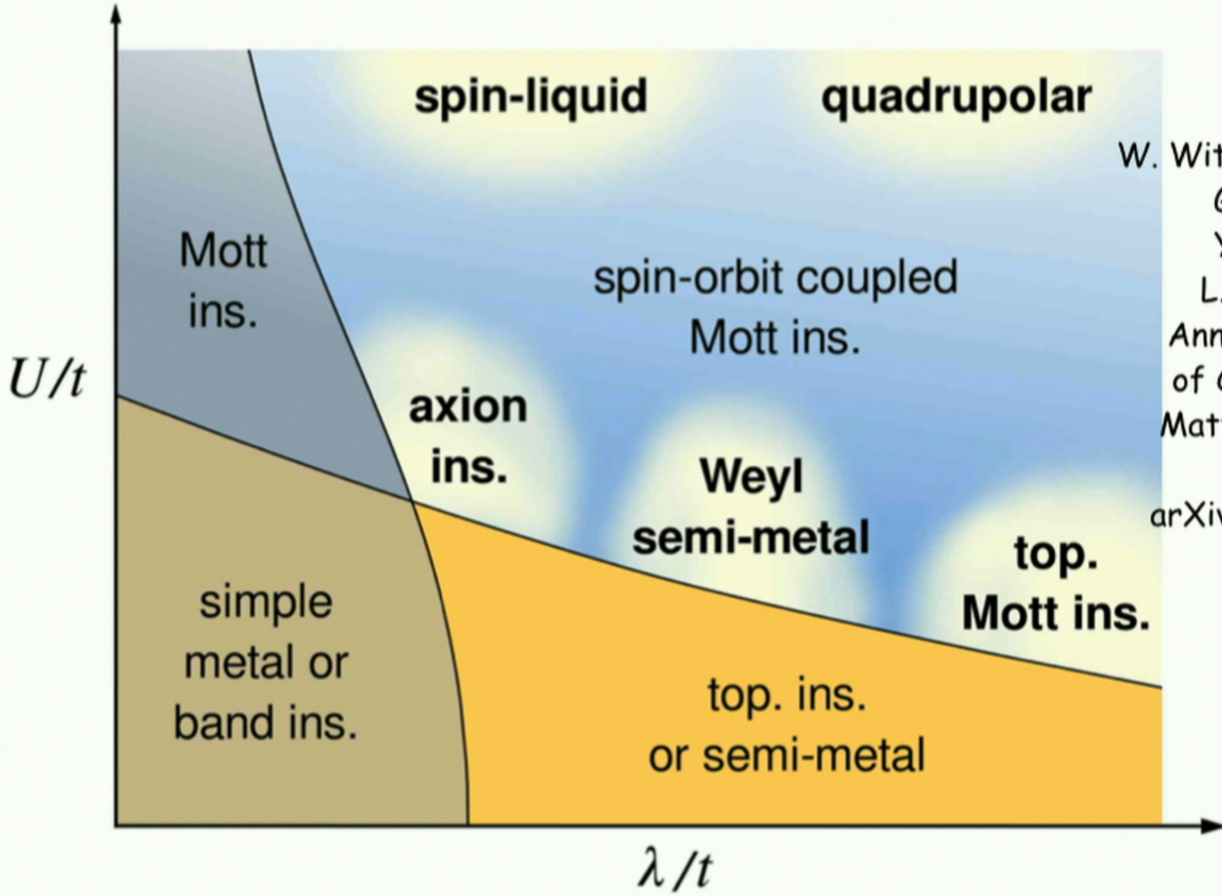
Title: Topological and Broken-Symmetry Phases in Three-dimensional Hyperhoneycomb Iridates

Date: Apr 30, 2015 04:30 PM

URL: http://pirsa.org/15040164

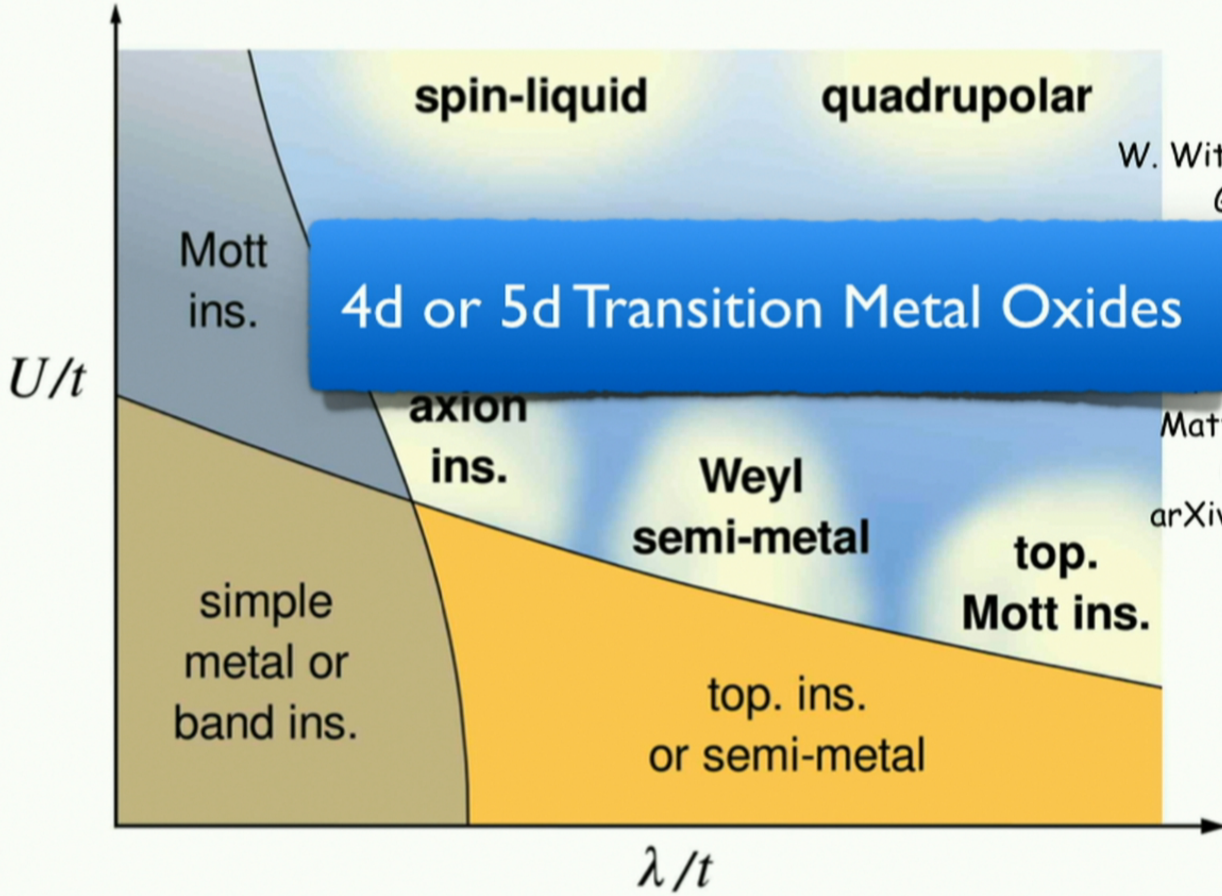
Abstract: Recently three-dimensional versions of honeycomb-lattice iridates, beta and gamma phases of Li2IrO3, have been discovered. It has been theoretically suggested that these hyperhoneycomb iridates may hold promise for the realization of the Kitaev spin liquid or the exactly solvable model for the elusive quantum spin liquid phase. Recent scattering experiments on these systems have, however, revealed highly non-trivial magnetic spiral phases. We propose a theory that may explain the emergence of this unusual magnetic order and discuss why the current experimental data may suggest that the hyperhoneycomb iridates are not too far from the Kitaev limit.

Correlations and Spin-Orbit Coupling



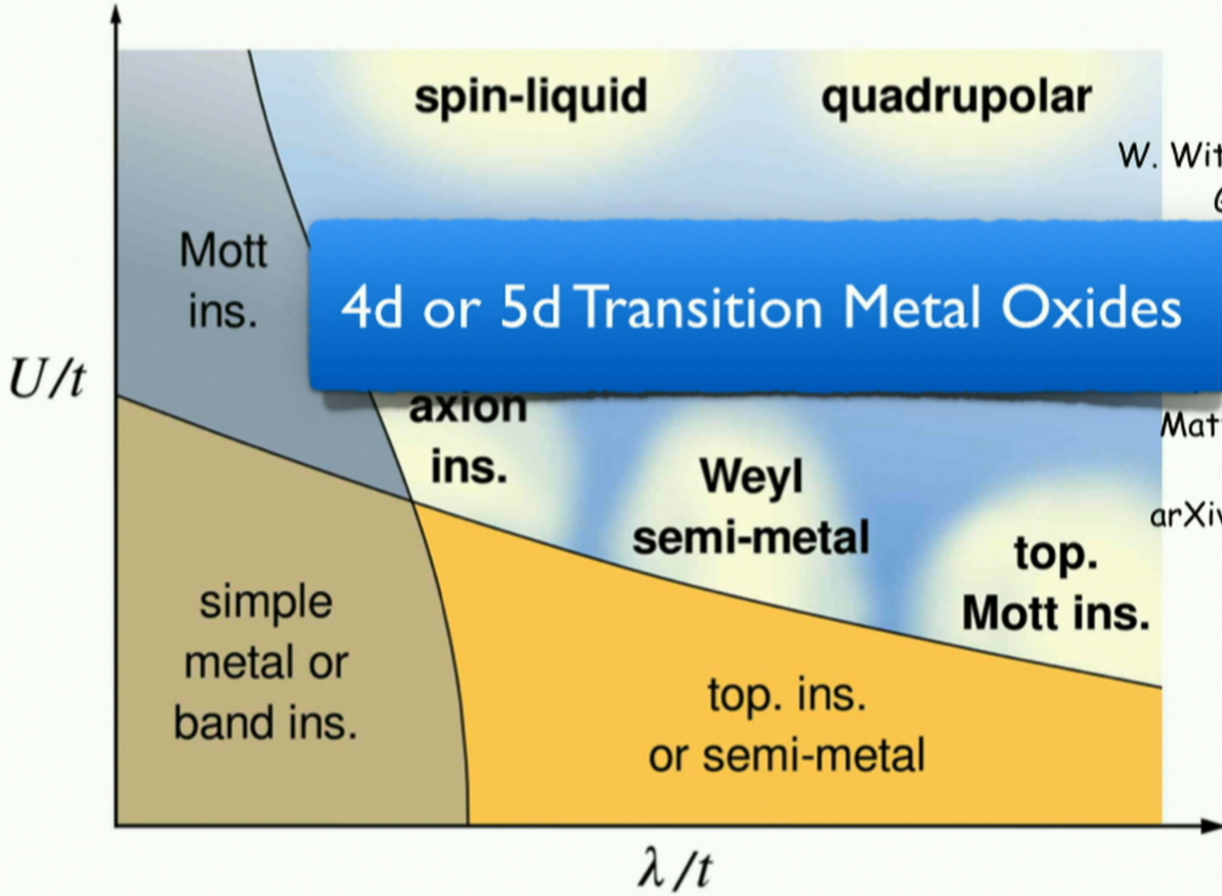
W. Witczak-Krempa,
G. Chen,
Y.B.Kim,
L. Balents
Annual Review
of Condensed
Matter Physics
(2014),
arXiv:1305.2193

