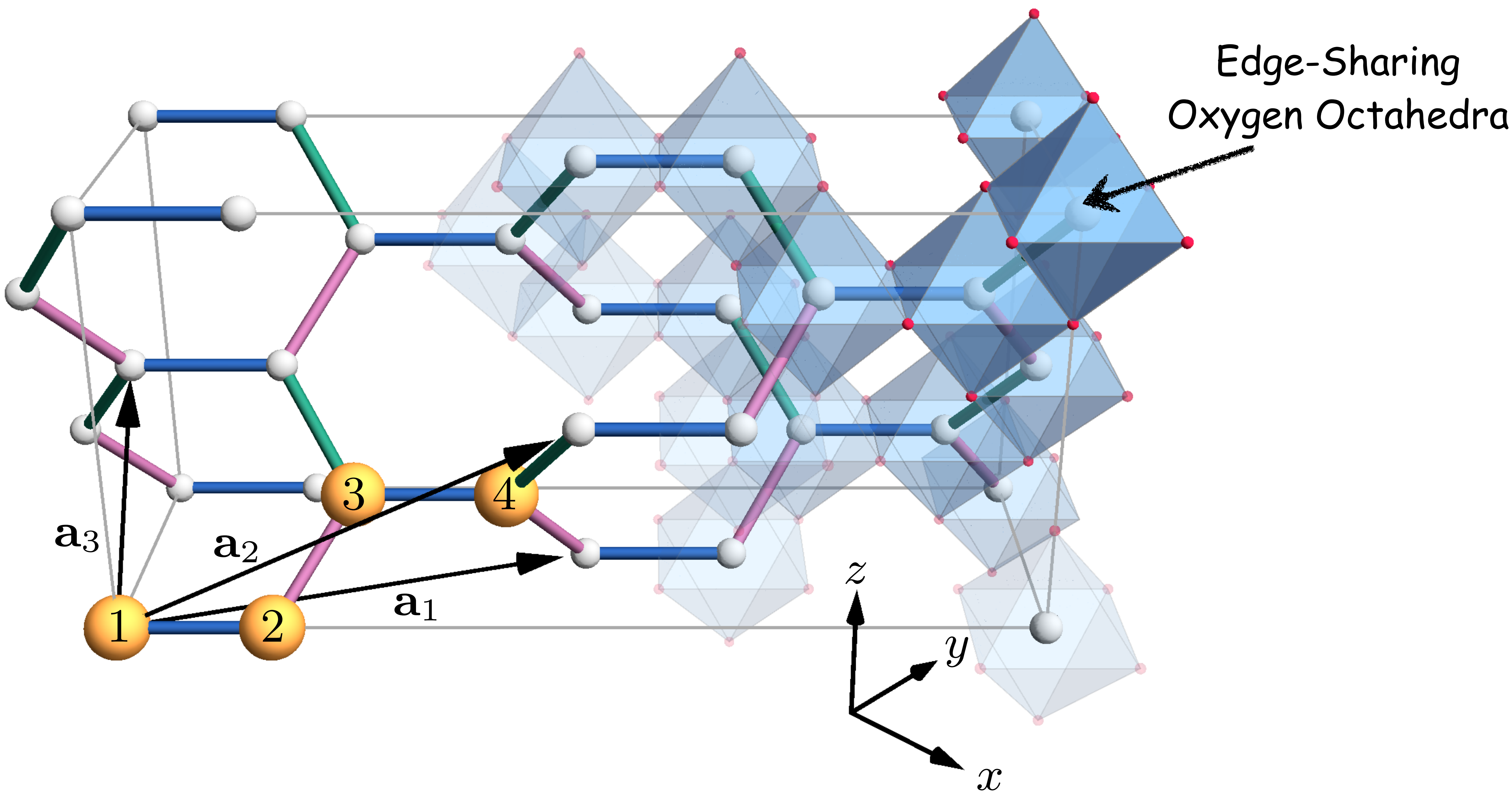
Trivial Band Insulator

Strong Topological Insulator

Heisenberg-Kitaev Model on Hyperhoneycomb lattice: Strong Coupling Limit

E. K.-H. Lee, R. Schaffer, S. Bhattacharjee, Y. B. Kim, PRB 89, 045117 (2013)
arXiv:1308.6592

Edge-sharing Oxygen Octahedra Structure

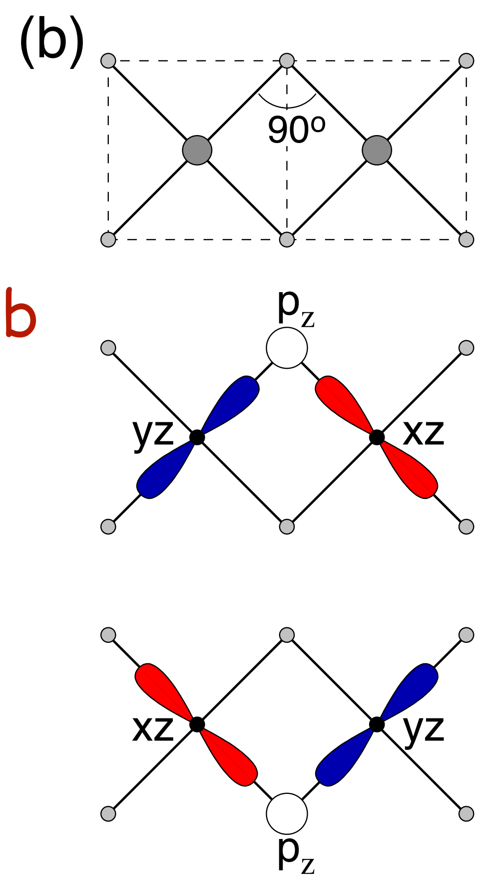


Strong Coupling Limit the Kitaev Model ?

Including Hund's coupling and projecting to J_{eff}=1/2 manifold

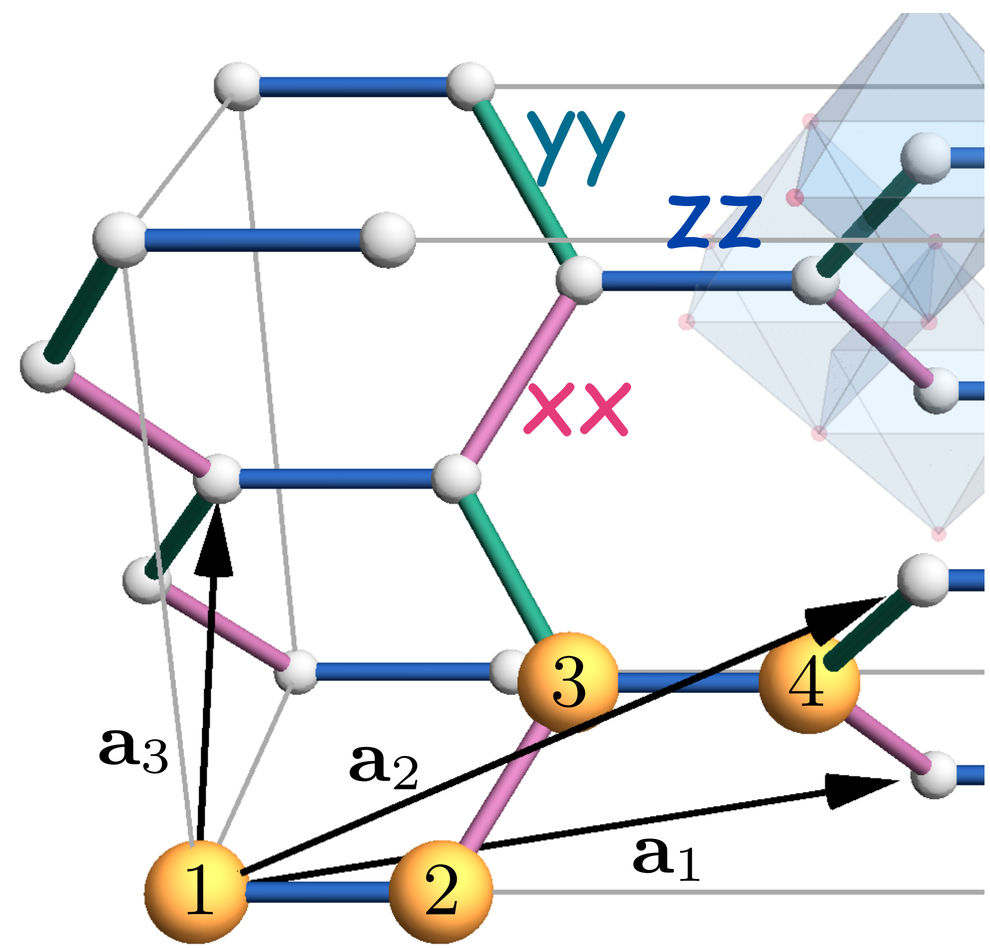
$$\mathcal{H}_{ij}^{(\gamma)} = -J S_i^\gamma S_j^\gamma \qquad \gamma = x, y, z$$

2D Honeycomb
G. Jackeli,
G. Khaliullin,
PRL (2009)



