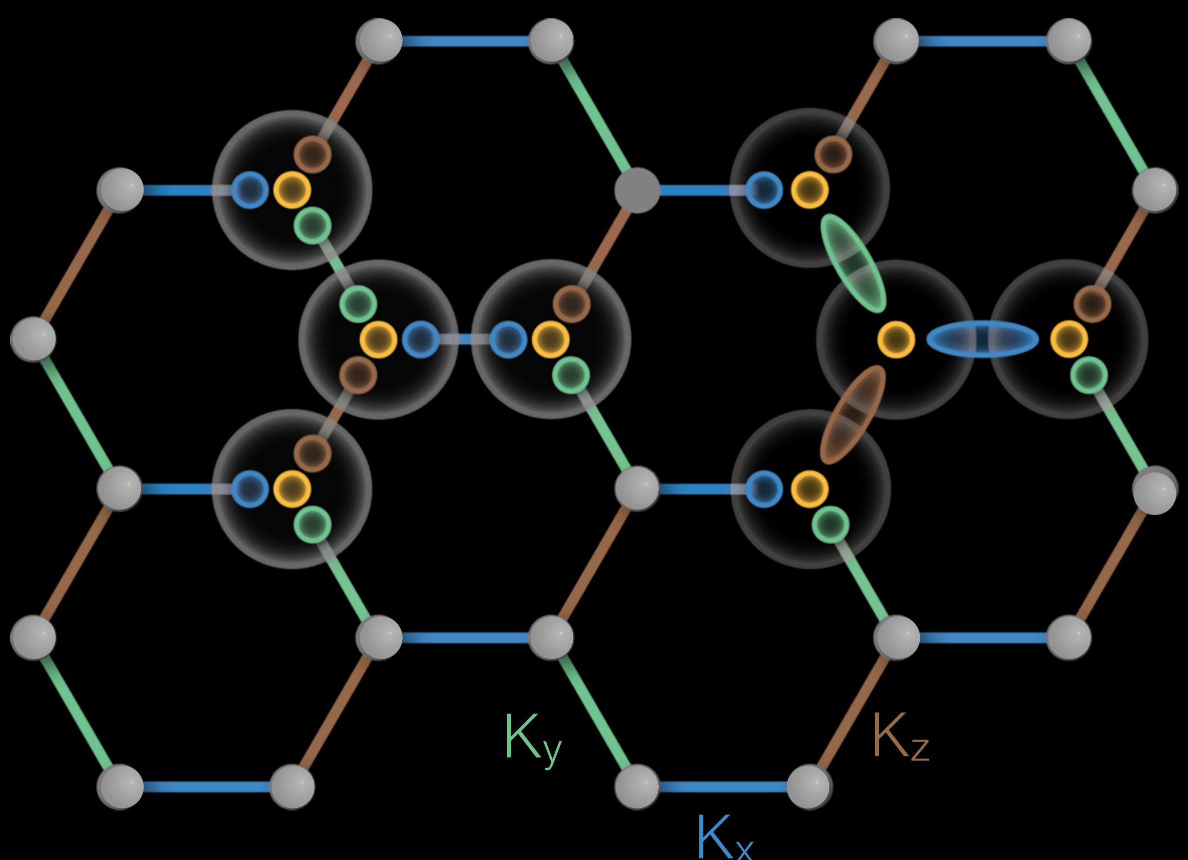
Kitaev materials

48th IFF Spring School “Topological Matter”
Jülich, April 2017



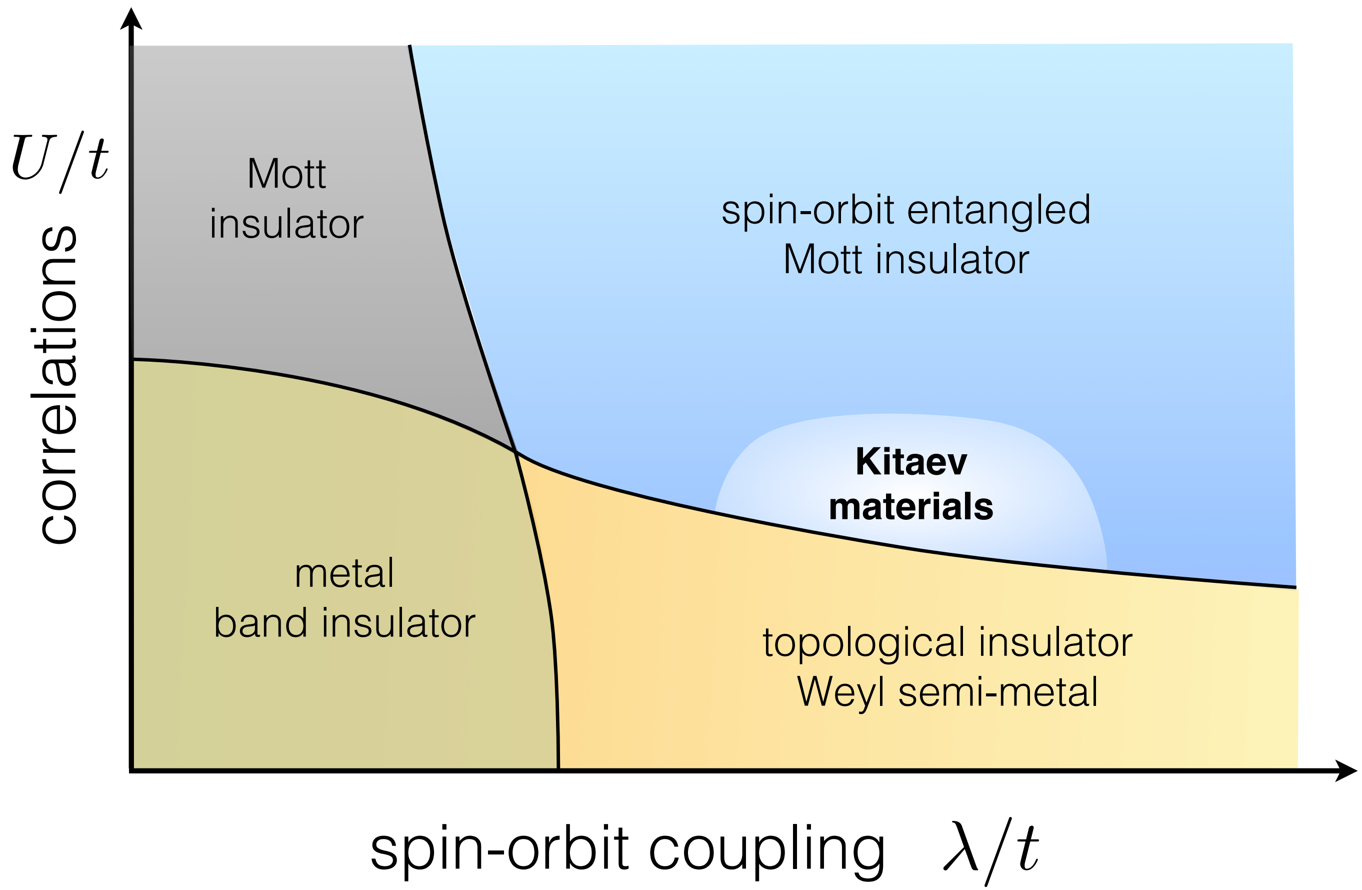
Simon Trebst
University of Cologne

lecture notes online at
arXiv:1701.07056

CRC 1238
Control and Dynamics of Quantum Materials

4d/5d transition metal compounds

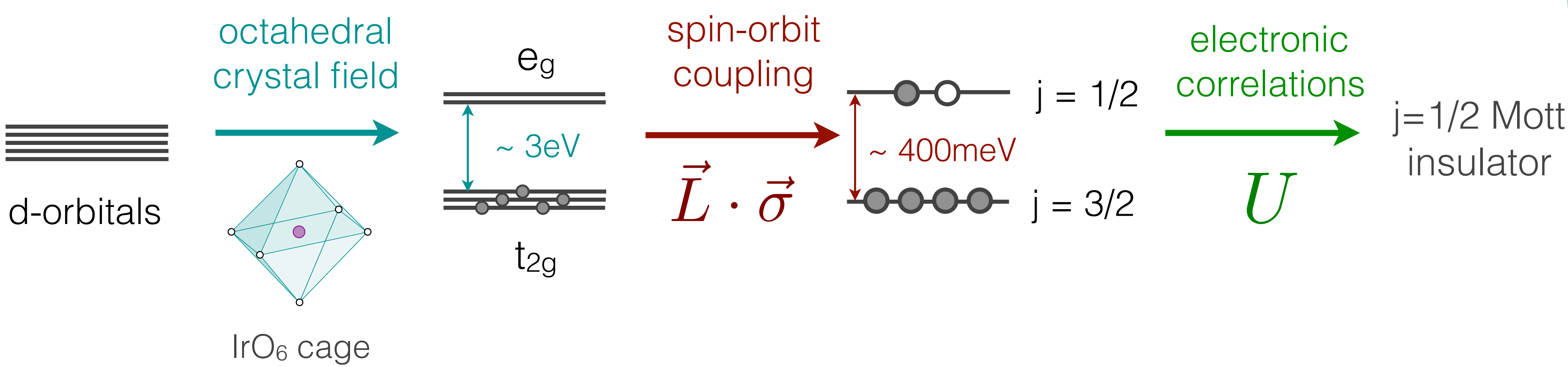
Transition metal oxides with **partially filled 4d/5d shells** exhibit an intricate interplay of **spin-orbit coupling**, **electronic correlations**, and **crystal field effects** resulting in a **broad variety of metallic and insulating states**.



W. Witczak-Krempa, G. Chen, Y. B. Kim, and L. Balents, Annual Review of Condensed Matter Physics 5, 57 (2014).

j=1/2 Mott insulators

most common **Iridium valence** Ir^{4+} $(5d^5)$



Why are these spin-orbit entangled j=1/2 Mott insulators **interesting?**

Sr_2IrO_4 — exhibits cuprate-like magnetism **superconductivity?**

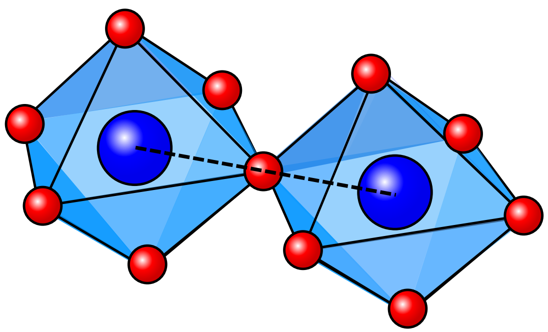
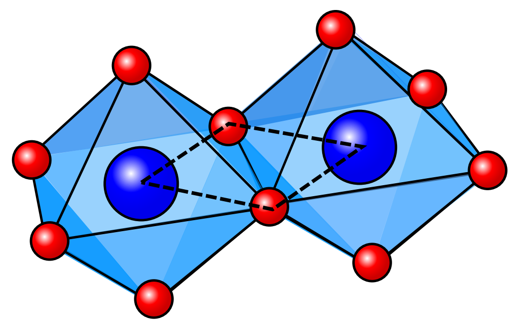
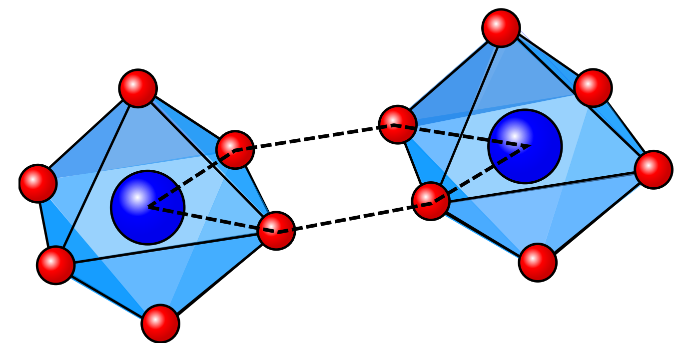
B.J. Kim et al. PRL 101, 076402 (2008)
B.J. Kim et al. Science 323, 1329 (2009)

$(Na,Li)_2IrO_3$ — exhibits Kitaev-like magnetism **spin liquids?**

G. Jackeli, G. Khaliullin, J. Chaloupka
PRL 102, 017205 (2009); PRL 105, 027204 (2010)

bond-directional exchange

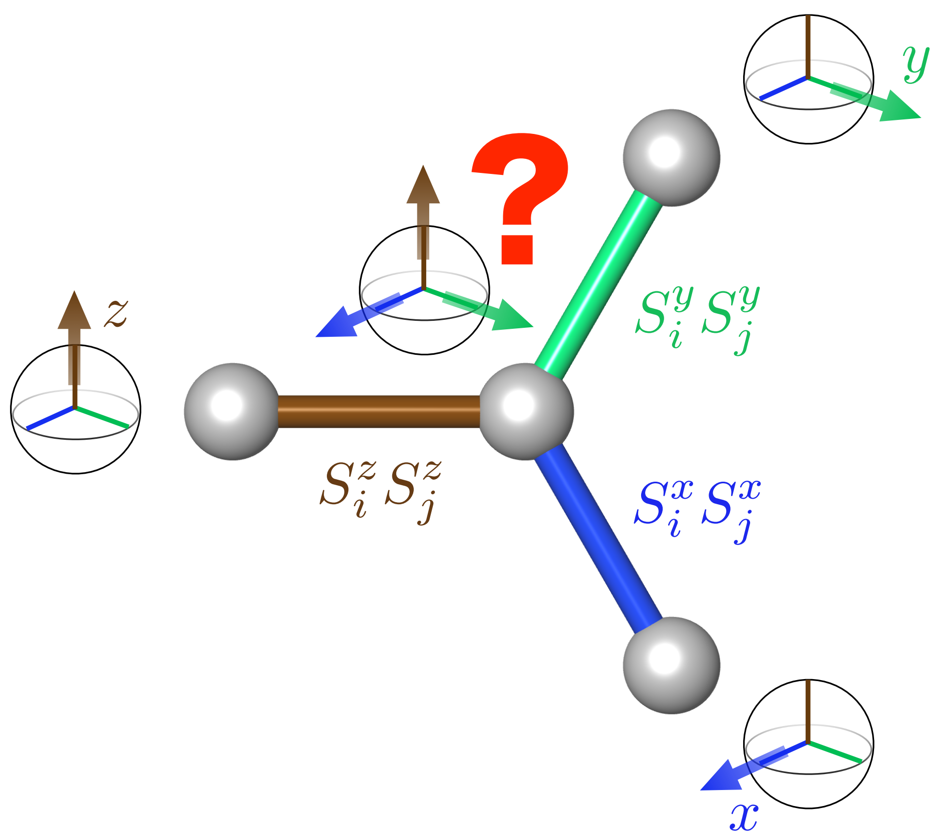
G. Jackeli and G. Khaliullin, PRL 102, 017205 (2009)
J. Chaloupka, G. Jackeli, and G. Khaliullin, PRL 105, 027204 (2010)

