Gapless Topological Phases and Unusual Magnetic Order in Iridates

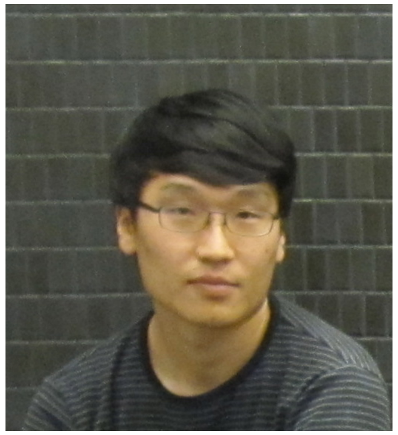
Yong Baek Kim
University of Toronto

Workshop on "Novel Materials and Novel Theories"

Trieste, Italy, August 17, 2015

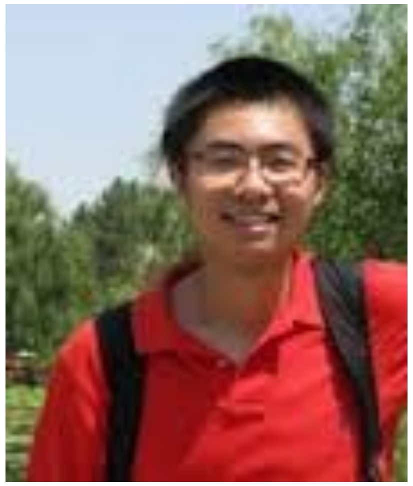
Eric K.-H. Lee
Toronto

Robert Schaffer
Toronto



Kyusung Hwang
Toronto

Subhro Bhattacharjee
Toronto
—> Assistant Prof.
ICTS Bangalore, India



Yuan-Ming Lu
Assistant Prof.
Ohio State Univ

Heung-Sik Kim
Toronto

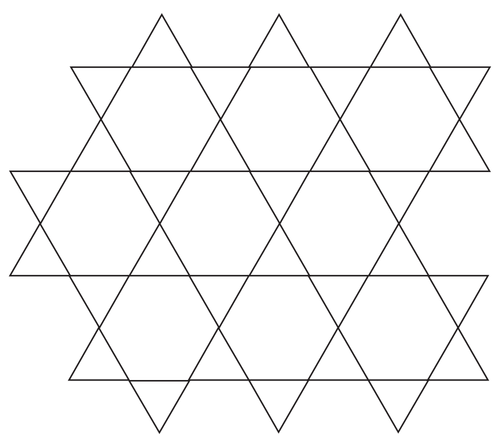
Hosub Jin
Assistant Prof.
UNIST, Korea

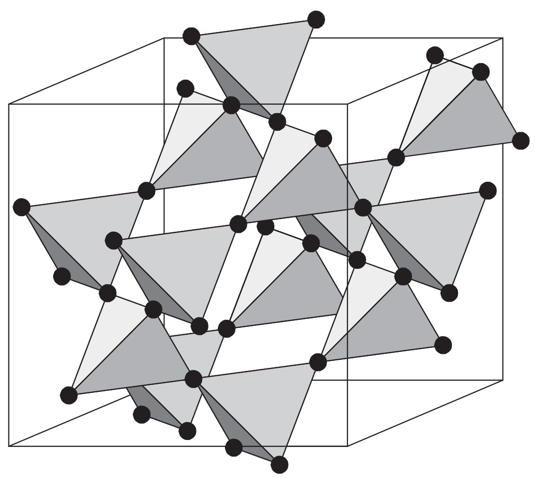
Two Routes to Quantum Spin Liquid

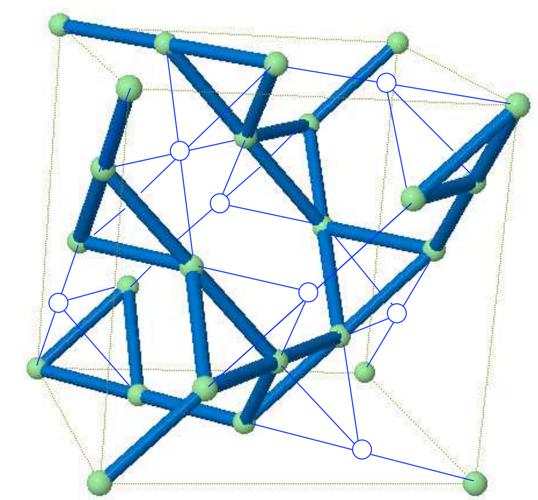
1. Geometric Frustration (spin-rotation invariant)

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = \frac{J}{2} \sum_{\text{simplex}} \left(\sum_{i \,\epsilon\, \text{simplex}} \mathbf{S}_i \right)^2 + \text{ constant}$$

$$\sum_{i \,\epsilon\, \text{simplex}} \mathbf{S}_i = 0$$ macroscopic degeneracy



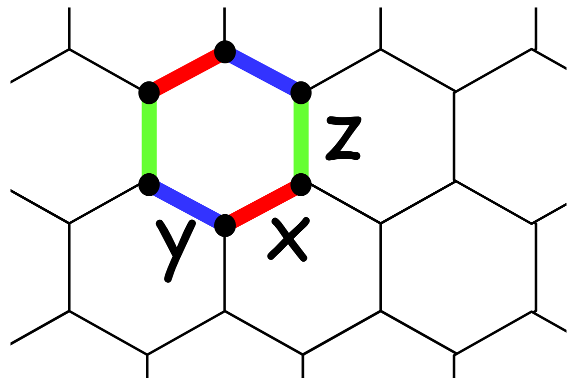




2. Frustrated Interactions (spin-orbit)

Spin interactions depend on spatial directions

Kitaev Model on Honeycomb Lattice: Exact Solution



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

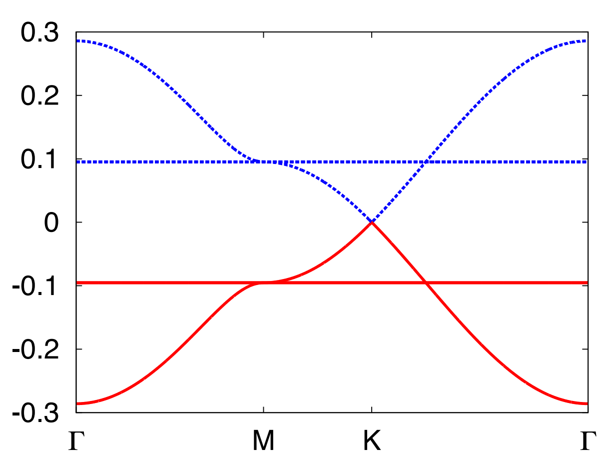
A. Kitaev (2006)

$S_i^\alpha = i b_i^\alpha c$ $\quad \{b_i^x, b_i^y, b_i^z, c\}$ 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 $u_{ij}^\alpha = +1 \, (\forall \langle ij \rangle)$



Majorana Fermions with Dirac Dispersion

Kitaev Spin Liquid as a Z_2 Spin Liquid

Making connection to Slave-fermion approach (more conventional)

$$f_{i\uparrow} = \frac{1}{\sqrt{2}}(c_i + i b_i^z) \qquad S_i^a = \frac{1}{2} f_{i\alpha}^\dagger \sigma_{\alpha\beta}^a f_{i\beta}$$

$$f_{i\downarrow} = \frac{i}{\sqrt{2}}(b_i^x + i b_i^y) \qquad \text{with} \quad \sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} = 1$$

$$H = \sum_{\langle ij\rangle \in a} \{ f_{i\alpha}^\dagger [T^a]_{\alpha\beta}^{ij} f_{j\beta} + f_{i\alpha} [\Delta^a]_{\alpha\beta}^{ij} f_{j\beta} \}$$

exactly one particle per site (insulator)