Correlations and Spin-Orbit Coupling



W. Witczak-Krempa, G. Chen, .B.Kim, Balents ıal Review ondensed Matter Physics (2014), arXiv:1305.2193

Correlations and Spin-Orbit Coupling



W. Witczak-Krempa,
G. Chen,
.B.Kim,
Balents
ıal Review
ondensed
Matter Physics
(2014),
arXiv:1305.2193

Phase	Symm.	Correlation	Properties	Proposed materials
Topological Insulator	TRS	W-I	Bulk gap, TME, protected surface states	many
Axion Insulator	P	I	Magnetic insulator, TME, no protected surface states	$R_2Ir_2O_7$, $A_2Os_2O_7$
WSM	TRS or P (not both)	W-I	Dirac-like bulk states, surface Fermi arcs, anomalous Hall	$R_2Ir_2O_7$, $HgCr_2Se_4$, ...
LAB Semi-metal	cubic + TRS	W-I	Non-Fermi liquid	$R_2Ir_2O_7$
Chern Insulator	broken TRS	I	Bulk gap, QHE	$Sr[Ir/Ti]O_3$, $R_2[B/B']_2O_7$
Fractional Chern Insulator	broken TRS	I-S	Bulk gap, FQHE	$Sr[Ir/Ti]O_3$
Fractional Topological Insulator, Topological Mott Insulator	TRS	I-S	Several possible phases. Charge gap, fractional excitations	$R_2Ir_2O_7$
Quantum spin liquid	any	S	Several possible phases. Charge gap, fractional excitations	$(Na,Li)_2IrO_3$, Ba_2YMoO_6
Multipolar order	various	S	Suppressed or zero magnetic moments. Exotic order parameters.	$A_2BB'O_6$

W. Witczak-Krempa, G. Chen, Y.-B.Kim, L. Balents, arXiv:1305.2193

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)

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)

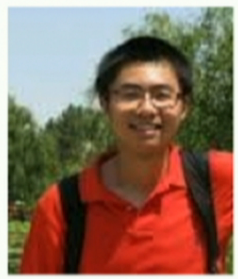
3D Harmonic-honeycomb γ- Li_2IrO_3 (3D)

Eric K.-H. Lee
Toronto

Robert Schaffer
Toronto

Kyusung Hwang
Toronto

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



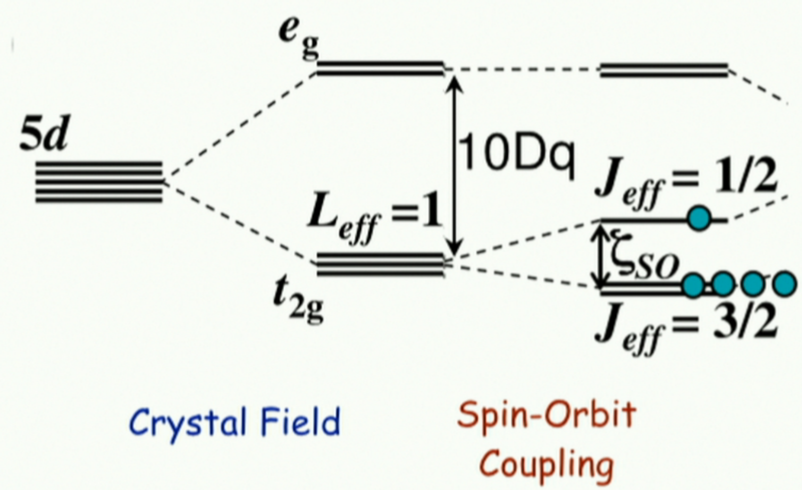
Yuan-Ming Lu
Assistant Prof.
Ohio State Univ

Heung-Sik Kim
Toronto

Hosub Jin
Assistant Prof.
UNIST, Korea

5d orbitals of Ir^{4+}: large spin-orbit coupling

Ir^{4+} = [Xe] $4f^{14}\, 5d^5$ $\qquad \mathcal{P}_{t2g}\mathbf{L}_{\ell=2}\mathcal{P}_{t2g} = -\mathbf{L}^{\text{eff}}_{\ell=1}$



B.J.Kim, T.W.Noh, G.Cao et al. PRL (2008)

B.J.Kim, H.Takagi, et al, Science (2009)

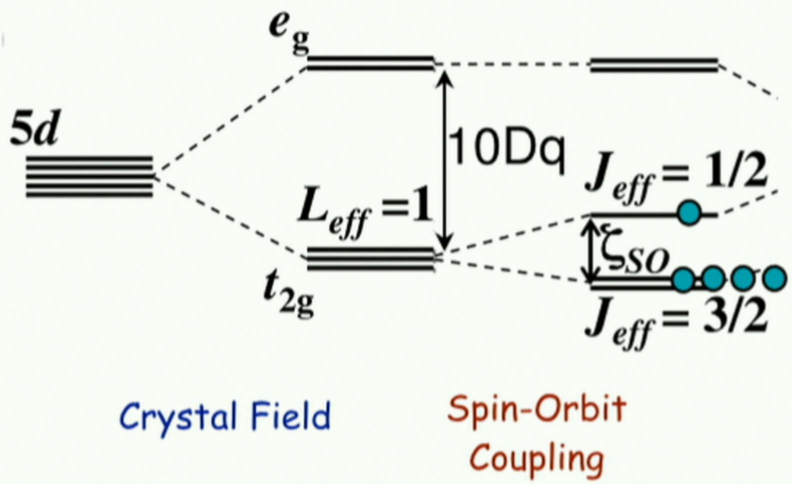
$$|\uparrow_j\rangle = \frac{1}{\sqrt{3}}(i|xz,\downarrow_s\rangle + |yz,\downarrow_s\rangle + |xy,\uparrow_s\rangle)$$
$$|\downarrow_j\rangle = -\frac{1}{\sqrt{3}}(i|xz,\uparrow_s\rangle - |yz,\uparrow_s\rangle + |xy,\downarrow_s\rangle)$$

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

5d orbitals of Ir^{4+}: large spin-orbit coupling

Ir^{4+} = [Xe] $4f^{14}$ $5d^5$

$$\mathcal{P}_{t2g}\mathbf{L}_{\ell=2}\mathcal{P}_{t2g} = -\mathbf{L}^{\text{eff}}_{\ell=1}$$



B.J.Kim, T.W.Noh, G.Cao et al. PRL (2008)

B.J.Kim, H.Takagi, et al, Science (2009)

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

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

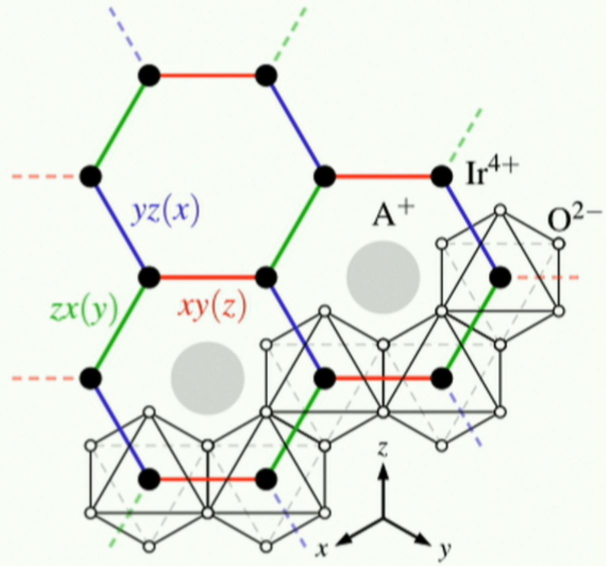
Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

α-A_2IrO_3 Heisenberg-Kitaev Model ?

$$\mathcal{H}_{ij}^{(\gamma)} = -J_1\ S_i^\gamma S_j^\gamma + J_2\ \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$
$$\gamma = x, y, z$$

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

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



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

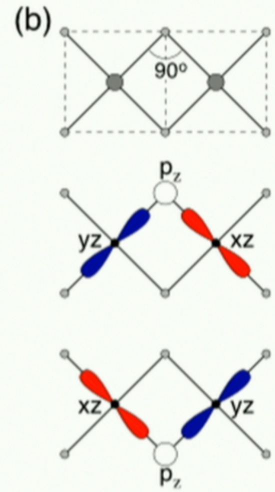
Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

α-A_2IrO_3 Heisenberg-Kitaev Model ?

$$\mathcal{H}_{ij}^{(\gamma)} = -J_1\ S_i^\gamma S_j^\gamma + J_2\ \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$
$$\gamma = x, y, z$$

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

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



Edge-Sharing Oxygen Octahedra

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

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

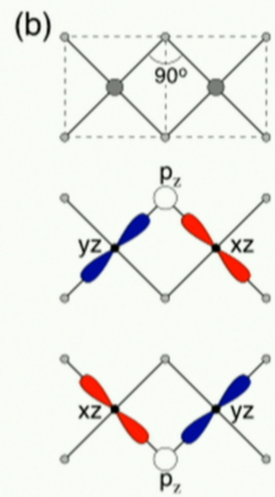
Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

α-A_2IrO_3 Heisenberg-Kitaev Model ?

$$\mathcal{H}_{ij}^{(\gamma)} = -J_1\, S_i^\gamma S_j^\gamma + J_2\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$
$$\gamma = x, y, z$$