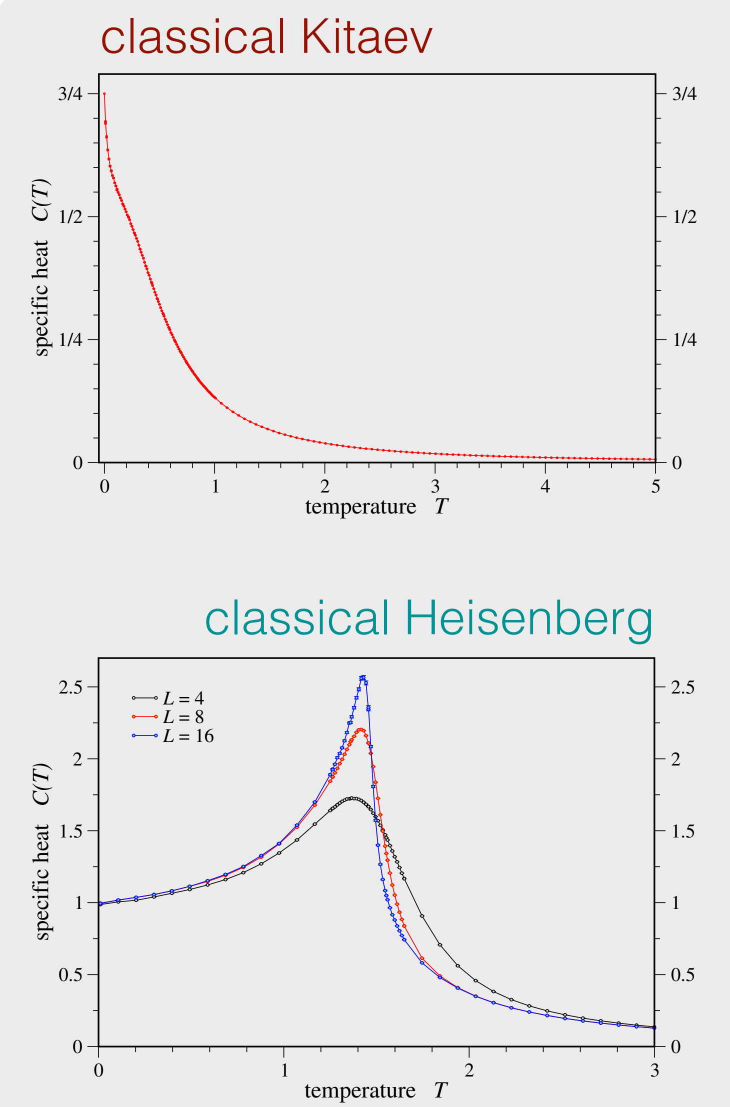
corner-sharing	**edge**-sharing	"**parallel edge**"-sharing
		
Sr_2IrO_4	$(Na,Li)_2IrO_3$ $RuCl_3$	$Ba_3IrTi_2O_9$
Heisenberg exchange	Heisenberg-Kitaev exchange	

$$H = -\sum_{\gamma-\text{bonds}} J\,\mathbf{S}_i\mathbf{S}_j + K\; S_i^\gamma S_j^\gamma + \Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)$$

exchange frustration

$$H = -\sum_{\gamma-\text{bonds}} J\, \mathbf{S}_i \mathbf{S}_j + K\, S_i^\gamma S_j^\gamma$$



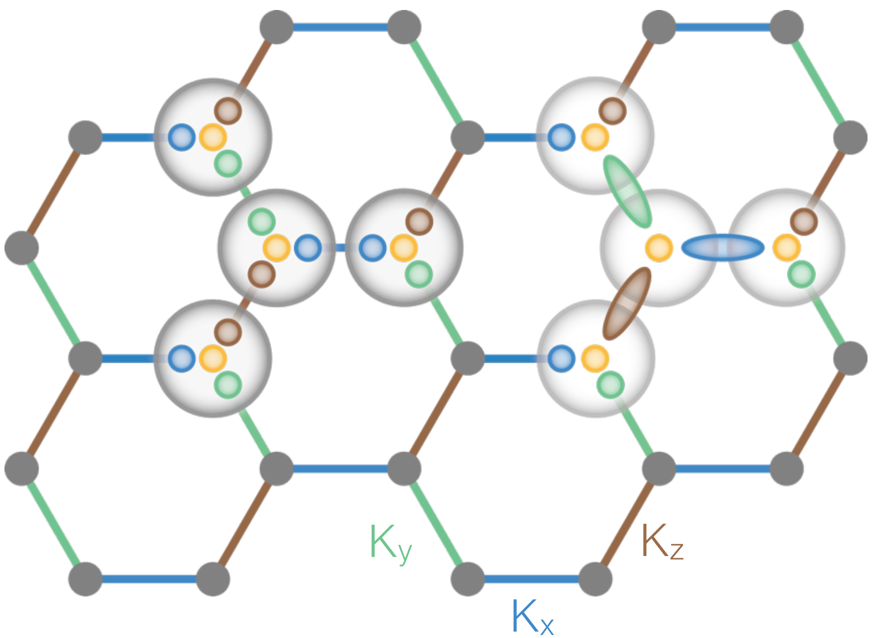


Kitaev model

fractionalization

Kitaev model

$$H = -\sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$



Represent spins in terms of four **Majorana fermions**

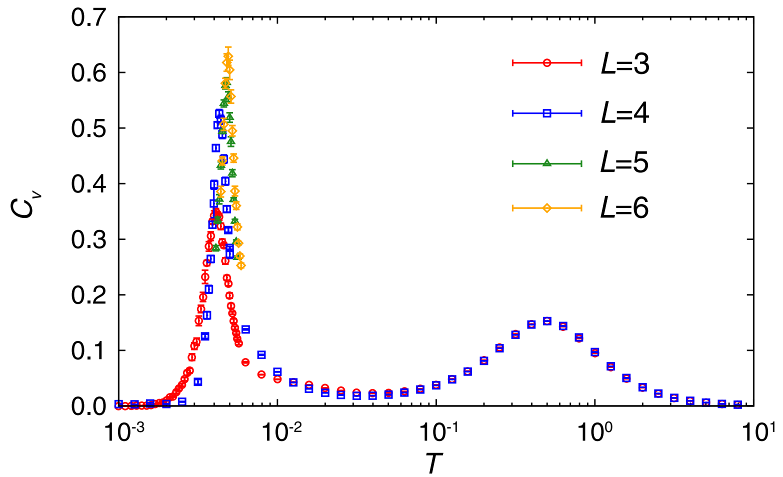
$$\sigma^\alpha = i a^\alpha c$$

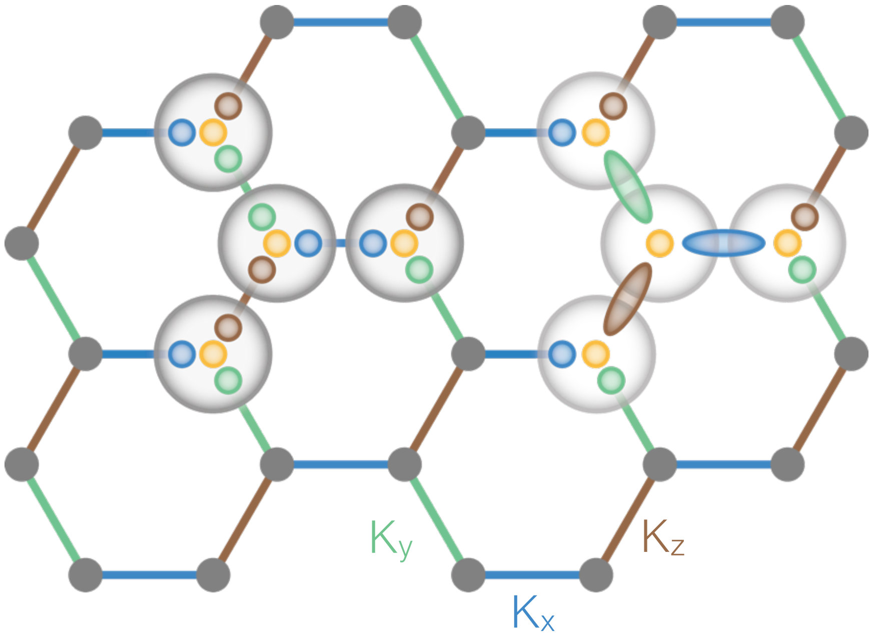
Bond operators

$$\hat{u}_{jk} = i a_j^\alpha a_k^\alpha$$

realize a **Z_2 gauge field**

Kitaev model





The $\mathbf{Z_2}$ **gauge fields** are **static** degrees of freedom.

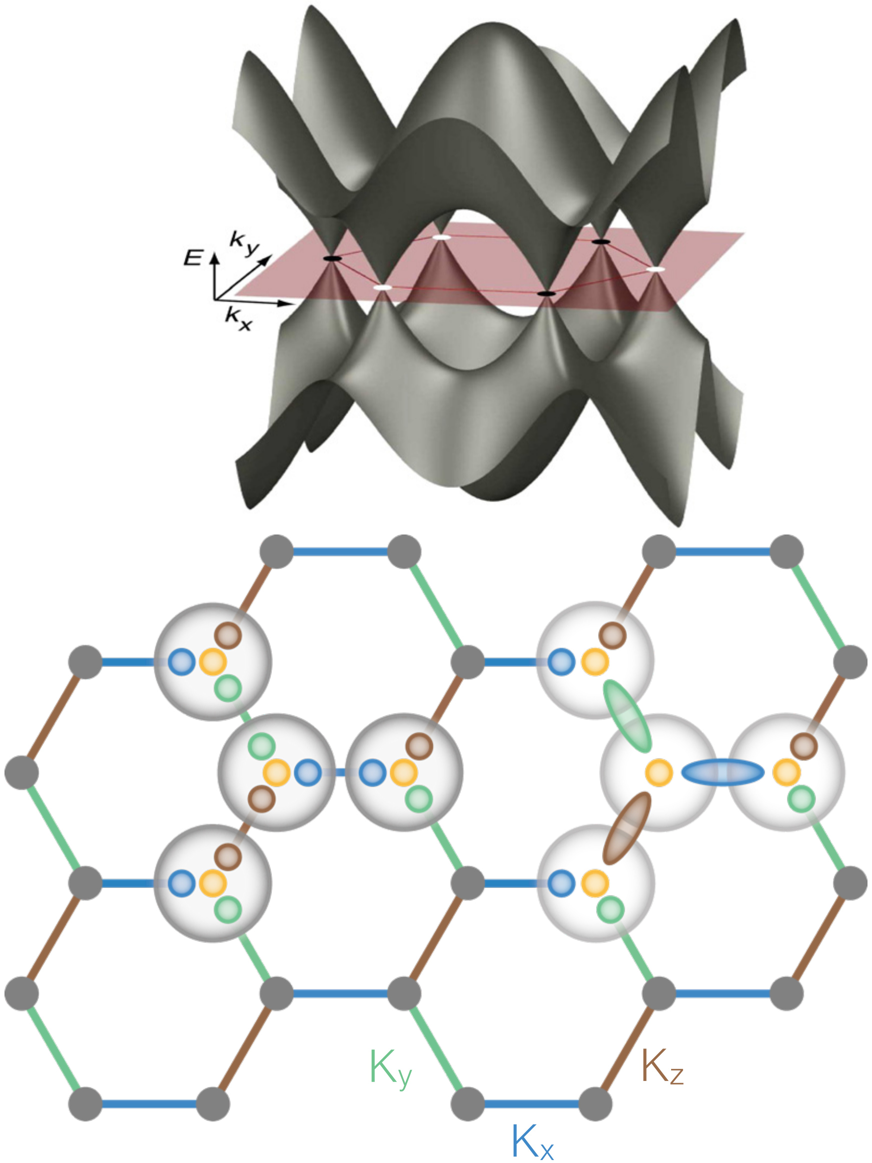
Generically, one has to find its **gapped ground-state** configuration via educated guesses, Monte Carlo sampling, or for some lattices via Lieb's theorem.