If $\Delta^a = 0$ $\quad f_{i\alpha} \longrightarrow f_{i\alpha} e^{i\theta_i} \qquad [T^a]_{ij} = |[T^a]_{ij}| e^{i a_{ij}}$ $\qquad$ U(1)

$$a_{ij} \longrightarrow a_{ij} + \theta_i - \theta_j$$

In general $\quad f_{i\alpha} \to f_{i\alpha} s_i \qquad s_i = \pm 1$ $\qquad$ Z_2

$$[T^a]_{ij}, \quad [\Delta^a]_{ij} \to s_i [T^a]_{ij} s_j, \quad s_i [\Delta^a]_{ij} s_j$$

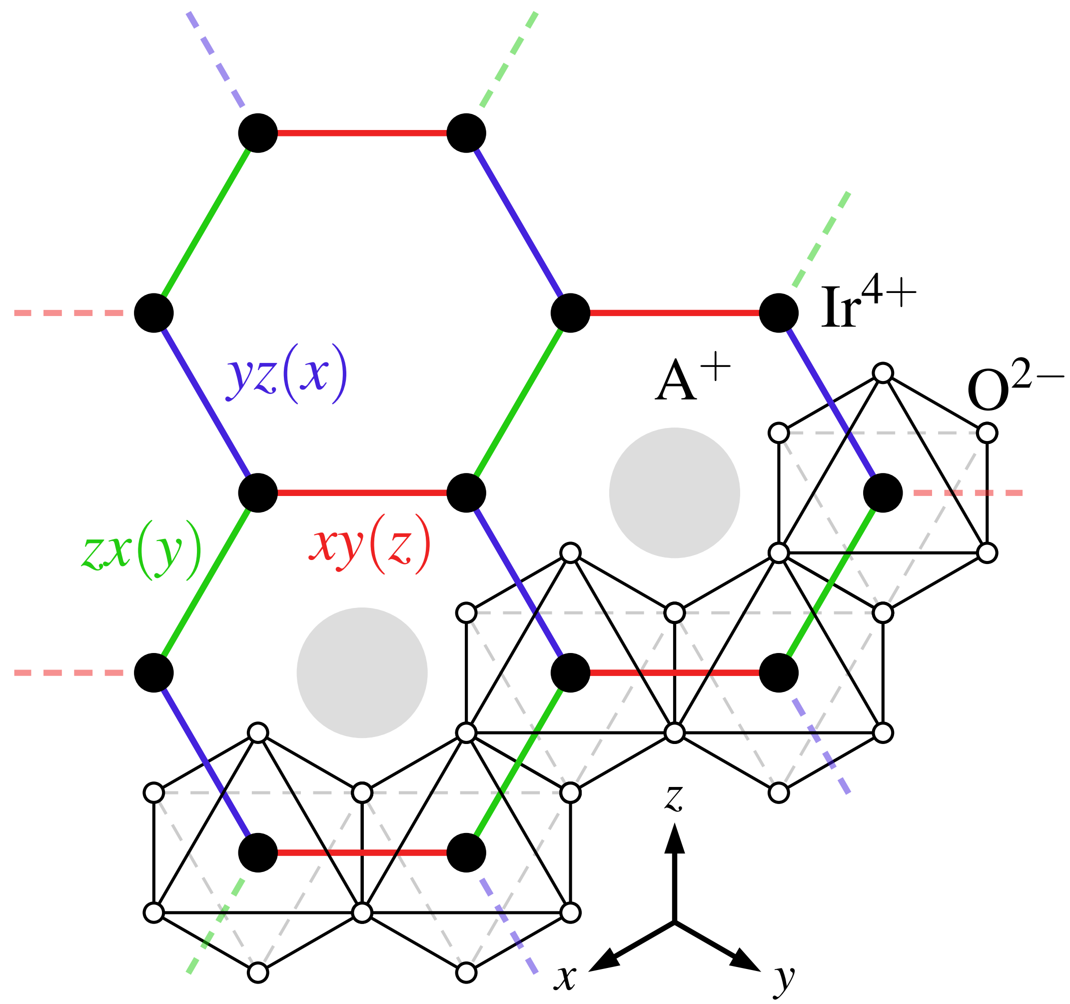
α-A_2IrO_3 Kitaev Interaction ?

$$H = \sum_{\langle ij \rangle \in \gamma} -K S_i^\gamma S_j^\gamma + J \vec{S}_i \cdot \vec{S}_j$$

$$\gamma = x, y, z$$

G. Jackeli and G. Khaliullin,
PRL 102, 256403 (2009)

J. Chaloupka, G. Jackeli
and G. Khaliullin,
PRL 105, 027204 (2010)



J_{eff}=1/2

$$|\uparrow_j\rangle = \frac{1}{\sqrt{3}}(i|xz,\downarrow_s\rangle + |yz,\downarrow_s\rangle + |xy,\uparrow_s\rangle)$$
$$|\downarrow_j\rangle = -\frac{1}{\sqrt{3}}(i|xz,\uparrow_s\rangle - |yz,\uparrow_s\rangle + |xy,\downarrow_s\rangle)$$

Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

Realization of Kitaev Quantum Spin Liquid ?

Honeycomb Iridates Family

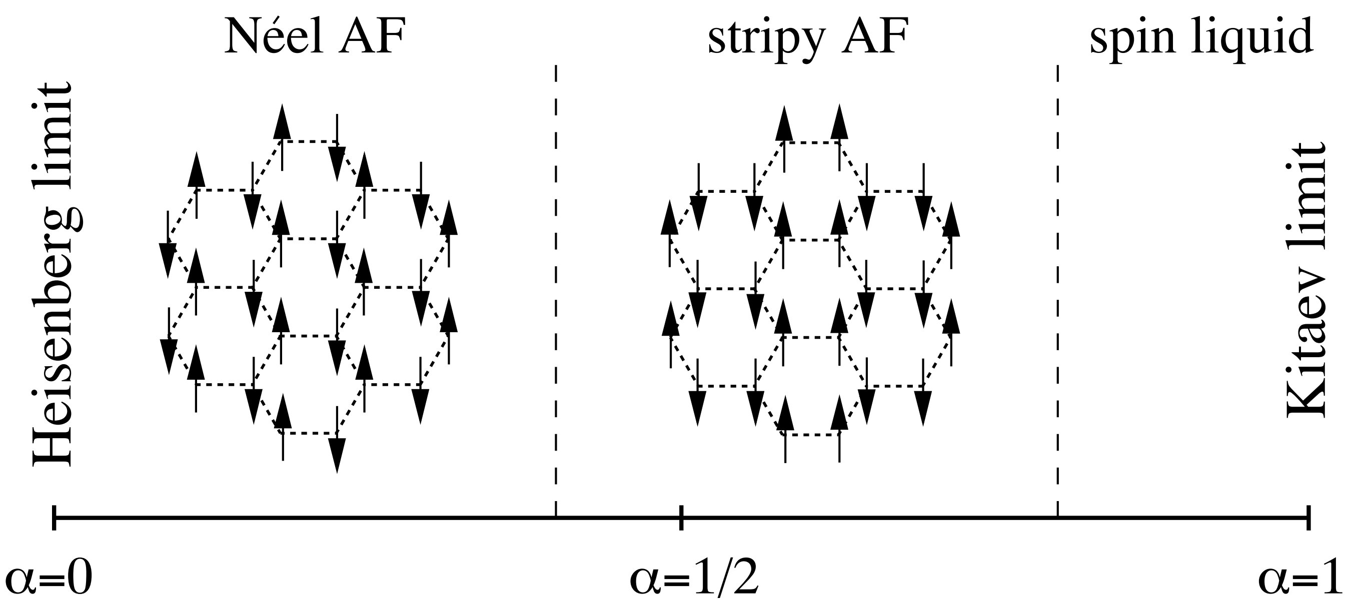
2D Honeycomb α- Na_2IrO_3 α- Li_2IrO_3 (2D)