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

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



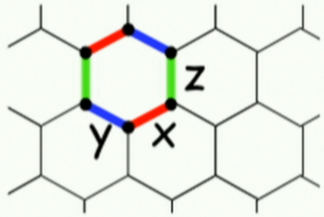
Edge-Sharing Oxygen Octahedra

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

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

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

Kitaev Model on Honeycomb Lattice: Exact Solution



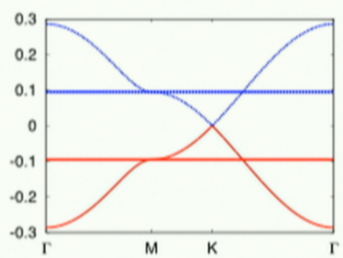
$$\mathcal{H}_{\rm K} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha$$ A. Kitaev (2006)

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

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

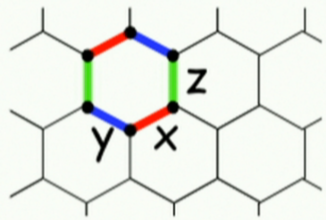
$\mathcal{W}_P = \prod_{\rm loop} u_{ij}^\alpha$ commute with the Hamiltonian $\Longrightarrow \mathcal{W}_P = \pm 1$

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



Majorana Fermions with Dirac Dispersion

Kitaev Model on Honeycomb Lattice: Exact Solution



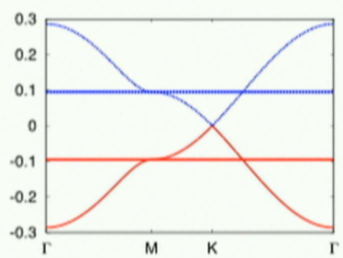
$$\mathcal{H}_{\rm K} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha$$ A. Kitaev (2006)

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

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

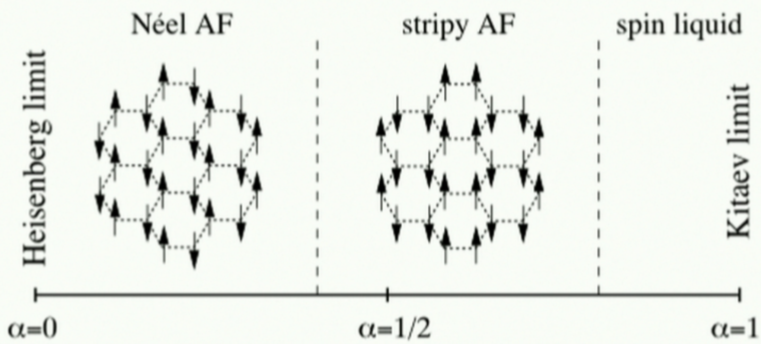
$\mathcal{W}_P = \prod_{\text{loop}} u_{ij}^\alpha$ commute with the Hamiltonian $\Longrightarrow \mathcal{W}_P = \pm 1$

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



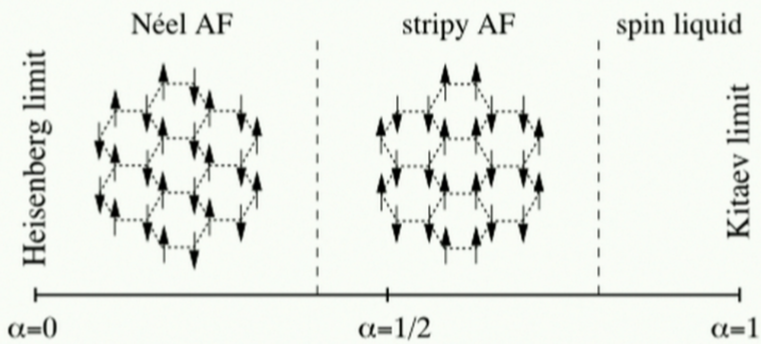
Majorana Fermions with
Dirac Dispersion

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



Quantum Spin Liquid robust
to small Heisenberg interaction

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

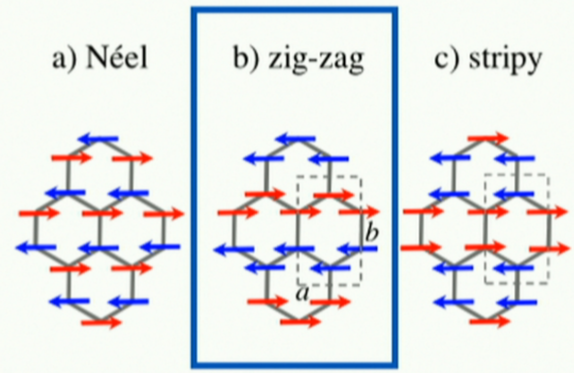


Quantum Spin Liquid robust
to small Heisenberg interaction

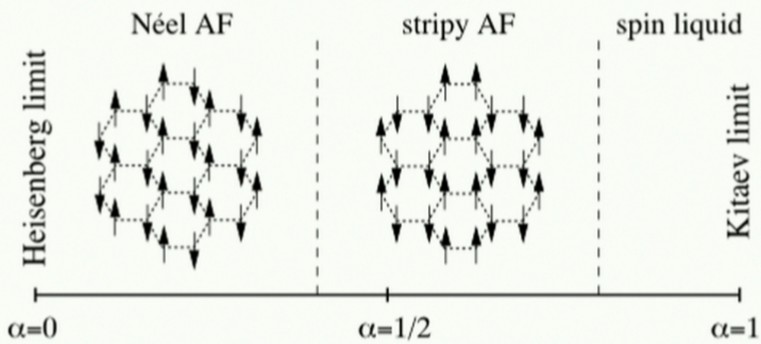
Radu Coldea
(Neutron Scattering)

α-Na_2IrO_3

Zig-Zag Order



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

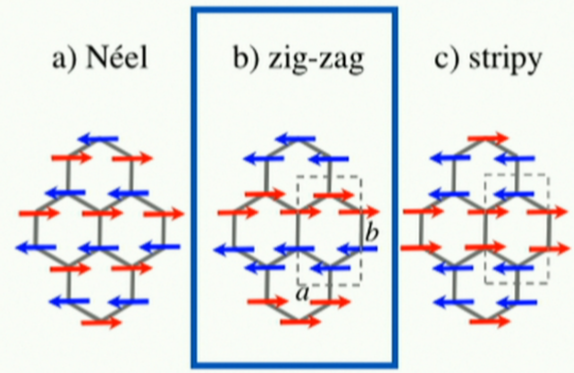


Quantum Spin Liquid robust
to small Heisenberg interaction

Radu Coldea
(Neutron Scattering)

α-Na_2IrO_3

Zig-Zag Order



Monoclinic Distortions
Strong Trigonal Distortions

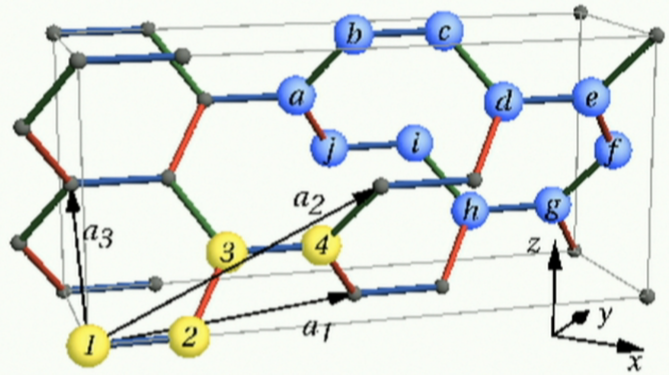
Discovery of Three dimensional "Honeycomb" lattice

β- Li_2IrO_3

arXiv:1403.3296

H. Takagi

Hyper-honeycomb



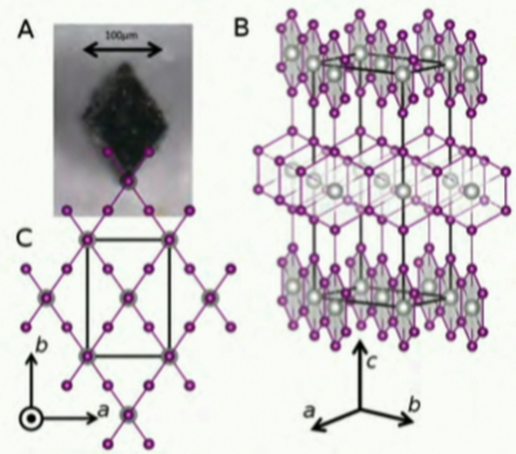
γ- Li_2IrO_3

arXiv:1402.3254

James Analytis

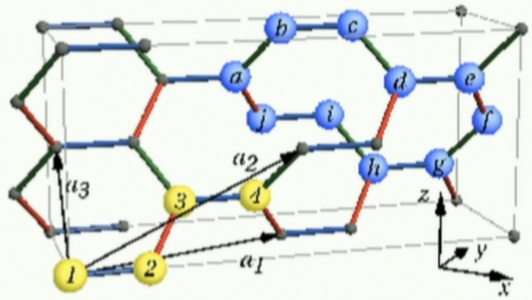
Radu Coldea

Harmonic-honeycomb



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

β- Li_2IrO_3 arXiv:1403.3296



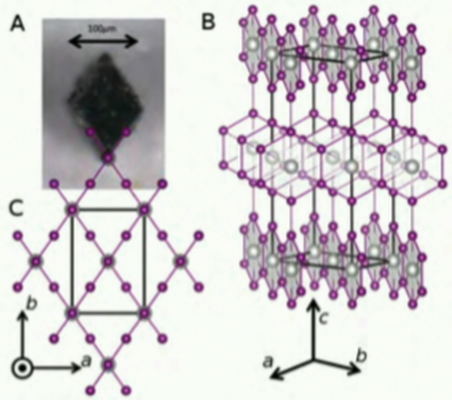
AF ordering (no net magnetization)
in zero magnetic field

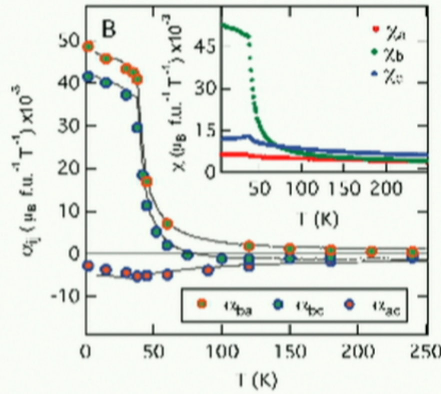
But with positive (ferro-like)
Curie-Weiss temperature