Bond operators

$$\hat{u}_{jk} = i a_j^\alpha a_k^\alpha$$

realize a $\mathbf{Z_2}$ **gauge field**

Kitaev model



Represent spins in terms of four **Majorana fermions**

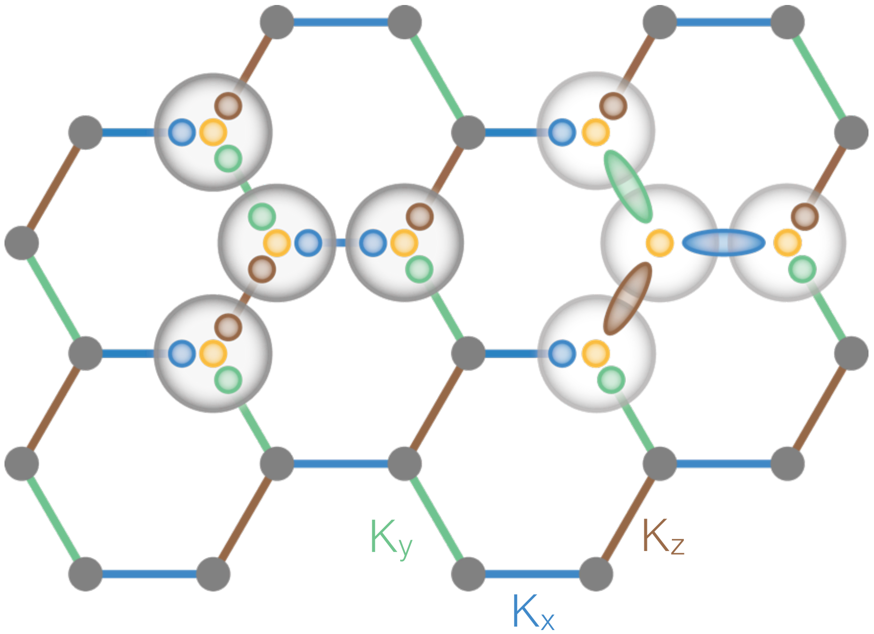
$$\sigma^\alpha = i a^\alpha c$$

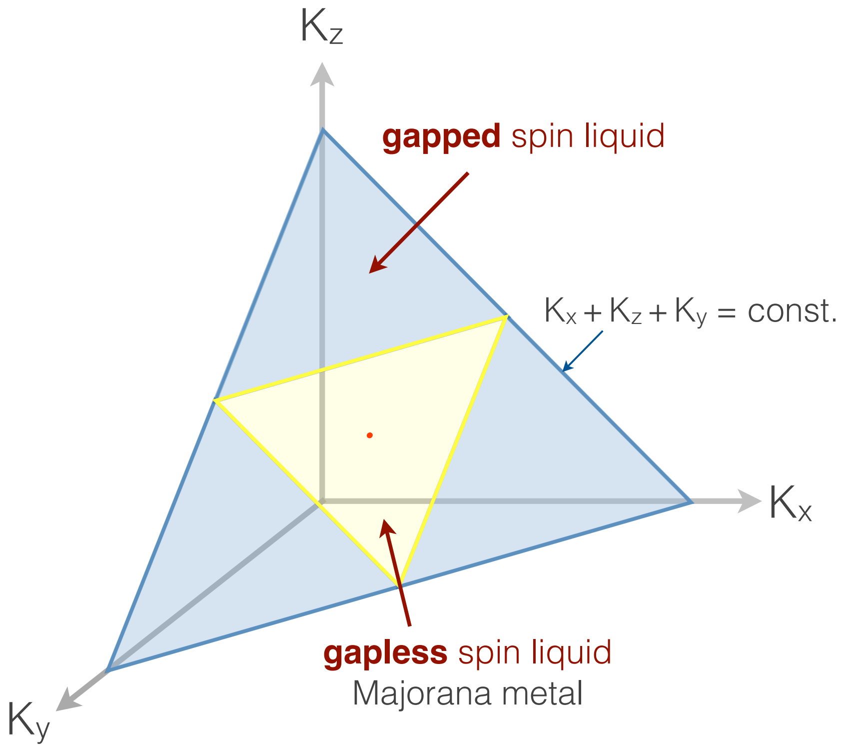
The emergent **Majorana fermions** are **itinerant** degrees of freedom.

Generically, they form a **gapless** collective state – a **Majorana metal**.

Kitaev model

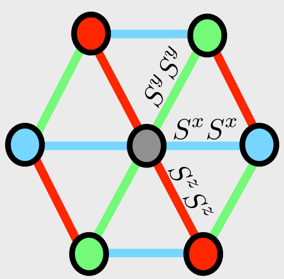
$$H = -\sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$





Heisenberg-Kitaev model

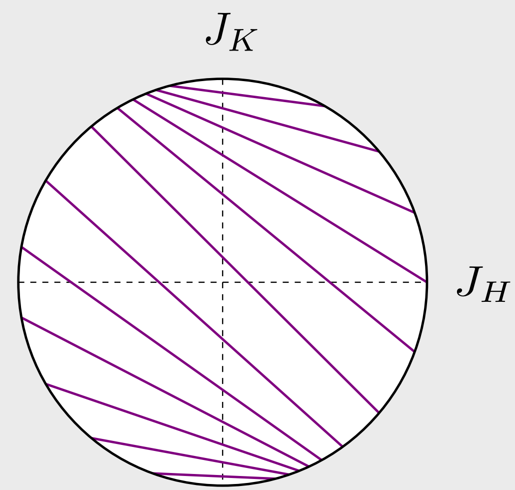
$$H = \sum_{\gamma-\text{bonds}} \cos\varphi \; \mathbf{S}_i \mathbf{S}_j + \sin\varphi \; S_i^\gamma S_j^\gamma$$



- id
- $S^x \mapsto -S^x$
- $S^y \mapsto -S^y$
- $S^z \mapsto -S^z$

Klein duality

- **mapping** between pairs of points (on left and right half-circle)
- **basis transformation** involves spin-rotations on four sublattices
- preserves **symmetry** of Hamiltonian, four SU(2) symmetric points



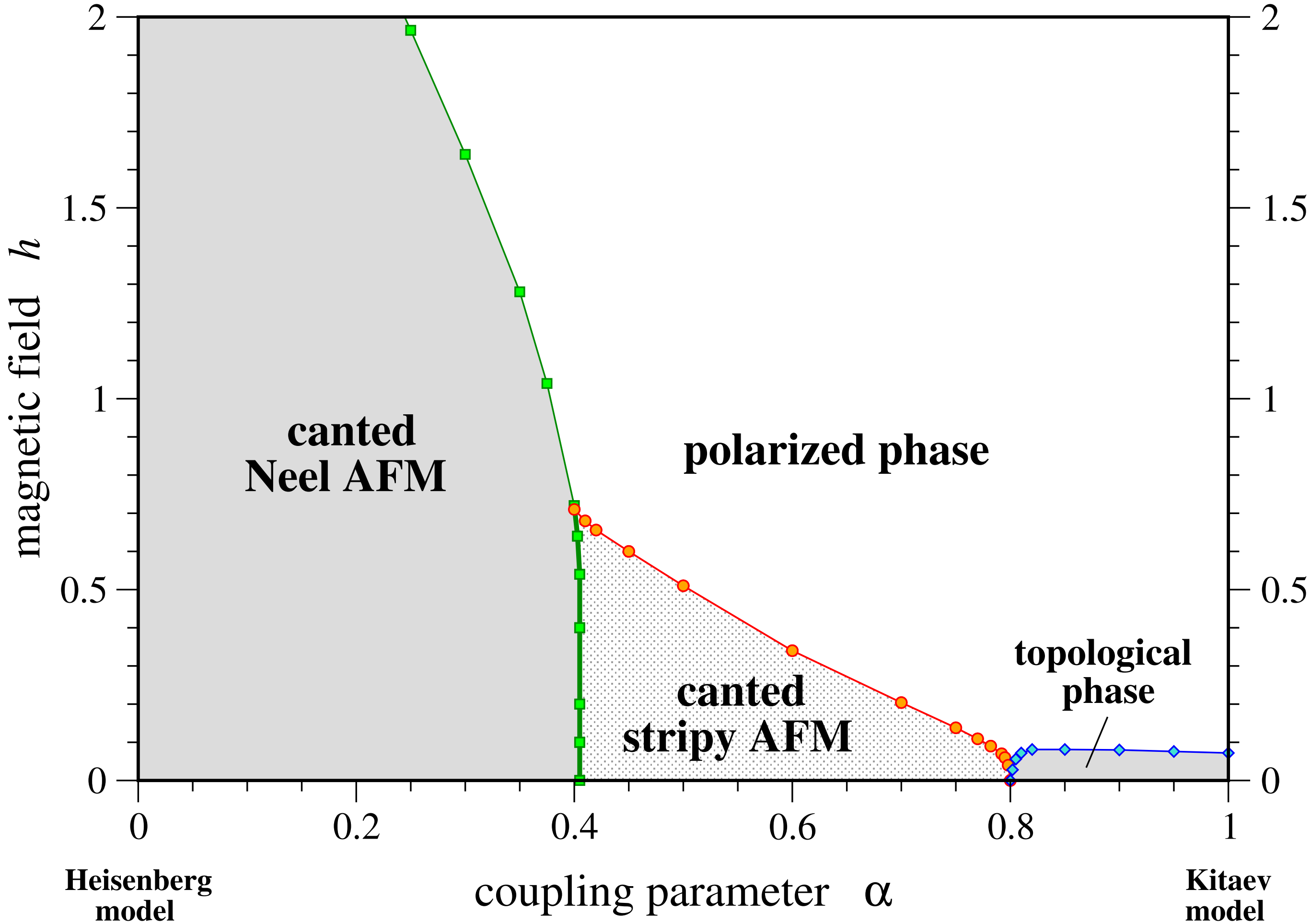
$$\tilde{J}_H = -J_H \qquad \tilde{J}_K = 2J_H + J_K$$

G. Khaliullin, Prog. Theor. Phys. Suppl. 160, 155 (2005)

Magnetic field & topological order

$$H = (1-\alpha)\sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - 2\alpha \sum_{\gamma-\text{bonds}} S_i^\gamma S_j^\gamma + \sum_i \mathbf{h} \cdot \mathbf{S}_i$$

H.-C. Jiang, Z.-C. Gu, X.-L. Qi, ST, PRB **83**, 245104 (2011).