3D Hyper-Honeycomb β- Li_2IrO_3 (3D)

3D Harmonic-Honeycomb γ- Li_2IrO_3 (3D)

J. Chaloupka, G. Jackeli and G. Khaliullin,
PRL 105, 027204 (2010)

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

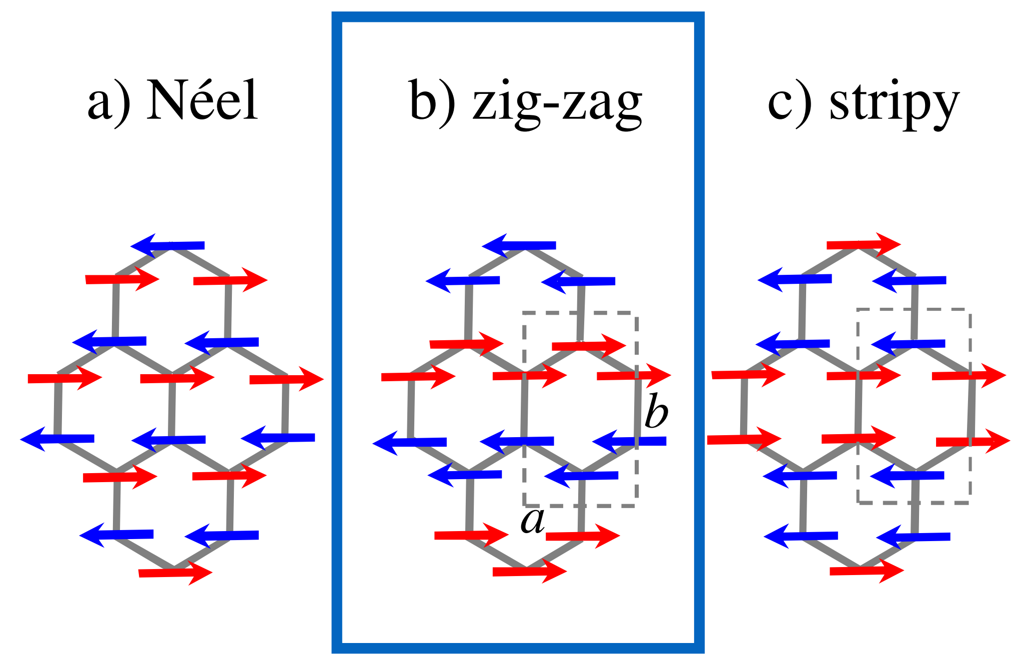


Quantum Spin Liquid robust
to small Heisenberg interaction

Radu Coldea
(Neutron Scattering)