Edge-Sharing
Oxygen Octahedra

Isotropic Heisenberg
Exchange suppressed



Kitaev-Heisenberg Model

$$\mathcal{H}_{\mathrm{HK}} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - K \sum_{\alpha-links} S_i^\alpha S_j^\alpha$$

e.g. In the limit of $U, J_H \gg \lambda \gg t$

$$J = \frac{4}{27}\left[\frac{6t_1(t_1+2t_3)}{U-3J_H} + \frac{2(t_1-t_3)^2}{U-J_H} + \frac{(2t_1+t_3)^2}{U+2J_H}\right]$$

$$K = \frac{8J_H}{9}\left[\frac{(t_1-t_3)^2 - 3t_2^2}{(U-3J_H)(U-J_H)}\right],$$

J. Chaloupka,
G. Jackeli
and G. Khaliullin,
(2010)

$$t_1 = \frac{t_{dd\pi} + t_{dd\delta}}{2}, \quad t_2 = \frac{t_{pd\pi}^2}{\Delta_{pd}} + \frac{t_{dd\pi} - t_{dd\delta}}{2}, \quad t_3 = \frac{3t_{dd\sigma} + t_{dd\delta}}{4},$$

Heisenberg-Kitaev Model on Hyper-Honeycomb Lattice:

Exactly Solvable Limits

$$\mathcal{H}_{\mathrm{HK}} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - K \sum_{\alpha-links} S_i^\alpha S_j^\alpha$$

Heisenberg-Kitaev Model on Hyper-Honeycomb Lattice:
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J=0 Limit: Kiatev Model

Exactly Solvable: Spin Liquid with Majorana fermions (Spinons)

Kitaev Model: Exact Solution

$$\mathcal{H}_{\mathrm{K}} = - \sum_{\alpha - links} S_i^\alpha S_j^\alpha$$

$$S_i^\alpha = i b_i^\alpha c \qquad \{b_i^x, b_i^y, b_i^z, c\}$$ **Four Majorana Fermions**

$$\mathcal{H}_{\mathrm{K}} = \frac{i}{2} \sum_{\alpha-\mathrm{links}} u_{ij}^\alpha c_i c_j \qquad (\text{where } \ u_{ij}^\alpha = i b_i^\alpha b_j^\alpha),$$

$\mathcal{W}_P = \prod_{\mathrm{loop}} u_{ij}^\alpha$ commute with the Hamiltonian $\Longrightarrow \mathcal{W}_P = \pm 1$

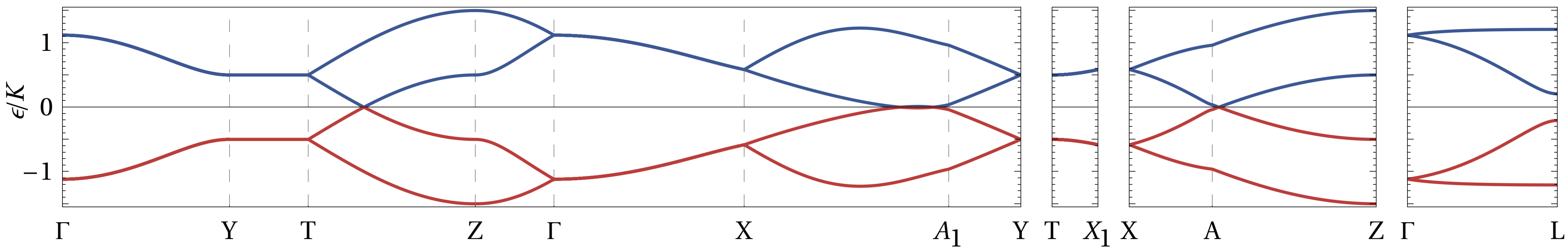
Ground state is in the zero-flux sector $u_{ij}^\alpha = +1 \; (\forall \langle ij \rangle)$

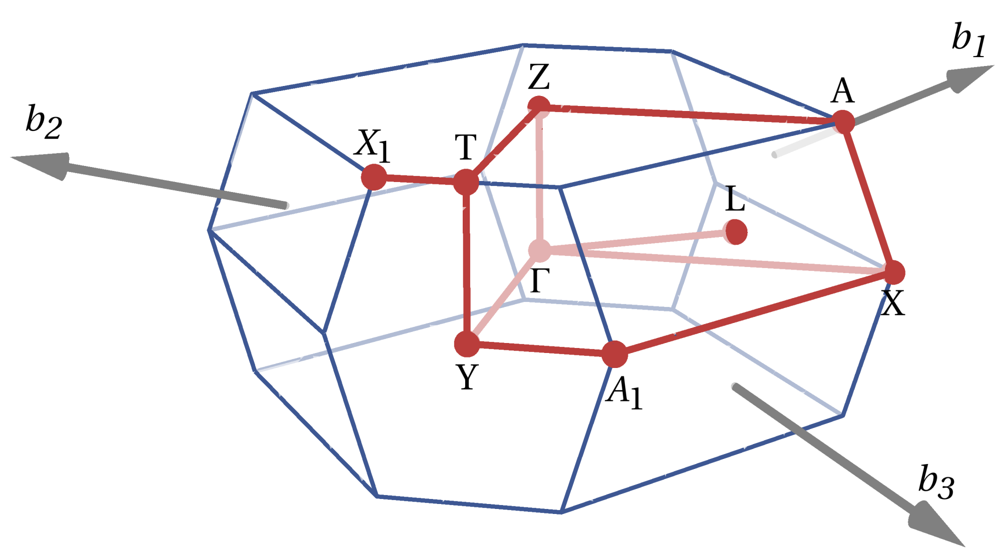
A. Kitaev (2006)

S. Mandal and N. Surendran (2009)

Kitaev Model: Exact Solution

$$\mathcal{H}_{\mathrm{K}} = - \sum_{\alpha-links} S_i^{\alpha} S_j^{\alpha}$$





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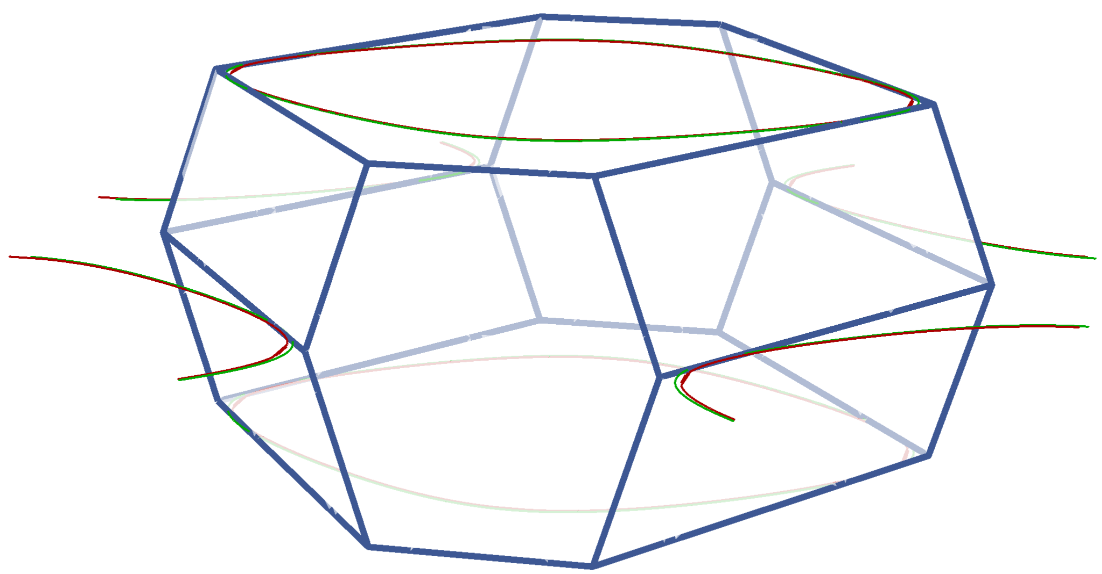
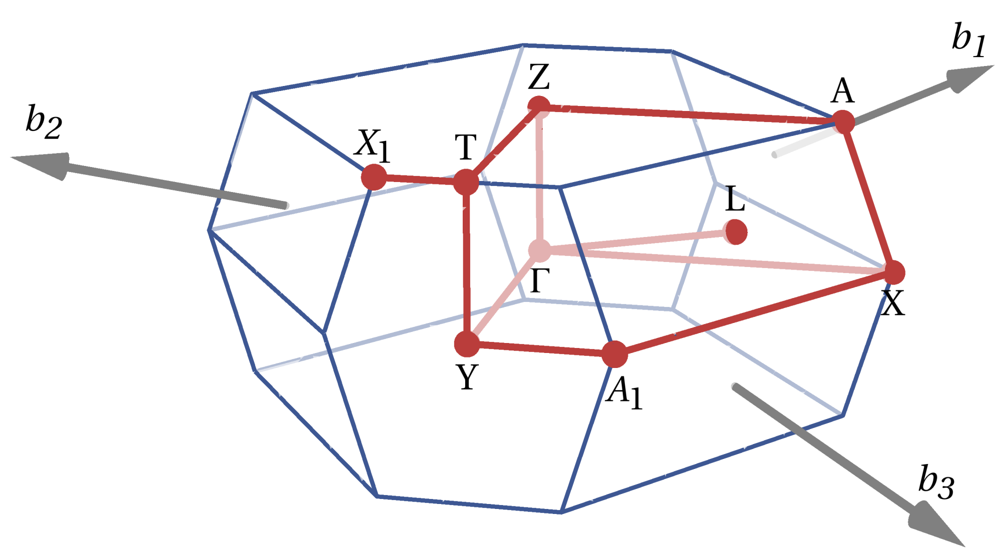