Radu Coldea James G. Analytis (Berkeley)

A different 3D structure of Li_2IrO_3 γ- Li_2IrO_3

space group: Cccm





$T_c = 38K$

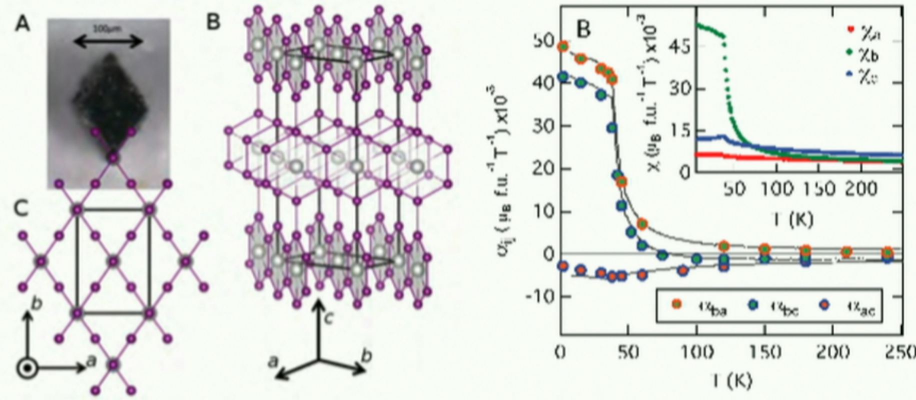
strong magnetic anisotropy

arXiv:1402.3254

Radu Coldea   James G. Analytis (Berkeley)

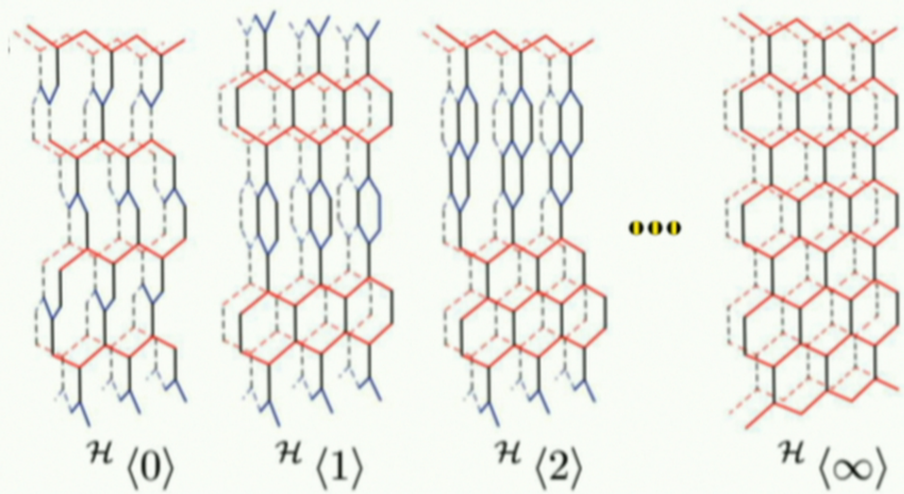
A different 3D structure of Li_2IrO_3 γ- Li_2IrO_3

space group: Cccm



strong magnetic anisotropy

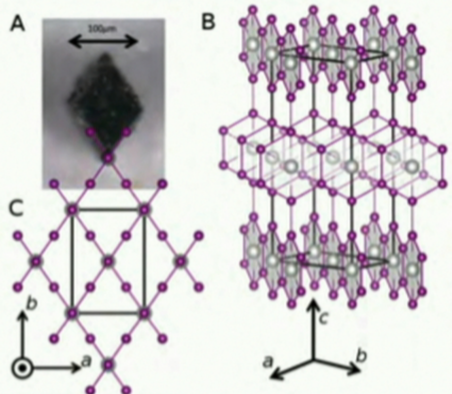
arXiv:1402.3254

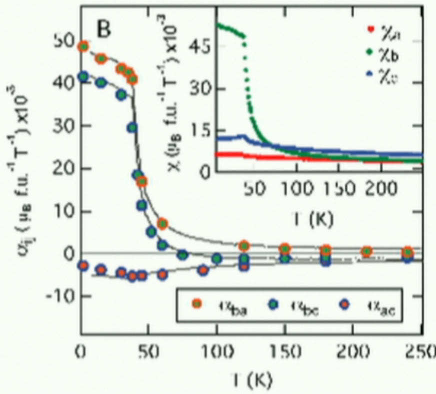


Radu Coldea James G. Analytis (Berkeley)

A different 3D structure of Li_2IrO_3 γ- Li_2IrO_3

space group: Cccm





$T_c = 38K$

strong magnetic anisotropy

arXiv:1402.3254

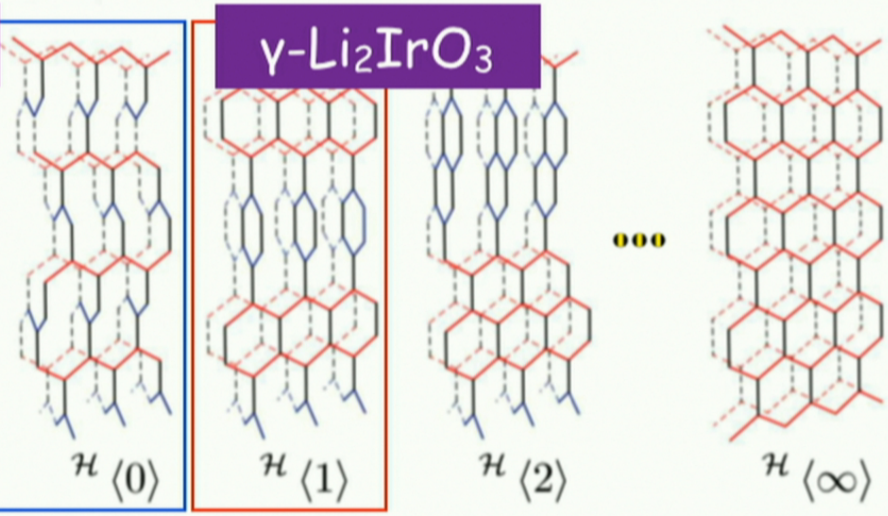
β-Li_2IrO_3

hyper-honeycomb

β- Na_2PtO_3

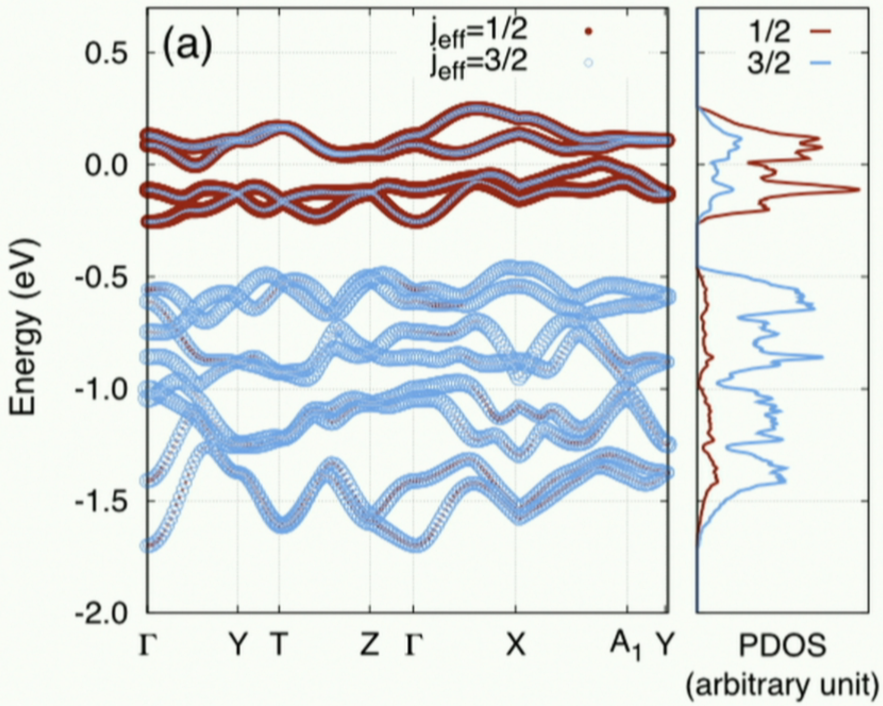
1972

γ-Li_2IrO_3



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

β- Li_2IrO_3



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)

Ab Initio
(OpenMx, PBE-GGA)

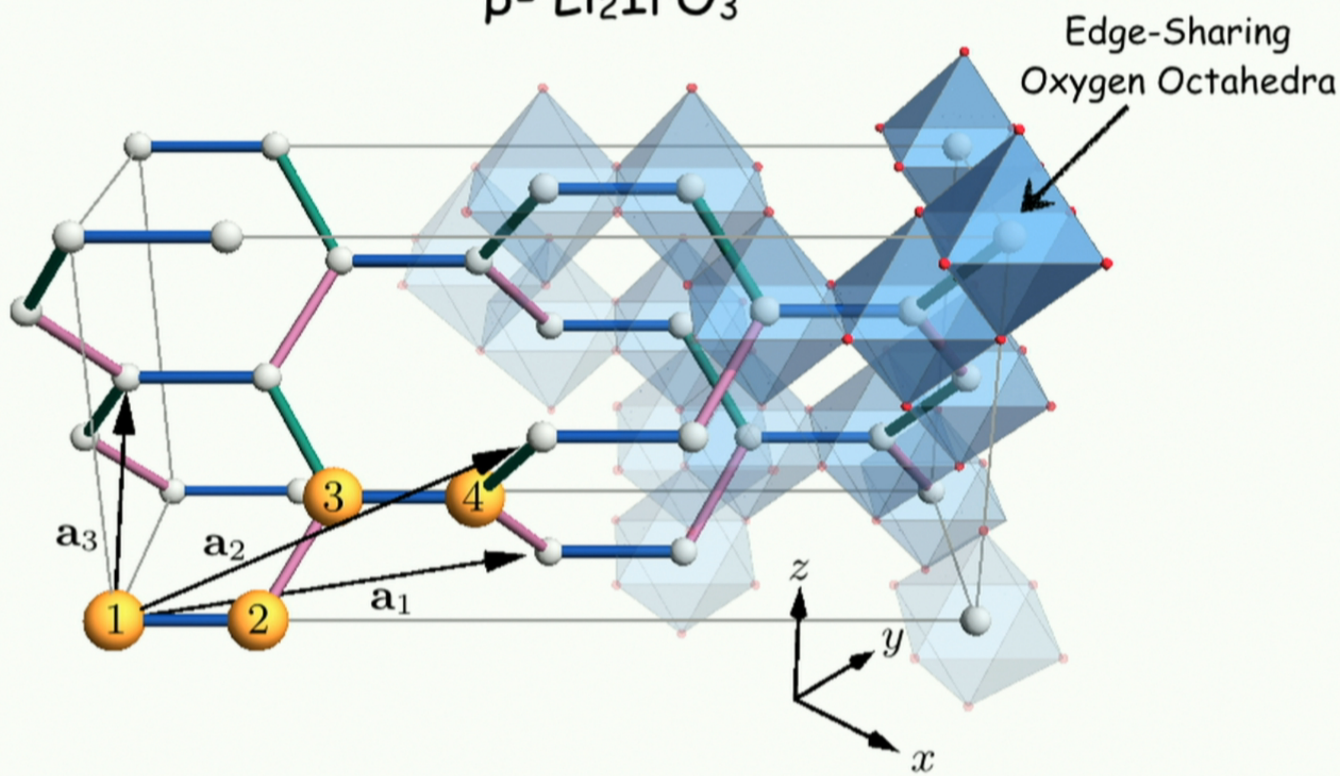
Localized Pseudo-Spin Model on Hyperhoneycomb Lattice: Strong Coupling Limit