α-Na_2IrO_3

Zig-Zag Order



Monoclinic Distortions
Strong Trigonal Distortions

Discovery of Three dimensional “Honeycomb” lattice

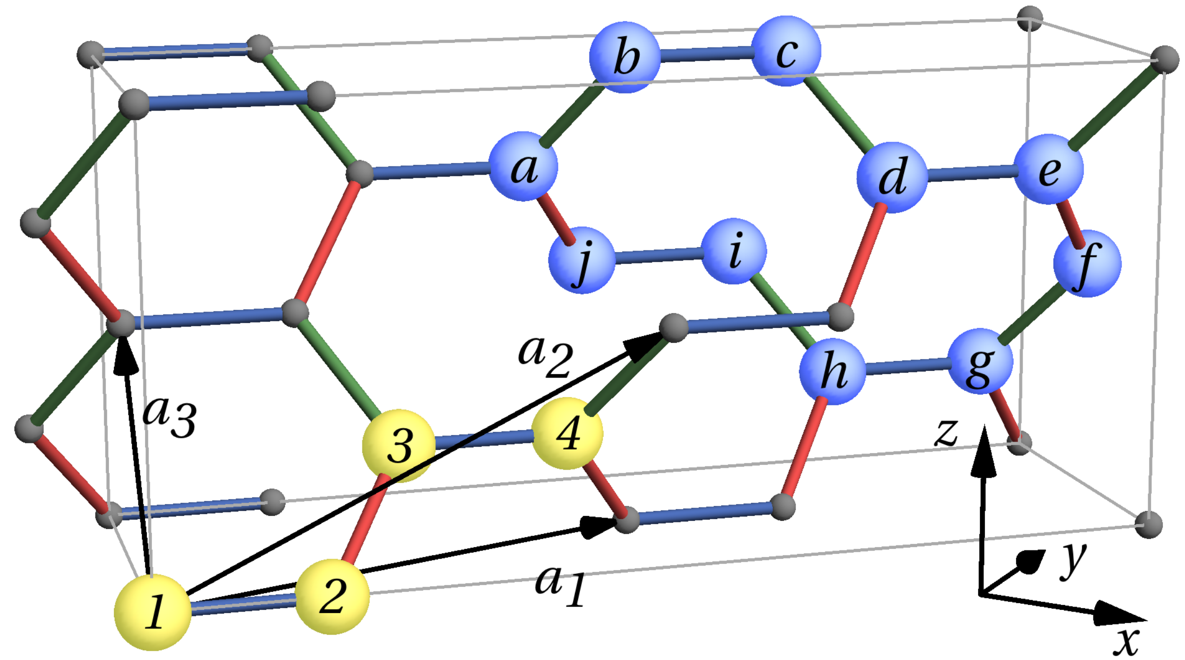
β- Li_2IrO_3

Dresden, July 2013

arXiv:1403.3296

H. Takagi

Hyper-Honeycomb



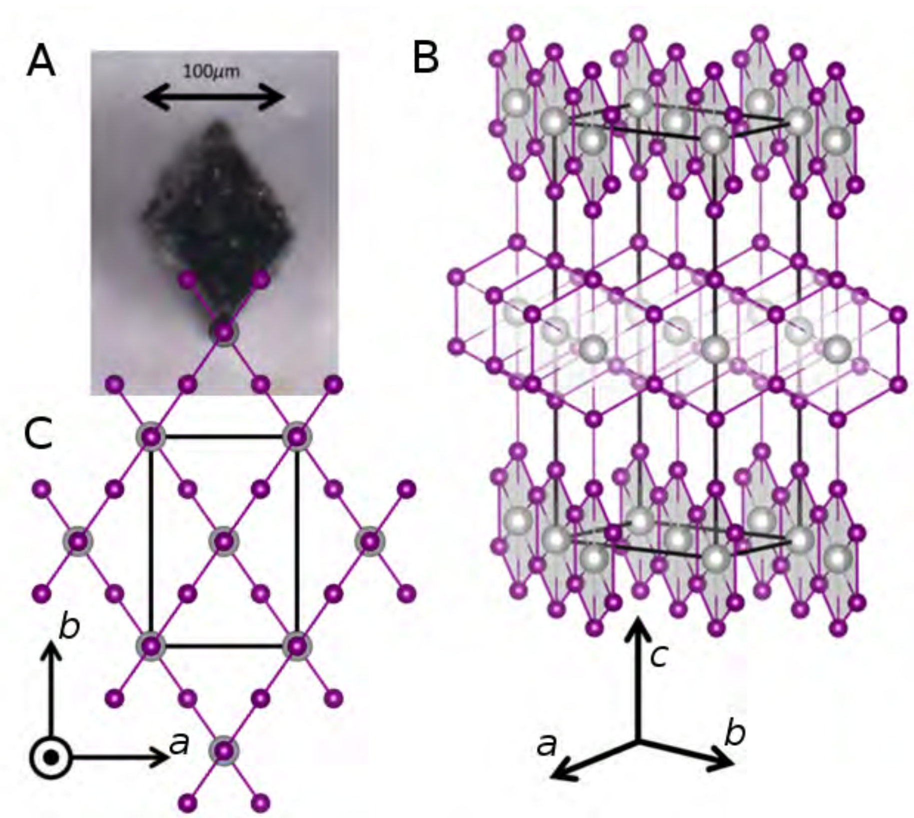
γ- Li_2IrO_3

arXiv:1402.3254

James Analytis

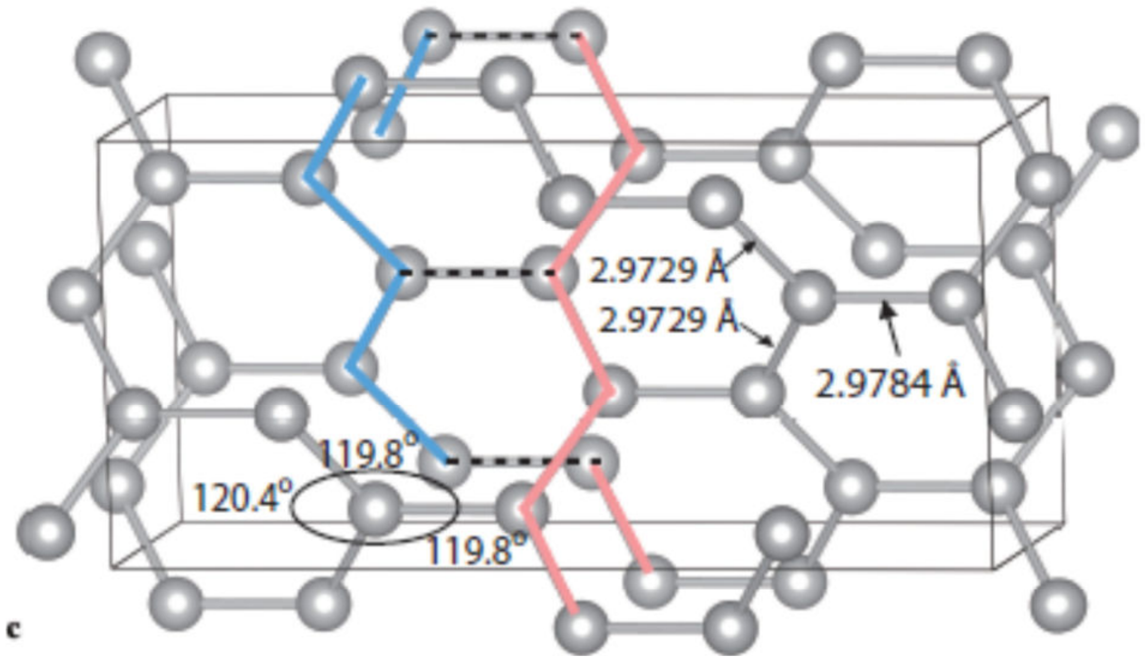
Radu Coldea

