Collective spin-orbital states in j=1/2 Mott insulators

Majorana metal on the hyperoctagon lattice

DPG Spring Meeting Dresden, April 2014

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University of Cologne

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University of Cologne

arXiv:1401.7678

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  (= the medial lattice of the hyperkagome lattice).

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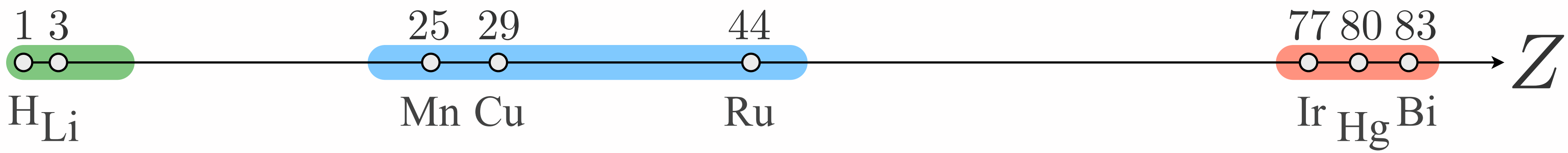
- The model is a **Kitaev model** on a 3D tri-coordinated lattice which we dubbed the **hyperoctagon lattice**
  (= the medial lattice of the hyperkagome lattice).

- Our original motivation to look into this is rooted in the physics of certain **spin-orbit entangled Iridates**
  (= really "heavy" 5d transition metal oxides).

Spin-orbit entanglement



$\lambda \propto Z^4$ $\frac{1}{2}$ 1 5 50 58 67

weak SOC	**moderate** SOC		**strong** SOC	
atomic fine structure	multiferroics	unconventional superconductors	SO-assisted Mott physics	topological insulators
	$TbMnO_3$	Sr_2RuO_4	Sr_2IrO_4 $Na_4Ir_3O_8$ $(Na,Li)_2IrO_3$	HgTe Bi_2Se_3

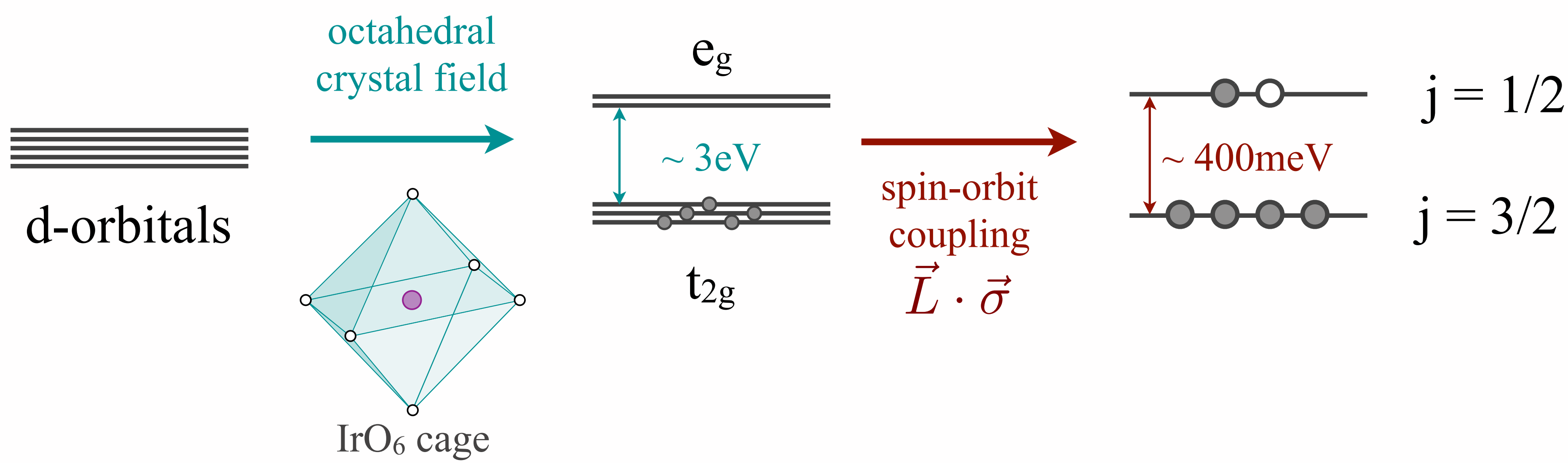
SOC induced DM interaction competes with **magnetic exchange**