Gapless Majorana Excitations:

Fermi "Circles" or Line Nodes



Heisenberg-Kitaev Model on Hyper-Honeycomb Lattice: Exactly Solvable Limits

$$\mathcal{H}_{\mathrm{HK}} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - K \sum_{\alpha-links} S_i^\alpha S_j^\alpha$$

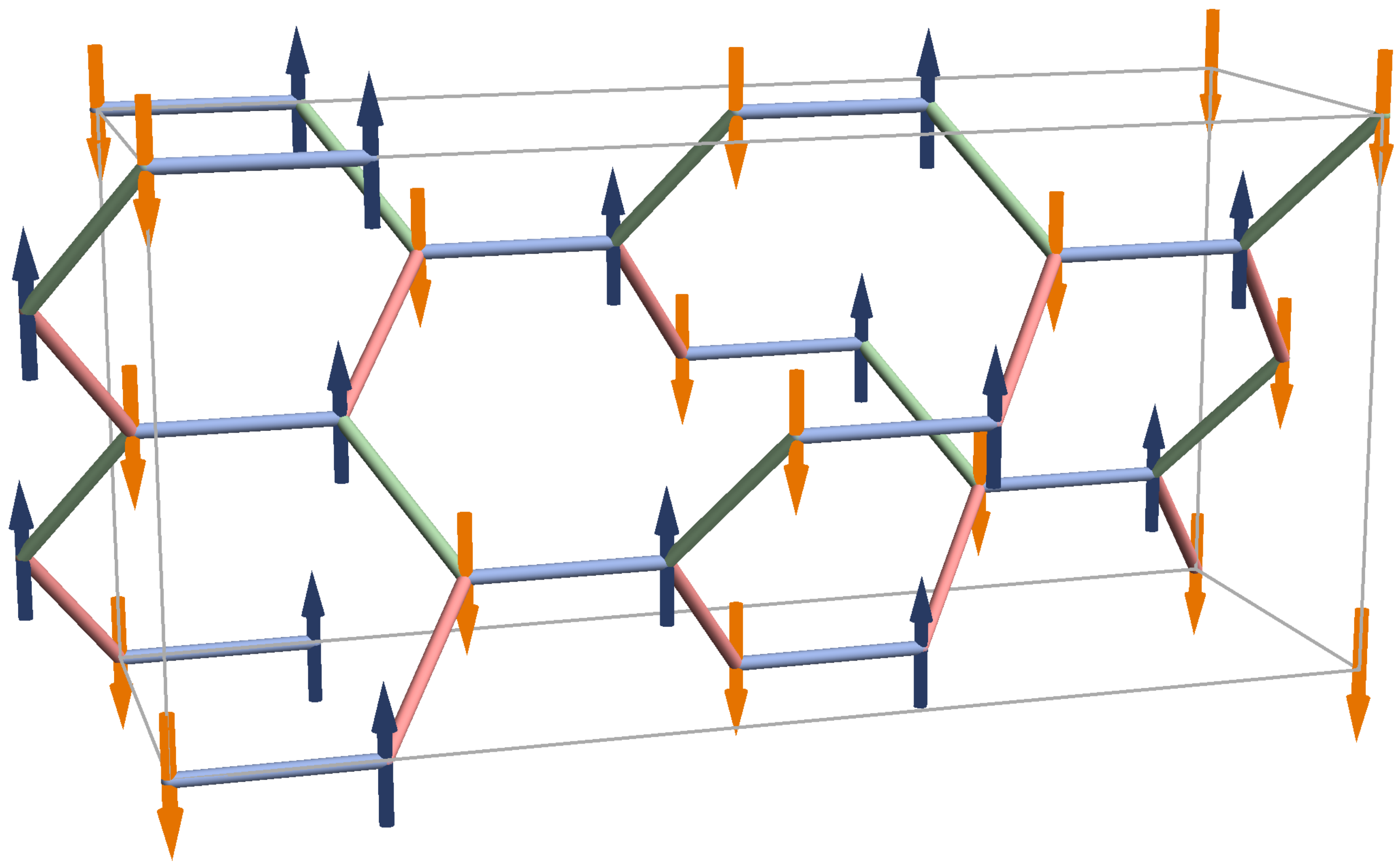
J=0 Limit: Kiatev Model

Exactly Solvable: Spin Liquid with Majorana fermions (Spinons)

K=0 Limit: Non-frustrated

Néel ordering

Néel Order



Heisenberg-Kitaev Model on Hyper-Honeycomb Lattice: Exactly Solvable Limits

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J=0 Limit: Kiatev Model

Exactly Solvable: Spin Liquid with Majorana fermions (Spinons)

K=0 Limit: Non-frustrated

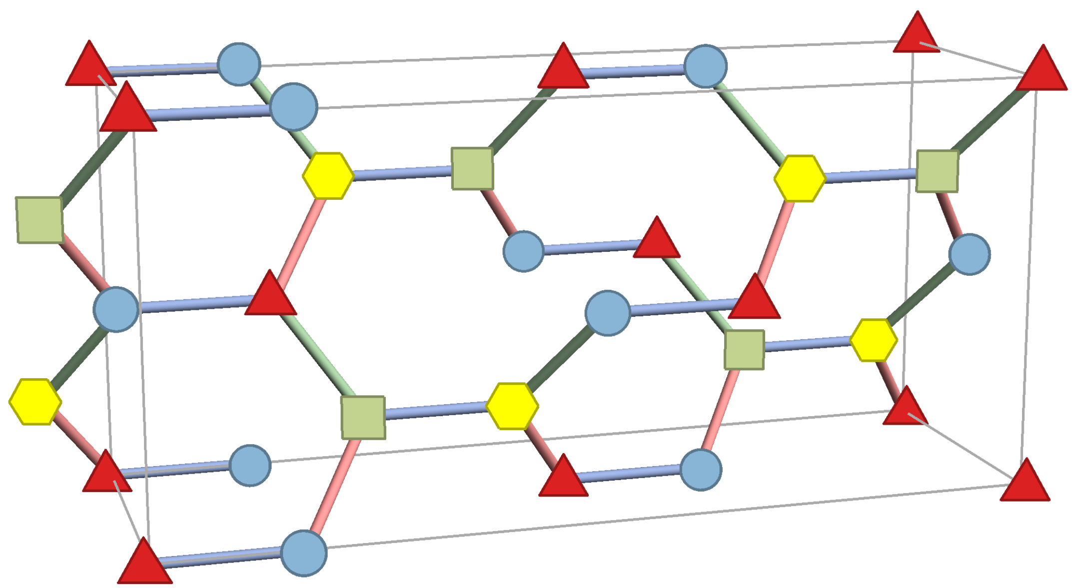
Néel ordering

K=2J: Can be mapped to ferromagnetic Heisenberg model by four-sublattice spin rotations (Jackeli and Khaliullin's Trick)

Magnetic order:

"Skew-Stripy" order when J > 0 and K > 0

Four-Sublattice Spin Rotation and Magnetic Order at K=2J



Mapped to
Heisenberg Ferromagnet

(Jackeli and Khaliullin's Trick)

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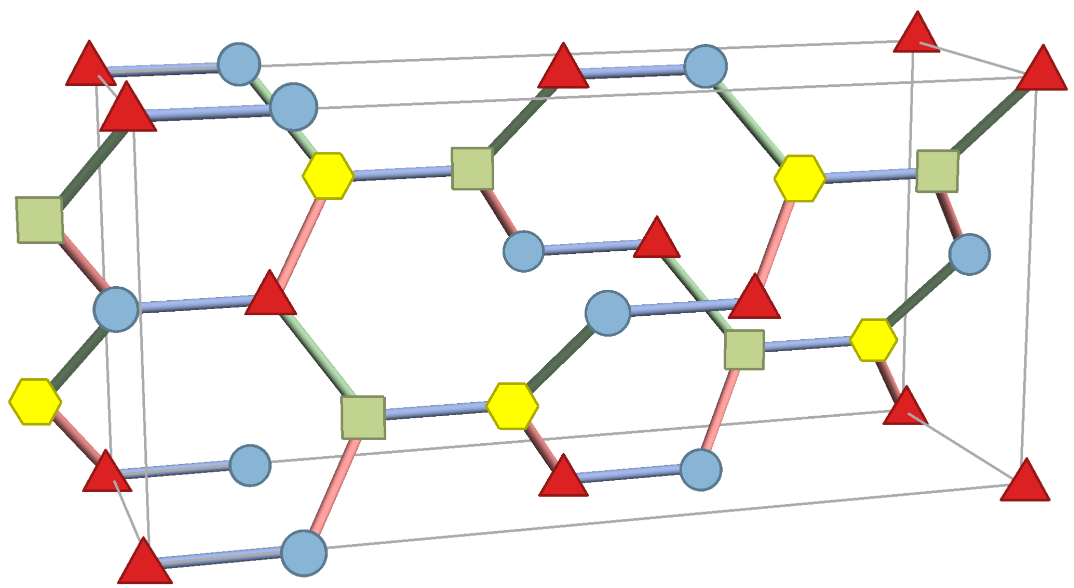

