Majorana metals
in spin-orbit entangled quantum matter

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PRB 89, 235102 (2014)
arXiv:1411.7379

Collaborators

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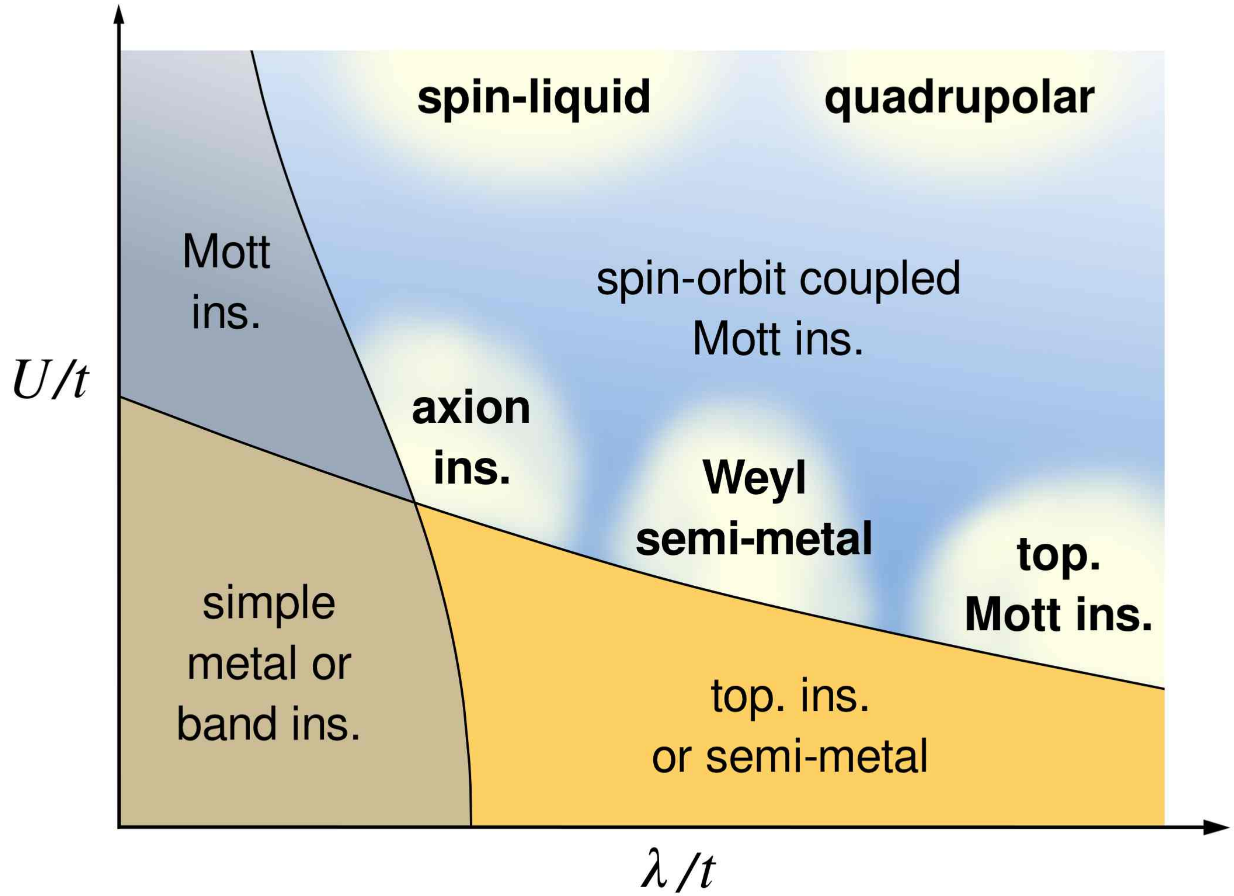
5d transition metal oxides

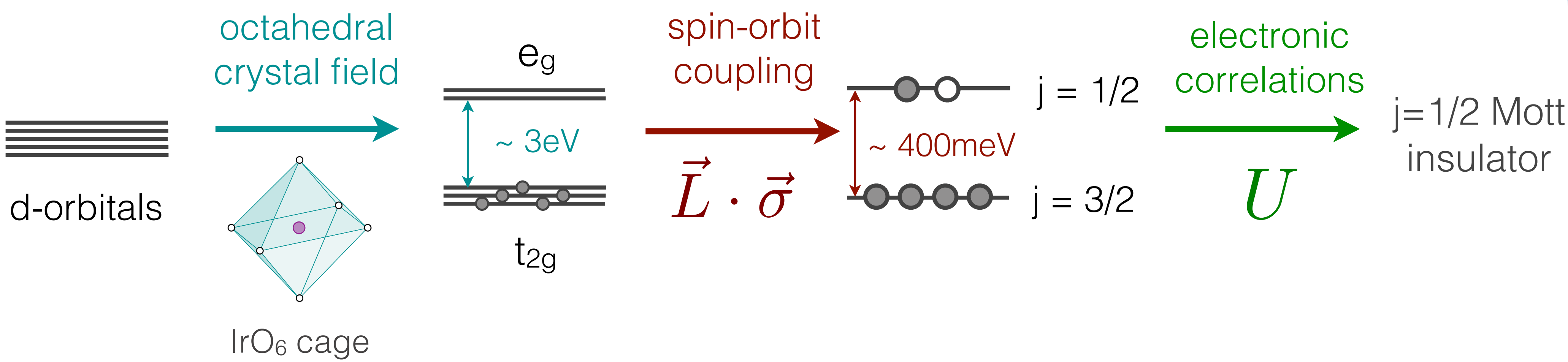
Largely *accidental* degeneracy of electronic correlations, spin-orbit entanglement, and crystal field effects results in a **broad variety of metallic and insulating states**.



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+} $(5d^5)$

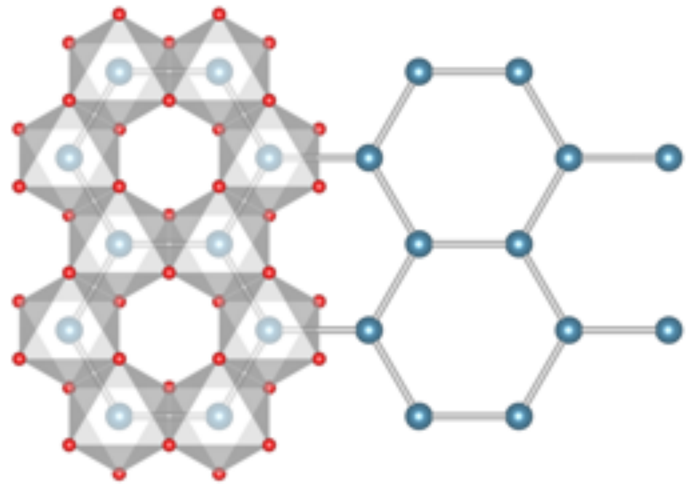


Why are these spin-orbit entangled j=1/2 Mott insulators **interesting?**

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)

Family of Li_2IrO_3 compounds

hexagonal layers

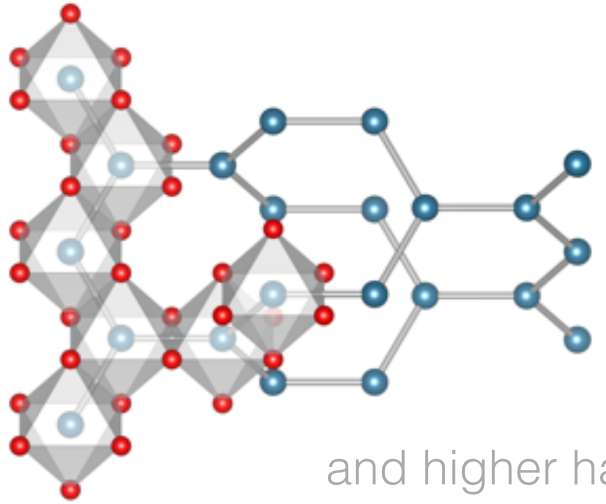


Na_2IrO_3

α-Li_2IrO_3

see also $RuCl_3$

hyper-honeycomb

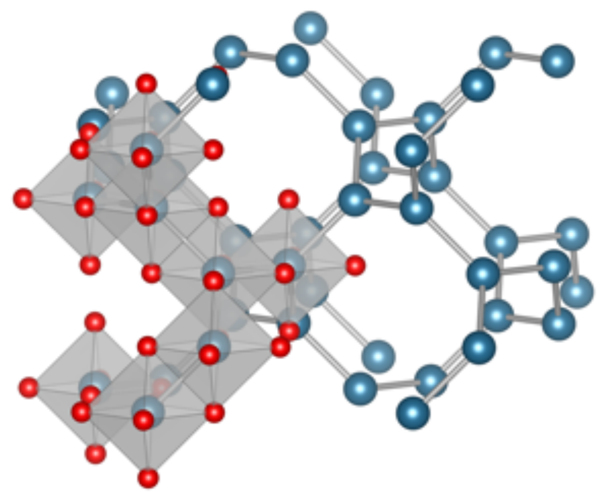


β-Li_2IrO_3

γ-Li_2IrO_3

and higher harmonics

hyper-octagon



Spin liquids in 3D Kitaev models

Spin-orbit entangled j=1/2 Mott insulators in Li_2IrO_3 realize two- and three-dimensional **Kitaev models**.

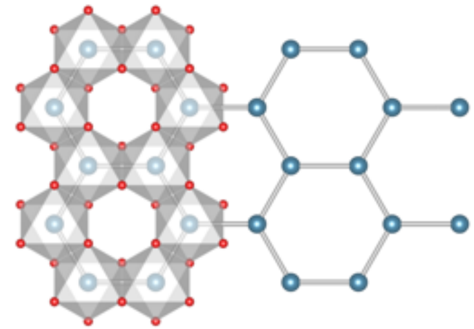
$$H_{\mathrm{Kitaev}} = -J_K \sum_{\gamma-\mathrm{bonds}} \sigma_i^\gamma \sigma_j^\gamma$$

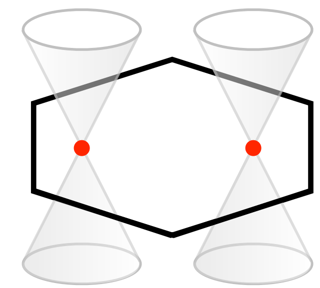
Kitaev models are paradigmatic examples for **spin fractionalization**.

spin-1/2 $\sigma_j^\gamma = i\, b_j^\gamma c_j$ Majorana fermion + Z_2 gauge field

Emergent Majorana fermions form
Majorana metals
reflecting the underlying lattice structure.