SOC competes directly with **Hubbard physics**

Spin-orbit entanglement in Iridates

most common
Iridium valence

Ir^{4+} $(5d^5)$



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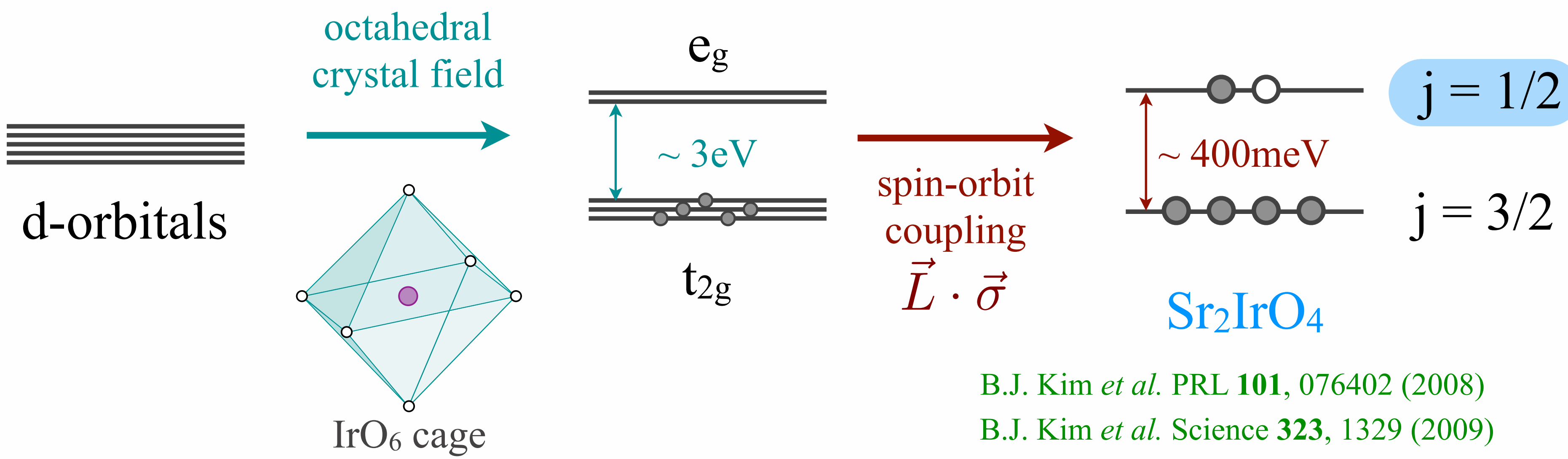


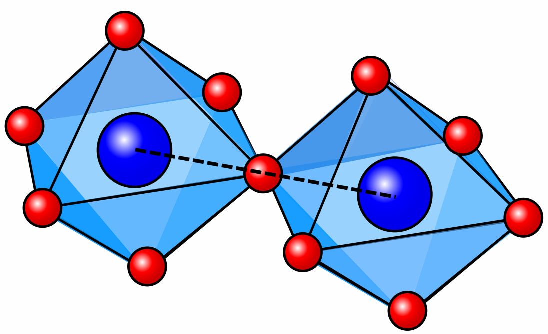
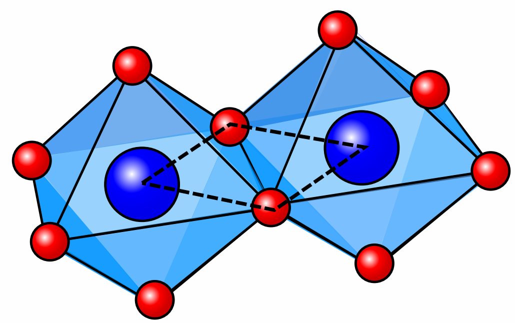
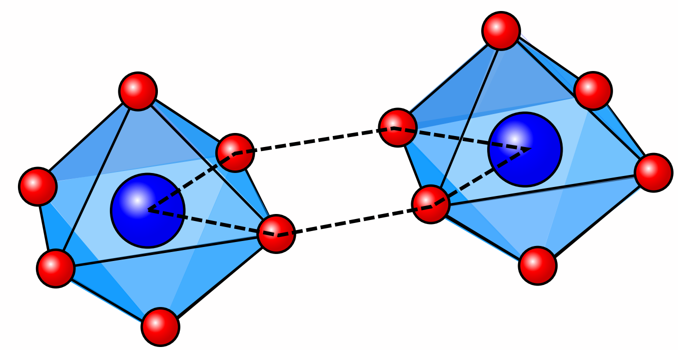
B.J. Kim *et al.* PRL **101**, 076402 (2008)
B.J. Kim *et al.* Science **323**, 1329 (2009)