Stripy-Honeycomb



Hyper-Honeycomb β- Li_2IrO_3 Hide Takagi

arXiv:1403.3296

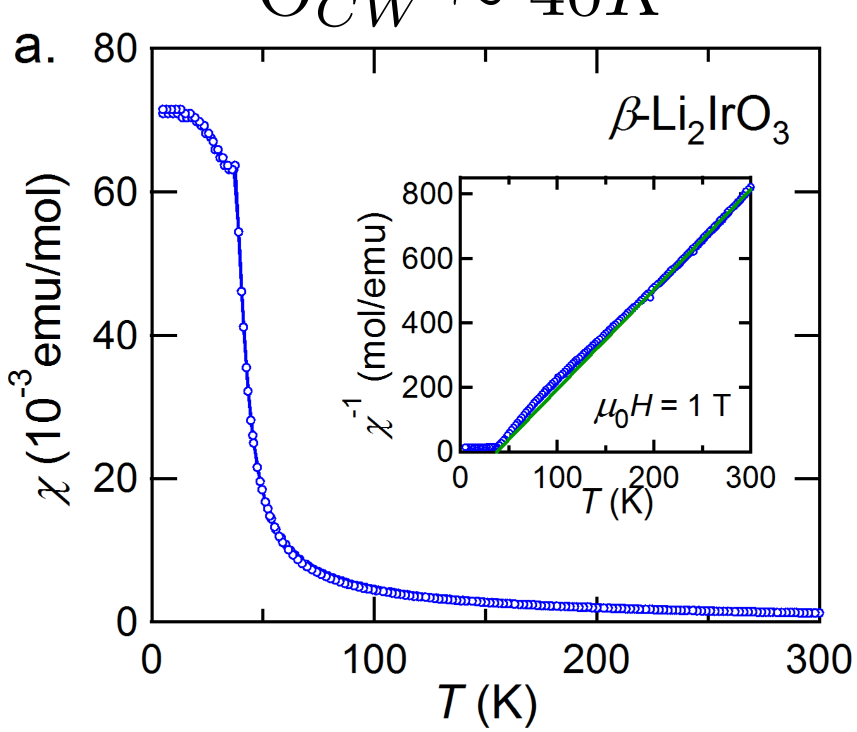


Close to ideal structure

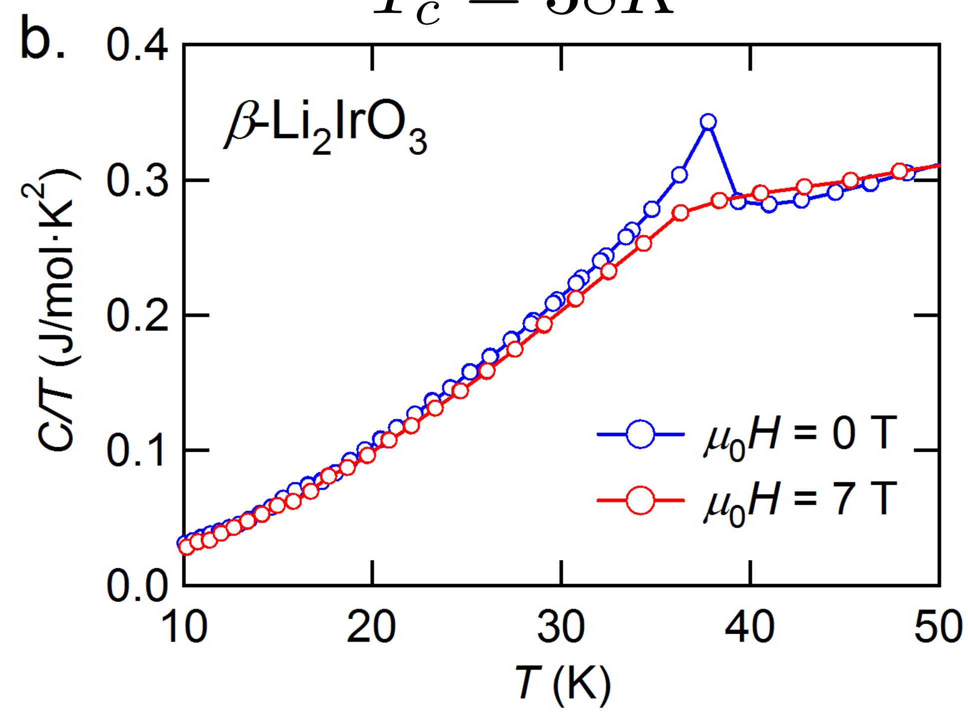
AF ordering

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

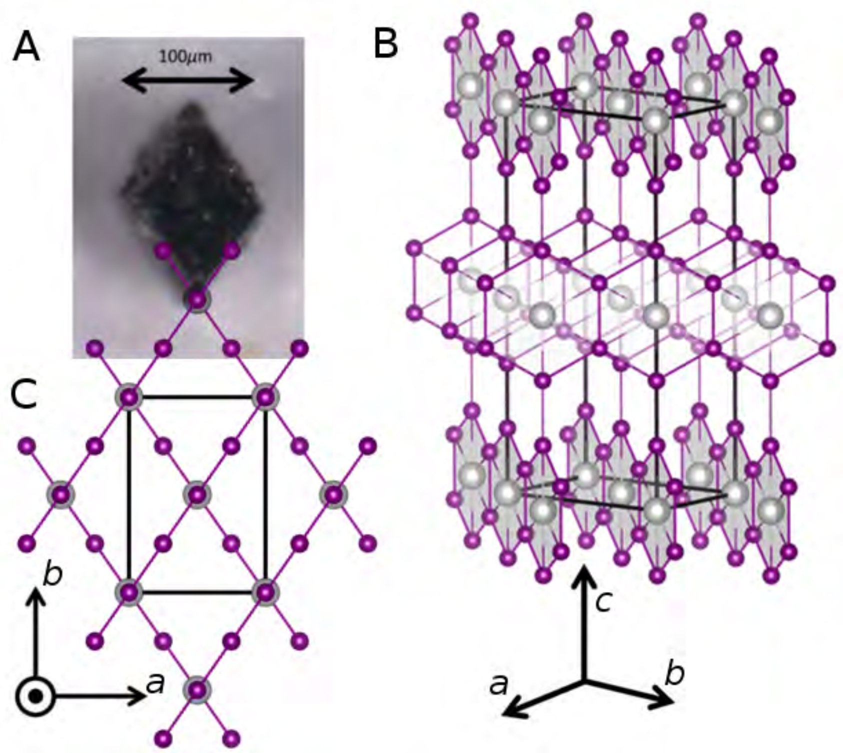
$$\Theta_{CW} \sim 40K$$



$$T_c = 38K$$

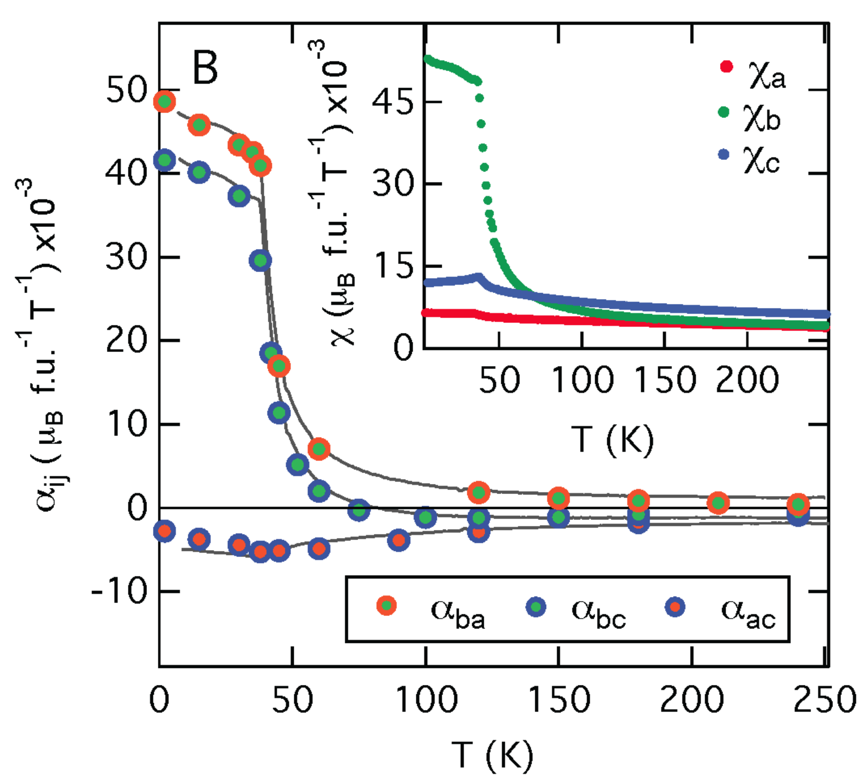


Stripy-Honeycomb γ- Li_2IrO_3 arXiv:1402.3254