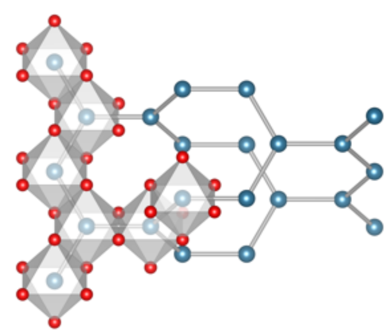
hexagonal layers

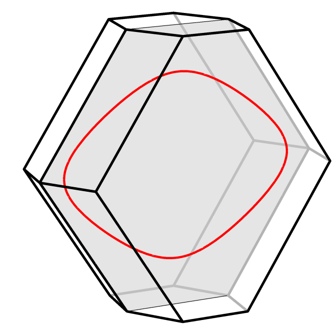




Dirac **points**

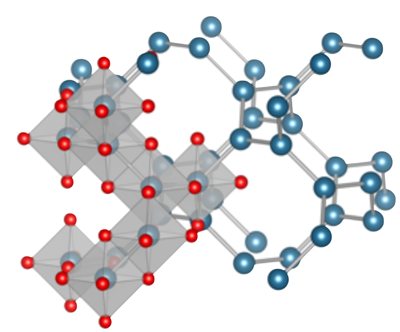
hyper-honeycomb

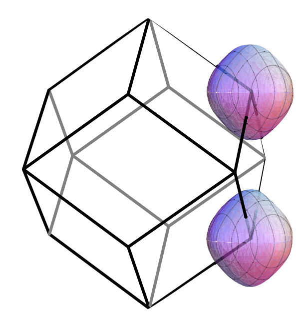




Fermi **lines**

hyper-octagon

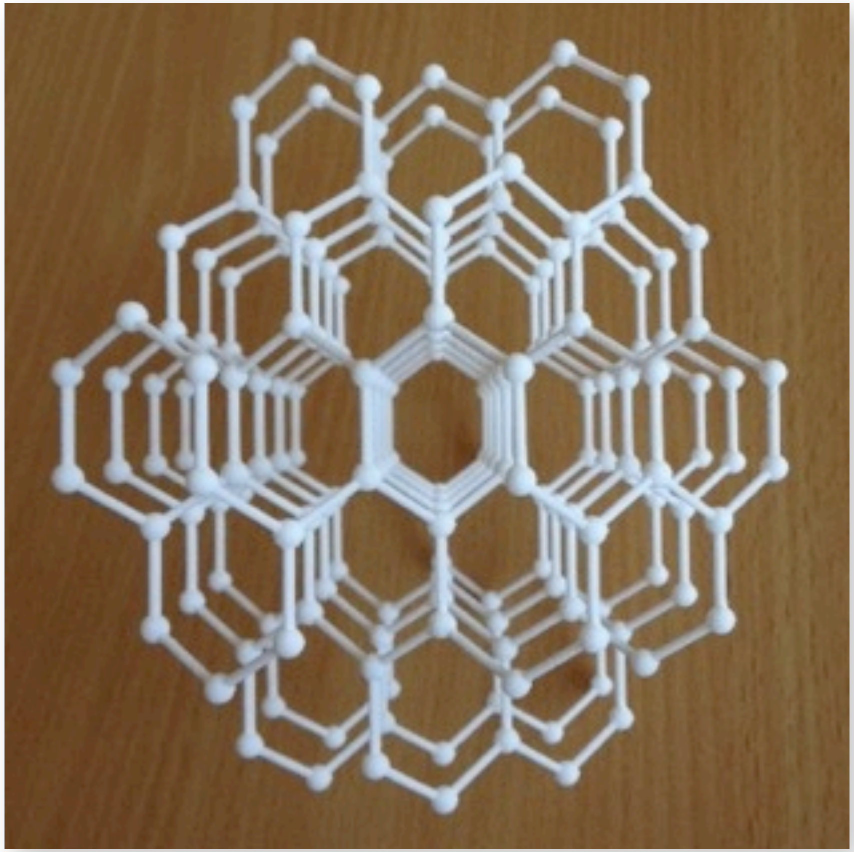




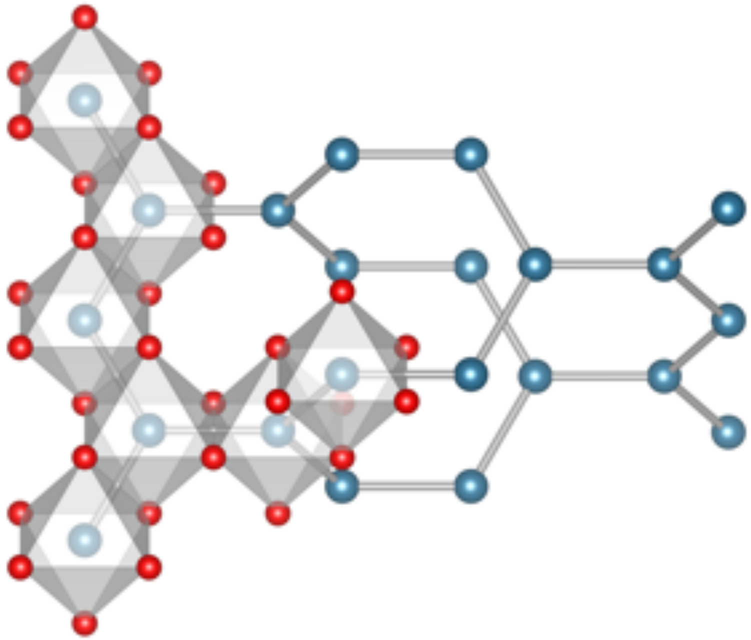
Fermi **surfaces**

The hyper-honeycomb lattice

β-Li_2IrO_3



3D prints @ www.shapeways.com/designer/trebst



novel crystalline form of Li_2IrO_3

Hide Takagi's group PRL (2015)

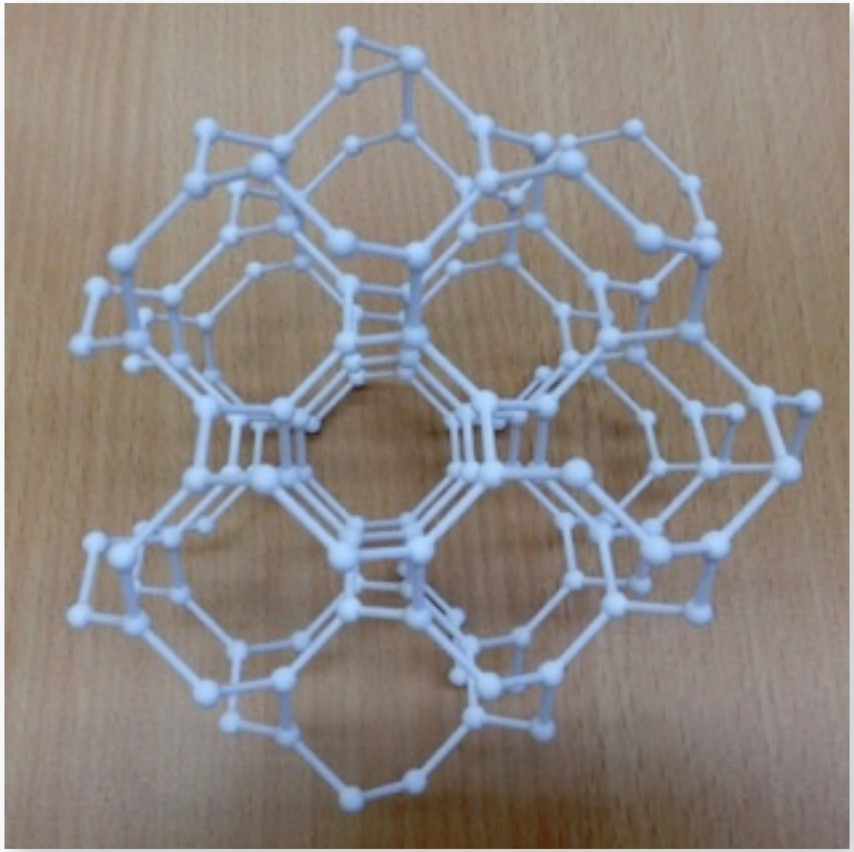
James Analytis's group Nature Comm. (2014)

3D tricoordinated Ir lattice

space group **Fddd** (no. 70)

The hyper-octagon lattice

δ-Li_2IrO_3 ?



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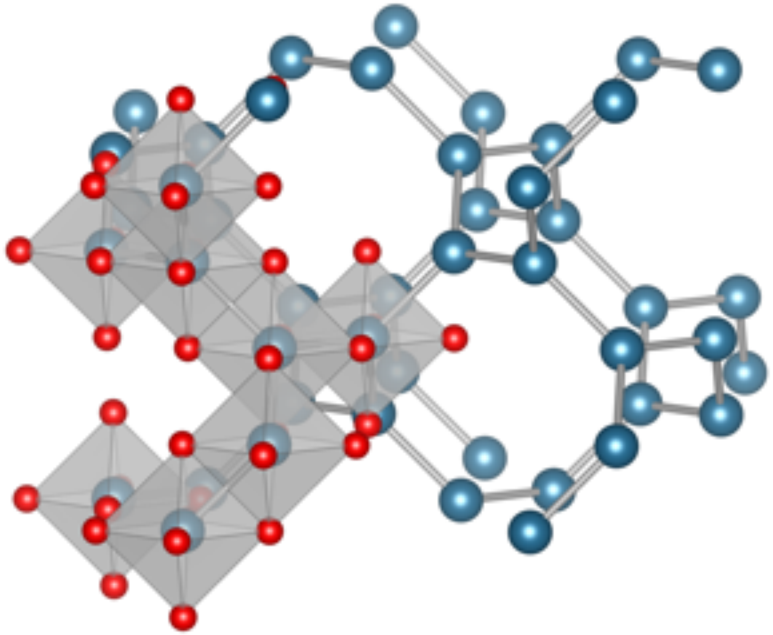