$(Na,Li)_2IrO_3$

Iridates – microscopic exchange

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

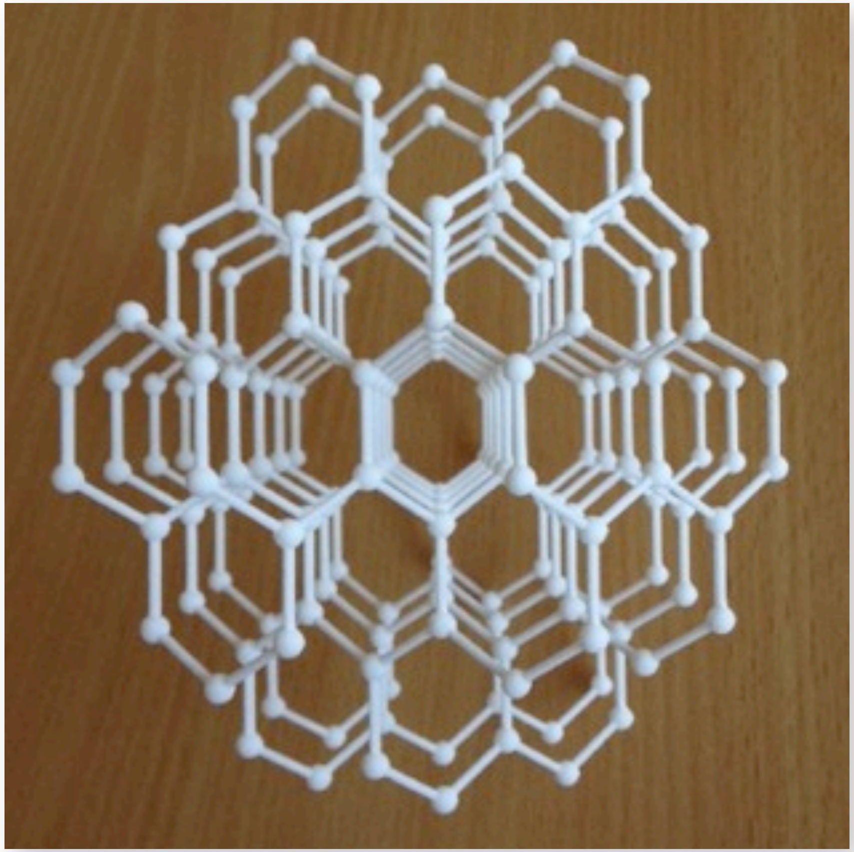
corner-sharing	edge-sharing	"parallel edge"-sharing
		
Sr_2IrO_4	$(Na,Li)_2IrO_3$	$Ba_3IrTi_2O_9$
square lattice	**honeycomb** lattices	**triangular** lattice