Radu Coldea

James G. Analytis



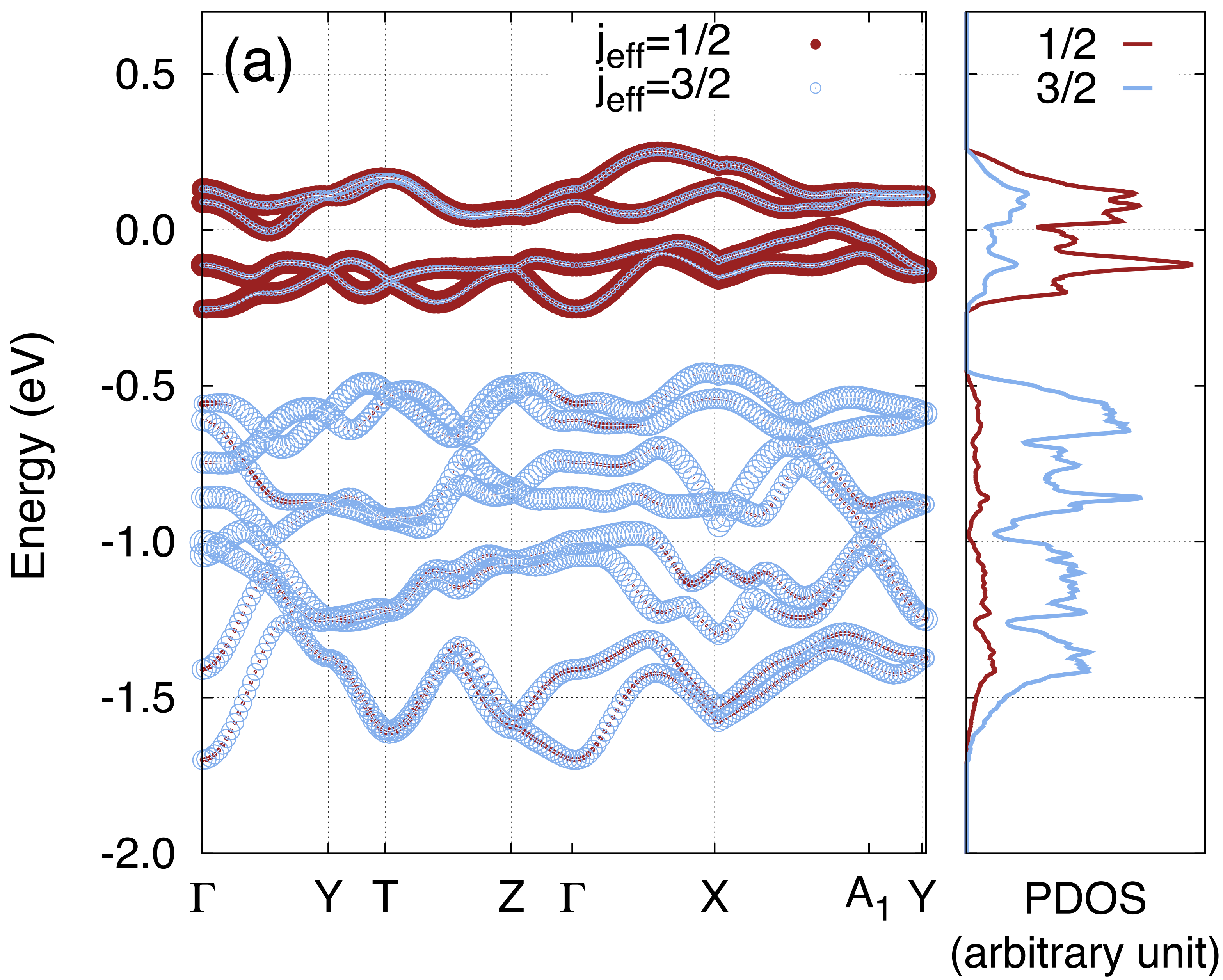
AF ordering

$T_c = 38K$

strong magnetic anisotropy

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

β- Li_2IrO_3



Ab Initio
(OpenMx, PBE-GGA)

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

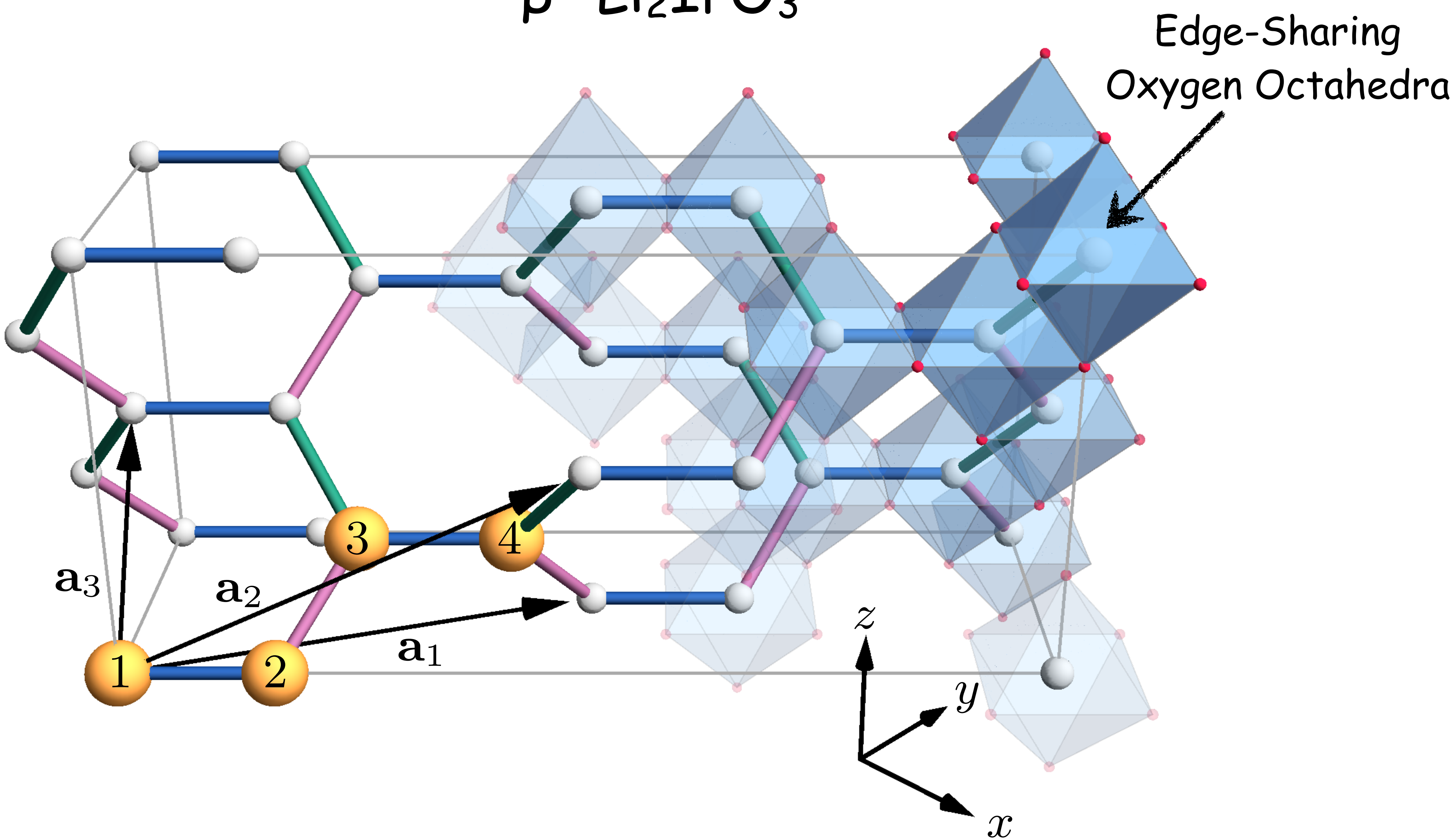
H.-S.Kim, E. K.-H. Lee,
Y. B. Kim,
arXiv:1502.00006 (2015)