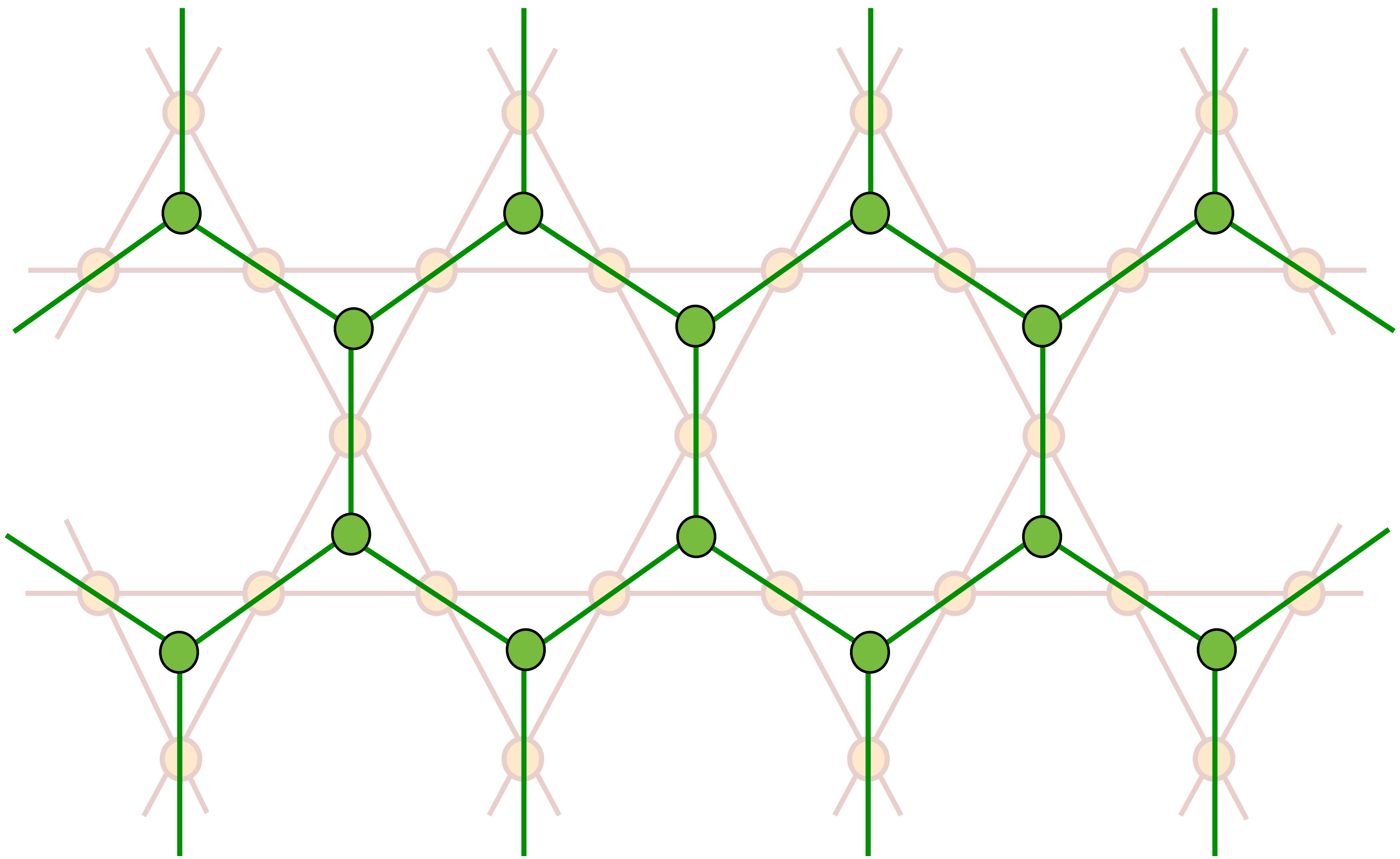
3D tricoordinated Ir lattice

space group **$I4_132$** (no. 214)

possibly **crystalline form** of Li_2IrO_3 ?

How do you find these lattices?

medial and premedial lattices



kagome lattice

medial lattice

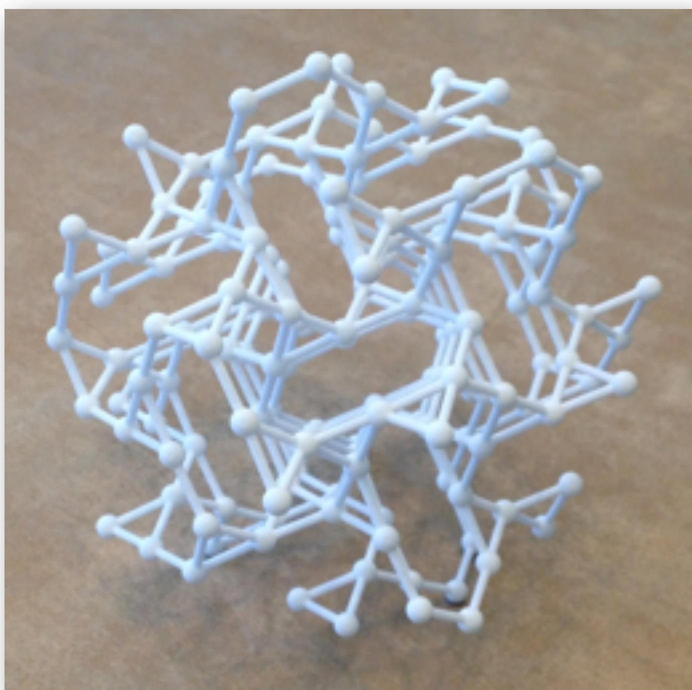
premedial lattice

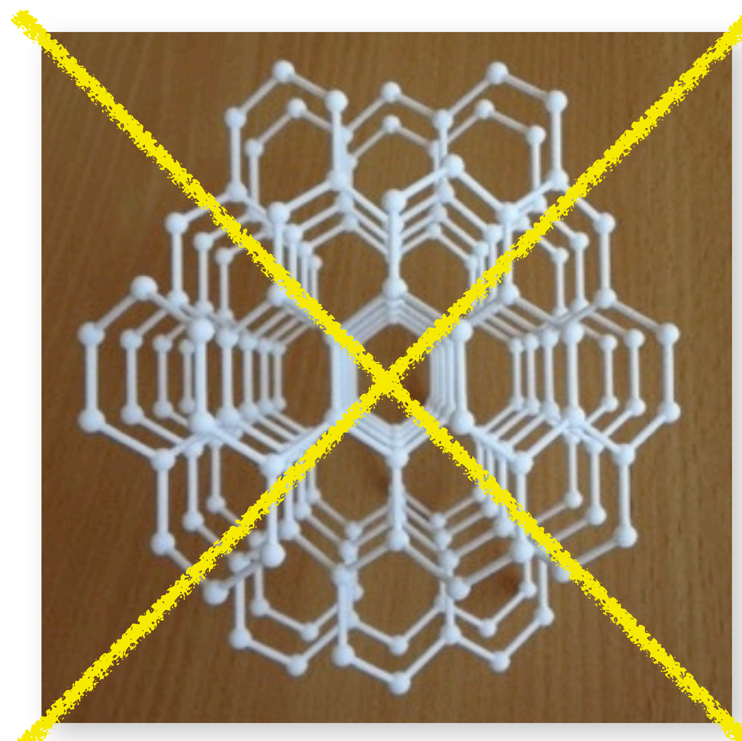
honeycomb lattice

Medial and premedial lattices

medial lattice
of triangles

hyperkagome → hyperhoneycomb





The hyperkagome is **chiral**.

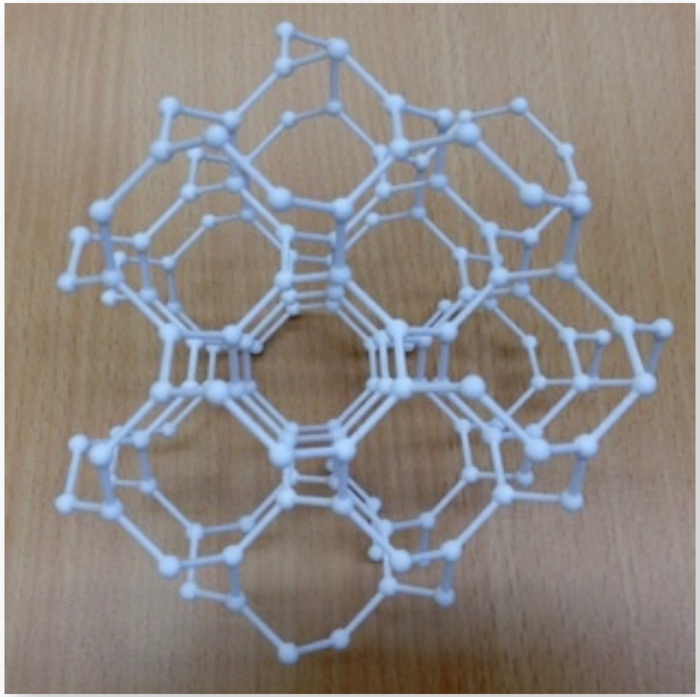
The hyperhoneycomb is **not chiral**!