Heisenberg exchange

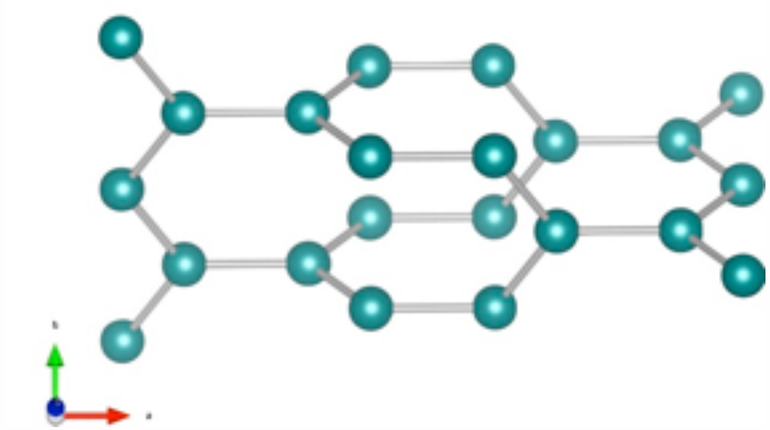
Heisenberg-Kitaev exchange

The hyperhoneycomb lattice

β-Li_2IrO_3



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



novel crystalline form of Li_2IrO_3

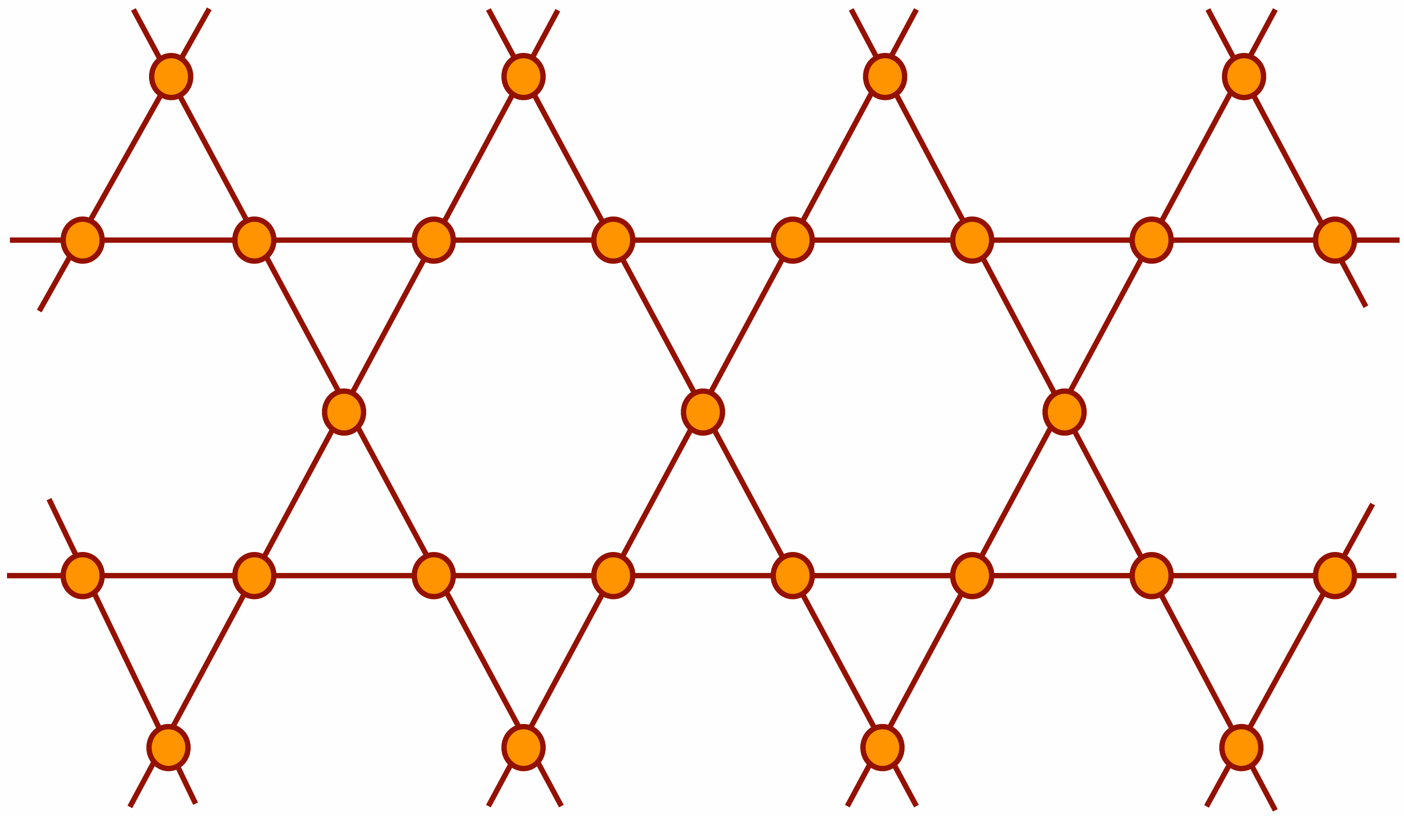
Hide Takagi's group, summer '13 arXiv:1403.3296