Kitaev materials

Kitaev materials

honeycomb Kitaev materials

Na_2IrO_3, α-Li_2IrO_3, $(H_{3/4}Li_{1/4})_2IrO_3$

$RuCl_3$

triangular Kitaev materials

$Ba_3IrTi_2O_9$, $Ba_3Ir_2TiO_9$, $Ba_3Ir_2InO_9$

more conventional (4d, 3d) triangular quantum magnets

three-dimensional Kitaev materials

β-Li_2IrO_3, γ-Li_2IrO_3, metal-organic compounds

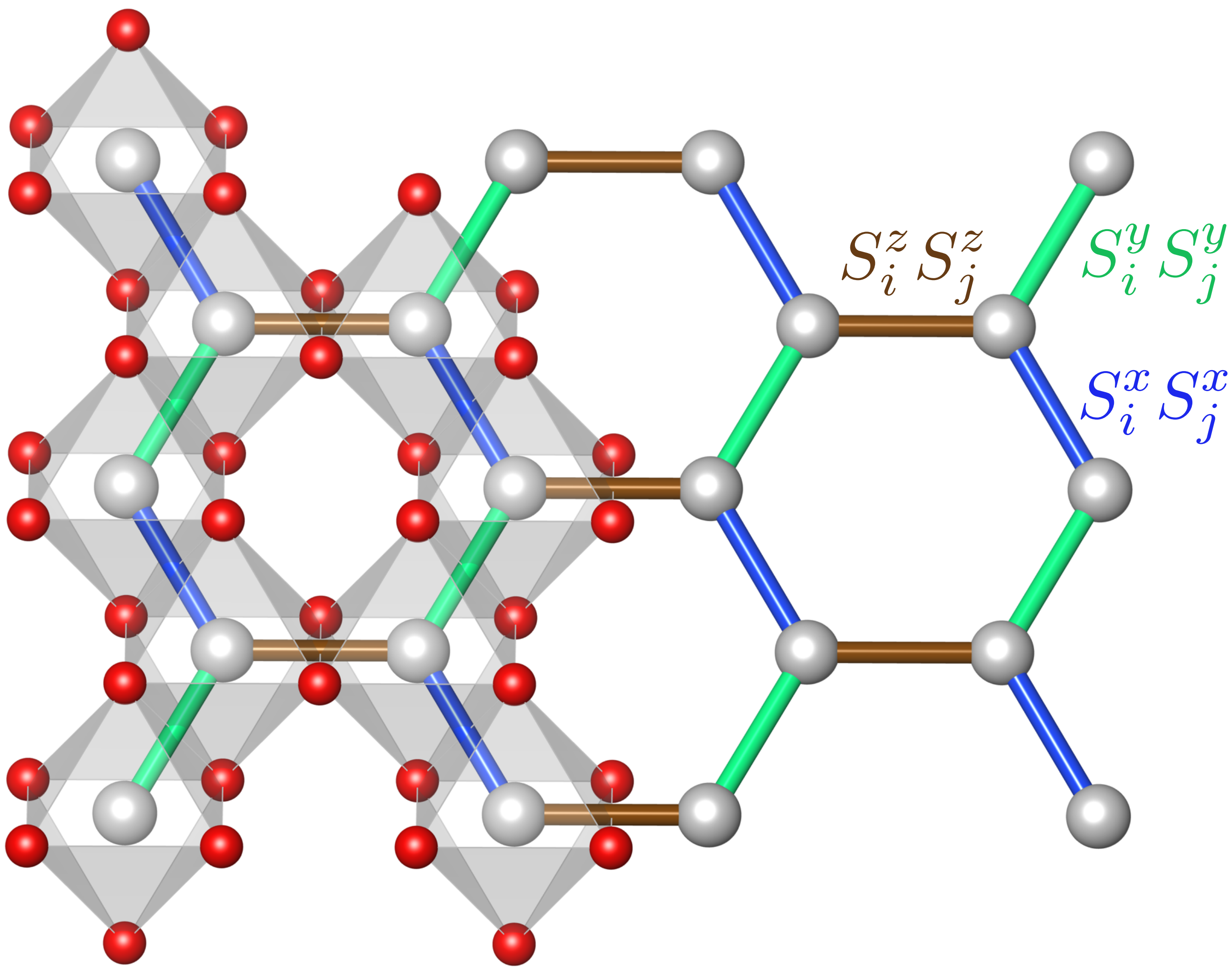
3D Dirac matter

honeycomb Kitaev materials

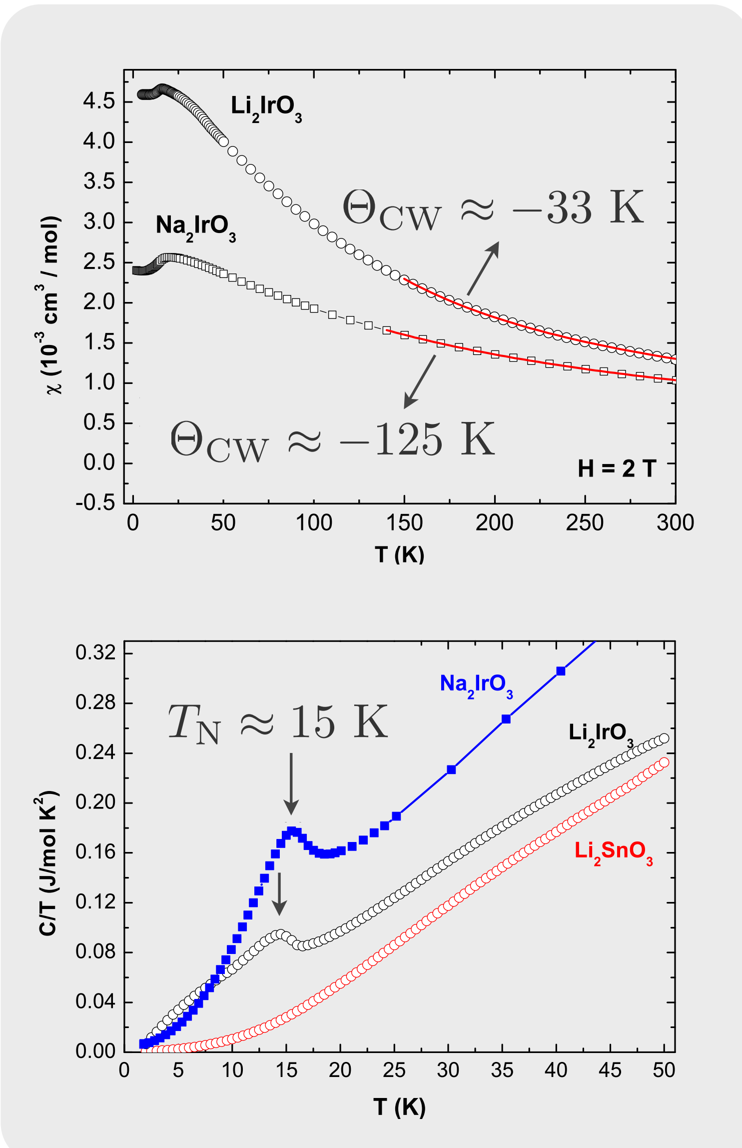
proximate spin liquids

honeycomb Kitaev materials

Na_2IrO_3, α-Li_2IrO_3, $RuCl_3$, $(H_{3/4}Li_{1/4})_2IrO_3$



Na_2IrO_3 and α-Li_2IrO_3



local moment formation
consistent with
j=1/2 spin-orbit entangled moments

these local moments form
magnetic order
at some finite temperature

honeycomb Kitaev materials

	magnetic moment μ_{eff}/μ_B	ordering temperature T_N	Curie-Weiss temperature Θ_{CW}
Na_2IrO_3	1.79(2)	15 K zig-zag order	-125 K
α-Li_2IrO_3	1.83(5)	15 K counterrotating spirals	-33 K
$RuCl_3$	2.2	7 K zig-zag order	-150 K
$(H_{3/4}Li_{1/4})_2IrO_3$	?	—	?

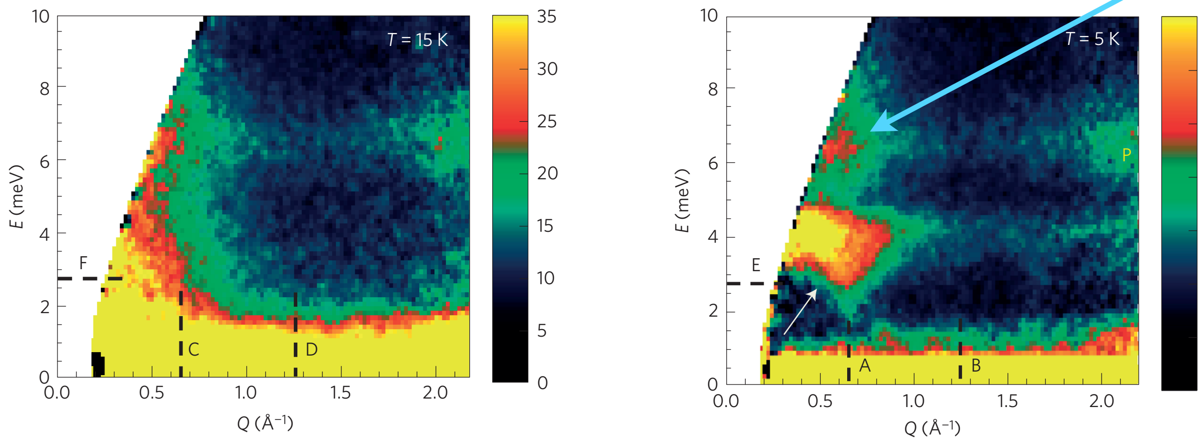
1.74 for spin 1/2

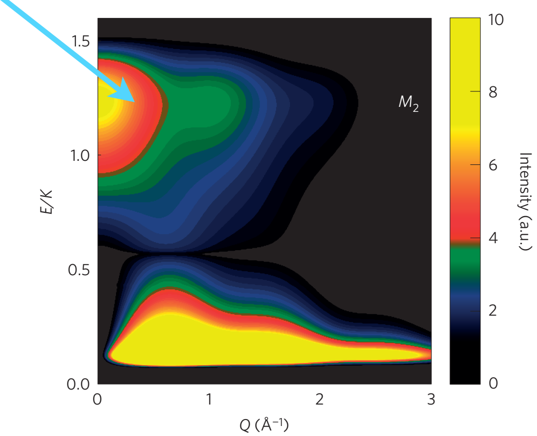
RuCl3

neutron scattering

Banerjee *et al.*, Nature Materials 4604 (2016)

broad **scattering continuum**

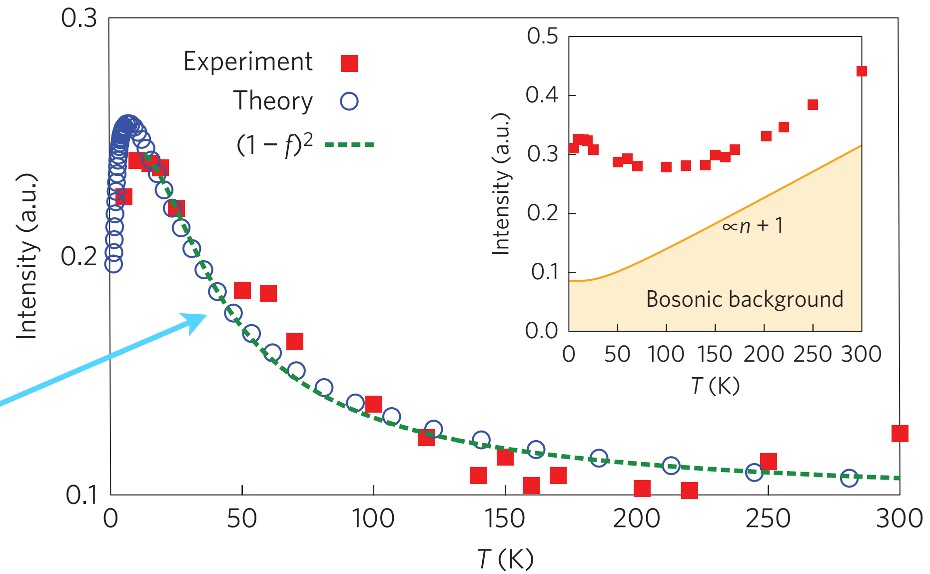




Raman scattering

Nasu *et al.*, Nature Physics **12**, 912 (2016)
Sandilands *et al.*, PRL **114**, 147201 (2015)

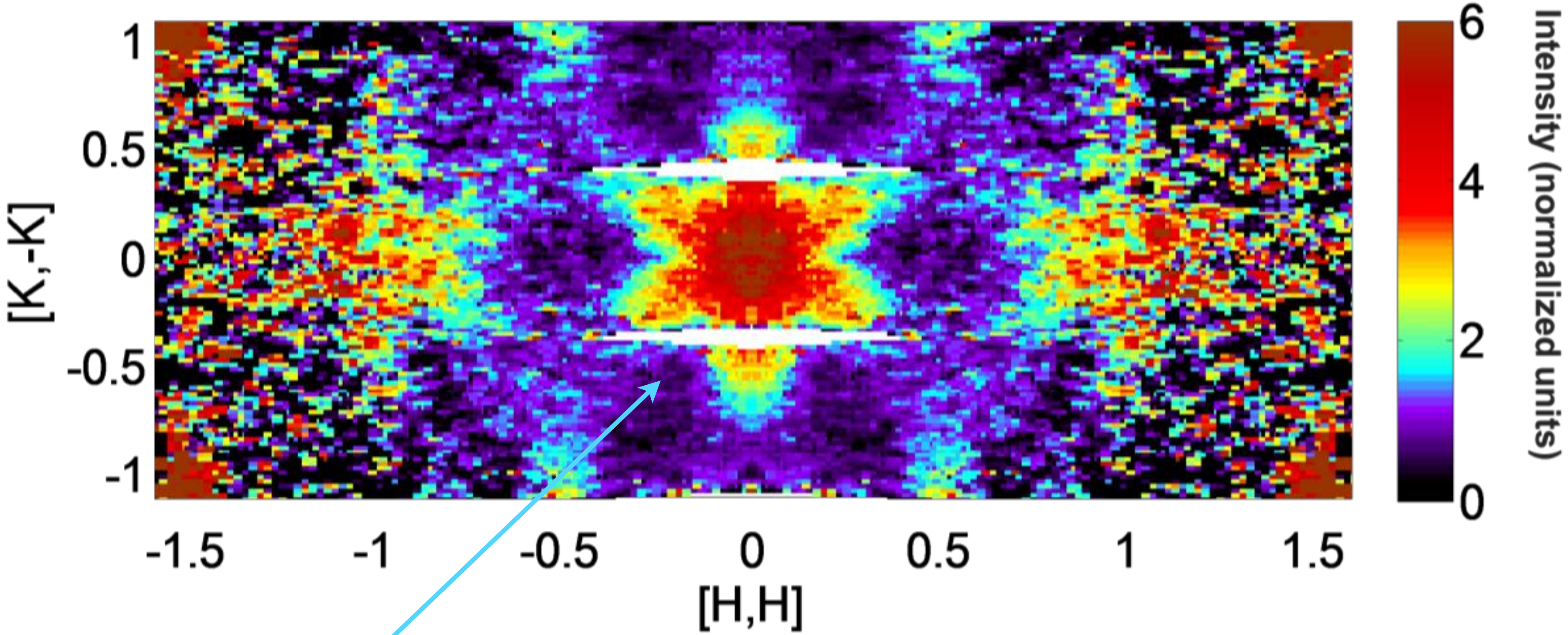
fermionic contribution



$RuCl_3$

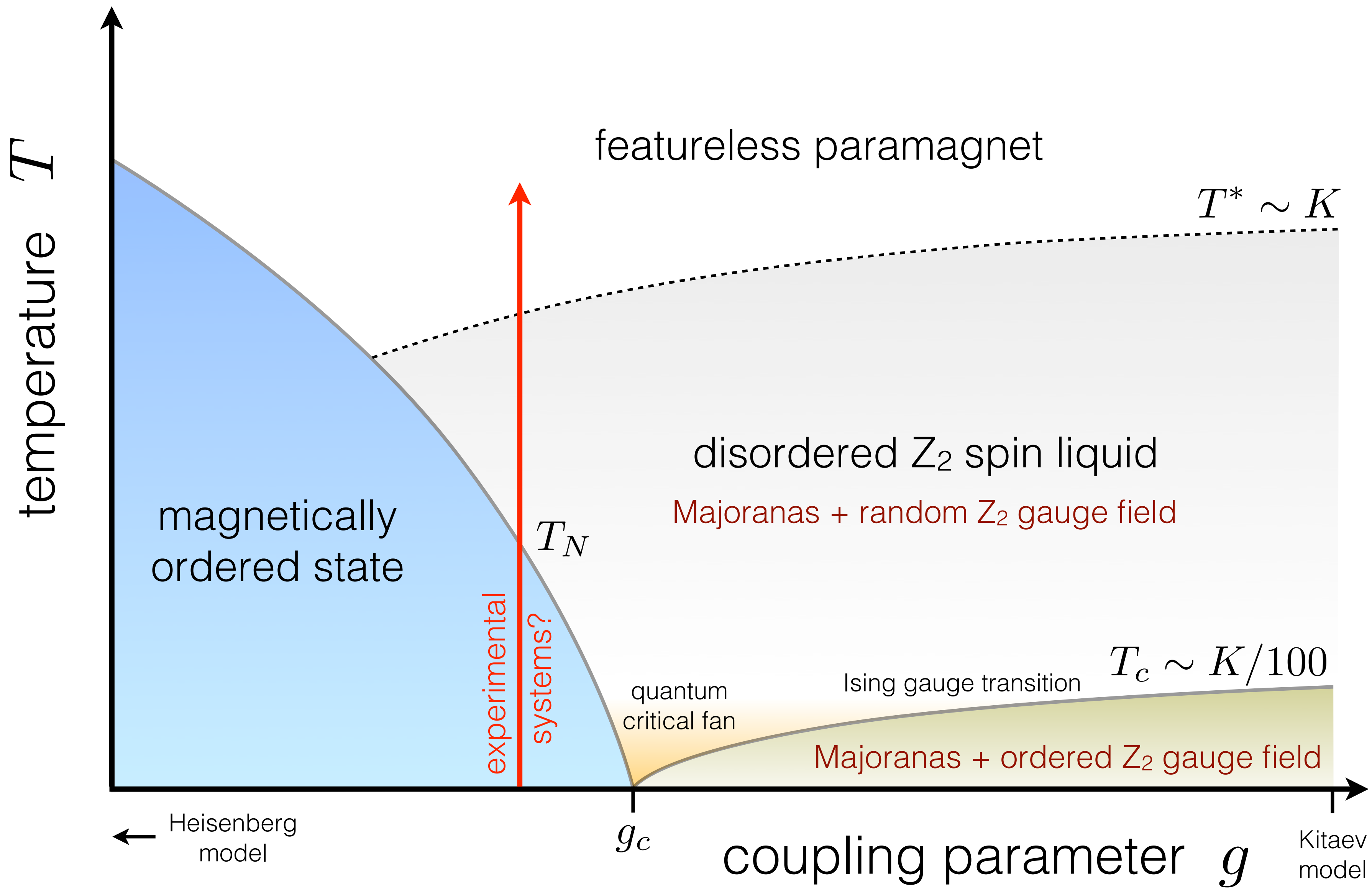
neutron scattering

Banerjee *et al.*, Nature Materials 4604 (2016)



star-like feature arises from
interplay of spin-wave and spin liquids physics
at intermediate energy scales.