Medial and premedial lattices

hyperkagome → hyperoctagon

medial lattice
of triangles

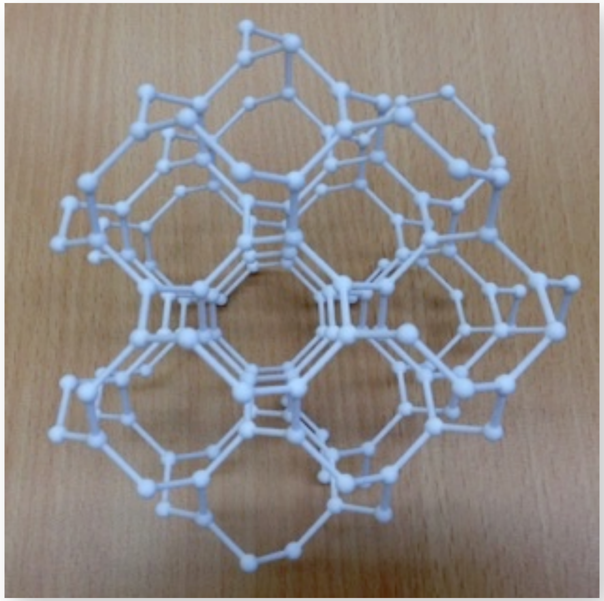
square-octagon projection



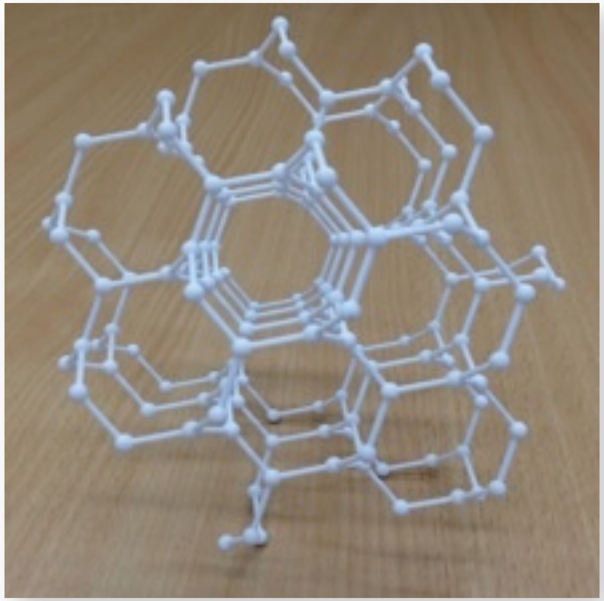
✓

square-octagon projection

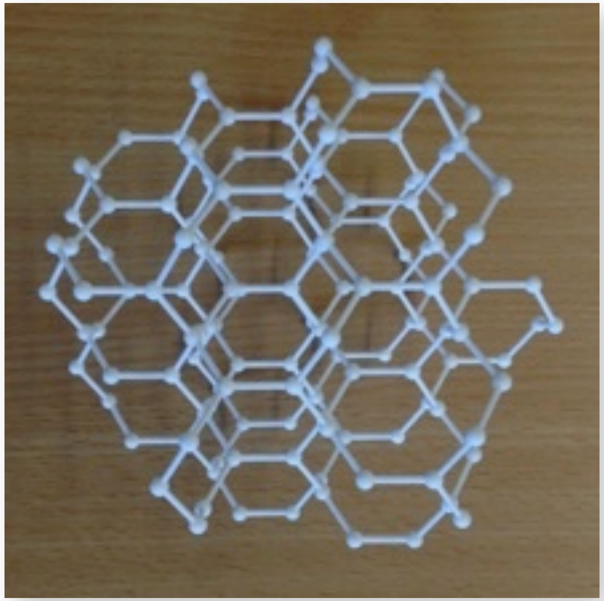
Hyperoctagon – space group symmetries



four-fold skew symmetry



three-fold symmetry



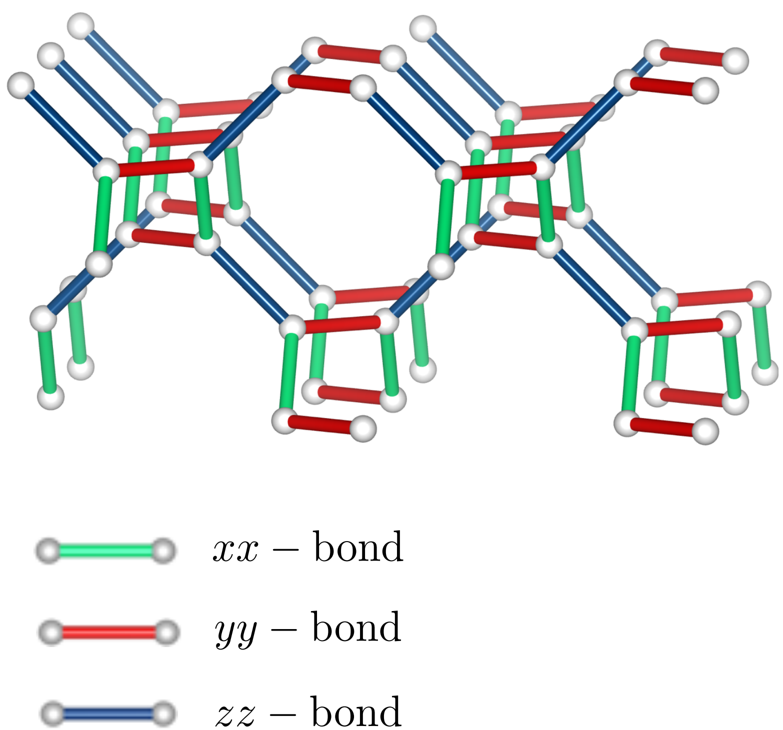
two-fold symmetry

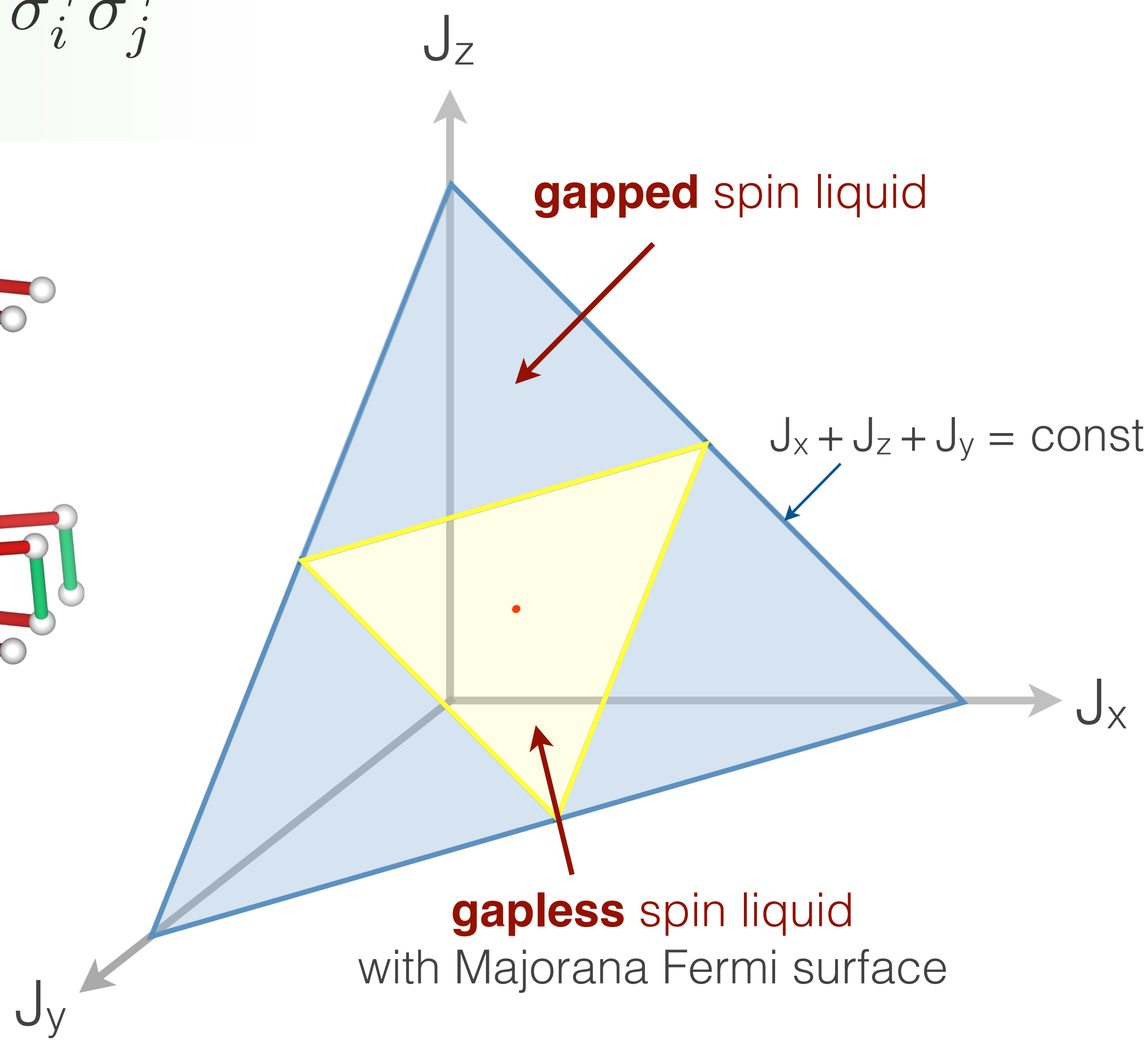
↓

space group **$I4_132$** (no. 214)

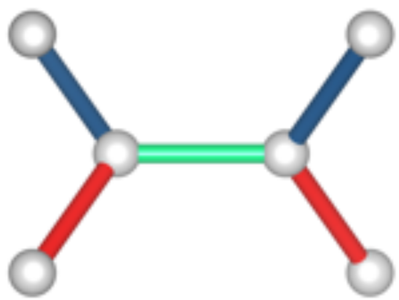
A three-dimensional Kitaev model

$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma$$

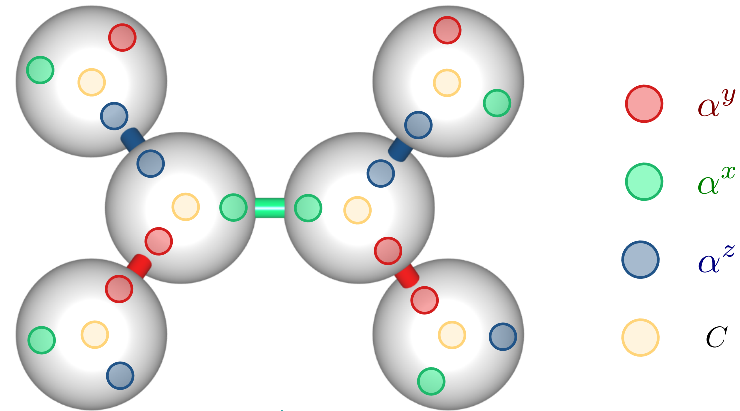




Let's solve this model



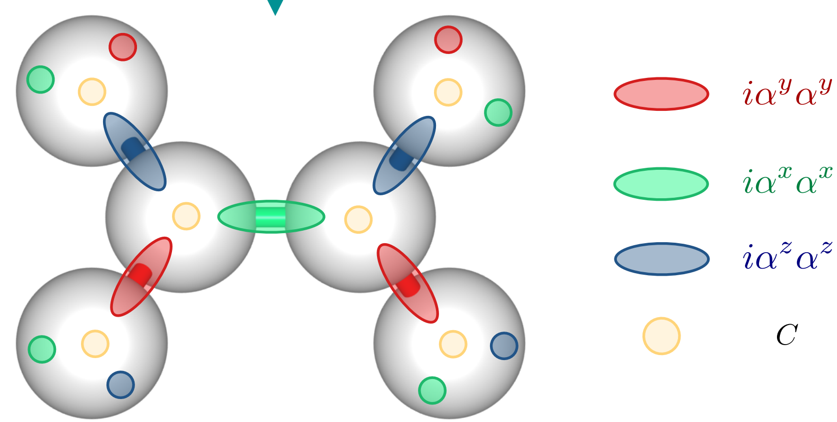
split spins



regroup
Majoranas

Step 1: Represent spins in terms of four **Majorana fermions** $\sigma^\alpha = i a^\alpha c$