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

E. K.-H. Lee, Y. B. Kim, PRB (2015), arXiv:1407.4145

Edge-sharing Oxygen Octahedra Structure

β- Li_2IrO_3



Strong Coupling Limit: Localized Pseudo-Spin Model

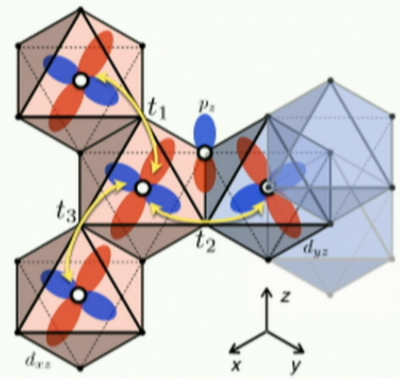
$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \boxed{\Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)} \right]$$

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

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

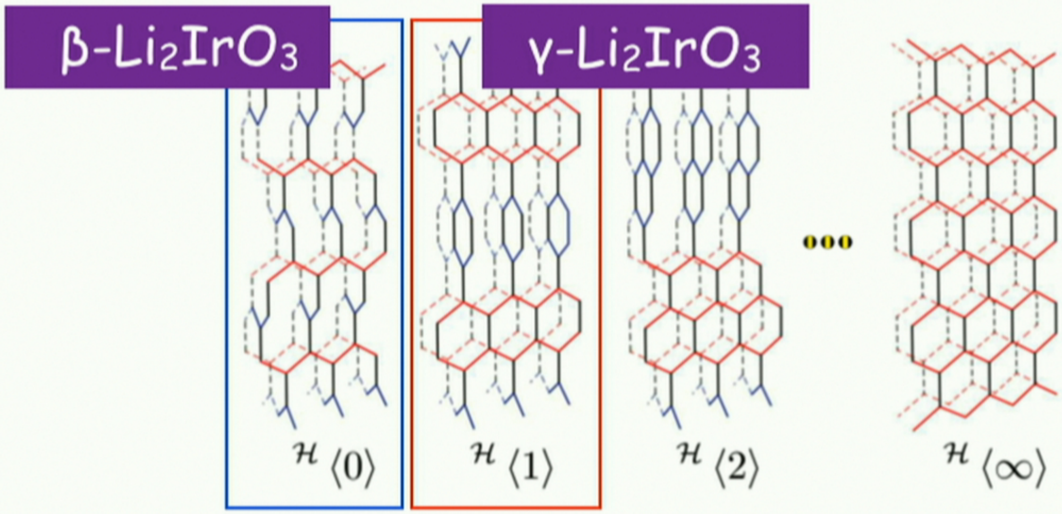
$$K = \frac{8J_H}{9}\left[\frac{(t_1-t_3)^2-3t_2^2}{(U-3J_H)(U-J_H)}\right],$$

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



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

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



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

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

BDI Class

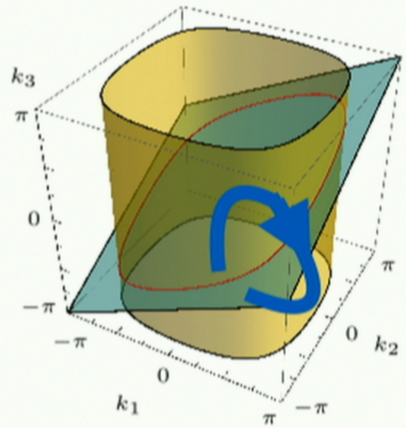
$$D_{0,k}^{0} = \begin{bmatrix} J_z & A_k e^{ik_3} \\ B_k & J_z \end{bmatrix}$$ β-lattice

$$D_{1,k}^{0} = \begin{bmatrix} J_z & 0 & 0 & A_k e^{ik_3} \\ A_k^* & J_z & 0 & 0 \\ 0 & B_k & J_z & 0 \\ 0 & 0 & B_k^* & J_z \end{bmatrix}$$

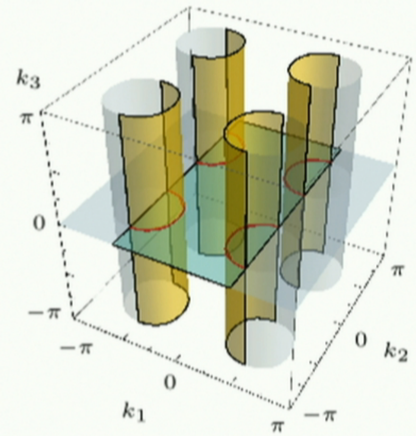
γ-lattice

β-lattice

γ-lattice



(a) $\mathcal{H}$–0: 0-flux, $\delta = 1$



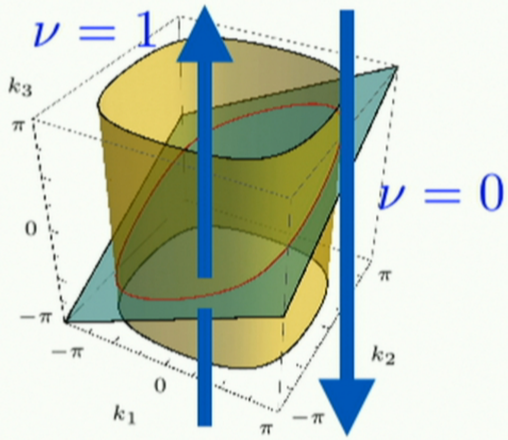
(c) $\mathcal{H}$–1: π-flux, $\delta = \{1, 7^{1/4}\}$

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

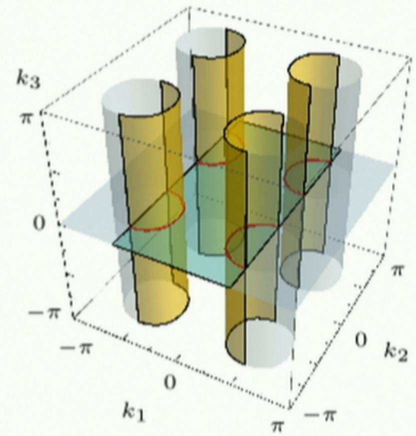
R. Schaffer, E. Lee, Y.-M. Lu, Y. B. Kim, PRL 2015

β-lattice



(a) $\mathcal{H}$–0: 0-flux, $\delta = 1$

γ-lattice



(c) $\mathcal{H}$–1: π-flux, $\delta = \{1, 7^{1/4}\}$

Topological Spinon "Semi-metal"

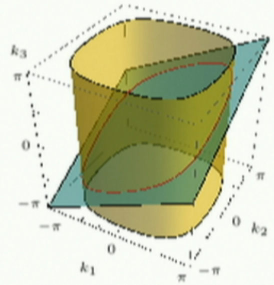
$$\nu = \frac{1}{4\pi i} \oint \mathrm{d}k \mathrm{Tr}[D_{\mathbf{k}}^{-1} \partial_k D_{\mathbf{k}} - (D^\dagger)_{\mathbf{k}}^{-1} \partial_k D_{\mathbf{k}}^\dagger]$$ Topological Invariant

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

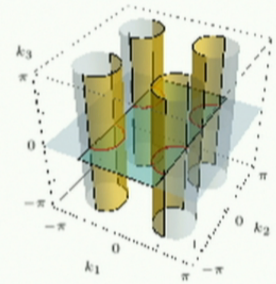
β-lattice

γ-lattice

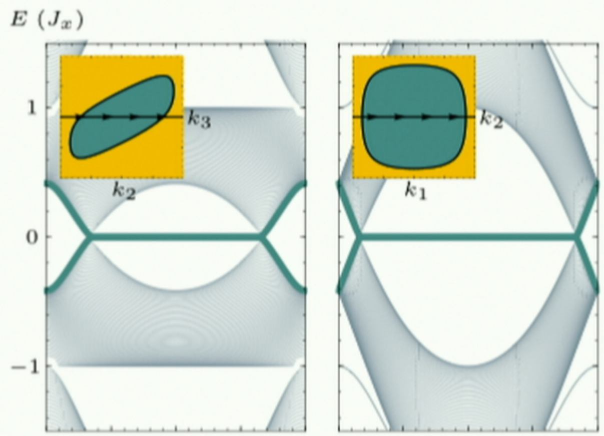
Surface Majorana States



(a) $\mathcal{H}$–0: 0-flux, $\delta = 1$

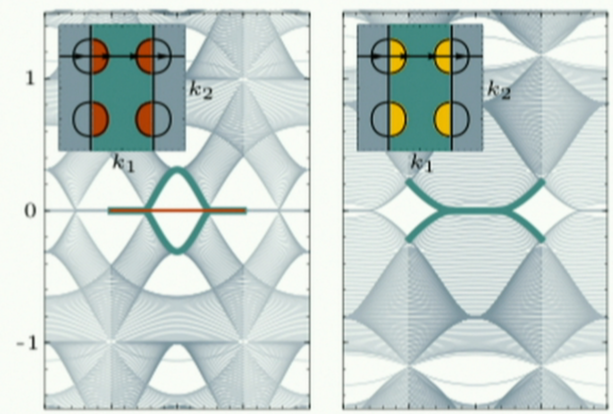


(c) $\mathcal{H}$–1: π-flux, $\delta = \{1, 7^{1/4}\}$



(d) (100) surface

(e) (001) surface



(g) (001) surface; $\delta = 1$

(h) (001) surface, $\delta = 7^{1/4}$

Magnetic Frustration and Spiral Magnetic Order

E. K.-H. Lee, Y. B. Kim, PRB (2015), arXiv:1407.4125 (2014)

Strong Coupling Limit: Localized Pseudo-Spin Model

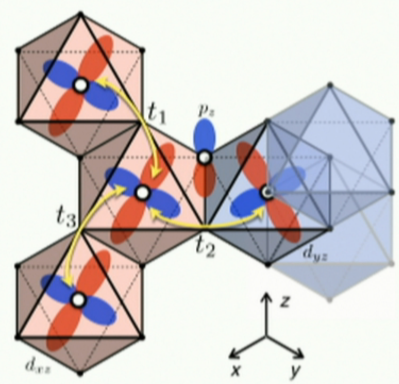
$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \boxed{\Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)} \right]$$