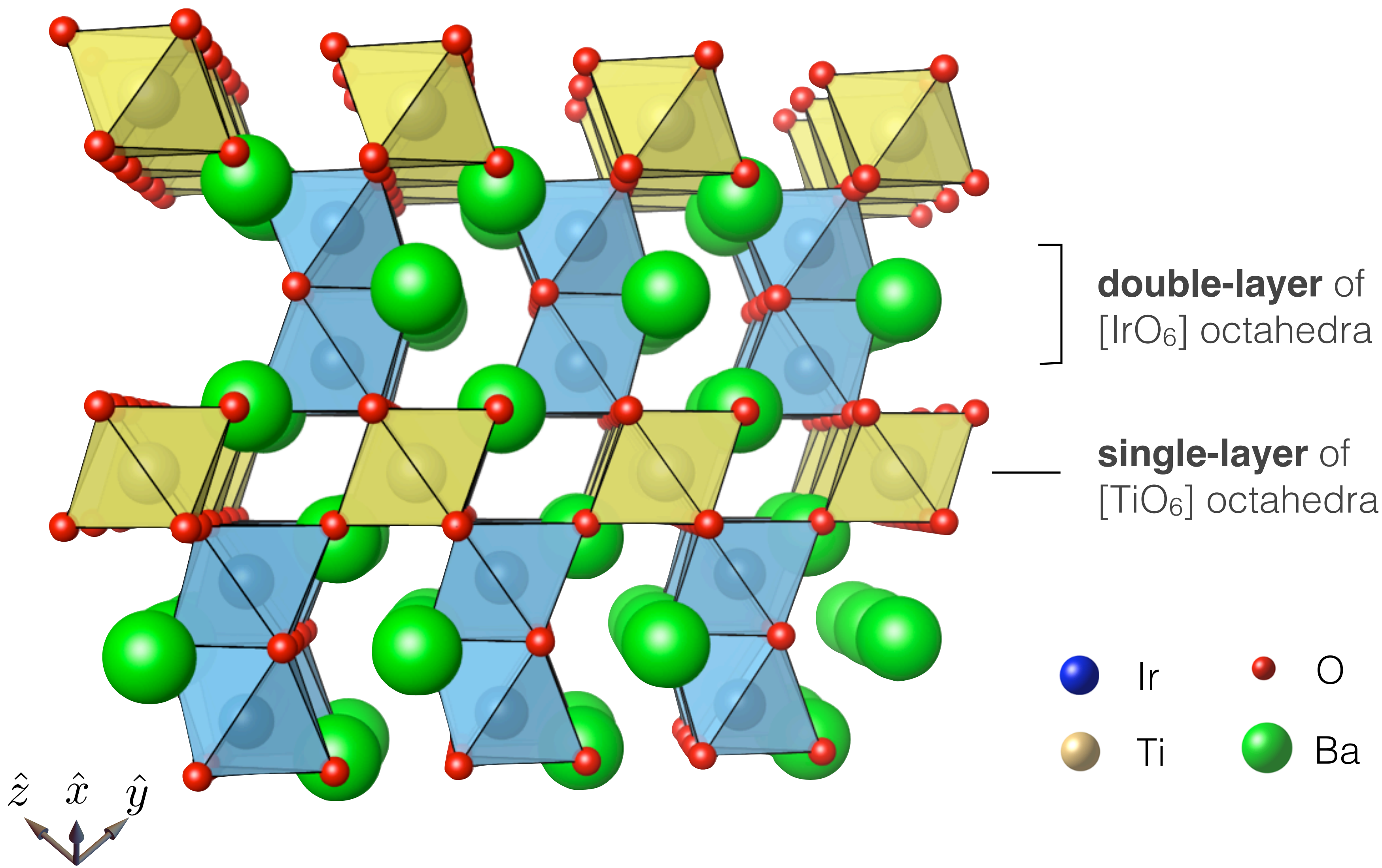
Proximate spin liquids



triangular Kitaev materials

spin textures

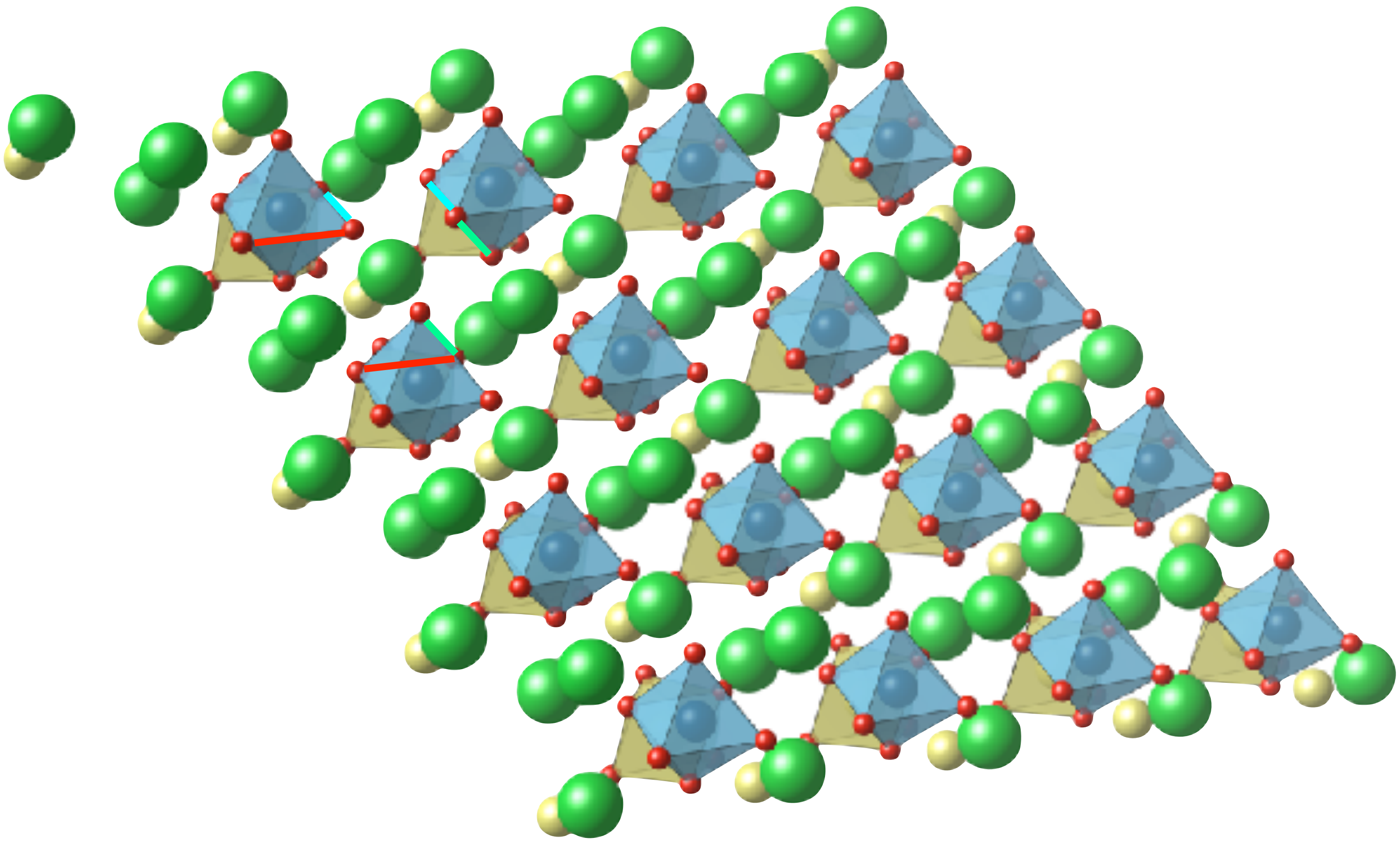
$Ba_3Ir_{2-x}Ti_xO_9$



$Ba_3Ir_{2-x}Ti_xO_9$

triangular lattice
Heisenberg-Kitaev
model

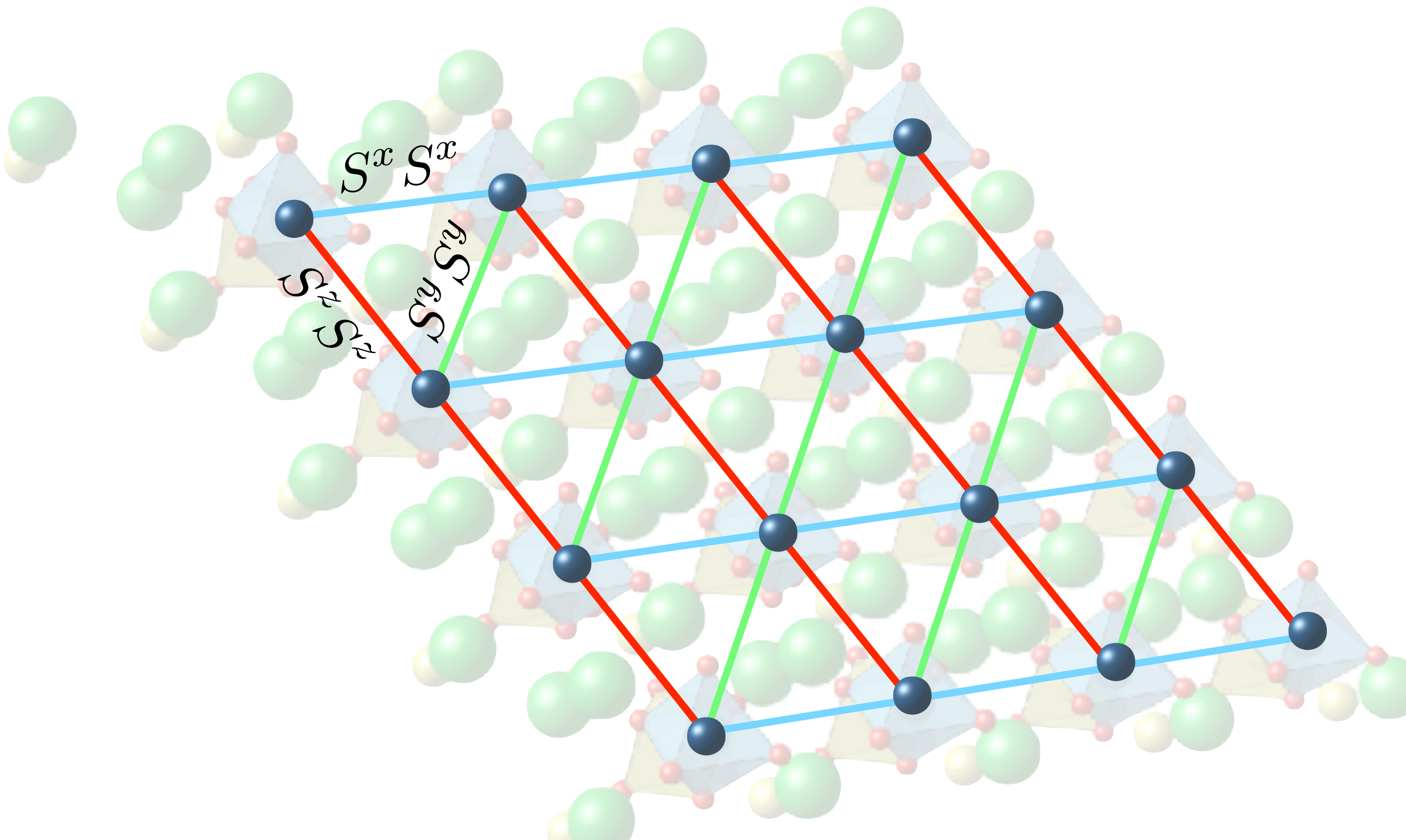
$$H = -\sum_{\gamma-\text{bonds}} J\, \mathbf{S}_i \mathbf{S}_j + K\, S_i^{\gamma} S_j^{\gamma}$$