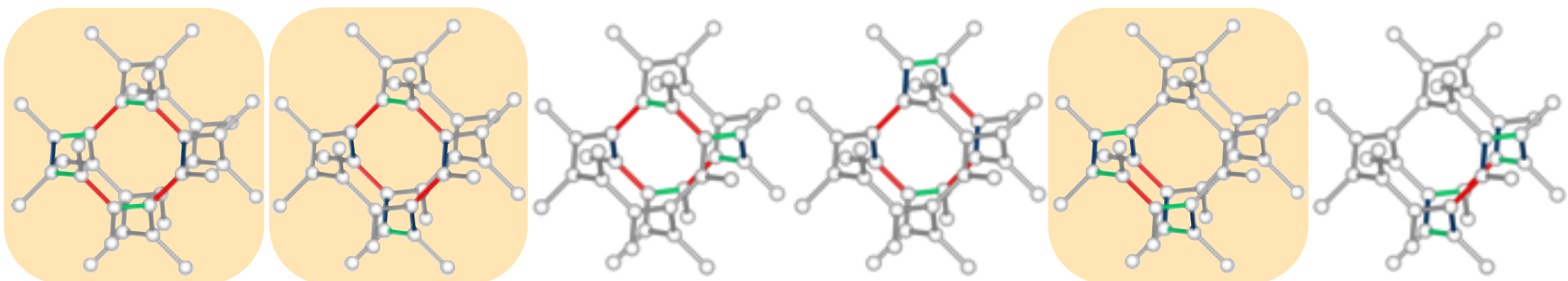
Step 2: Bond operators $\hat{u}_{jk} = i a_j^\alpha a_k^\alpha$ realize an emergent **Z_2 gauge field**



Physics of the Z_2 gauge field

Z_2 gauge field is **static** due to presence of additional conserved quantities

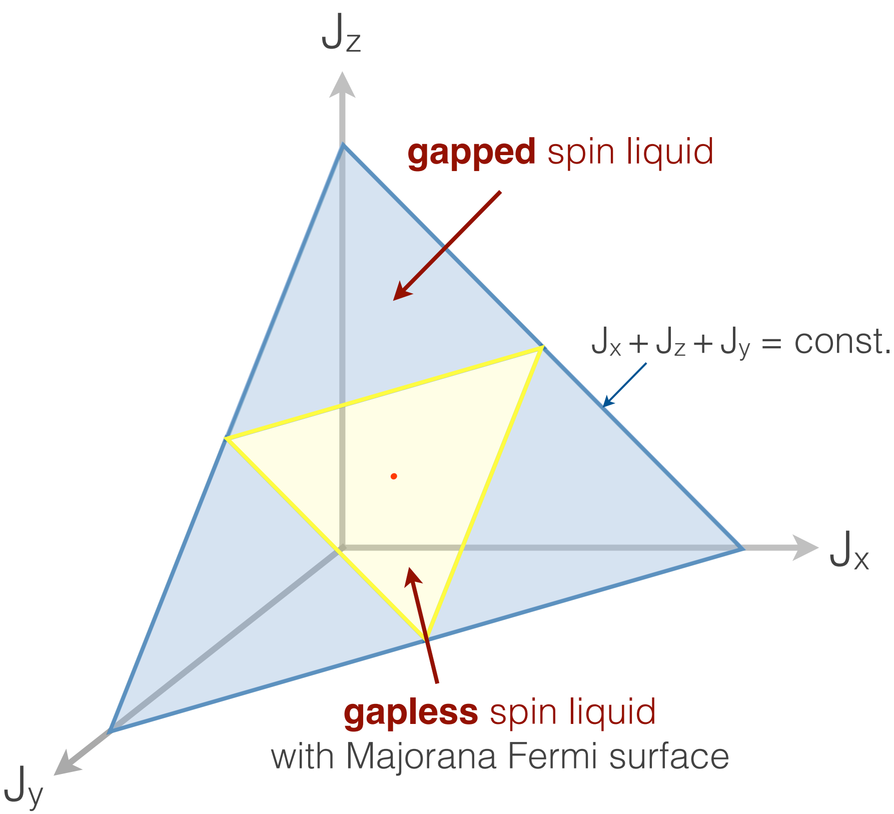
Six fundamental **loop operators** (per unit cell) $W_l = \prod_{\langle \alpha,\beta \rangle \in l} \sigma_\alpha^{\gamma_{\alpha\beta}} \sigma_\beta^{\gamma_{\alpha\beta}}$

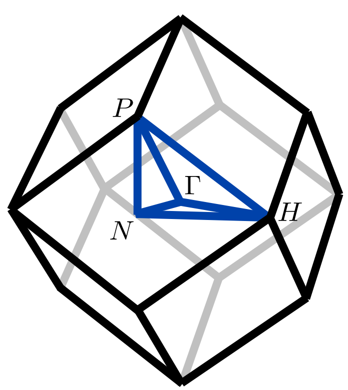


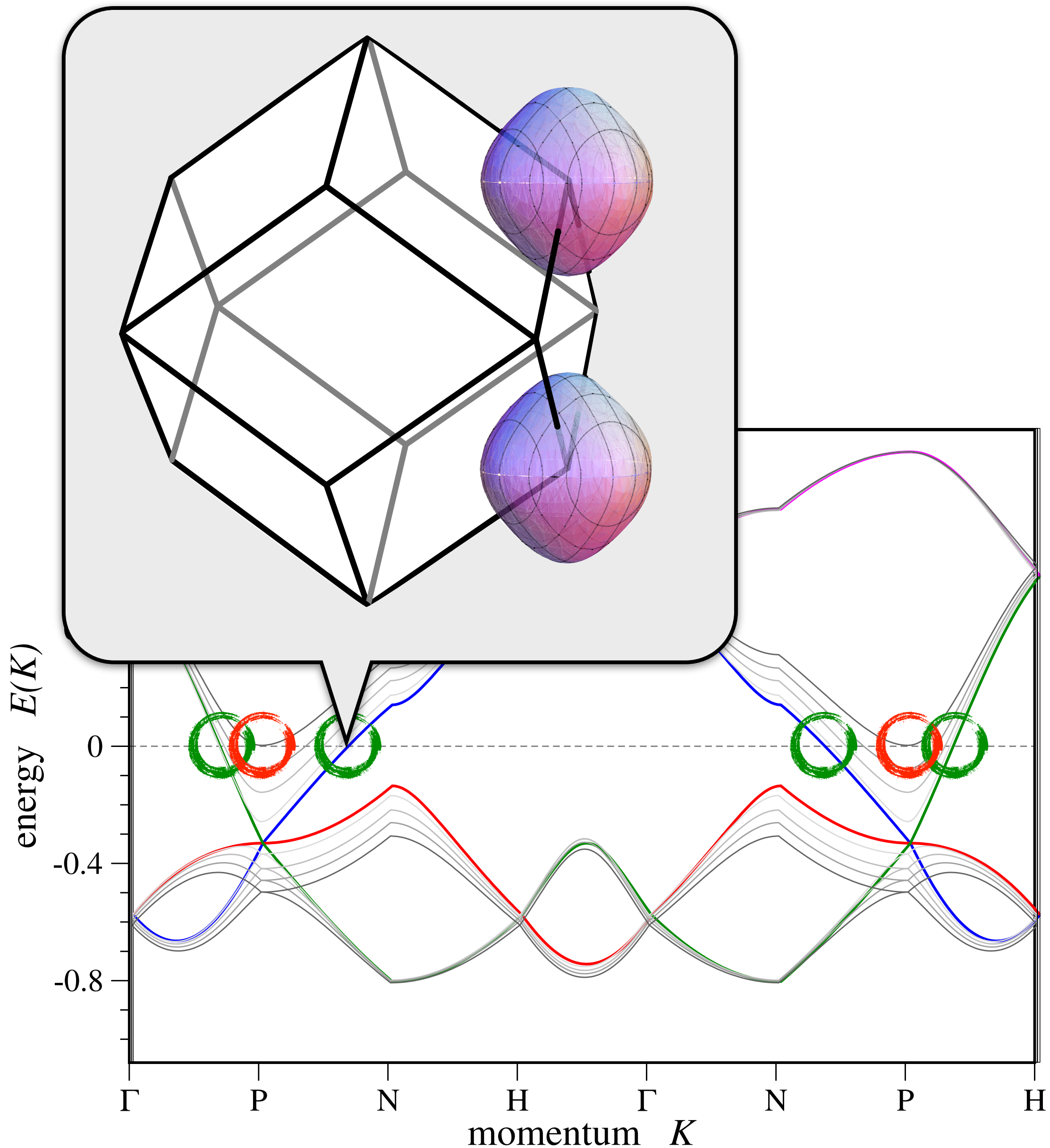
only two loop operators per unit cell are linearly independent