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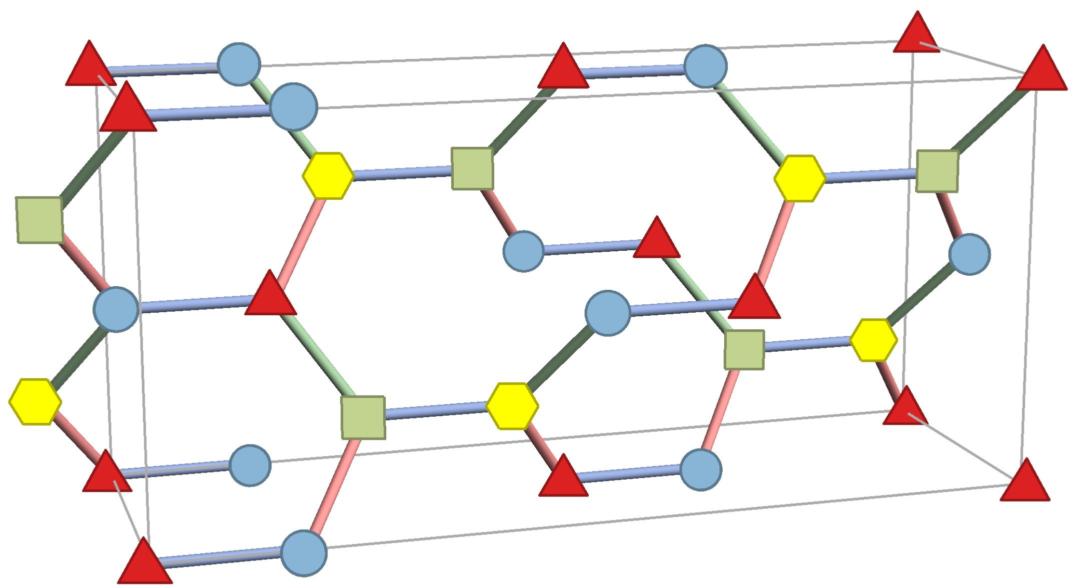
$$J = 1 - \alpha, \quad K = 2\alpha$$

$$H_{\mathrm{H}} \to -H_{\mathrm{H}} + 2H_{\mathrm{K}} \qquad\qquad H_{\mathrm{K}} \to H_{\mathrm{K}}$$

$$H \to H = -(1-\alpha)H_{\mathrm{H}} - 4(\alpha - \frac{1}{2})H_{\mathrm{K}}$$

Four-Sublattice Spin Rotation and Magnetic Order at K=2J



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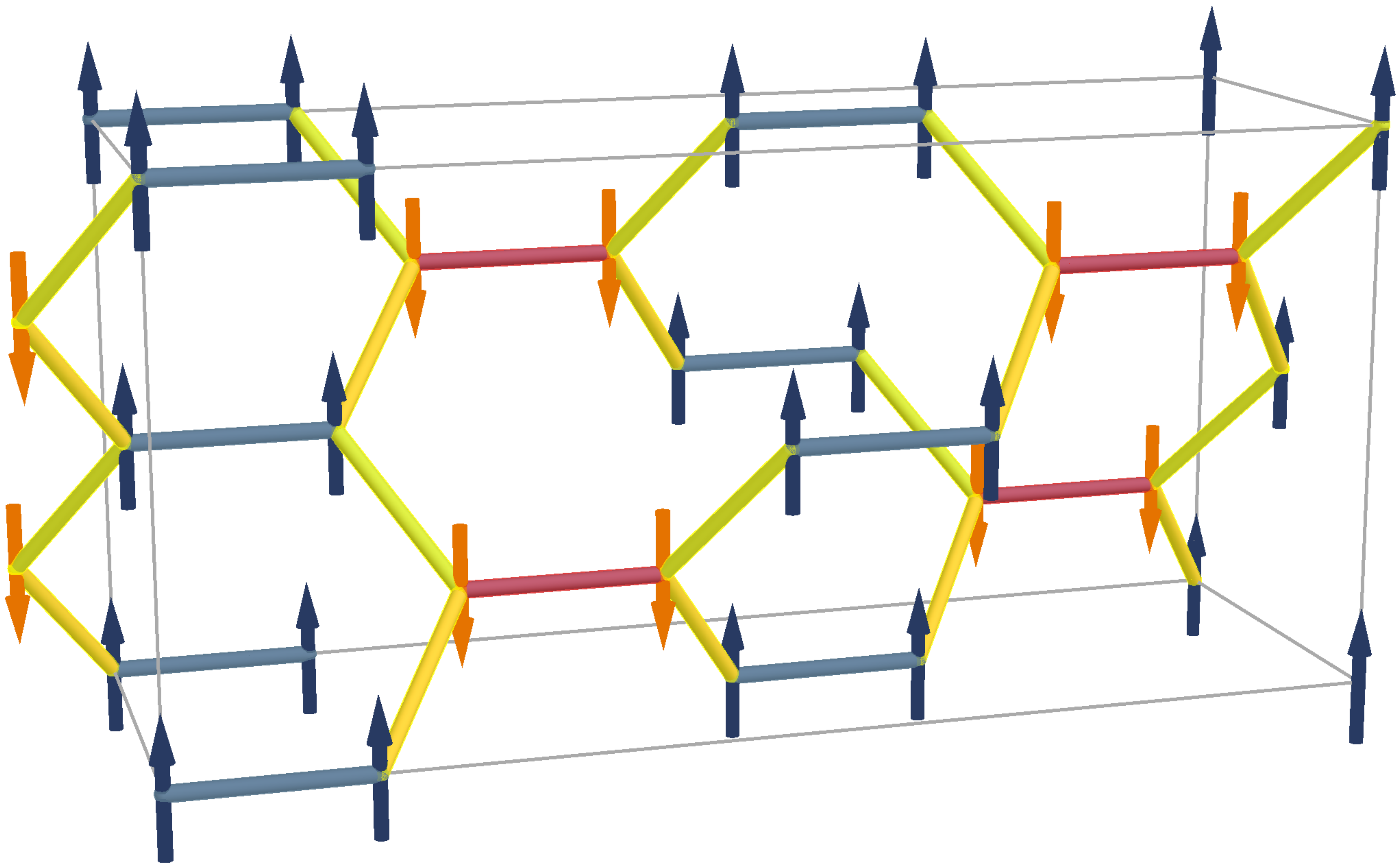
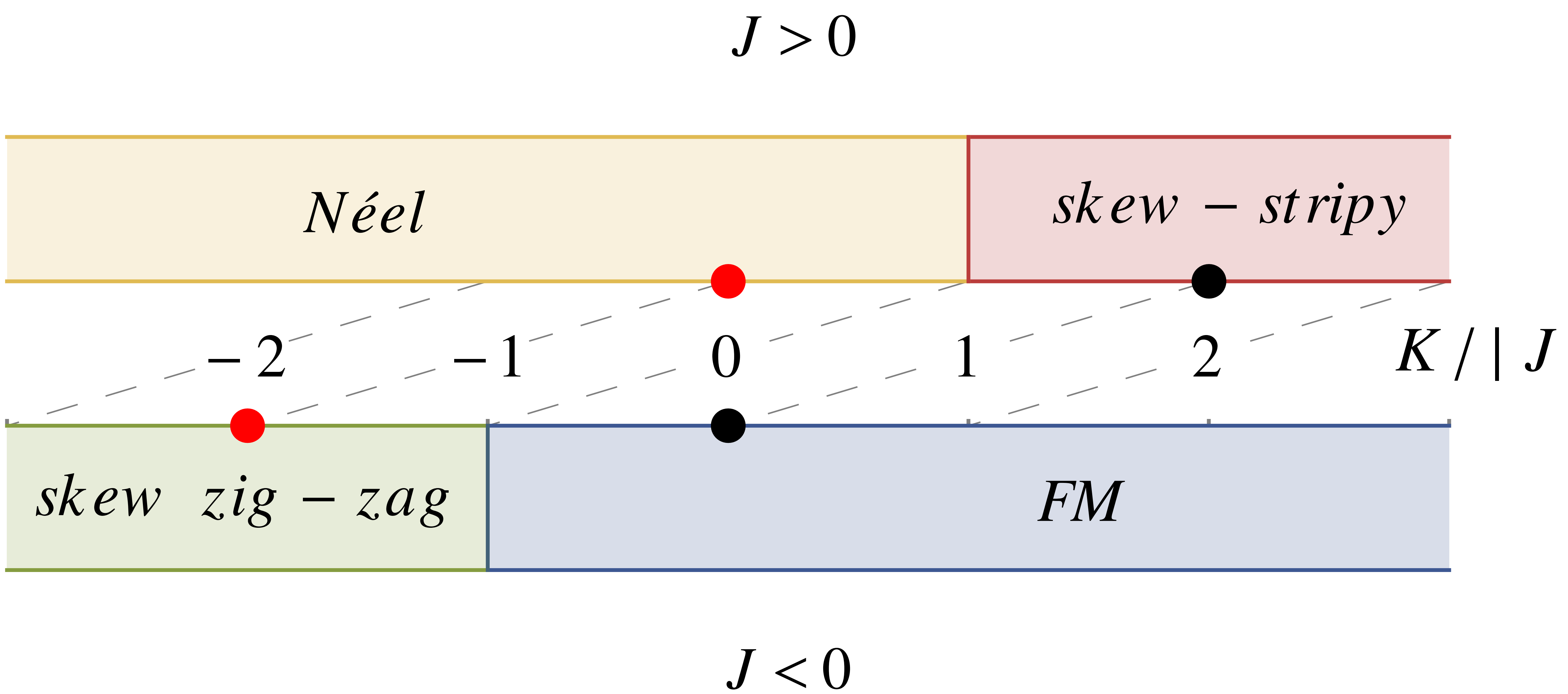
$\alpha = 0.5$ is the SU(2) invariant ferromagnetic Heisenberg model