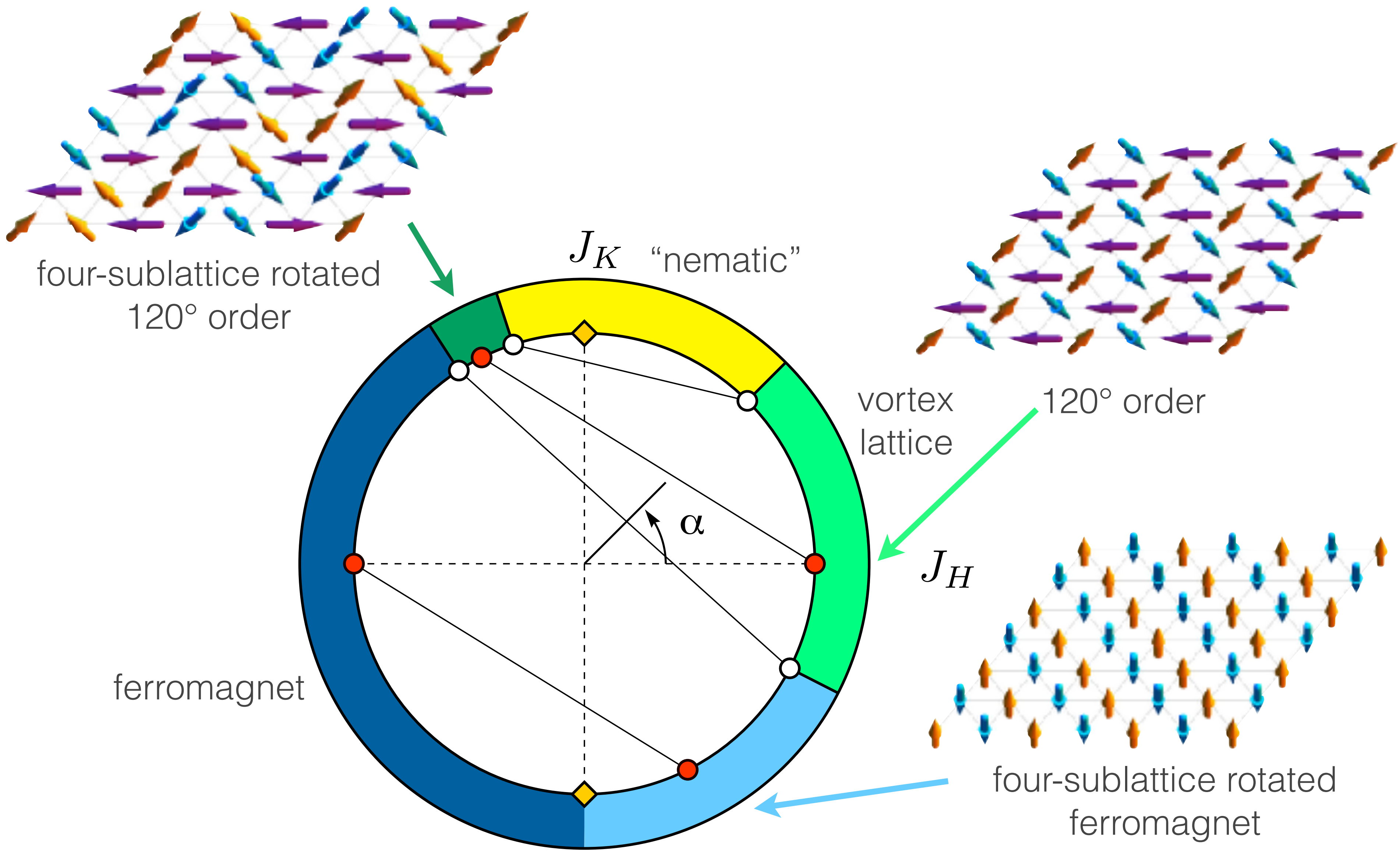
$Ba_3Ir_{2-x}Ti_xO_9$

triangular lattice
Heisenberg-Kitaev
model

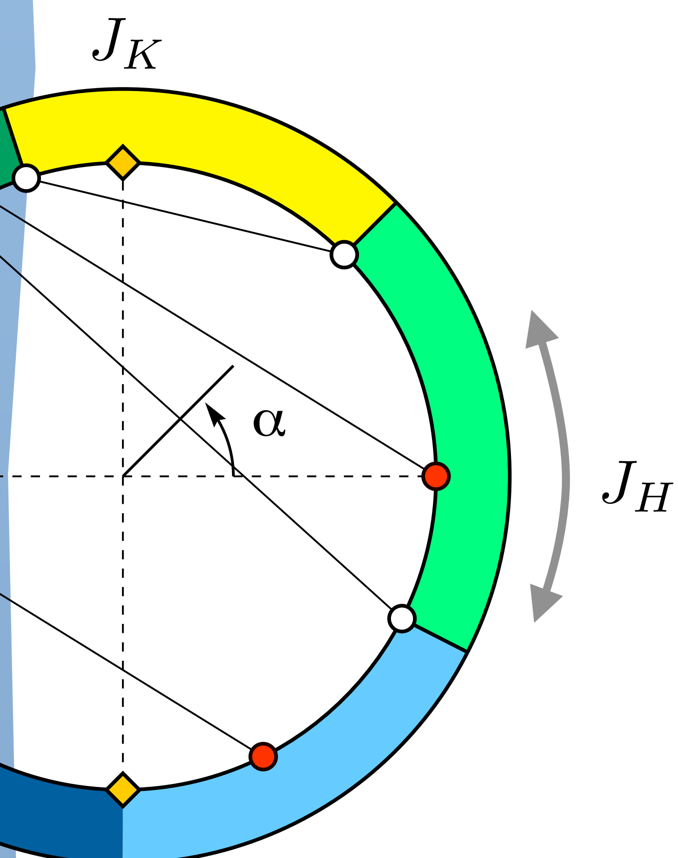
$$H = - \sum_{\gamma-\text{bonds}} J\, \mathbf{S}_i \mathbf{S}_j + K\, S_i^\gamma S_j^\gamma$$



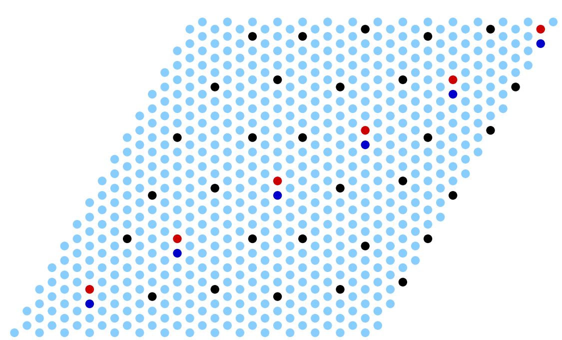
Triangular lattice Heisenberg-Kitaev model