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

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

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

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

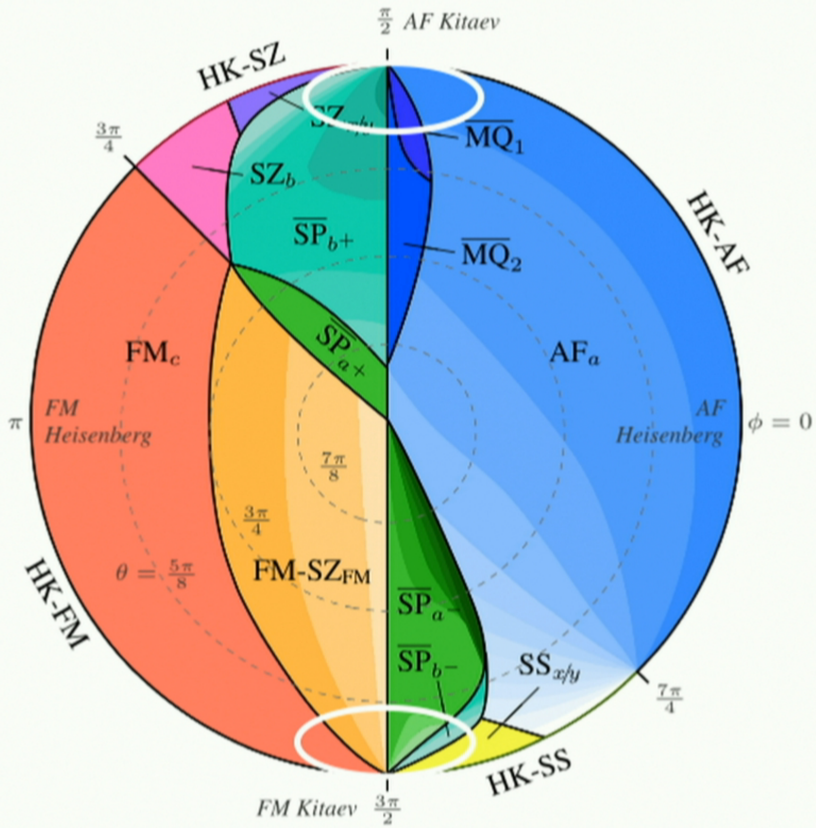


$$t_1 = \frac{t_{dd\pi} + t_{dd\delta}}{2}, \quad t_2 = \frac{t_{pd\pi}^2}{\Delta_{pd}} + \frac{t_{dd\pi} - t_{dd\delta}}{2}, \quad t_3 = \frac{3t_{dd\sigma} + t_{dd\delta}}{4},$$

β-Li_2IrO_3

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

Two possible sign choices



$$J = \cos\phi \sin\theta$$

$$K = \sin\phi \sin\theta$$

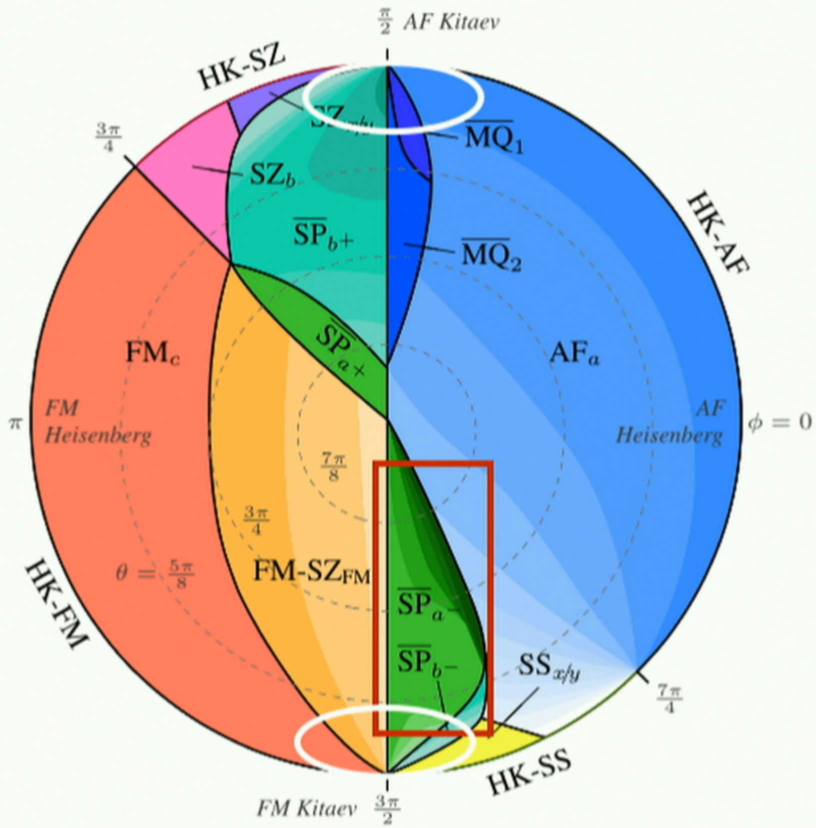
$$\Gamma = \cos\theta$$

E. K.-H. Lee, Y. B. Kim, arXiv:1407.4125 (2014)

β-Li_2IrO_3

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

Two possible sign choices



$$J = \cos\phi \sin\theta$$

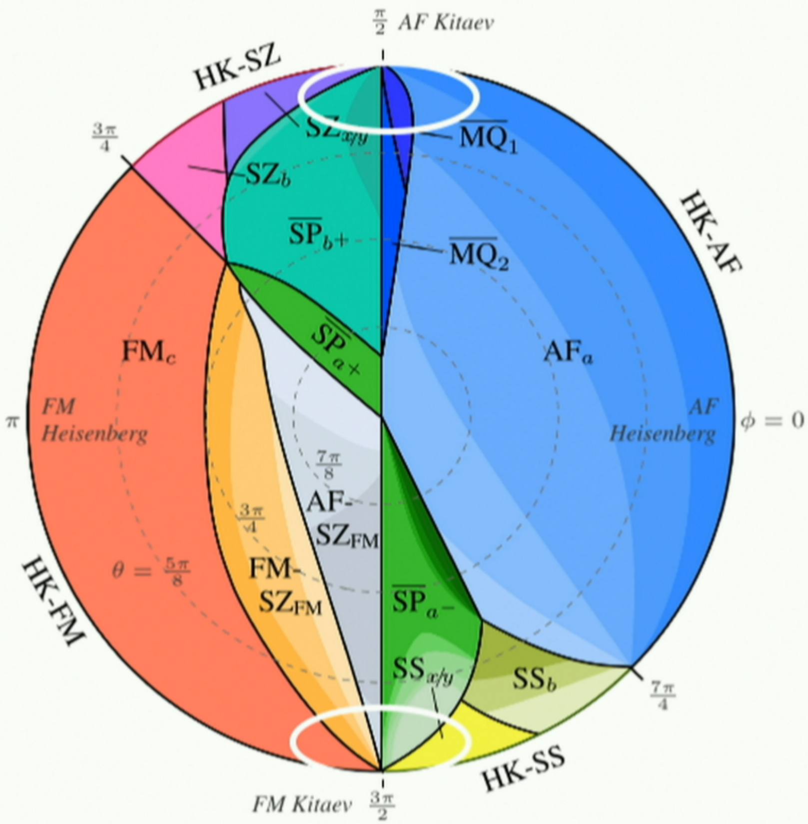
$$K = \sin\phi \sin\theta$$

$$\Gamma = \cos\theta$$

E. K.-H. Lee, Y. B. Kim, arXiv:1407.4125 (2014)

γ-Li_2IrO_3

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



Two possible sign choices

$$J = \cos\phi \sin\theta$$

$$K = \sin\phi\sin\theta$$

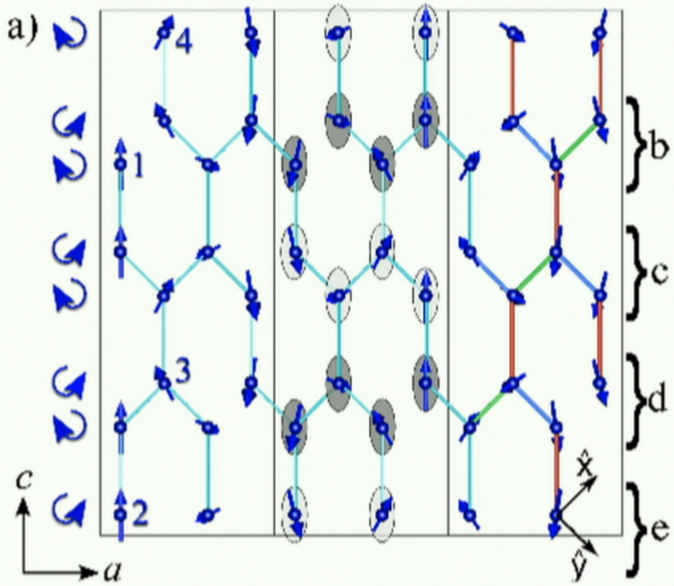
$$\Gamma = \cos\theta$$

E. K.-H. Lee, Y. B. Kim, arXiv:1407.4125 (2014)

β-Li_2IrO_3

Counter-propagating Incommensurate Non-Coplanar Spiral Orders

$$(iA_a, iC_b, F_c)$$



$$F = \begin{bmatrix} 1 \\ 1 \\ \delta \\ \delta \end{bmatrix}, C = \begin{bmatrix} 1 \\ 1 \\ -\delta \\ -\delta \end{bmatrix}, A = \begin{bmatrix} 1 \\ -1 \\ -\delta \\ \delta \end{bmatrix}, G = \begin{bmatrix} 1 \\ -1 \\ \delta \\ -\delta \end{bmatrix}$$