Skew-Stripy Order



Phase Diagram: Luttinger-Tisza Analysis for Classical Model



$$\boxed{J = 1 - \alpha, \quad K = 2\alpha}$$

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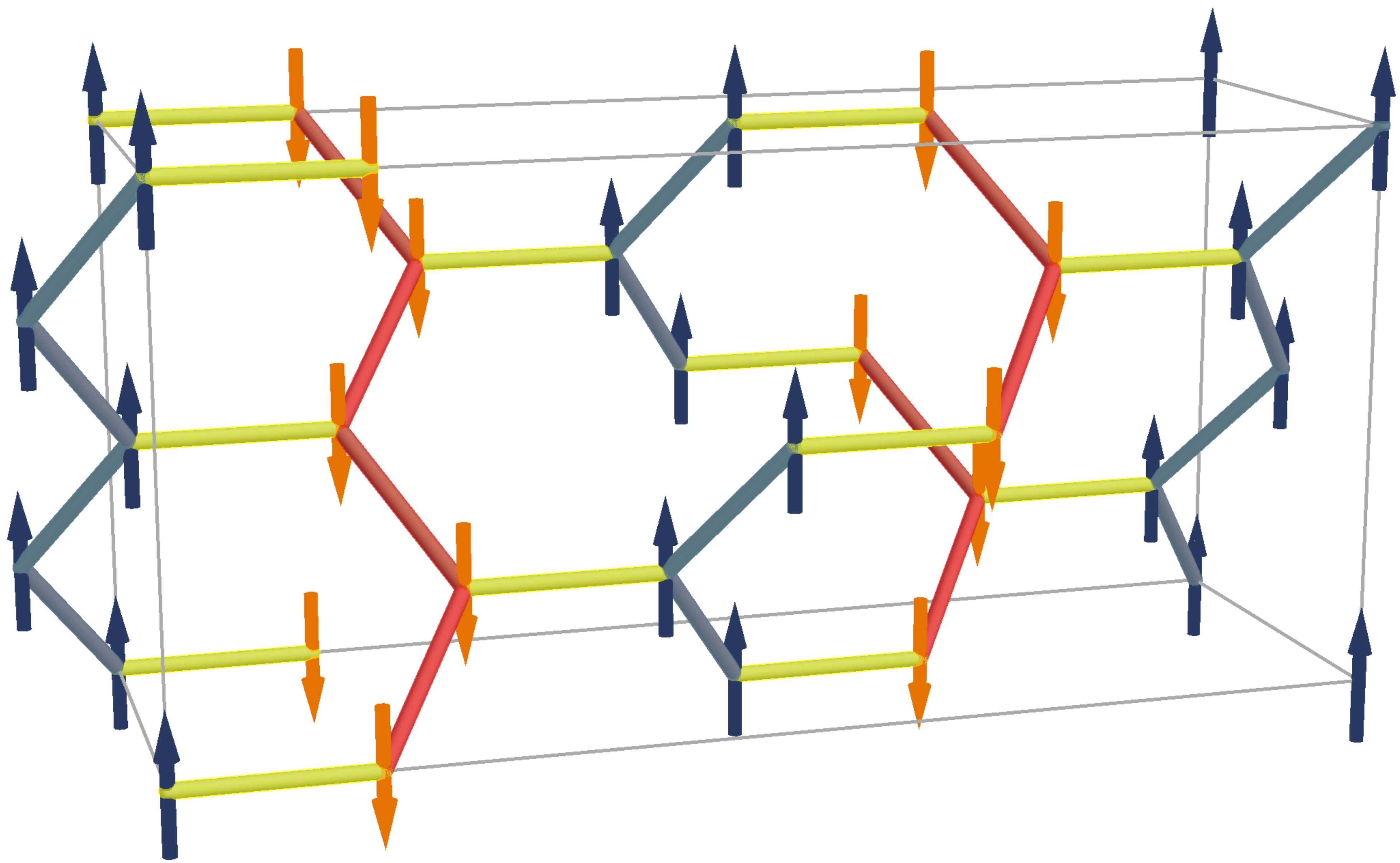
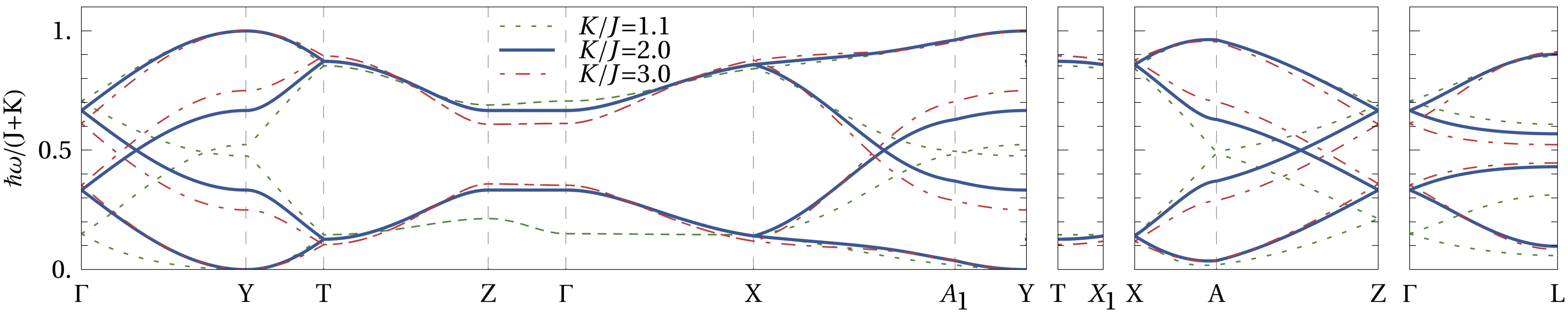
Skew-Zig-Zag Order



Quantum Fluctuations via Spin-Wave Analysis (z-Skew-Stripy Order)



Quantum Order by Disorder: Zero point quantum fluctuations prefer z-Skew-Stripy phase over x- and y-Skew-Stripy phase

Approaching the Kitaev Limit: Transition to Spin Liquid

E. K.-H. Lee, R. Schaffer, S. Bhattacharjee, Y. B. Kim, PRB 89, 045117 (2013)
arXiv:1308.6592

Slave Fermion Mean-Field Theory (in the rotated basis)

$$\boxed{J = 1 - \alpha, \quad K = 2\alpha}$$

$$\boxed{H \to H = -(1-\alpha)H_{\mathrm{H}} - 4(\alpha - \frac{1}{2})H_{\mathrm{K}}}$$

$\alpha = 0.5$ Hidden SU(2)

$\alpha = 1$ Kitaev limit

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$$S_j^\mu = \frac{1}{2} f_{j\alpha}^\dagger [\sigma^\mu]_{\alpha\beta} f_{j\beta} \qquad f_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger f_{i\downarrow} = 1$$