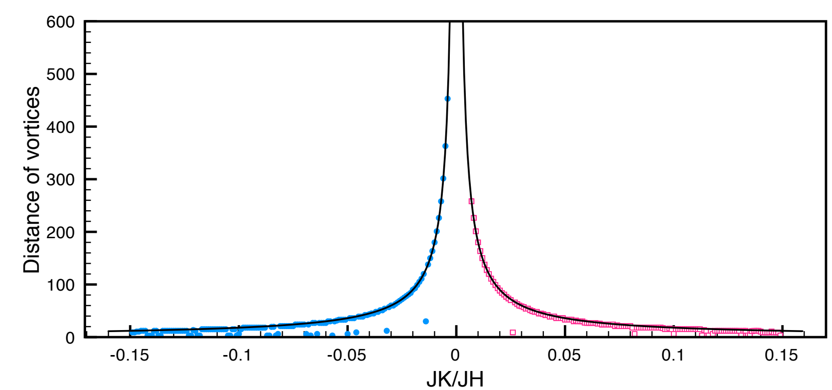
Spin textures – vortex lattice



Monte Carlo



vorticity

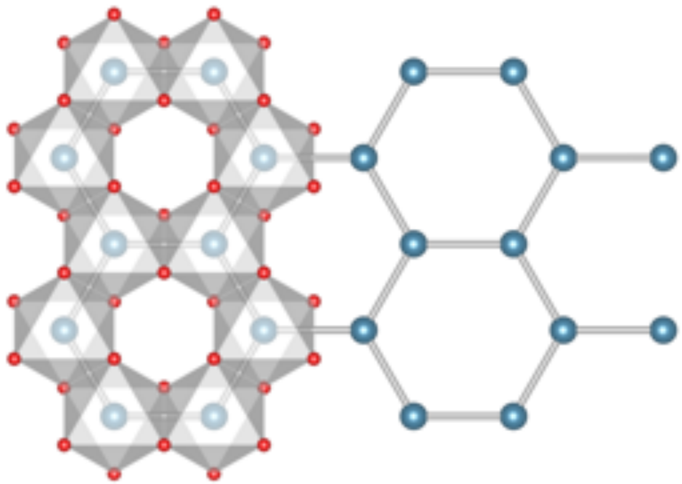


3D Kitaev materials

Majorana metals

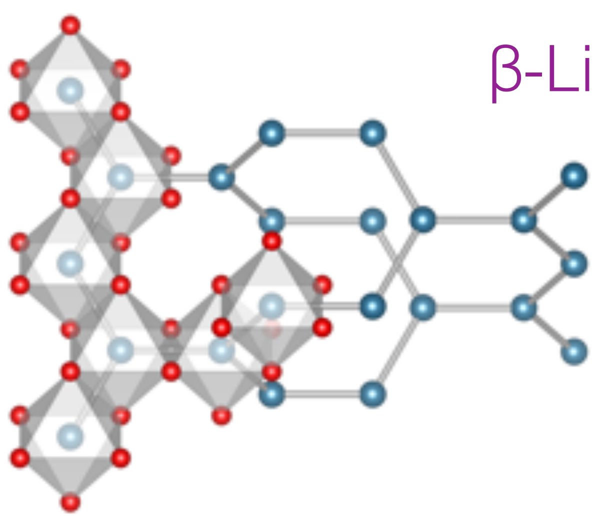
Family of Li_2IrO_3 compounds

hexagonal layers



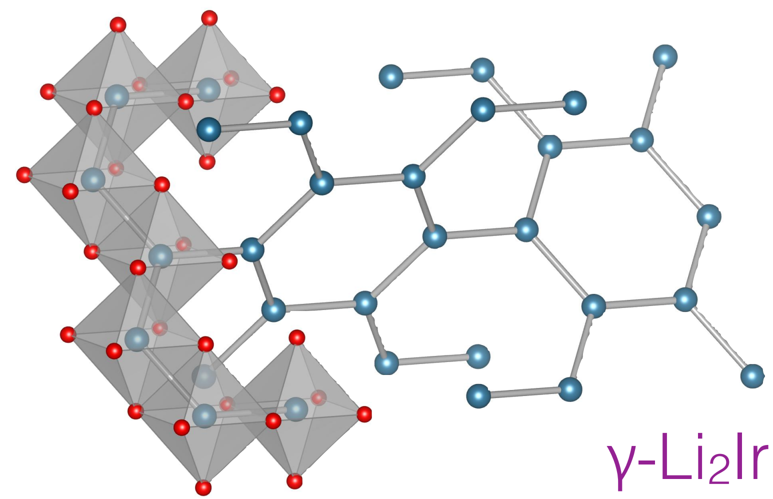
α-Li_2IrO_3

hyperhoneycomb



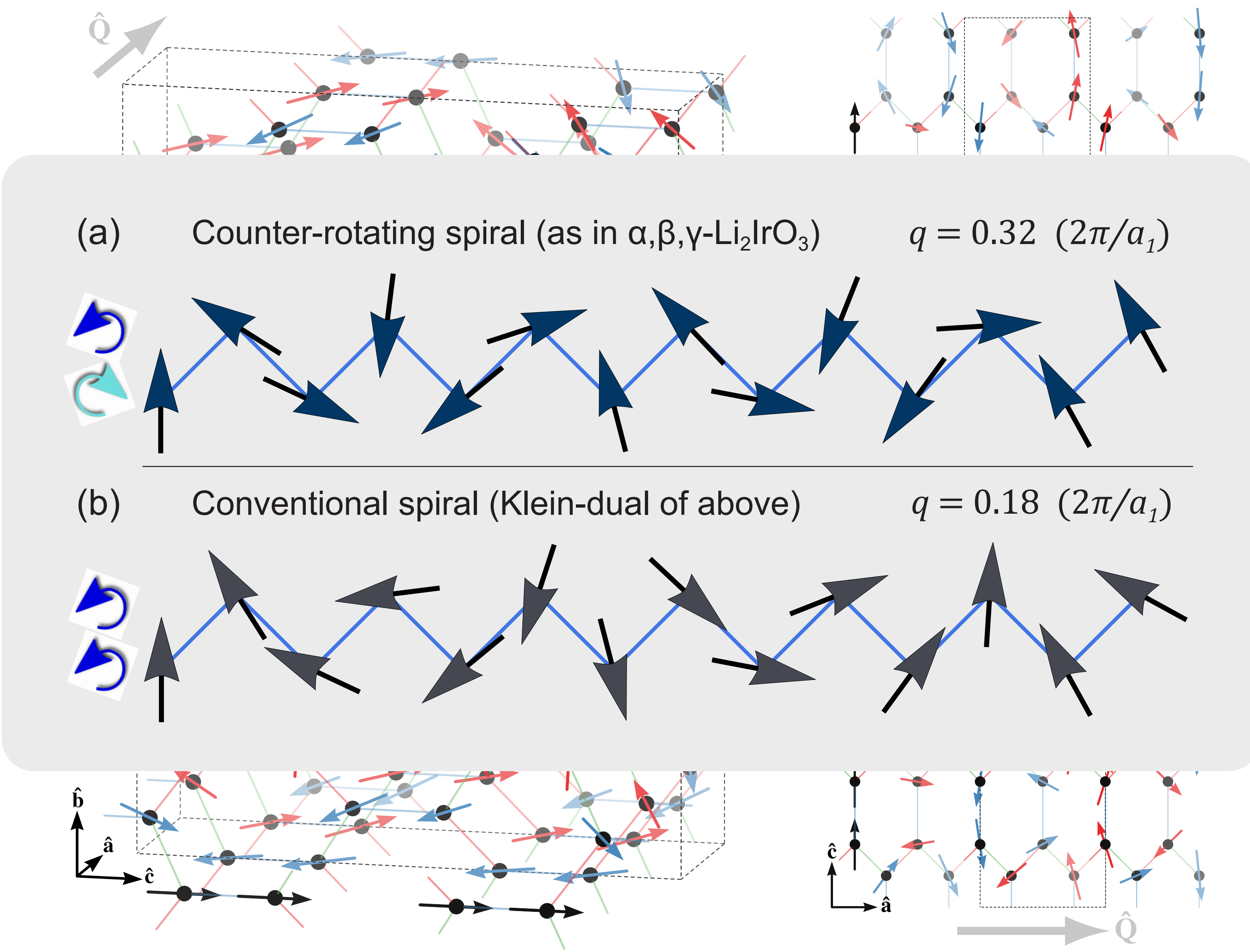
β-Li_2IrO_3

harmonic honeycomb

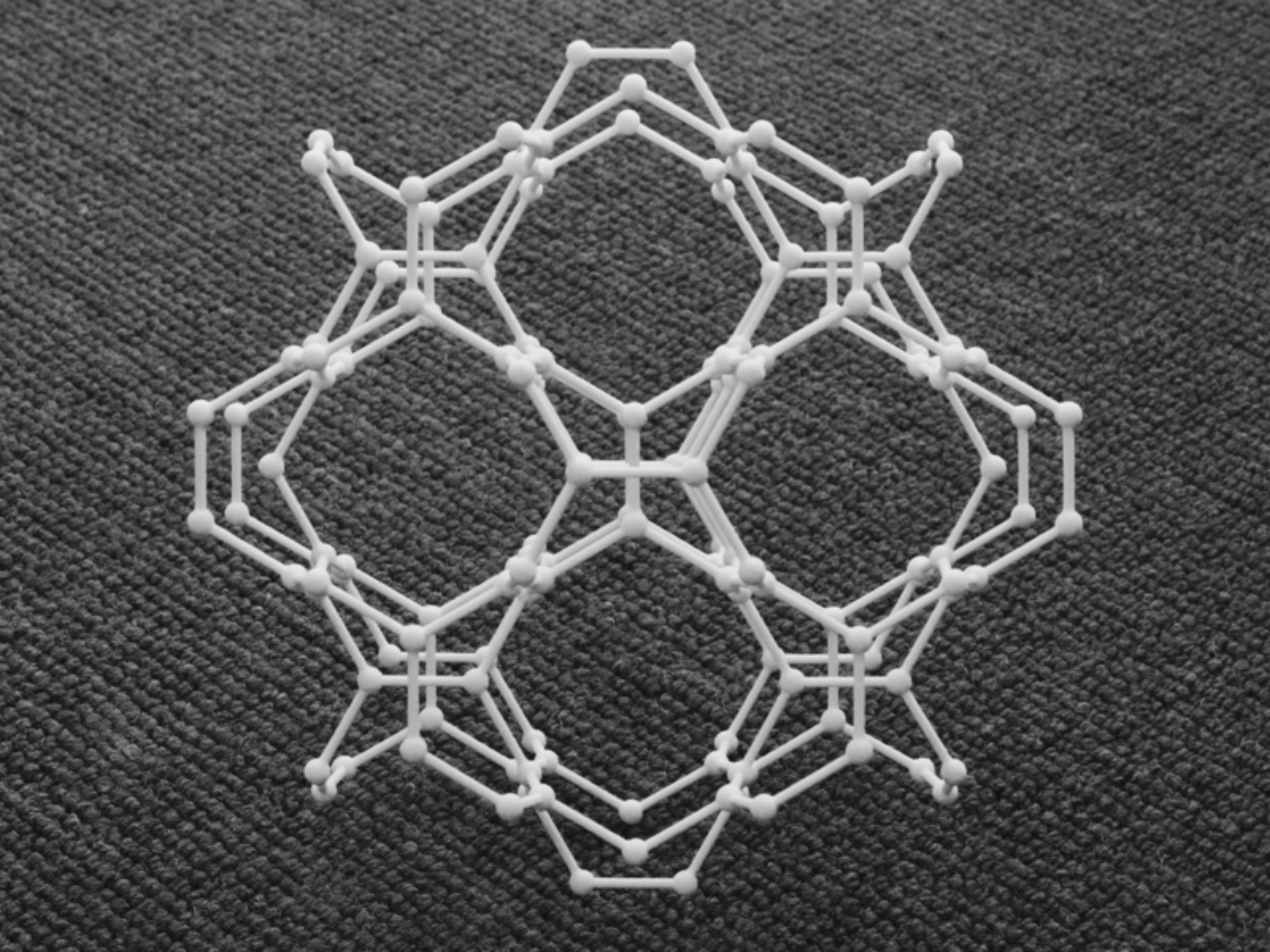


γ-Li_2IrO_3

Counter-rotating spiral order



(b) Ordering in γ-Li_2IrO_3



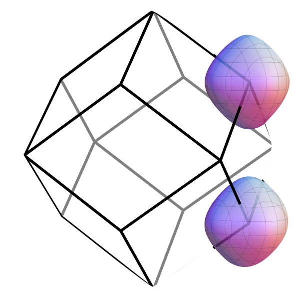
Tricoordinated lattices

		other names	Z	inversion	space group	
3D lattices	(10,3)a	hyperoctagon, K4 crystal	4	✗	$I4_132$	214
	(10,3)b	hyperhoneycomb	4	✓	Fddd	70
	(10,3)c	—	6	✗	$P3_112$	151
	(9,3)a	—	12	✓	$R\bar{3}m$	166
	(8,3)a	—	6	✗	$P6_222$	180
	(8,3)b	—	6	✓	$R\bar{3}m$	166
	(8,3)c	—	8	✓	$P6_3$ / mmc	194
	(8,3)n	—	16	✓	I4 / mmm	139
2D	(6,3)	honeycomb	2	✓		

Majorana metals

PRB **93**, 085101 (2016)

		Majorana metal	TR breaking
3D lattices	(10,3)a	Fermi surface	Fermi surface
	(10,3)b	nodal line	Weyl nodes
	(10,3)c	nodal line	Fermi surface
	(9,3)a	Weyl nodes	Weyl nodes
	(8,3)a	Fermi surface	Fermi surface
	(8,3)b	Weyl nodes	Weyl nodes
	(8,3)c	nodal line	Weyl nodes
	(8,3)n	gapped	gapped
2D	(6,3)	Dirac nodes	gapped

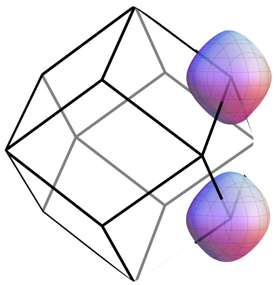


Majorana Fermi surfaces

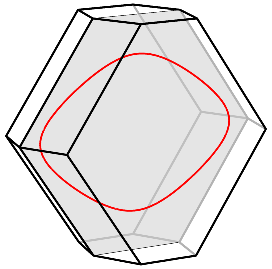
Majorana metals

PRB **93**, 085101 (2016)

		Majorana metal	TR breaking
3D lattices	(10,3)a	Fermi surface	Fermi surface
	(10,3)b	nodal line	Weyl nodes
	(10,3)c	nodal line	Fermi surface
	(9,3)a	Weyl nodes	Weyl nodes
	(8,3)a	Fermi surface	Fermi surface
	(8,3)b	Weyl nodes	Weyl nodes
	(8,3)c	nodal line	Weyl nodes
	(8,3)n	gapped	gapped
2D	(6,3)	Dirac nodes	gapped



Majorana Fermi surfaces

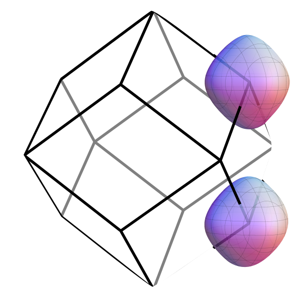


nodal lines

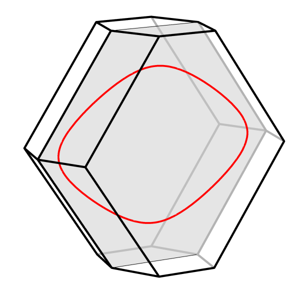
Majorana metals

PRB **93**, 085101 (2016)

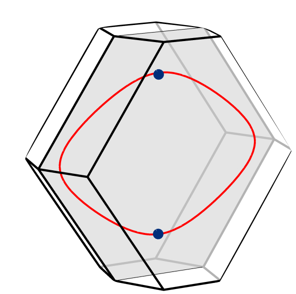
		Majorana metal	TR breaking
3D lattices	(10,3)a	Fermi surface	Fermi surface
	(10,3)b	nodal line	Weyl nodes
	(10,3)c	nodal line	Fermi surface
	(9,3)a	Weyl nodes	Weyl nodes
	(8,3)a	Fermi surface	Fermi surface
	(8,3)b	Weyl nodes	Weyl nodes
	(8,3)c	nodal line	Weyl nodes
	(8,3)n	gapped	gapped
2D	(6,3)	Dirac nodes	gapped



Majorana Fermi surfaces



nodal lines

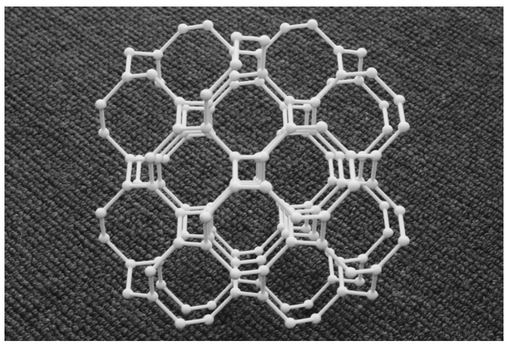


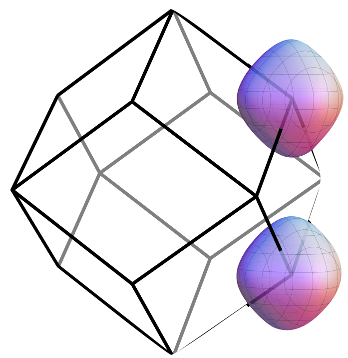
Weyl nodes

Breaking time-reversal symmetry

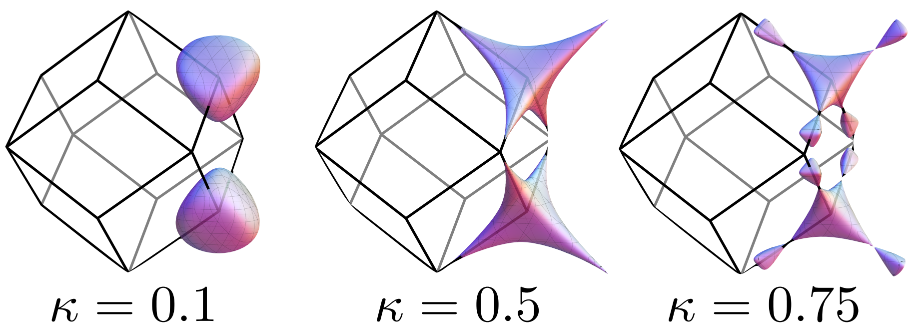
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma - \sum_j \vec{h} \cdot \vec{\sigma}_j$$

(10,3)a – hyperoctagon



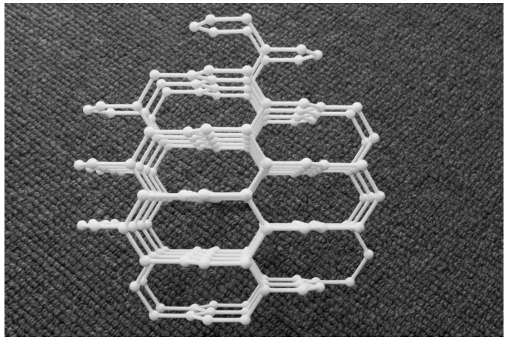


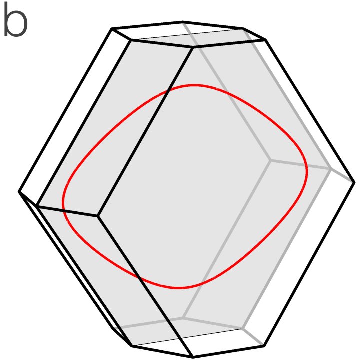
Fermi **surface**



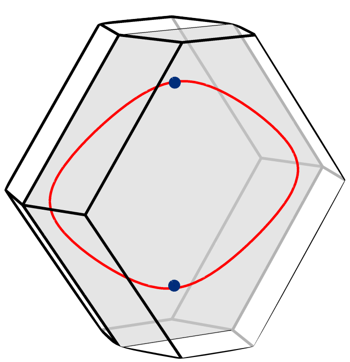
Fermi surface **deforms**

(10,3)b – hyperhoneycomb





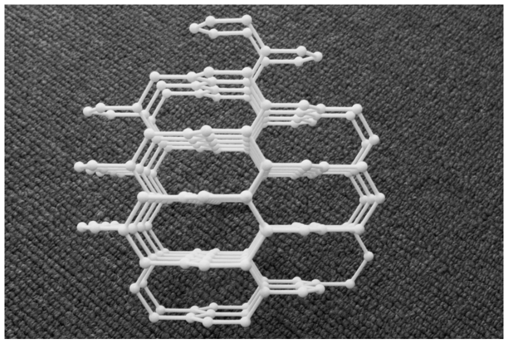
Fermi **line**



Fermi line **gaps out**, but two **Weyl nodes remain**

Weyl physics – energy spectrum

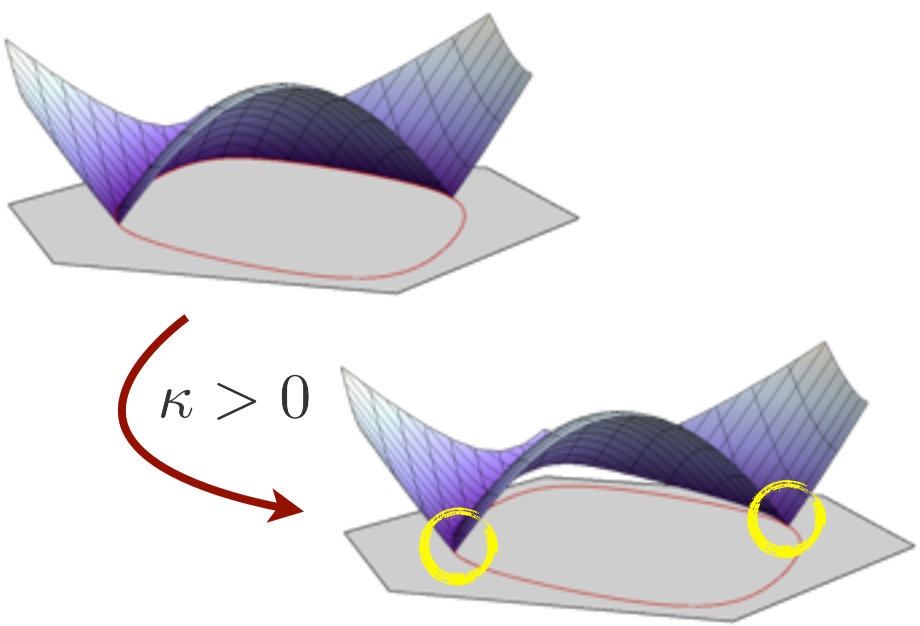
(10,3)b – hyperhoneycomb

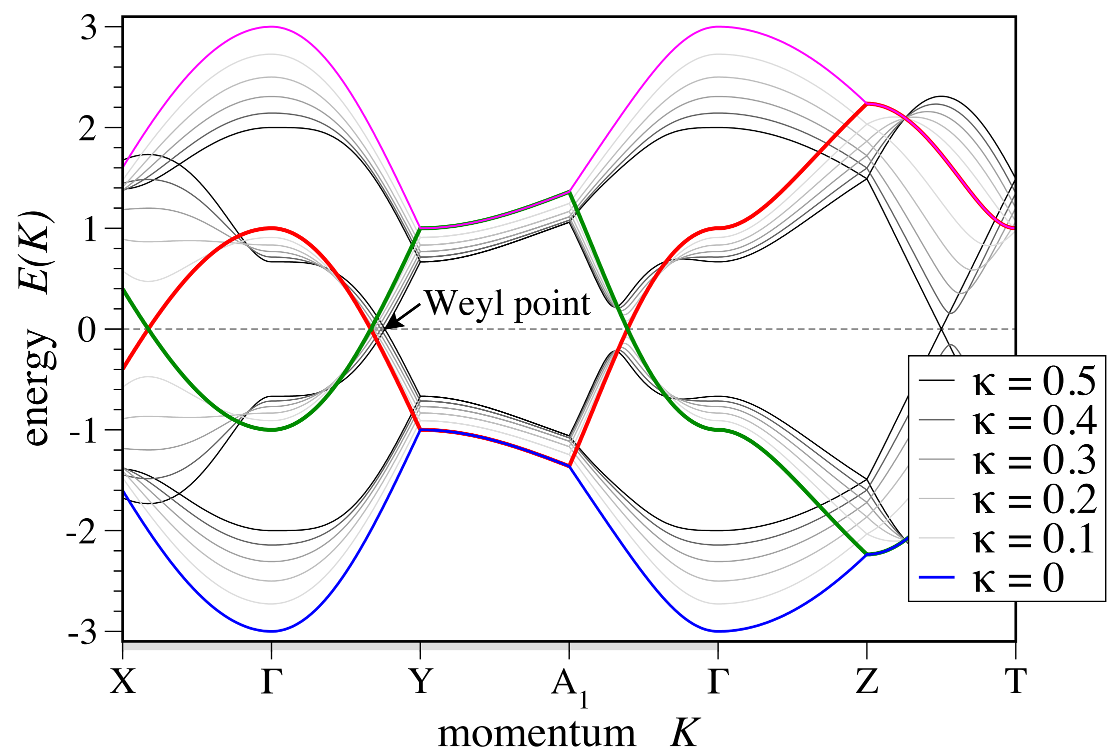


Touching of two bands in 3D is **linear**

$$\hat{H} = \vec{v}_0 \cdot \vec{q}\,\mathbb{1} + \sum_{i=1}^{3} \vec{v}_j \cdot \vec{q}\,\sigma_j$$