Irreducible Representation	Basis Vectors
Γ_1	F_x, G_y, A_z
Γ_2	C_x, A_y, G_z
Γ_3	G_x, F_y, C_z
Γ_4	A_x, C_y, F_z

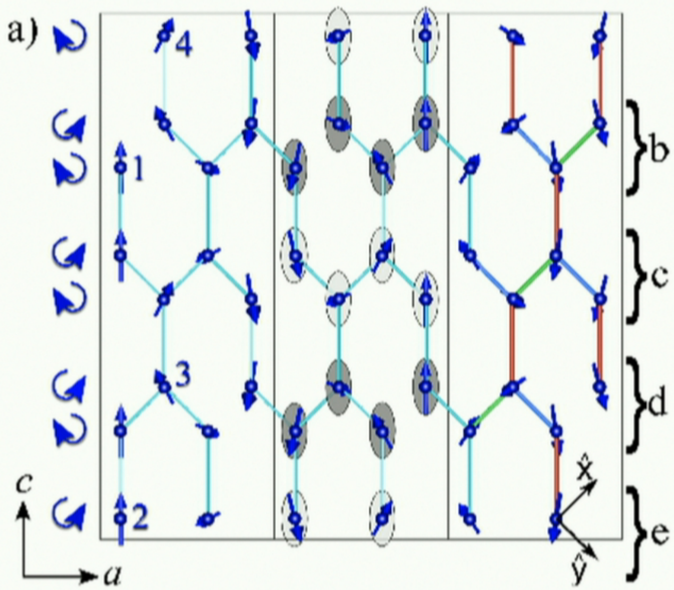
$$\mathbf{Q}_{\text{exp}} = (0.57, 0, 0)$$

Radu Coldea, P. Gegenwart (2014)

β-Li_2IrO_3

Counter-propagating Incommensurate Non-Coplanar Spiral Orders

$$(iA_a, iC_b, F_c)$$



$$F = \begin{bmatrix} 1 \\ 1 \\ \delta \\ \delta \end{bmatrix}, C = \begin{bmatrix} 1 \\ 1 \\ -\delta \\ -\delta \end{bmatrix}, A = \begin{bmatrix} 1 \\ -1 \\ -\delta \\ \delta \end{bmatrix}, G = \begin{bmatrix} 1 \\ -1 \\ \delta \\ -\delta \end{bmatrix}$$

Irreducible Representation	Basis Vectors
Γ_1	F_x, G_y, A_z
Γ_2	C_x, A_y, G_z
Γ_3	G_x, F_y, C_z
Γ_4	A_x, C_y, F_z

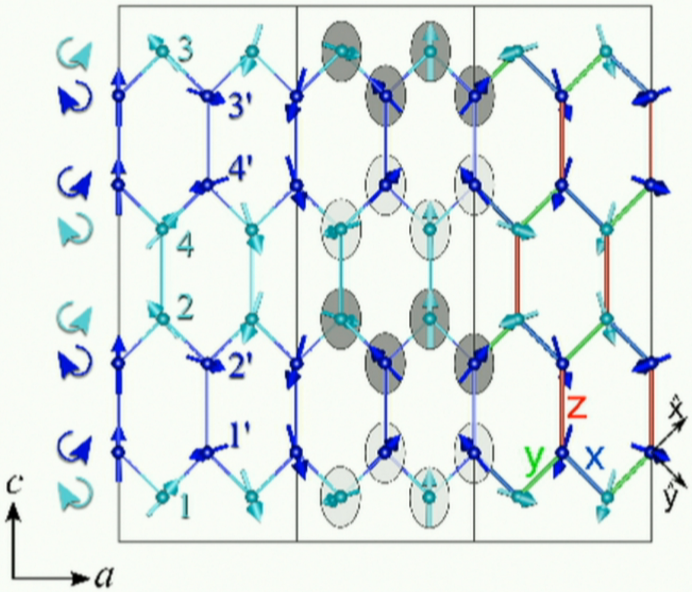
$$\mathbf{Q}_{\mathrm{exp}} = (0.57, 0, 0)$$

Radu Coldea, P. Gegenwart (2014)

γ-Li_2IrO_3

Counter-propagating Incommensurate Non-Coplanar Spiral Orders

$$[i(A,-A)_a, (-1)^m i(F,-F)_b, (F,F)_c] \quad m=1$$



$$F = \begin{bmatrix} 1 \\ 1 \\ \delta \\ \delta \end{bmatrix}, C = \begin{bmatrix} 1 \\ 1 \\ -\delta \\ -\delta \end{bmatrix}, A = \begin{bmatrix} 1 \\ -1 \\ -\delta \\ \delta \end{bmatrix}, G = \begin{bmatrix} 1 \\ -1 \\ \delta \\ -\delta \end{bmatrix}$$

Irreducible Representation	Basis Vectors
Γ_1	F_x, G_y, A_z
Γ_2	C_x, A_y, G_z
Γ_3	G_x, F_y, C_z
Γ_4	A_x, C_y, F_z

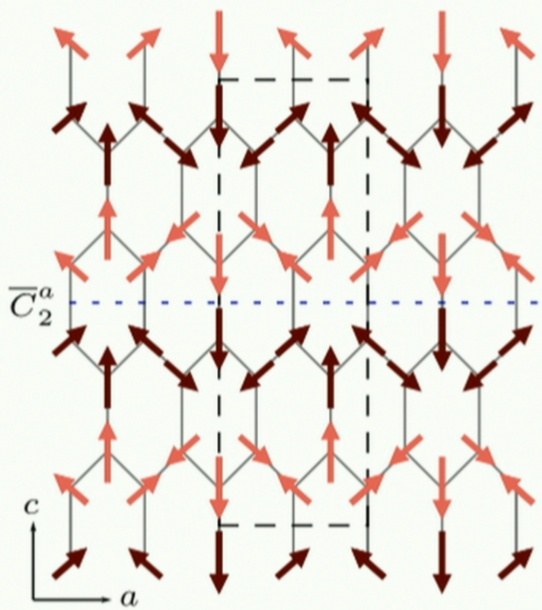
$$\mathbf{Q}_{\text{exp}} = (0.57, 0, 0)$$

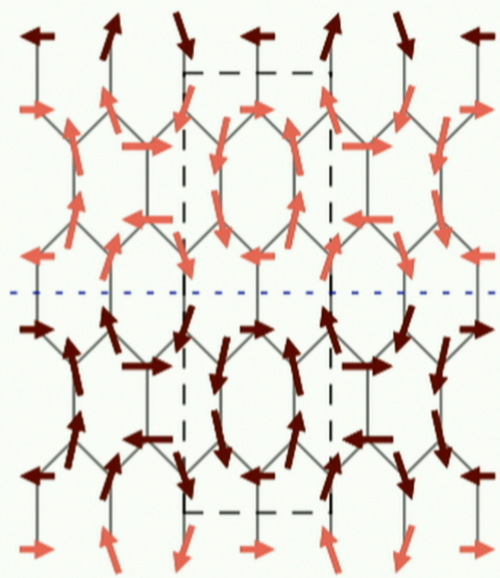
Radu Coldea, James Analytis (2014)

Theory ?

$$(iA_a, iC_b, F_c)$$

$$[i(A,-A)_a, \boxed{-i(C,-C)_b}, (F,F)_c] \neq$$
$$[i(A,-A)_a, \boxed{(-1)^m i(F,-F)_b}, (F,F)_c]$$





β-Li_2IrO_3 $\overline{\mathrm{SP}}_{a-}$

γ-Li_2IrO_3 $\overline{\mathrm{SP}}_{a-}$

$$\boxed{\mathbf{Q} = (h'00) \quad 0.53 \lesssim h' \lesssim 0.80}$$

$$\mathbf{Q}_{\mathrm{exp}} = (0.57, 0, 0)$$

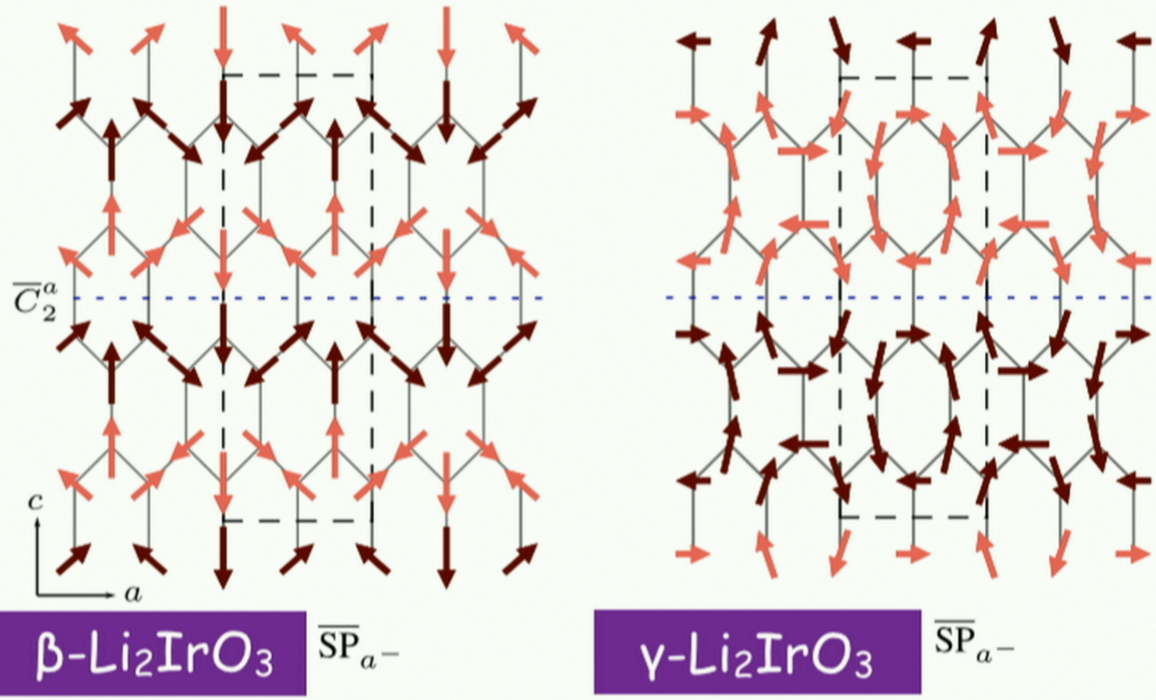
Radu Coldea (2014)

Theory ?