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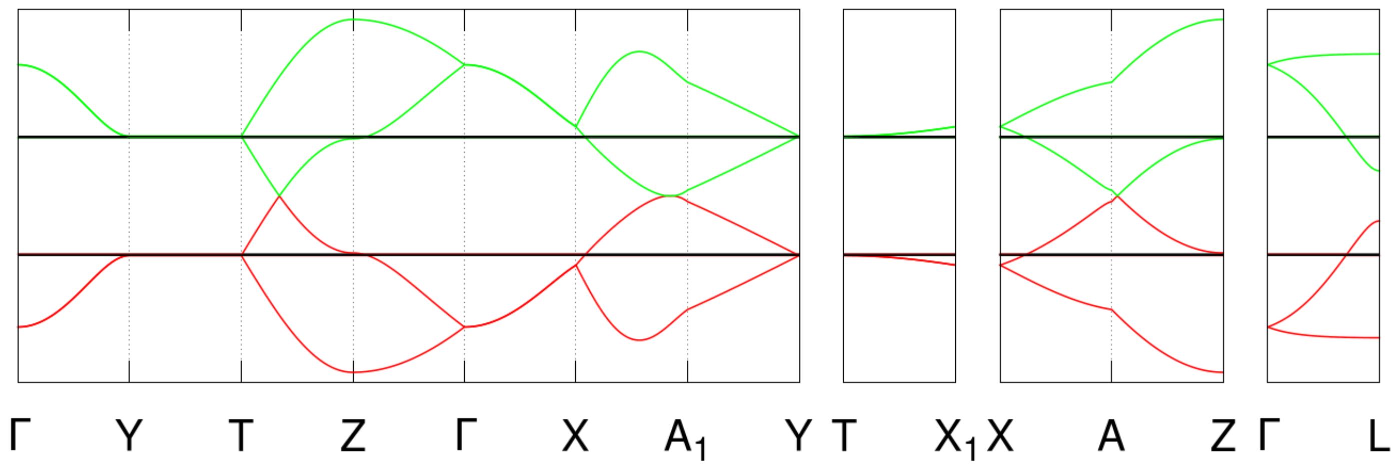
α-th component in the link-p

$$S_i^{\alpha} S_{i+p}^{\alpha} = \frac{1}{2} \sum_{\beta = x,y,z} (1 - \delta_{\alpha,\beta}) \left[E_{i,p}^{\beta\dagger} E_{i,p}^{\beta} + D_{i,p}^{\beta\dagger} D_{i,p}^{\beta} \right] - \frac{n_i}{4}$$

$$E_{i,p}^{\mu} = \frac{1}{2} f_{i+p\alpha}^{\dagger} [\sigma^{\mu}]_{\alpha\beta} f_{i\beta} \qquad D_{i,p}^{\mu} = \frac{1}{2} f_{i+p\alpha} [i\sigma^{y}\sigma^{\mu}]_{\alpha\beta} f_{i\beta}$$

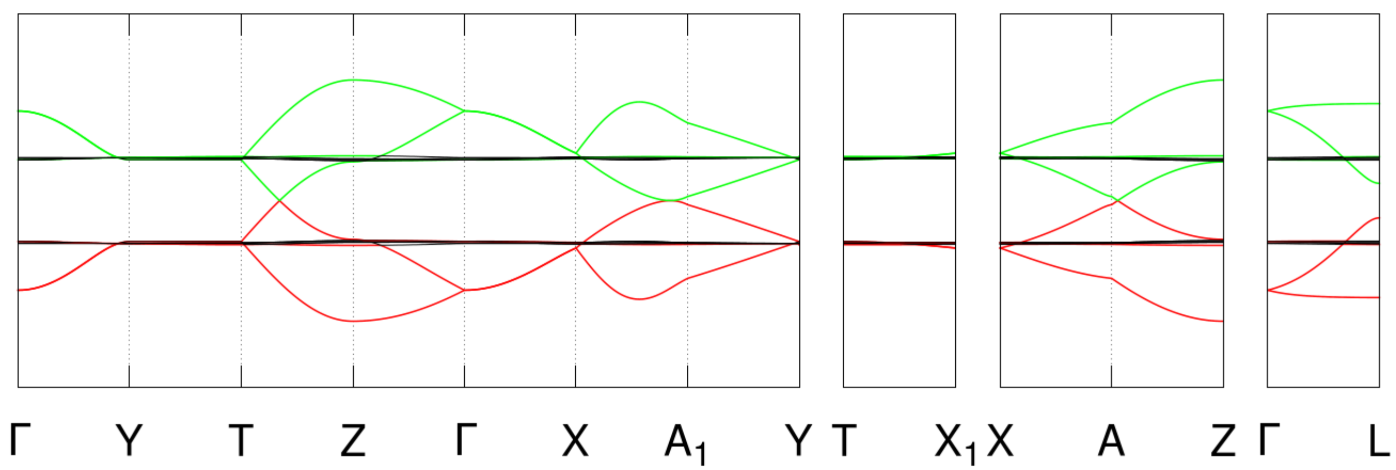
$$m_j = \frac{1}{2} \langle f_{j\alpha}^{\dagger} [\sigma^{z}]_{\alpha\beta} f_{j\beta} \rangle$$ magnetic order



(a)The spinon band structure at the exactly solvable point J=0, K>0.

J=0, K > 0

Kitaev Spin Liquid

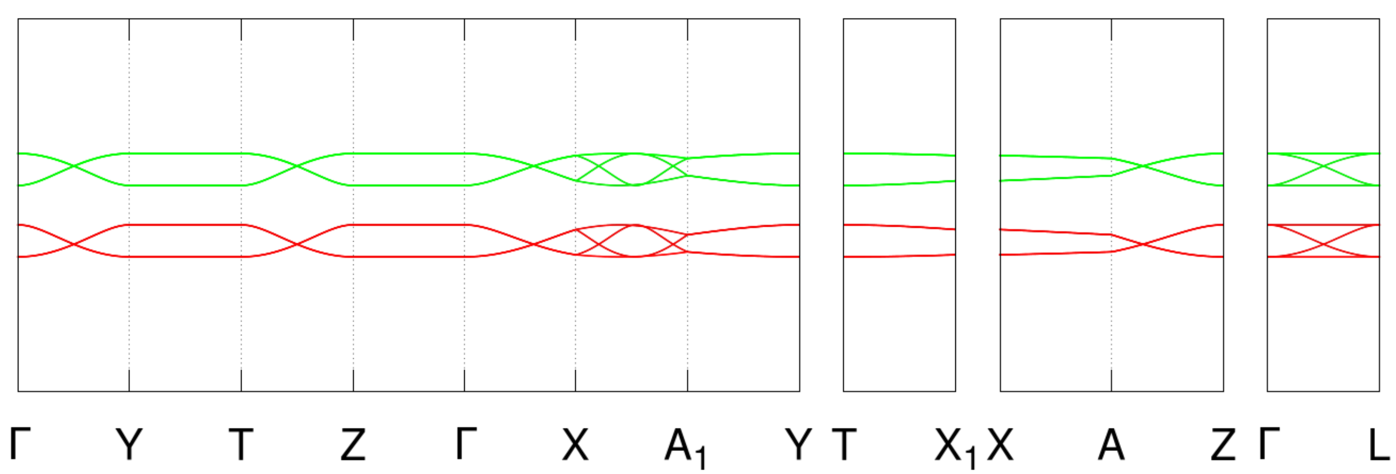


(b)The spinon band structure at the point K=8J. At this point, magnetic order has not yet stabilized.

K=8J

Kitaev Spin Liquid

$K_c \approx 7.7J$

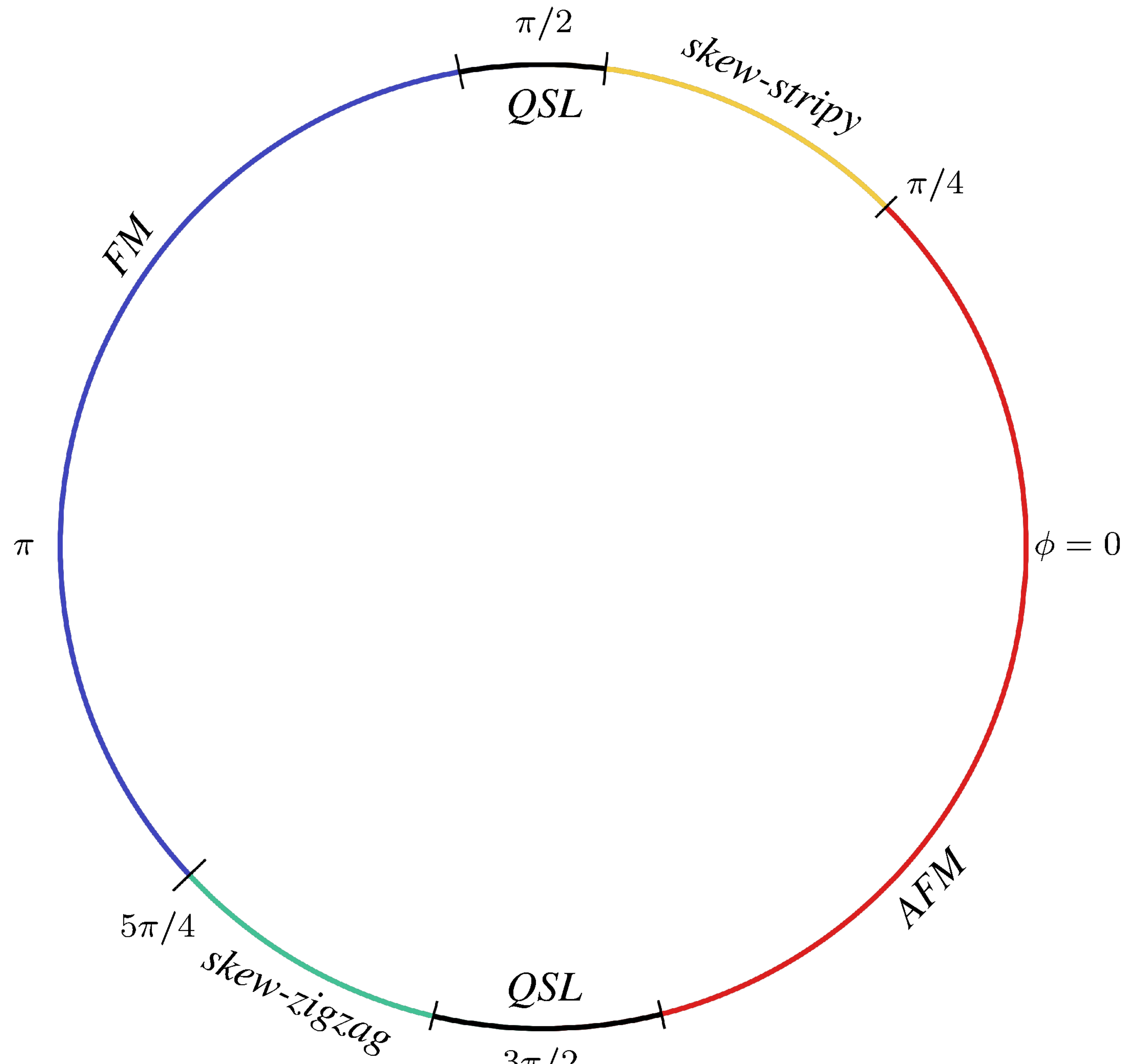


(c)The spinon band structure at the point K=4.9J. At this point, magnetic order is present.