Weyl nodes



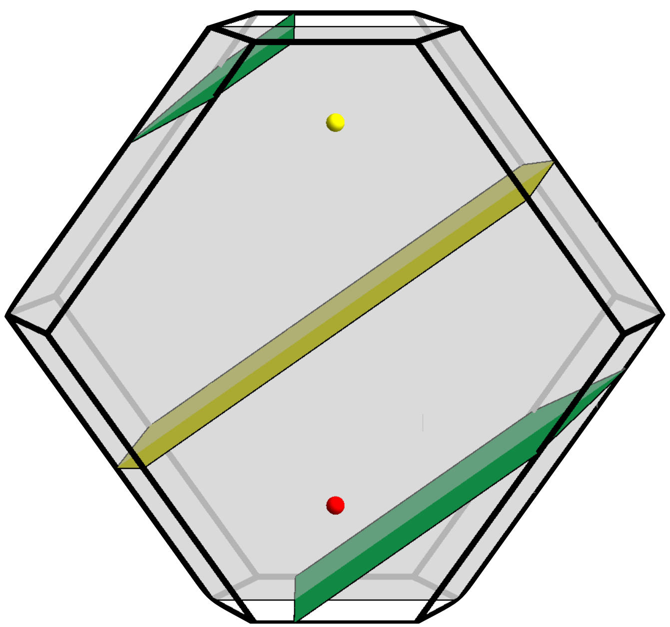


Weyl physics – Chern numbers

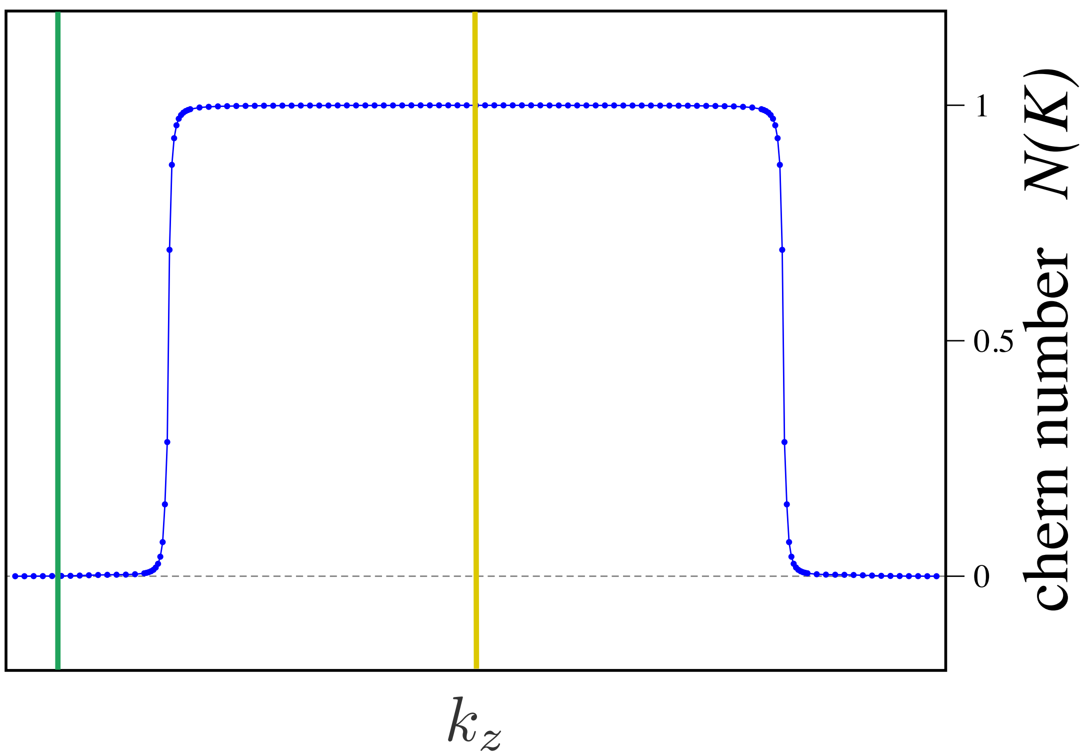
Weyl nodes are **sources or sinks of Berry flux**

$$\vec{B}_n(\vec{k}) = \nabla_{\vec{k}} \times \left(i \langle n(\vec{k}) | \nabla_{\vec{k}} | n(\vec{k}) \rangle \right)$$

with chirality $\text{sign}[\vec{v}_1 \cdot (\vec{v}_2 \times \vec{v}_3)]$



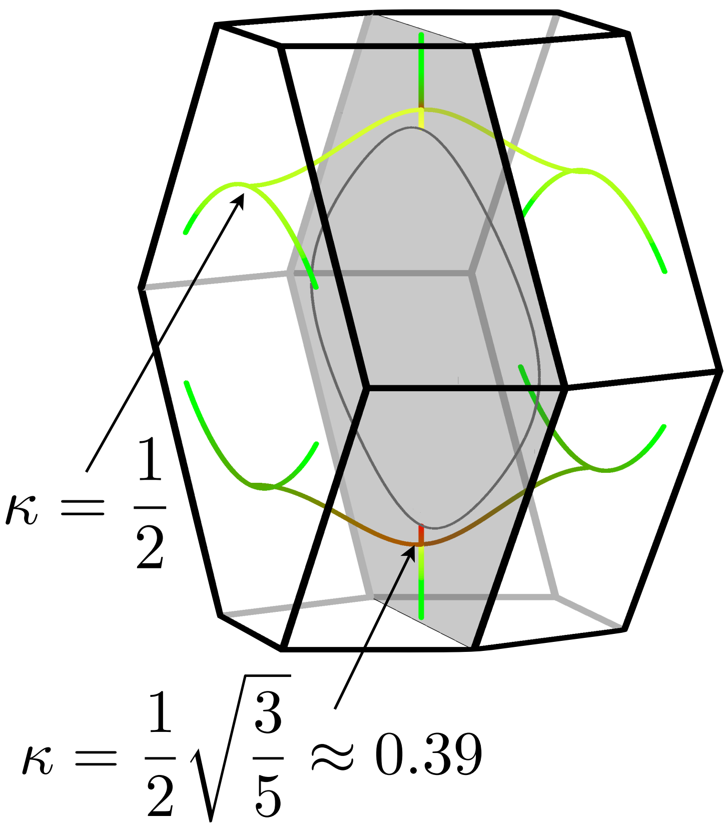
$\kappa = 0.05$

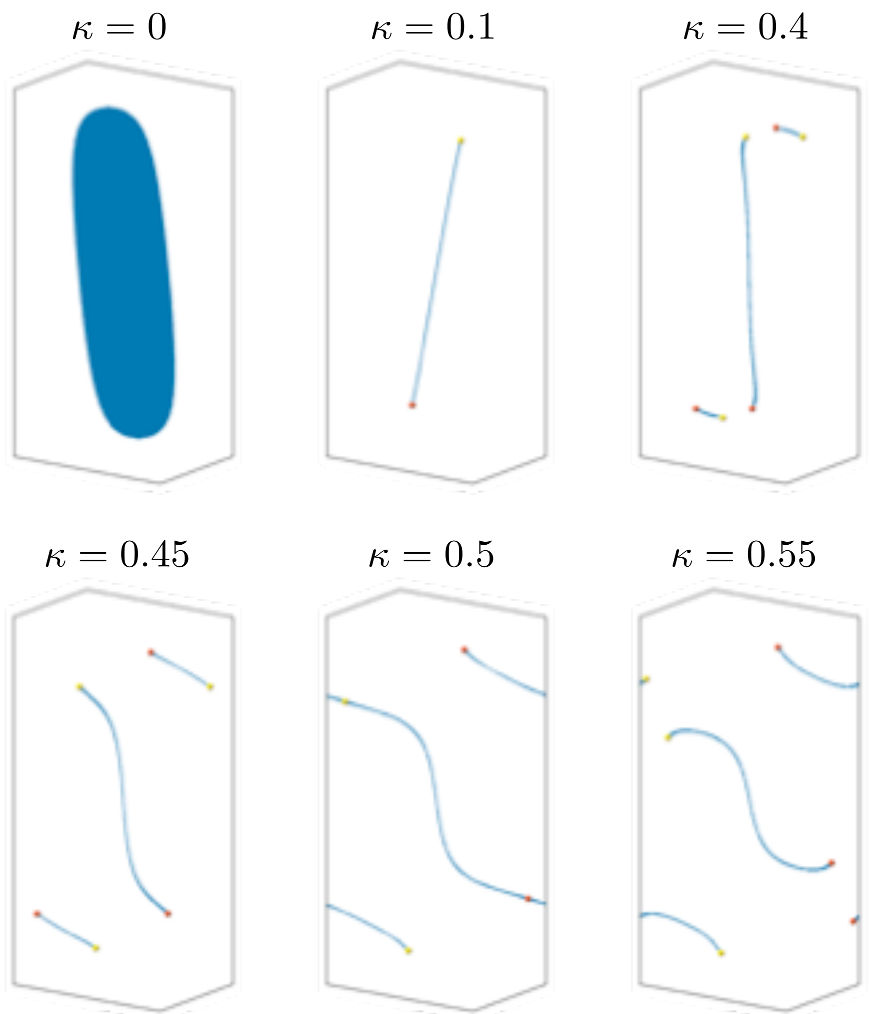


Weyl physics – surface states

evolution of **Weyl nodes** in the bulk

evolution of **Fermi arcs** on the **surface**





Experimental signatures?

specific heat

Specific heat has bulk and surface contributions

$$C(T) \sim a_{\text{bulk}} \cdot L^3 \cdot T^3 + a_{\text{surf}} \cdot L^2 \cdot T$$

Could be distinguished via sample size variation.

thermal Hall effect

Applying a thermal gradient to the system, a net heat current perpendicular to the gradient arises due to the chiral nature of the surface modes.

Thermal Hall conductance given by

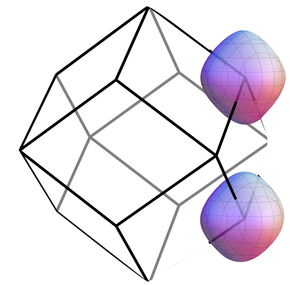
$$K = \frac{1}{2} \frac{k_B^2 \pi^2 T}{3h} \frac{d}{2\pi} L_z$$

see also T. Meng and L. Balents, Phys. Rev. B 86, 054504 (2012).

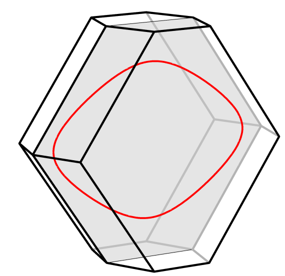
Majorana metals

PRB **93**, 085101 (2016)

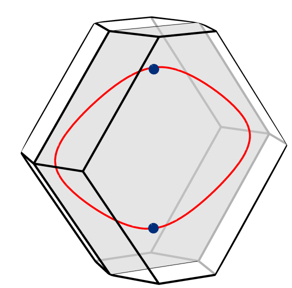
		Majorana metal	TR breaking
3D lattices	(10,3)a	Fermi surface	Fermi surface
	(10,3)b	nodal line	Weyl nodes
	(10,3)c	nodal line	Fermi surface
	(9,3)a	Weyl nodes	Weyl nodes
	(8,3)a	Fermi surface	Fermi surface
	(8,3)b	Weyl nodes	Weyl nodes
	(8,3)c	nodal line	Weyl nodes
	(8,3)n	gapped	gapped
2D	(6,3)	Dirac nodes	gapped



Majorana Fermi surfaces



nodal lines



Weyl nodes

Summary

lecture notes
arXiv:1701.07056

Kitaev materials

- a family of spin-orbit assisted j=1/2 Mott insulators
- bond-directional exchange induces frustration
- unconventional forms of magnetism

Bond-directional exchange

- (proximate) spin liquids
- signatures of Majorana fermions and Z_2 gauge field
- spin textures

Family of lattice geometries

- honeycomb – Na_2IrO_3, α-Li_2IrO_3, $(H_{3/4}Li_{1/4})_2IrO_3$, $RuCl_3$
- triangular – $Ba_3IrTi_2O_9$, $Ba_3Ir_2TiO_9$, $Ba_3Ir_2InO_9$
- 3D – β-Li_2IrO_3, γ-Li_2IrO_3, metal-organic compounds

Thanks!