(iA_a, iC_b, F_c)

$[i(A,-A)_a, \boxed{-i(C,-C)_b}, (F,F)_c] \neq$

$[i(A,-A)_a, \boxed{(-1)^m i(F,-F)_b}, (F,F)_c]$



$$\boxed{\mathbf{Q} = (h'00) \quad 0.53 \lesssim h' \lesssim 0.80}$$

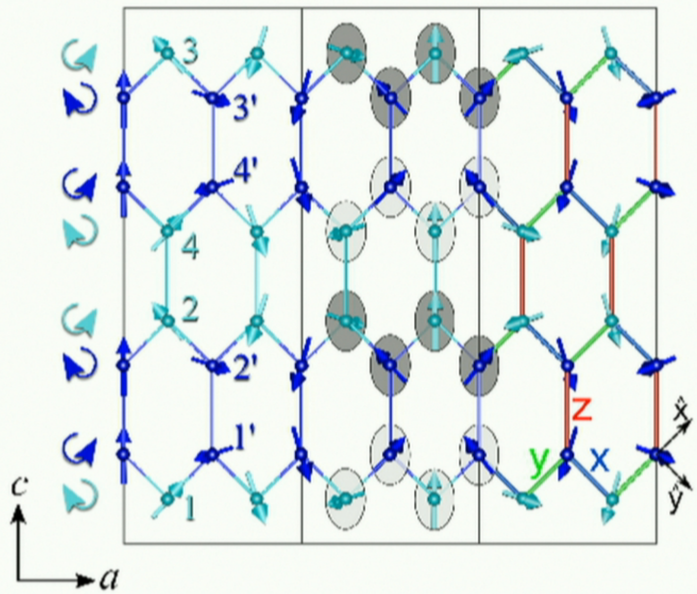
$\mathbf{Q}_{\mathrm{exp}} = (0.57, 0, 0)$

Radu Coldea (2014)

γ-Li_2IrO_3

Counter-propagating Incommensurate Non-Coplanar Spiral Orders

$$[i(A,-A)_a, (-1)^m i(F,-F)_b, (F,F)_c] \quad m=1$$



$$F=\begin{bmatrix}1\\1\\\delta\\\delta\end{bmatrix}, C=\begin{bmatrix}1\\1\\-\delta\\-\delta\end{bmatrix}, A=\begin{bmatrix}1\\-1\\-\delta\\\delta\end{bmatrix}, G=\begin{bmatrix}1\\-1\\\delta\\-\delta\end{bmatrix}$$

Irreducible Representation	Basis Vectors
Γ_1	F_x, G_y, A_z
Γ_2	C_x, A_y, G_z
Γ_3	G_x, F_y, C_z
Γ_4	A_x, C_y, F_z

$$\mathbf{Q}_{\rm exp} = (0.57, 0, 0)$$

Radu Coldea, James Analytis (2014)

Microscopics ?
From ab-initio to Spin Model

β- Li_2IrO_3

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

Other Models (Berkeley Model)

$$H = \sum_{\langle ij \rangle} \left[K \; S_i^{\gamma_{ij}} S_j^{\gamma_{ij}} + J \; \vec{S}_i \cdot \vec{S}_j + I_c \; S_i^{r_{ij}} S_j^{r_{ij}} \right]$$

Γ non-zero only along z-direction

Instability Analysis ?

> Soft-spin model (Luttinger-Tisza with no constraint):
> Mix the lowest eigenmode (co-planar spiral) + fifth eigenmode = non-coplanar spiral

Can get the experimentally determined magnetic structures for both lattices

I. Kimchi, R. Coldea, A. Vishwanath (2014)

Other Models (Berkeley Model)

$$H = \sum_{\langle ij \rangle} \left[K \; S_i^{\gamma_{ij}} S_j^{\gamma_{ij}} + J \; \vec{S}_i \cdot \vec{S}_j + I_c \; S_i^{r_{ij}} S_j^{r_{ij}} \right]$$

Γ non-zero only along z-direction

Instability Analysis ?

Soft-spin model (Luttinger-Tisza with no constraint):
Mix the lowest eigenmode (co-planar spiral) + fifth eigenmode = non-coplanar spiral

Can get the experimentally determined magnetic structures for both lattices

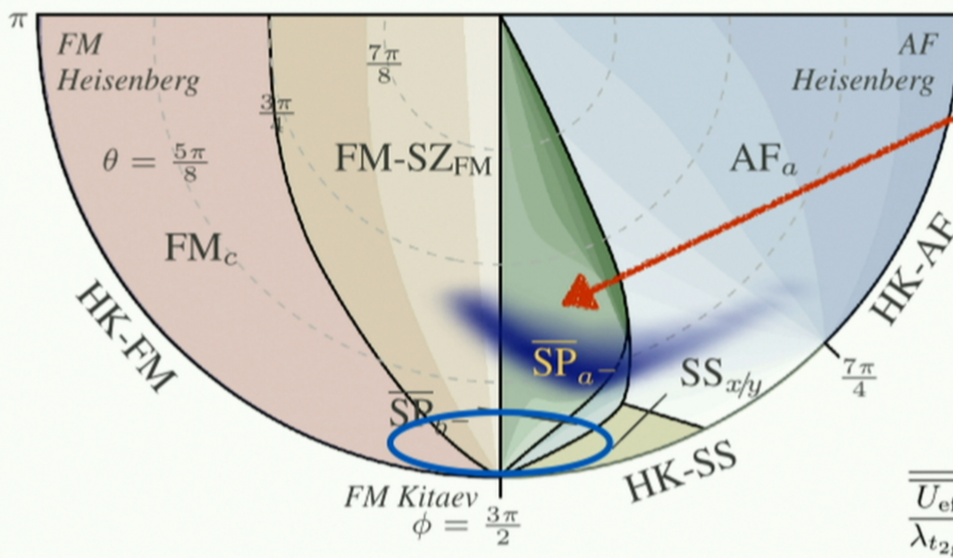
I. Kimchi, R. Coldea, A. Vishwanath (2014)

Comparison Analysis

E.K.-H. Lee, J. G. Rau, Y. B. Kim (2015)

	Classical Model: Simulated Annealing, Monte Carlo	Soft-spin model, Mixing eigenmodes
Toronto Model	Non-coplanar spiral (lowest energy solution) β (same as exp) γ (different from exp)	
Berkeley Model		Can construct Non-coplanar spiral β (same as exp) γ (same as exp)

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



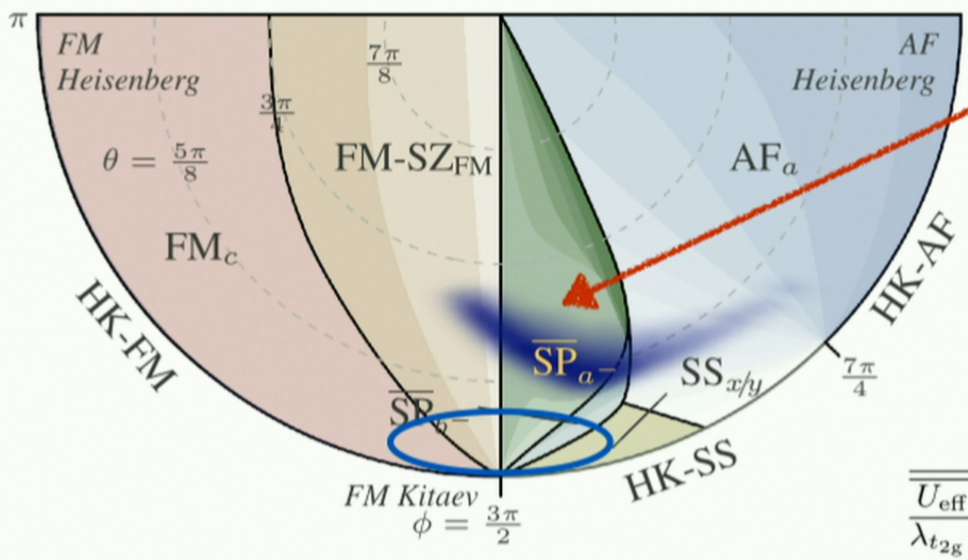
Counter-propagating
Incommensurate
Non-Coplanar
Spiral Order

Interpolation and
statistical analysis for

$U_{\mathrm{eff}} \sim 1\text{–}3\ eV \qquad J_H \sim 50\text{–}300\ meV$

U_{eff} (eV)		0.0	1.5	3.0
$\lambda_{t_{2g}}$		0.401	0.482	0.516
t_1	Z	+0.085	+0.077	+0.064
	X	+0.083	+0.074	+0.058
$\lvert t_2 \rvert$	Z	0.238	0.255	0.270
	X	0.260	0.276	0.289
t_3	Z	-0.162	-0.119	-0.060
	X	-0.153	-0.110	-0.055

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



(iA_a, iC_b, F_c)

Counter-propagating
Incommensurate
Non-Coplanar
Spiral Order

Interpolation and
statistical analysis for

$U_{\mathrm{eff}} \sim 1\text{–}3\ eV \qquad J_H \sim 50\text{–}300\ meV$

U_{eff} (eV)		0.0	1.5	3.0
$\lambda_{t_{2g}}$		0.401	0.482	0.516
t_1	Z	+0.085	+0.077	+0.064
	X	+0.083	+0.074	+0.058
$\lvert t_2 \rvert$	Z	0.238	0.255	0.270
	X	0.260	0.276	0.289
t_3	Z	-0.162	-0.119	-0.060
	X	-0.153	-0.110	-0.055