Localized Pseudo-Spin Model in the Strong Coupling Limit

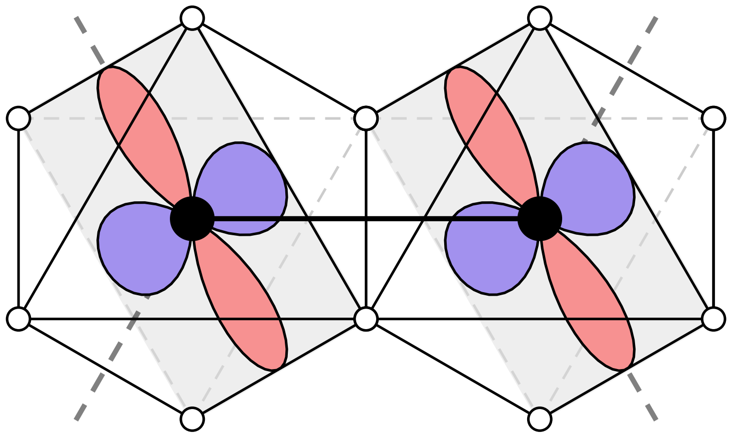
$J_{eff}=1/2$

Edge-sharing Oxygen Octahedra Structure

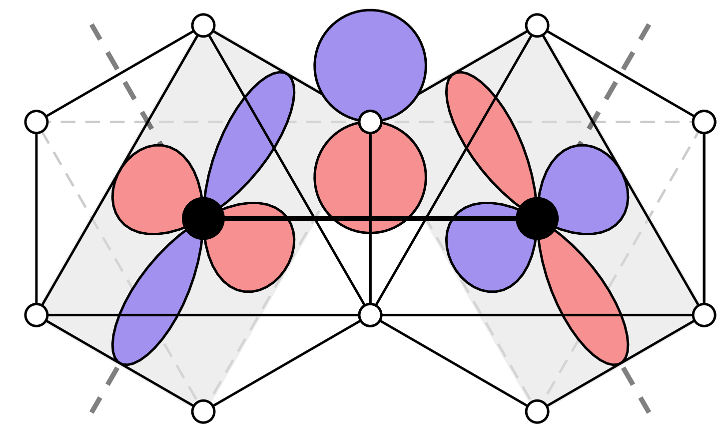
β- Li_2IrO_3



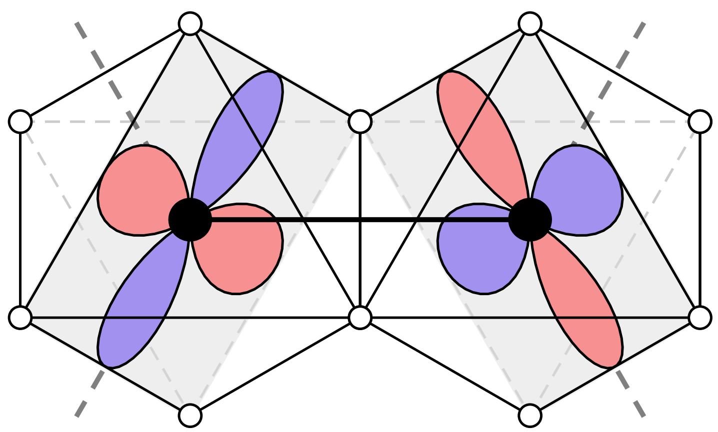
Strong Coupling Limit: Localized Pseudo-Spin Model



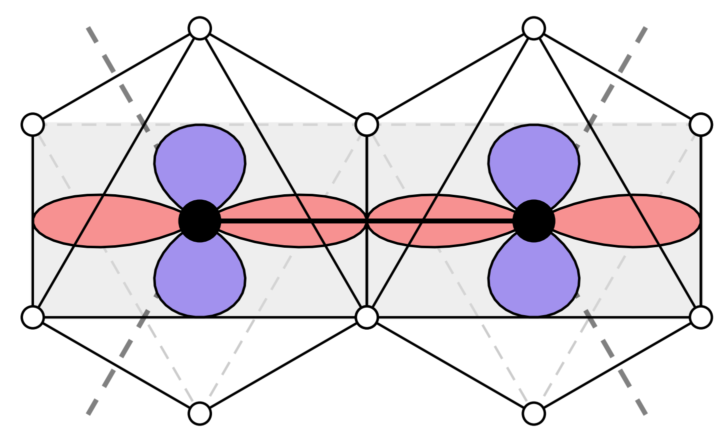
(a) Ir-Ir overlap for t_1



(b) Ir-O-Ir overlap for t_2



(c) Ir-Ir overlap for t_2



(d) Ir-Ir overlap for t_3

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

Strong Coupling Limit: Localized Pseudo-Spin Model

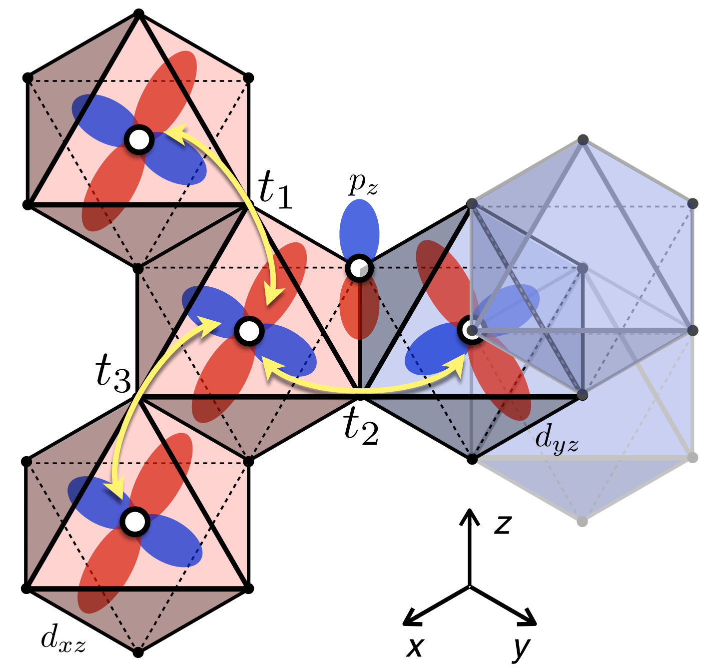
$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[J \vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \boxed{\Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right)} \right]$$

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

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

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

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



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

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

Kitaev Model: Exact Solution

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

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

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

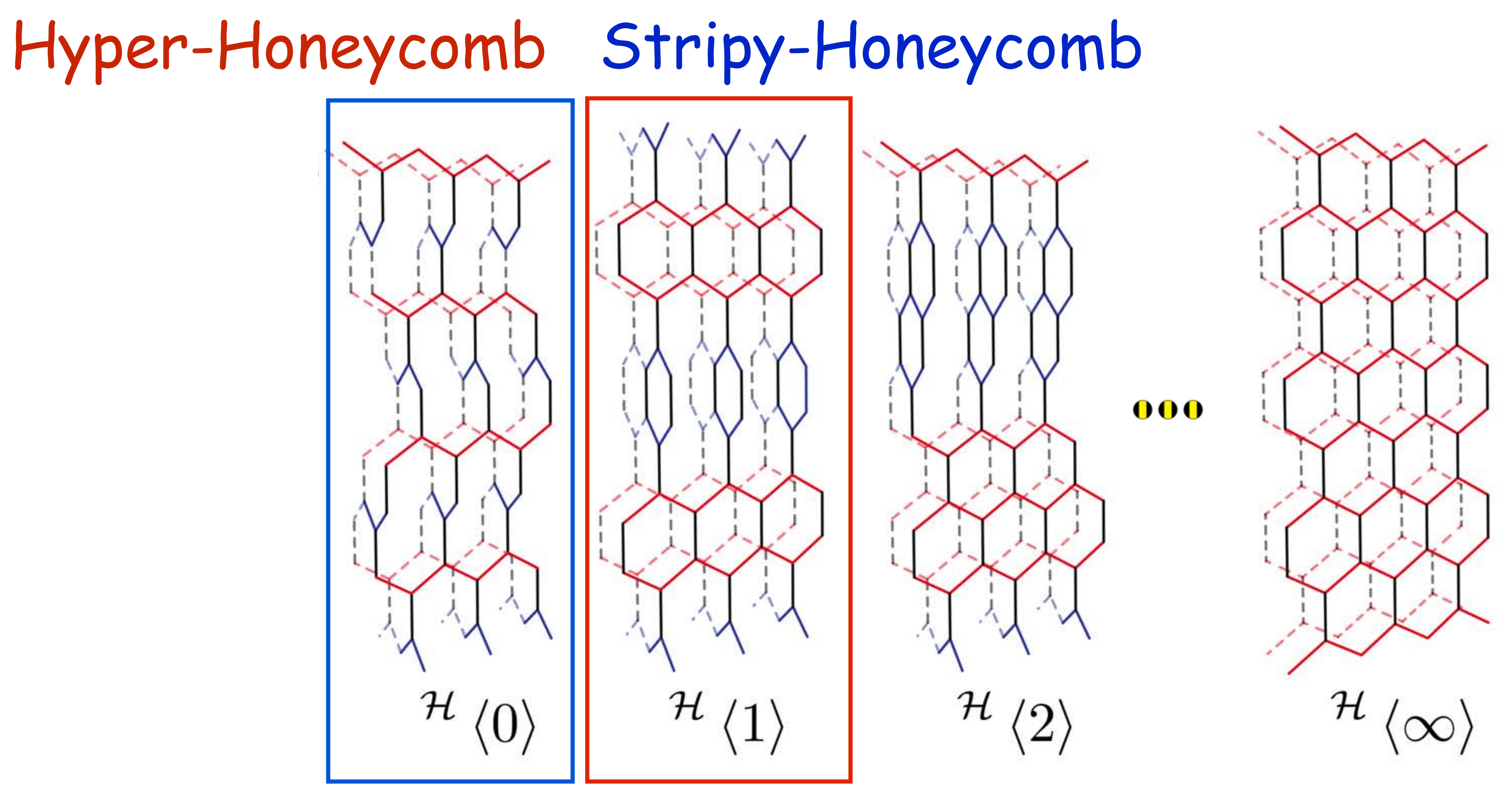
$\mathcal{W}_P = \prod_{\text{loop}} u_{ij}^\alpha$ commute with the Hamiltonian $\Longrightarrow \mathcal{W}_P = \pm 1$