$$W_{l_a} W_{l_b} W_{l_c} = 1$$

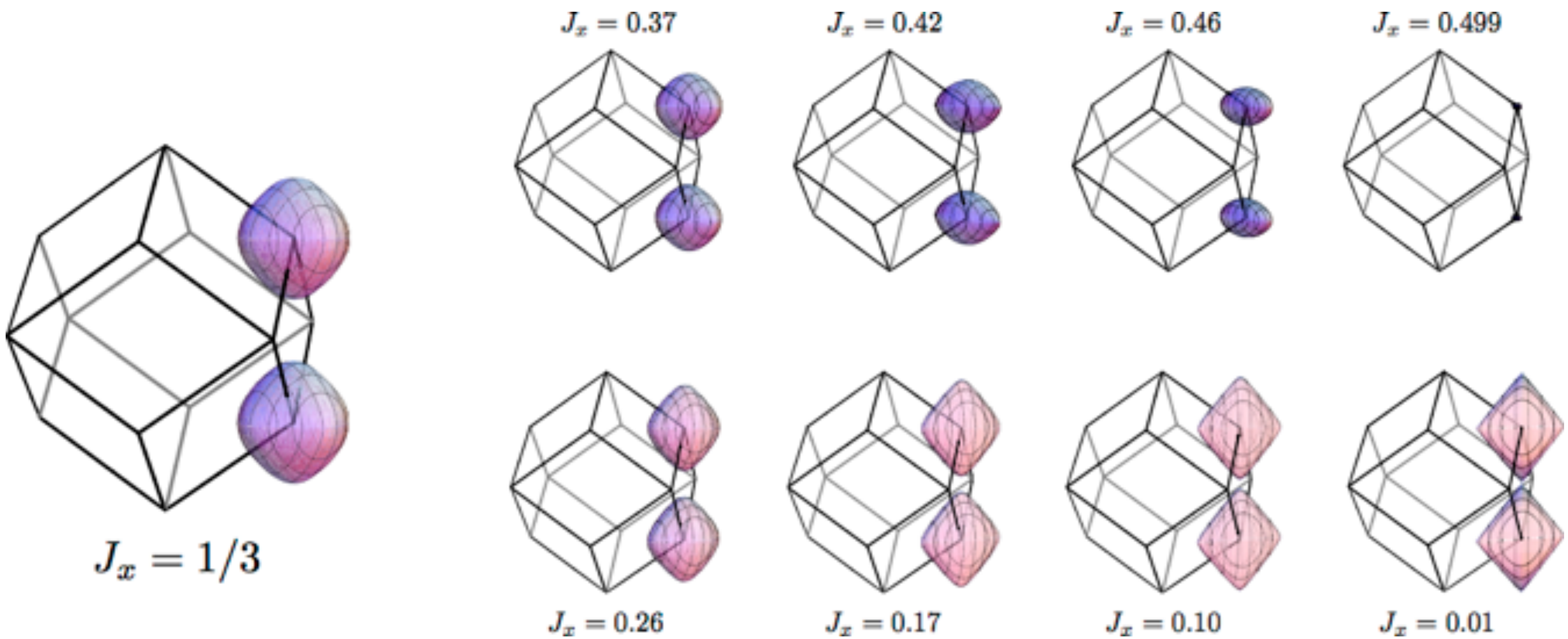
Majorana Fermi surface





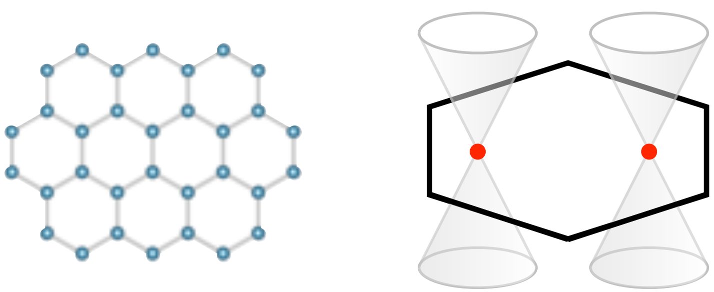


Majorana Fermi surface

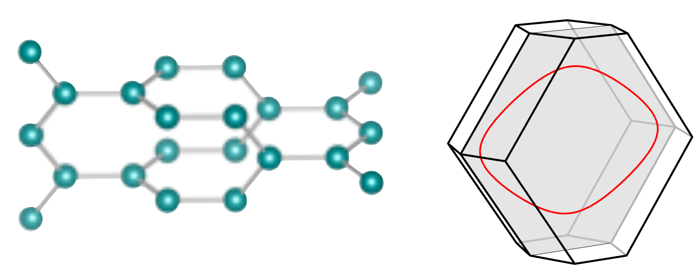


The hyperoctagon Kitaev model exhibits a full **two-dimensional Majorana Fermi surface**.

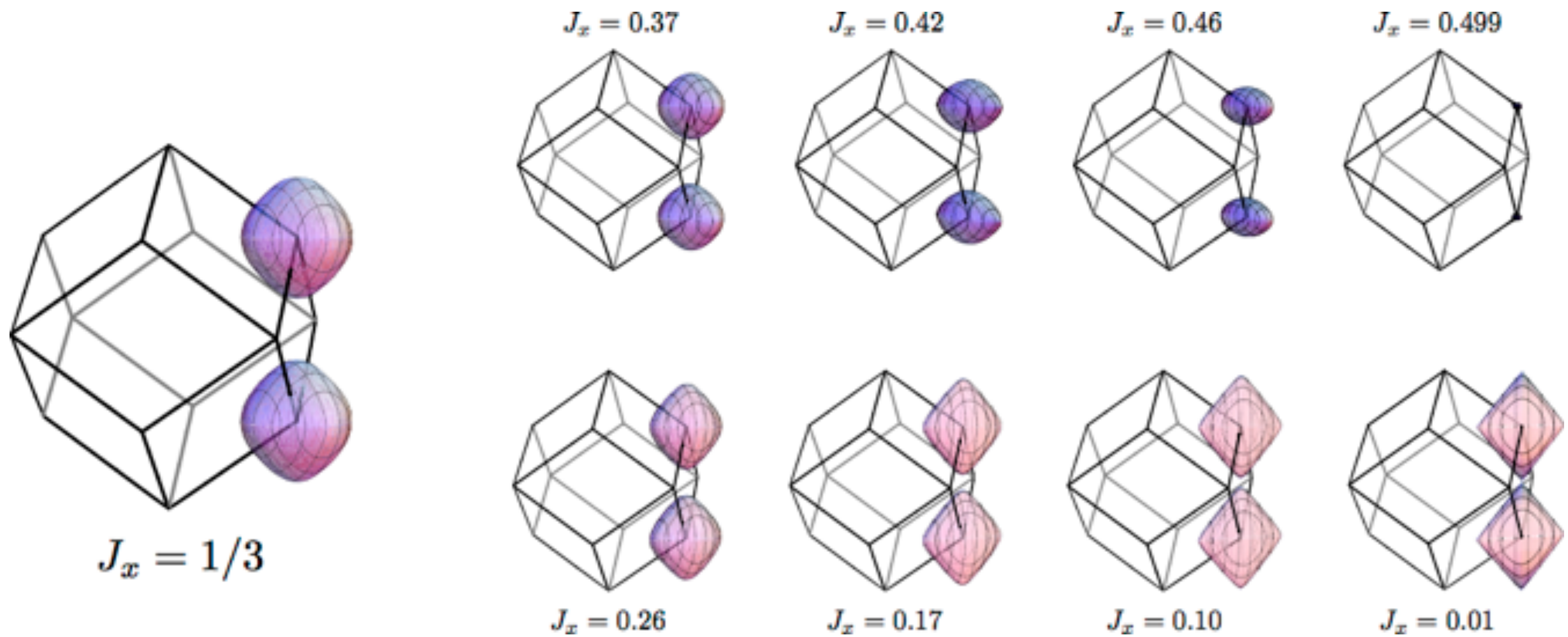
honeycomb – Fermi **points**



hyperhoneycomb – Fermi **lines**



Majorana Fermi surface



The hyperoctagon Kitaev model exhibits a full **two-dimensional Majorana Fermi surface**.

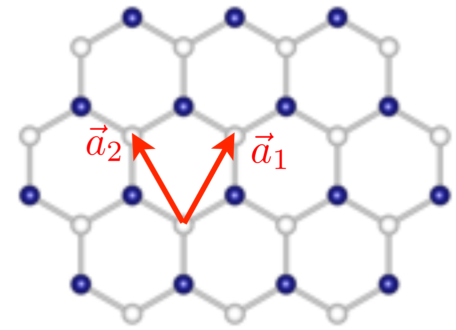
Recasting our result in the language of spin liquids, what we have found is the first **exactly solvable microscopic model** of a spin liquid with a **spinon Fermi surface**.

Why is the Fermi surface stable?

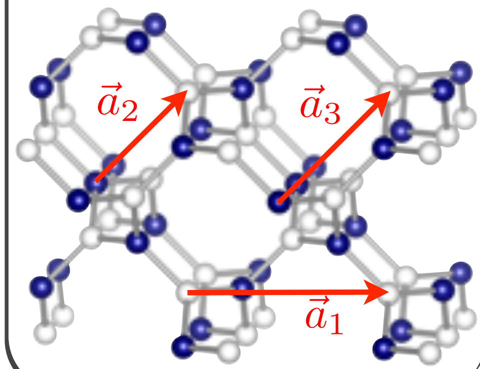
Symmetry relations

Particle-hole symmetry	$\epsilon(\mathbf{k}) = -\epsilon(-\mathbf{k})$
Sublattice symmetry	$\epsilon(\mathbf{k}) = -\epsilon(\mathbf{k} - \mathbf{k}_0)$
Time-reversal symmetry	$\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k} + \mathbf{k}_0)$
Inversion symmetry	$\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k} + \mathbf{k}_0)$

honeycomb lattice



hyperoctagon lattice



$\mathbf{k}_0$ is the reciprocal lattice vector
of the translation vector of the sublattice

Why is the Fermi surface stable?

Stability of gapless modes in the **honeycomb** model

$$H = \begin{pmatrix} \mathbf{0} & if(\mathbf{k}) \\ -if^\star(\mathbf{k}) & \mathbf{0} \end{pmatrix}$$

→ complex-valued function

$$E(\mathbf{k}) = \pm|f(\mathbf{k})|$$

Stability of gapless modes in the **hyperhoneycomb** model

$$H = \begin{pmatrix} \mathbf{0} & \mathbf{A} \\ \mathbf{A}^\dagger & \mathbf{0} \end{pmatrix}$$

→ complex matrix

$$E(\mathbf{k}) = \pm|\lambda_j(\mathbf{k})|$$

Stability of gapless modes in the **hyperoctagon** model

$$H = \begin{pmatrix} 0 & & \mathbf{A} \\ & \ddots & \\ \mathbf{A}^\dagger & & 0 \end{pmatrix}$$

→ generic band Hamiltonian with TR symmetry

However, there is only a **single** Majorana zero-mode at a given momentum.

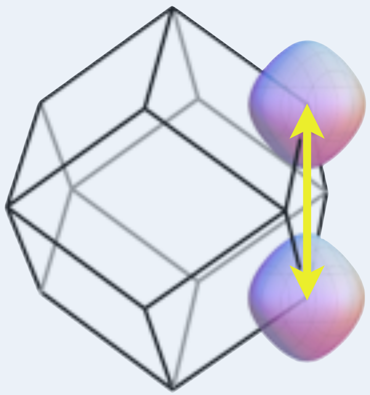
Peierls instability of Fermi surface

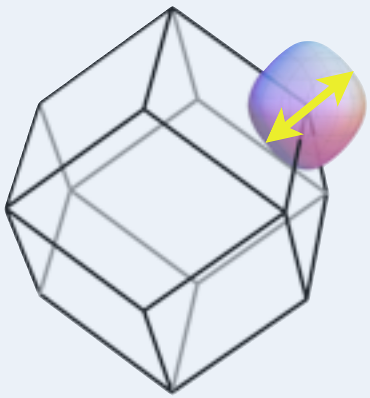
Fermi surface instabilities arise from additional spin interactions (e.g. a Heisenberg term), which introduce interactions between the Majorana fermions.

The generic instability is a **spin-Peierls instability**, i.e. the system spontaneously dimerizes at exponentially small temperatures and forms a spin liquid with a Fermi line.

Majorana fermions

perfect nesting
between the two surfaces





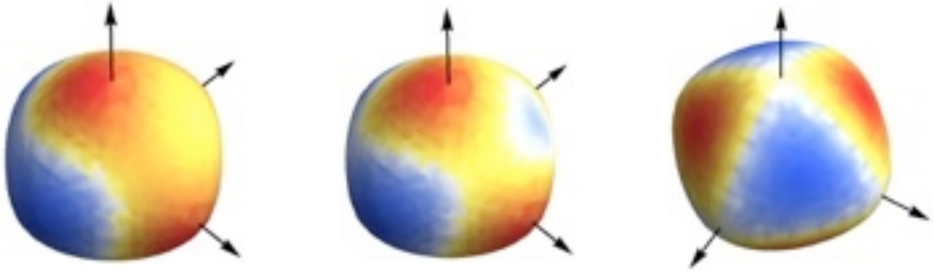
(complex) fermion

conventional
BCS instability

Generic form of the induced interactions between Majorana fermions

$$H_{\text{int}} = -U\Big(\cos\alpha \sum_{\vec{R}} c_1(\vec{R})c_2(\vec{R})c_3(\vec{R})c_1(\vec{R}+\vec{a}_2) + \sin\alpha \sum_{\vec{R}} c_1(\vec{R})c_2(\vec{R})c_3(\vec{R})c_4(\vec{R}) + \text{sym.}\Big)$$

order parameter distribution



M. Hermanns, S. Trebst & A. Rosch, in preparation

Experimental signatures?

correlation functions

spin-spin correlations $\langle S_i^z S_j^z \rangle$ decay exponentially.

bond-bond energy correlations $\langle (S_i^z)^2 (S_j^z)^2 \rangle$ exhibit algebraic divergence on Majorana Fermi surface.