K=4.9J

Skew-Stripy Order

Phase Diagram



$$J = \cos\phi$$

$$K = \sin\phi$$

Connections to Experiments ?

$$\Theta_{\mathrm{CW}} = \frac{1}{4}(K - 3J)$$

$\Theta_{CW} > 0$ when $K > 3J$

But the ground State is AF (Skew-Stripy) when $K \lesssim 7.7J$

Possible to have ferro-like Curie-Weiss temperature with AF ordering

Connections to Experiments ?

$$\Theta_{\mathrm{CW}} = \frac{1}{4}(K - 3J)$$

$\Theta_{CW} > 0$ when $K > 3J$

But the ground State is AF (Skew-Stripy) when $K \lesssim 7.7J$

Possible to have ferro-like Curie-Weiss temperature with AF ordering

When external magnetic field is applied in the perpendicular direction to x-, y-, or z-directions,
the saturation field is h = J, independent of K

can be used to extract the values of J and K

Magnetic Frustration and Spiral Magnetic Order

E. K.-H. Lee, Y. B. Kim, unpublished (2014)

S. Lee, J.-S. Jeong, K. Hwang, Y. B. Kim, arXiv:1403.2724 (2014)

Extended Kitaev-Heisenberg Model

$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + KS_i^\gamma S_j^\gamma + \boxed{\Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right)]}\right.$$

e.g. In the limit of $U, J_H \gg \lambda \gg t$

$$J = \frac{4}{27}\left[\frac{6t_1(t_1+2t_3)}{U-3J_H} + \frac{2(t_1-t_3)^2}{U-J_H} + \frac{(2t_1+t_3)^2}{U+2J_H}\right]$$

$$K = \frac{8J_H}{9}\left[\frac{(t_1-t_3)^2 - 3t_2^2}{(U-3J_H)(U-J_H)}\right],$$

$$\boxed{\Gamma = \frac{16J_H}{9}\left[\frac{t_2(t_1-t_3)}{(U-3J_H)(U-J_H)}\right].}$$

$$t_1 = \frac{t_{dd\pi} + t_{dd\delta}}{2}, \quad t_2 = \frac{t_{pd\pi}^2}{\Delta_{pd}} + \frac{t_{dd\pi} - t_{dd\delta}}{2}, \quad t_3 = \frac{3t_{dd\sigma} + t_{dd\delta}}{4},$$

Extended Kitaev-Heisenberg Model

$$H = \sum_{\langle ij\rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) \right]$$

e.g. In the limit of $U, J_H \gg \lambda \gg t$

$$J = \frac{4}{27}\left[\frac{6t_1(t_1+2t_3)}{U-3J_H} + \frac{2(t_1-t_3)^2}{U-J_H} + \frac{(2t_1+t_3)^2}{U+2J_H} \right]$$

$$K = \frac{8J_H}{9}\left[\frac{(t_1-t_3)^2 - 3t_2^2}{(U-3J_H)(U-J_H)} \right],$$

$$\Gamma = \frac{16J_H}{9}\left[\frac{t_2(t_1-t_3)}{(U-3J_H)(U-J_H)} \right].$$

$$t_1 = \frac{t_{dd\pi} + t_{dd\delta}}{2}, \quad t_2 = \frac{t_{pd\pi}^2}{\Delta_{pd}} + \frac{t_{dd\pi} - t_{dd\delta}}{2}, \quad t_3 = \frac{3t_{dd\sigma} + t_{dd\delta}}{4},$$

S. Bhattacharjee, S. S. Lee, Y. B. Kim (2012)

E. K.-H. Lee, Y. B. Kim (2013)

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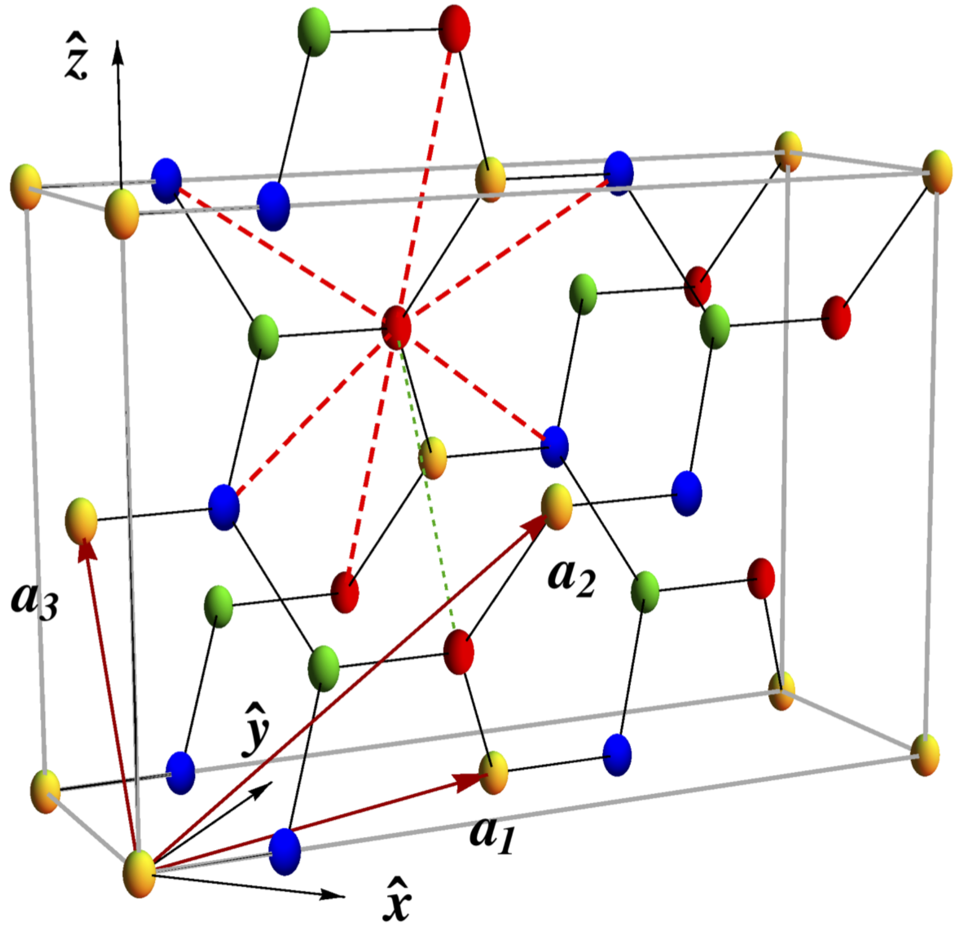
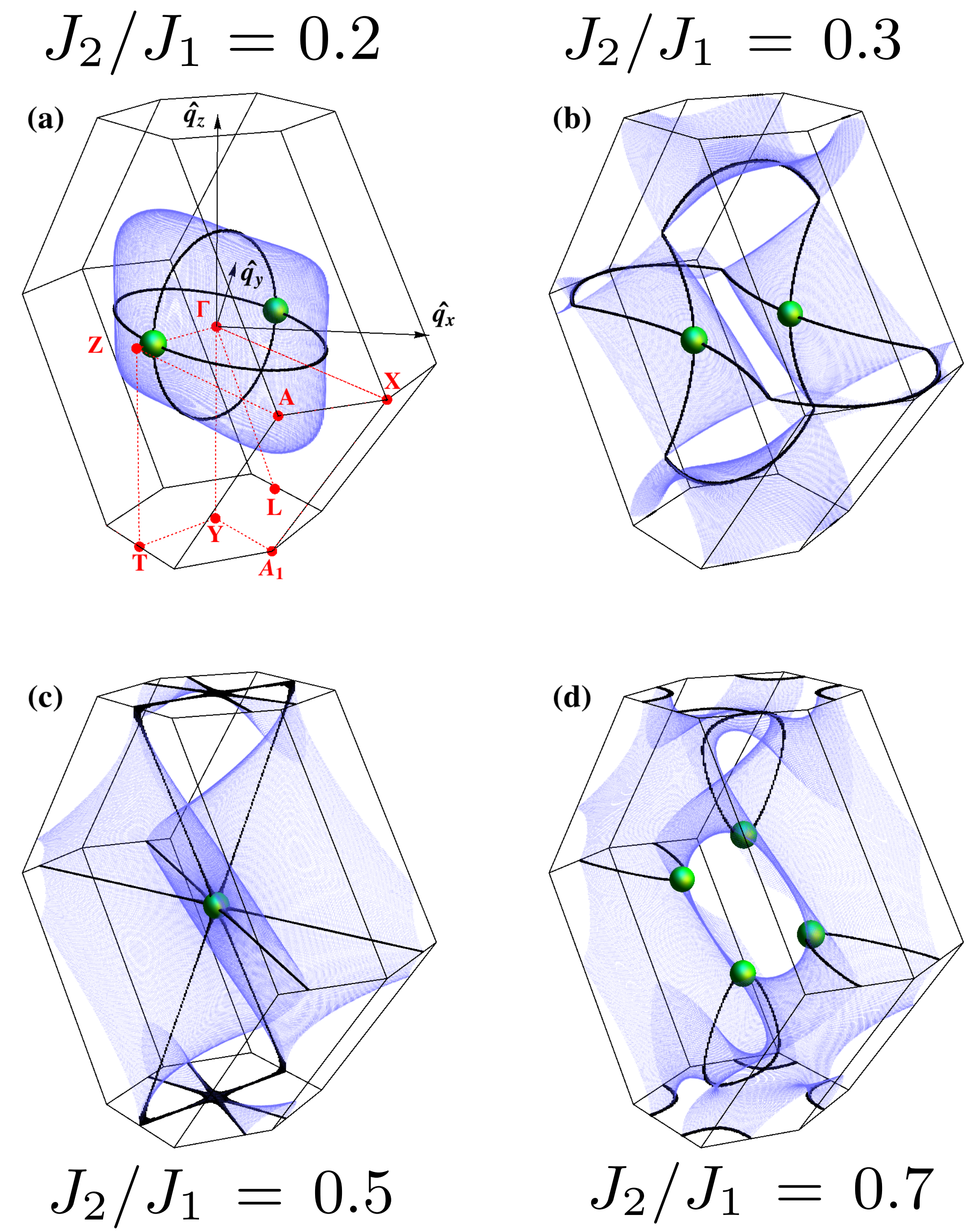
Frustrated Further Neighbor Interactions