Hyper-Honeycomb S. Mandal and N. Surendran (2009)

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

Stripy-Honeycomb R. Schaffer, E. Lee, Y.-M. Lu, Y. B. Kim, PRL 2015

Ground state is in a π-flux sector some $\mathcal{W}_p = -1$



$$\mathbf{H}_n^{\Phi} = \sum_k \vec{c}_{n,-k}^{\,T} H_{n,k}^{\Phi} \vec{c}_{n,k}$$

$$H_{n,k}^{\Phi} = \begin{bmatrix} 0 & -iD_{n,k}^{\Phi} \\ i\left(D_{n,k}^{\Phi}\right)^{\dagger} & 0 \end{bmatrix}$$

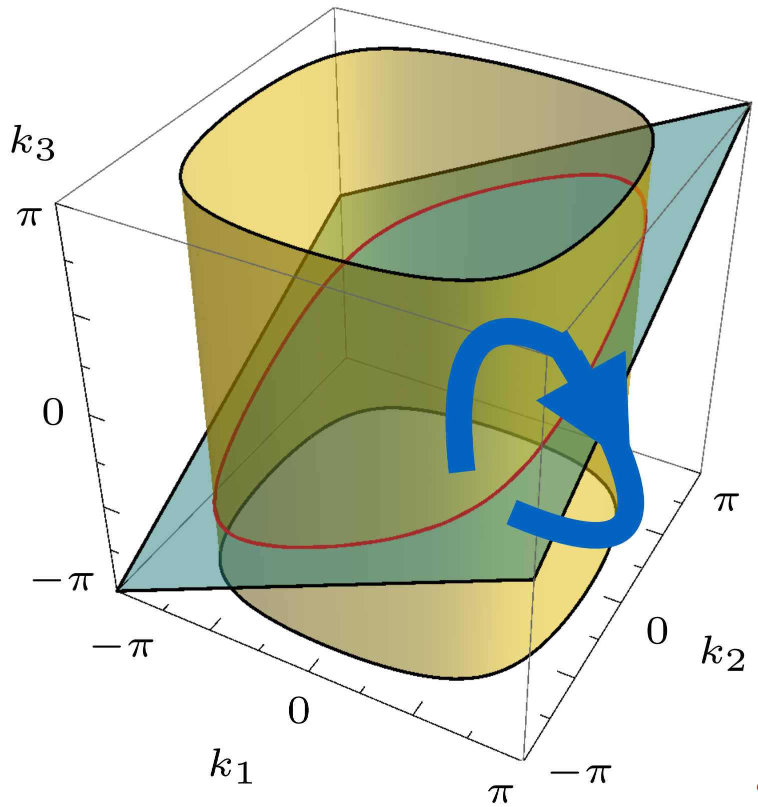
BDI Class

Gapless Modes determined by two equations

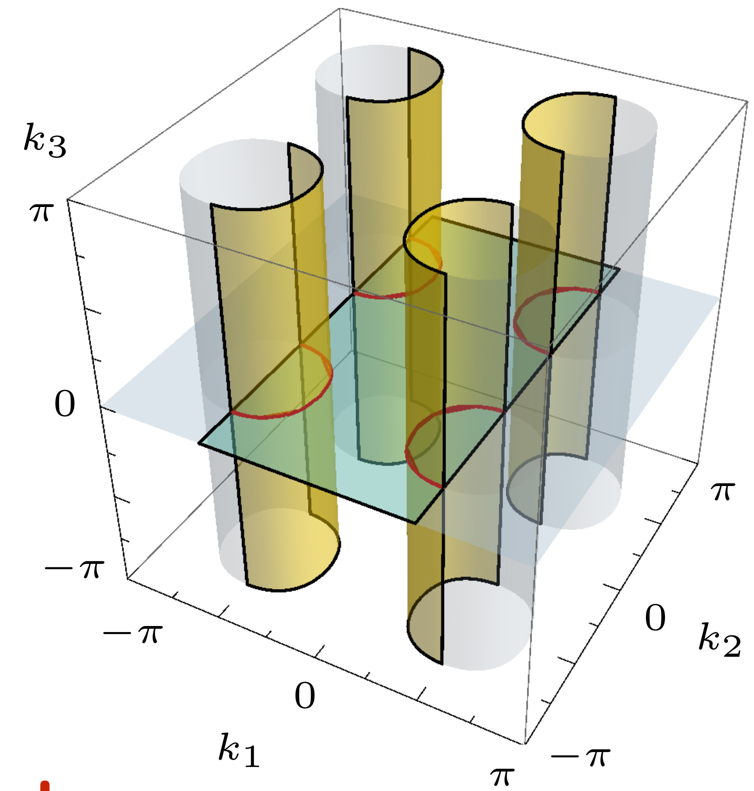
$$\mathrm{Re}\left[\det(D_k)\right] = 0$$
$$\mathrm{Im}\left[\det(D_k)\right] = 0$$

Nodal Ring in 3D

0-FLUX SECTOR
HYPERHONEYCOMB



π-FLUX SECTOR
STRIPYHONEYCOMB



Topological Spinon "Semi-metal"

$$\nu = \frac{1}{4\pi i}\oint \mathrm{d}k \mathrm{Tr}[D_{\mathbf{k}}^{-1}\partial_k D_{\mathbf{k}} - (D^\dagger)_{\mathbf{k}}^{-1}\partial_k D_{\mathbf{k}}^\dagger],$$

Topological Invariant

R. Schaffer, E. Lee, Y.-M. Lu, Y. B. Kim, PRL 2015