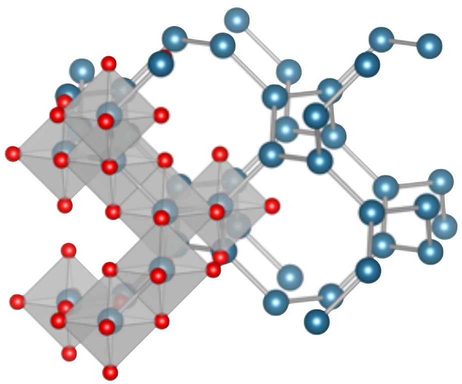
specific heat

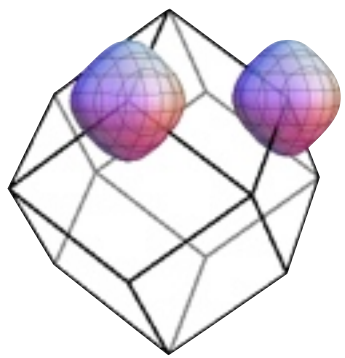
U(1) spin liquid	$C(T) \propto T \ln(1/T)$	γ = C/T diverges
Z_2 spin liquid with spinon Fermi surface	$C(T) \propto T$	γ = C/T constant
Z_2 spin liquid with spinon Fermi line	$C(T) \propto T^2$	γ = C/T vanishes

Breaking time-reversal symmetry

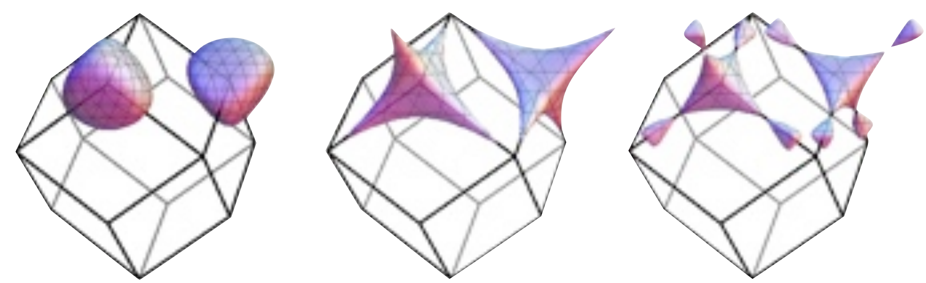
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma - \sum_j \vec{h} \cdot \vec{\sigma}_j$$