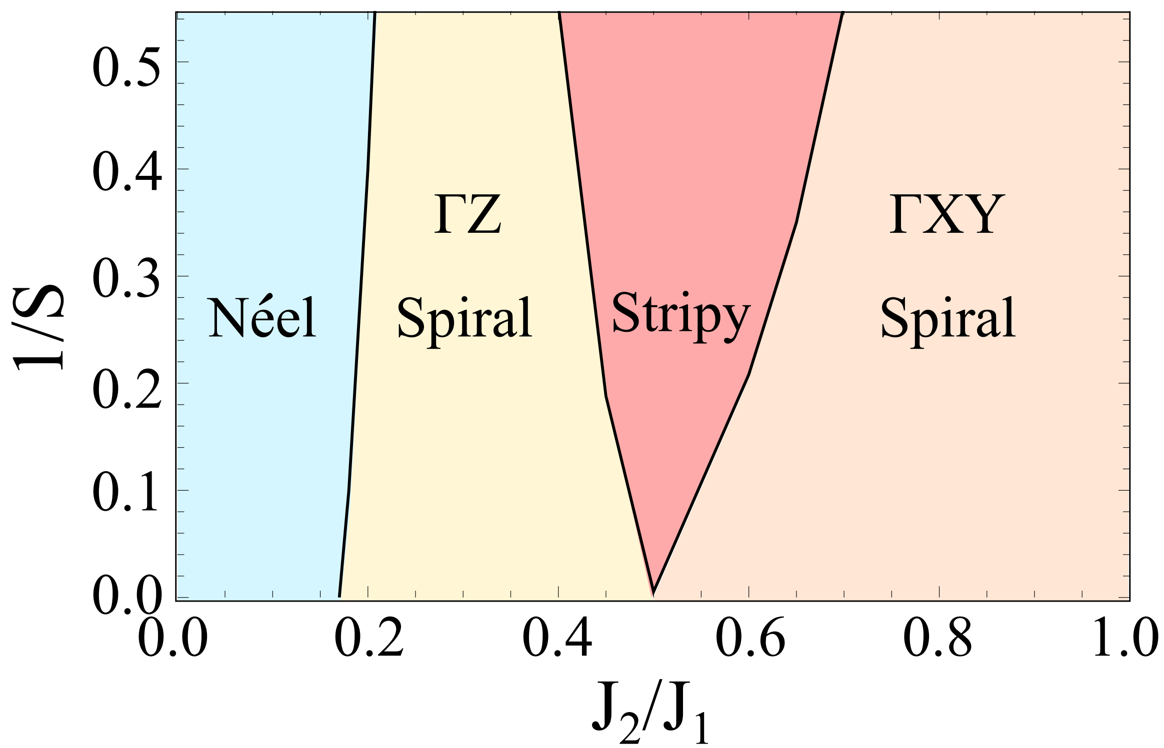


$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

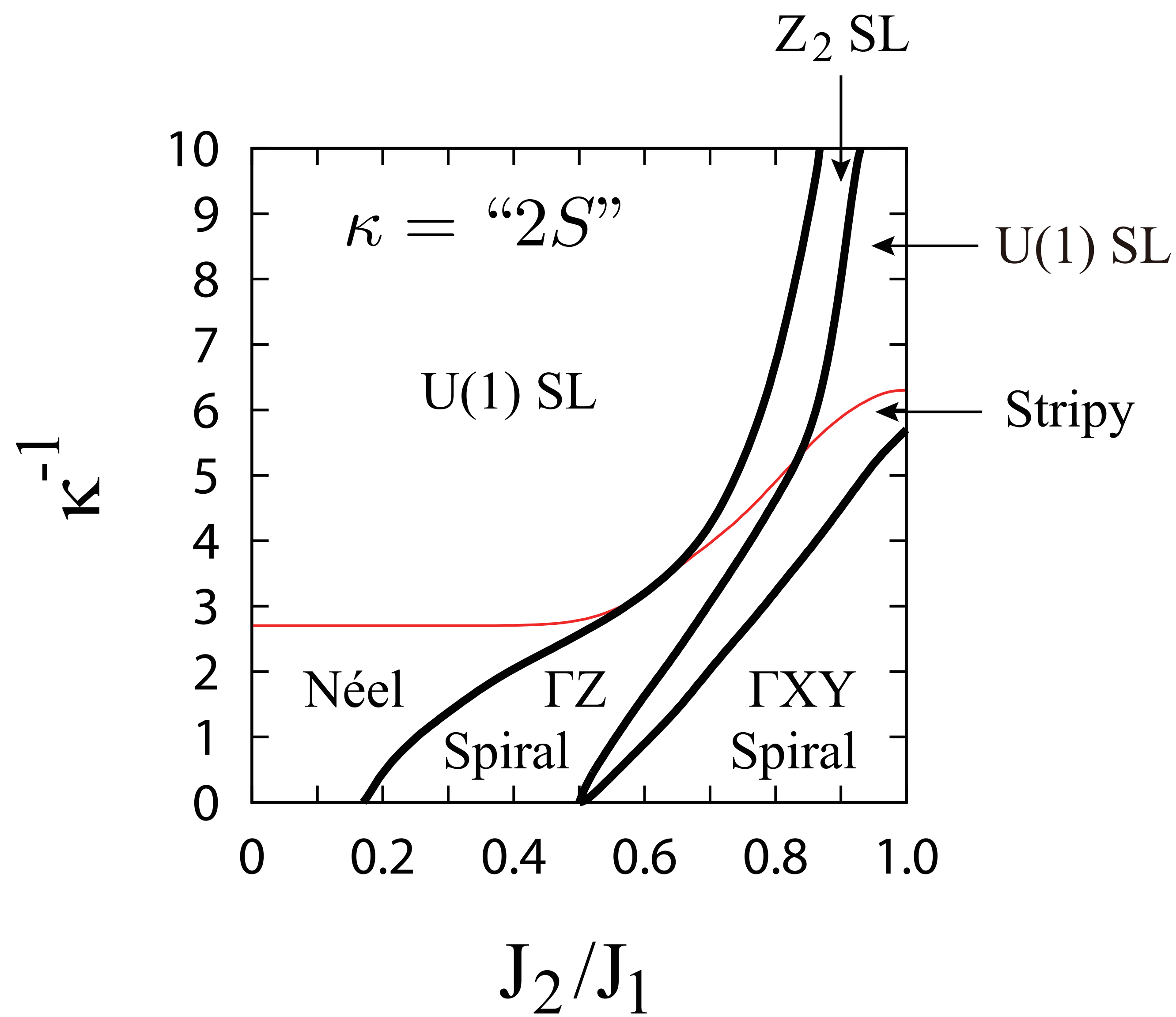
$$\mathbf{S}_i^{0,2(1,3)} \rightarrow -\mathbf{S}_i^{0,2(1,3)}, \quad J_1 \rightarrow -J_1 \ ,$$

Classical Line Degeneracy

Quantum Order-by-Disorder



Linear Spin-Wave



Schwinger Boson

Emergent Spiral and Skew-Stripy (or Skew-Zigzag) Order