hyper-octagon





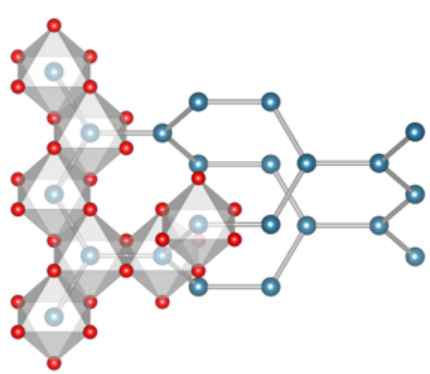
Fermi **surface**

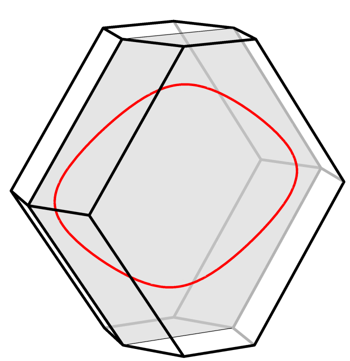


$\kappa = 0.1$ $\kappa = 0.5$ $\kappa = 0.75$

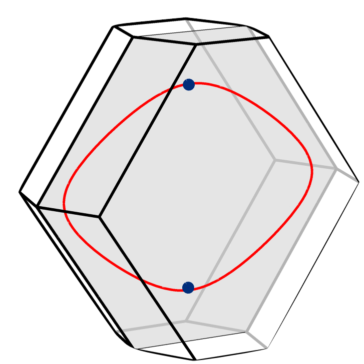
Fermi surface **deforms**

hyper-honeycomb





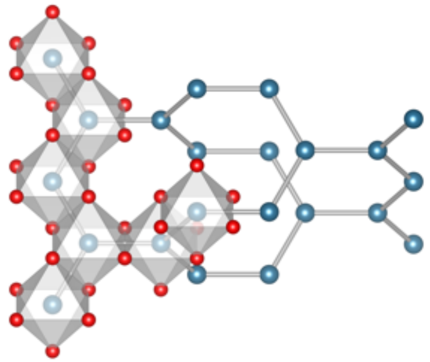
Fermi **line**



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

Weyl physics – energy spectrum

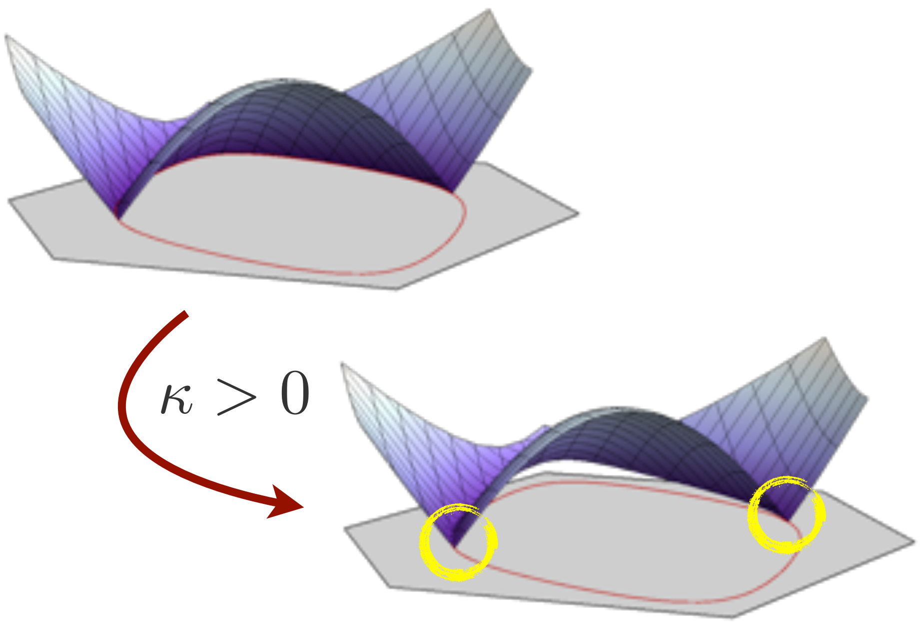
hyper-honeycomb

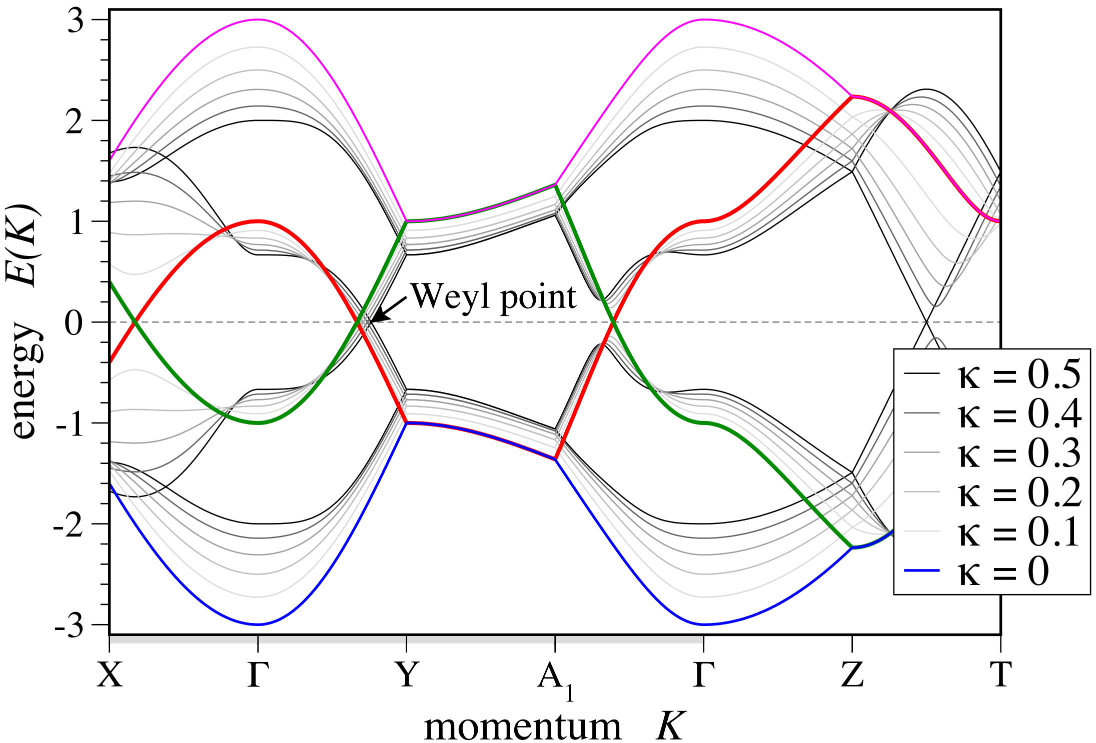


Touching of two bands in 3D is generically **linear**

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

Weyl nodes



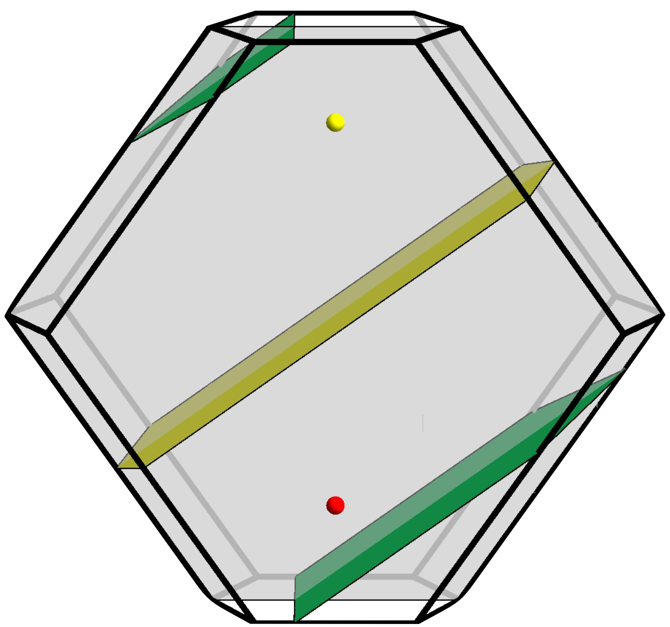


Weyl physics – Chern numbers

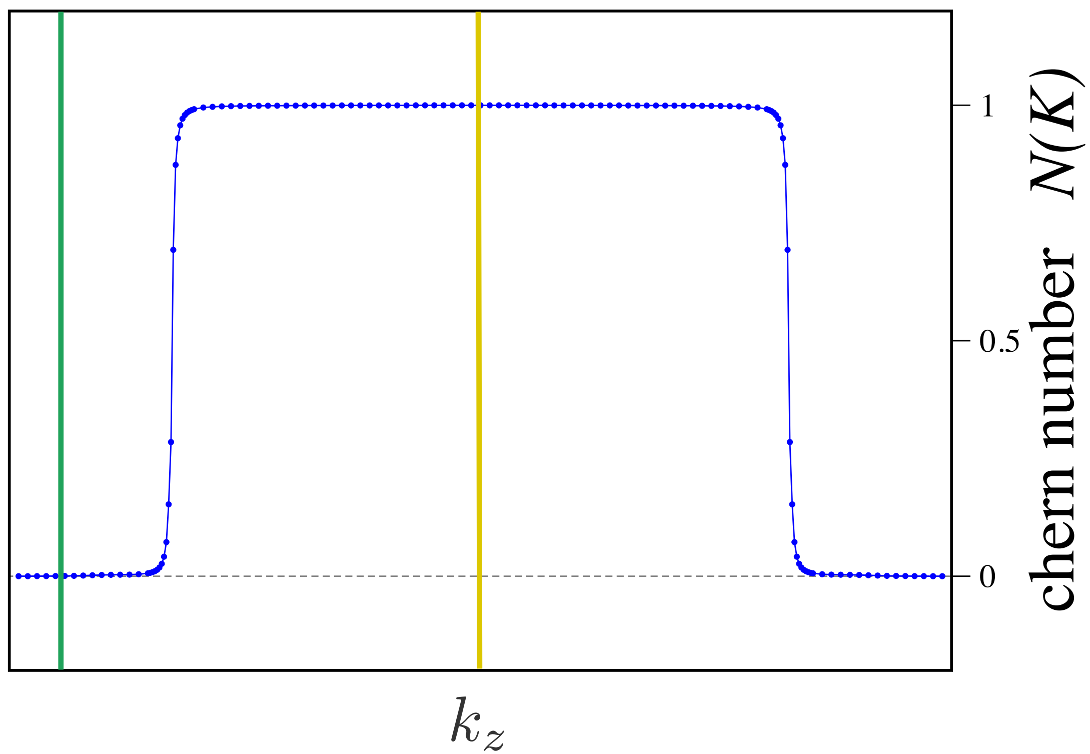
Weyl nodes are **sources or sinks of Berry flux**

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

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



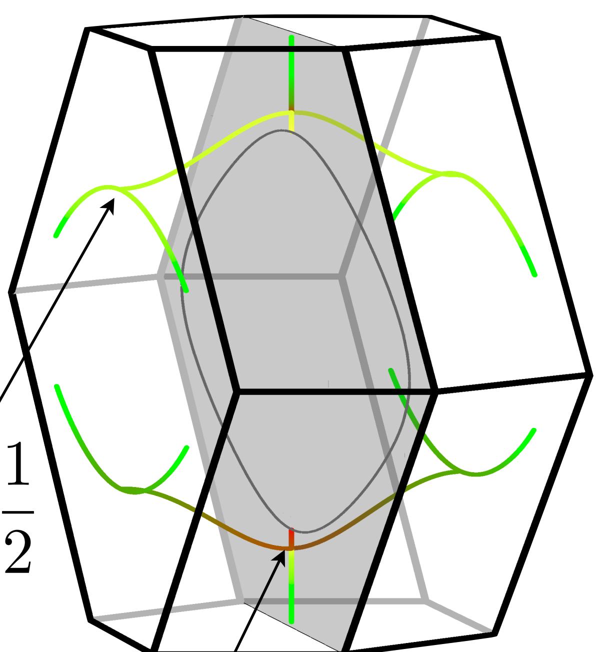
$\kappa = 0.05$



Weyl physics – surface states

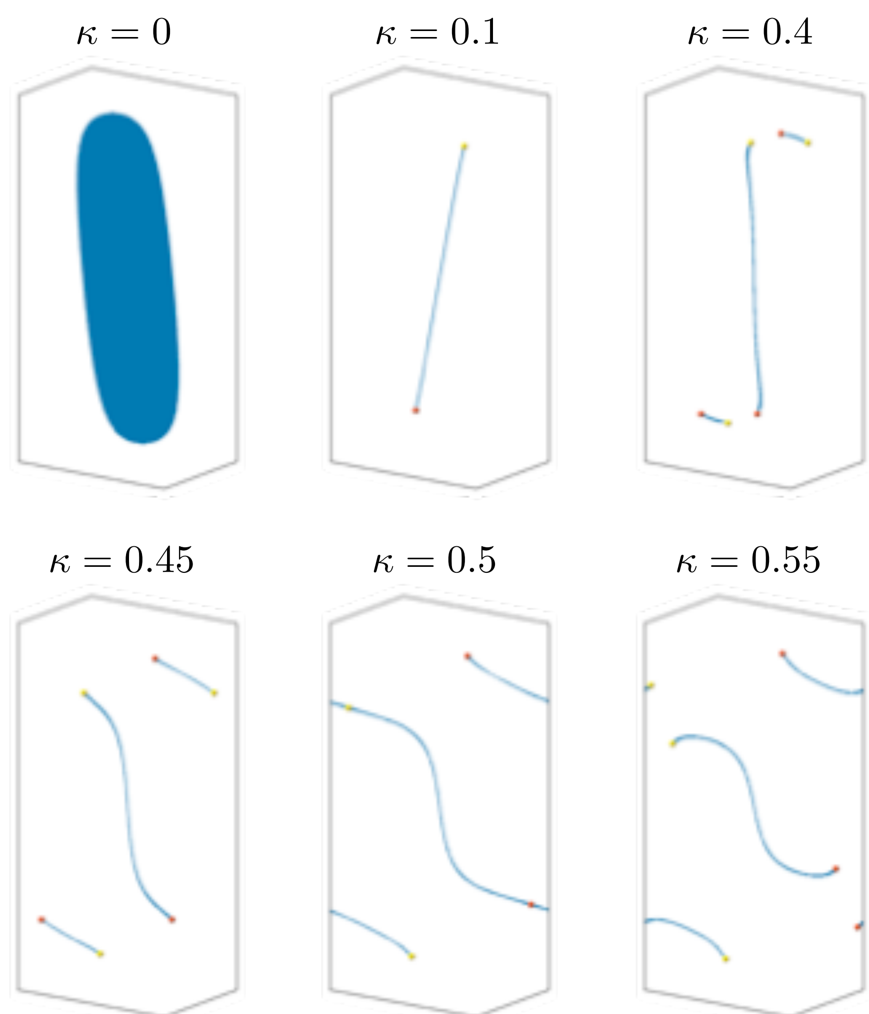
evolution of **Weyl nodes**
in the **bulk**

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



$\kappa = \frac{1}{2}$

$\kappa = \frac{1}{2}\sqrt{\frac{3}{5}} \approx 0.39$



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).

Summary

PRB 89, 235102 (2014)
arXiv:1411.7379

Spin-orbit entangled j=1/2 Mott insulators in Li_2IrO_3 realize two- and three-dimensional **Kitaev models**.

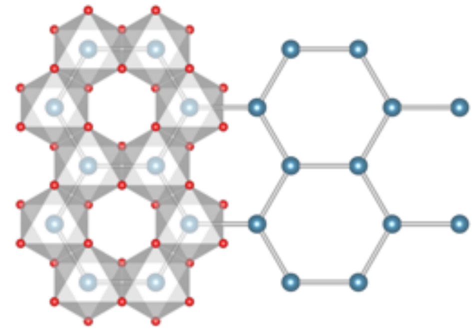
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma$$

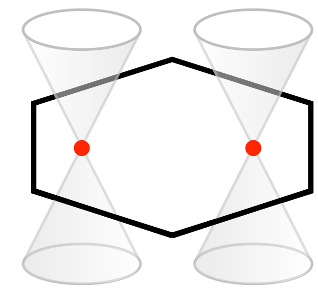
Kitaev models are paradigmatic examples for **spin fractionalization**.

spin-1/2 $\sigma_j^\gamma = i\, b_j^\gamma c_j$ Majorana fermion + Z_2 gauge field

Emergent Majorana fermions form a remarkably **rich variety of Majorana metals** reflecting the underlying lattice structure.

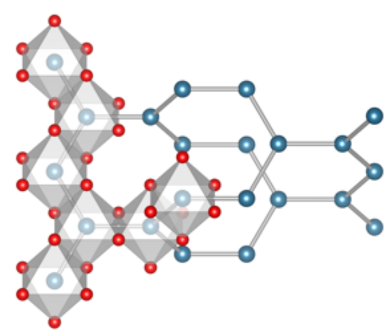
hexagonal layers

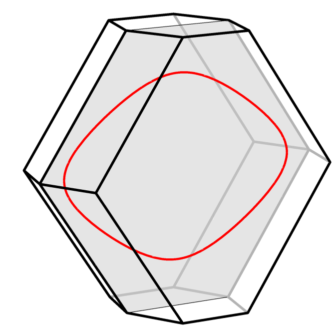




Dirac **points**

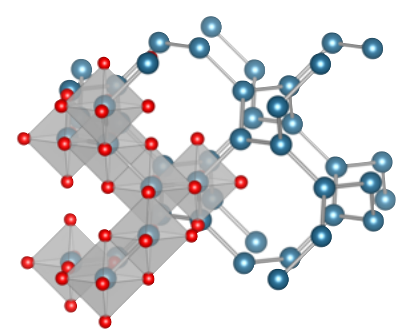
hyper-honeycomb

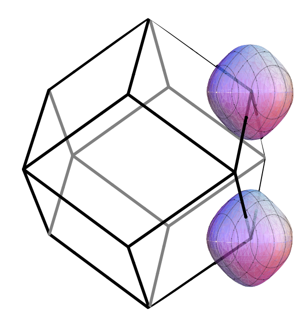




Fermi **lines**
Weyl **nodes** + Fermi **arcs**

hyper-octagon





Fermi **surfaces**