James Analytis's group, spring '14 arXiv:1402.3254

truly **3D tricoordinated** Ir lattice

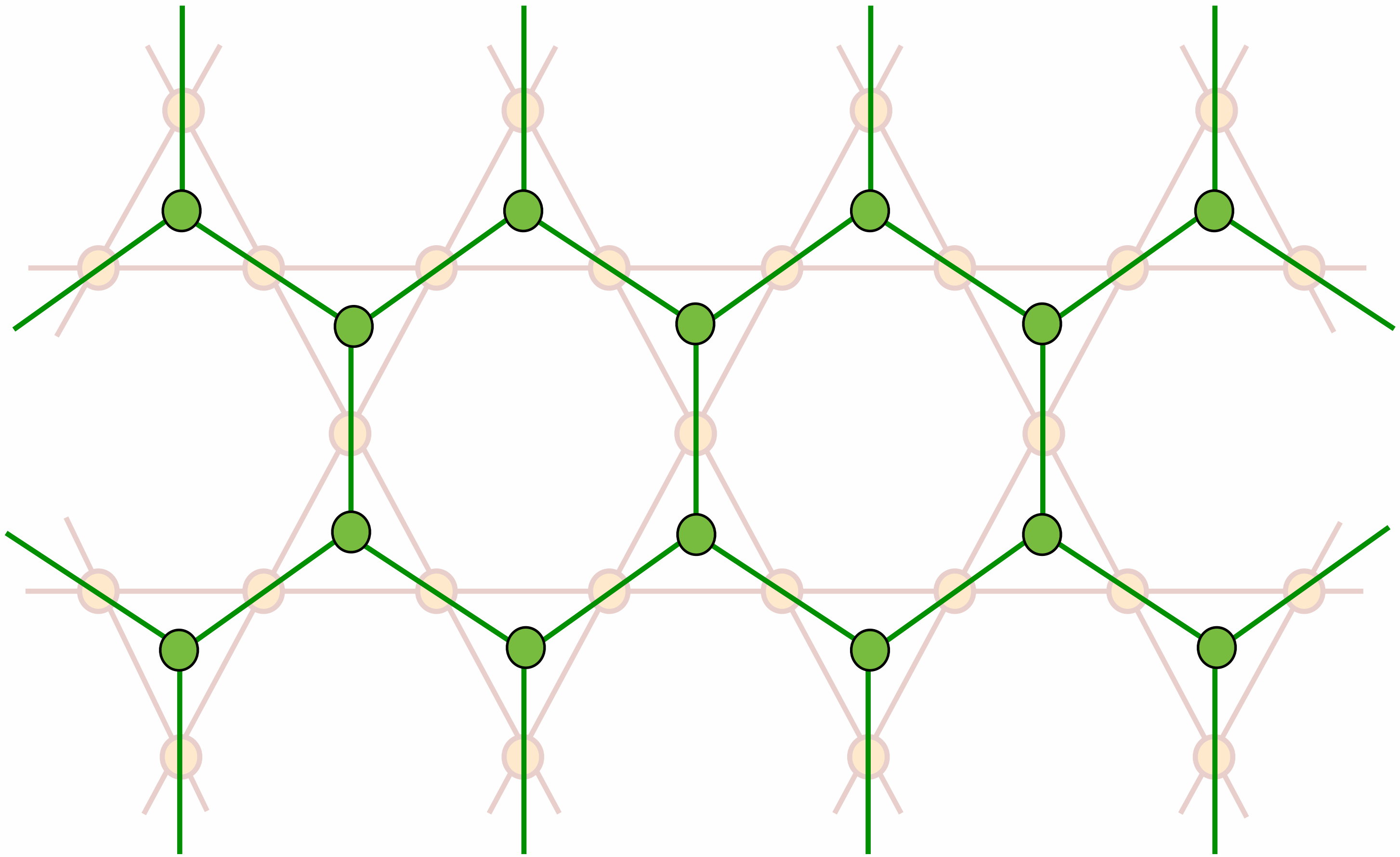
space group **Fddd** (no. 70)

Medial and premedial lattices



kagome lattice

Medial and premedial lattices

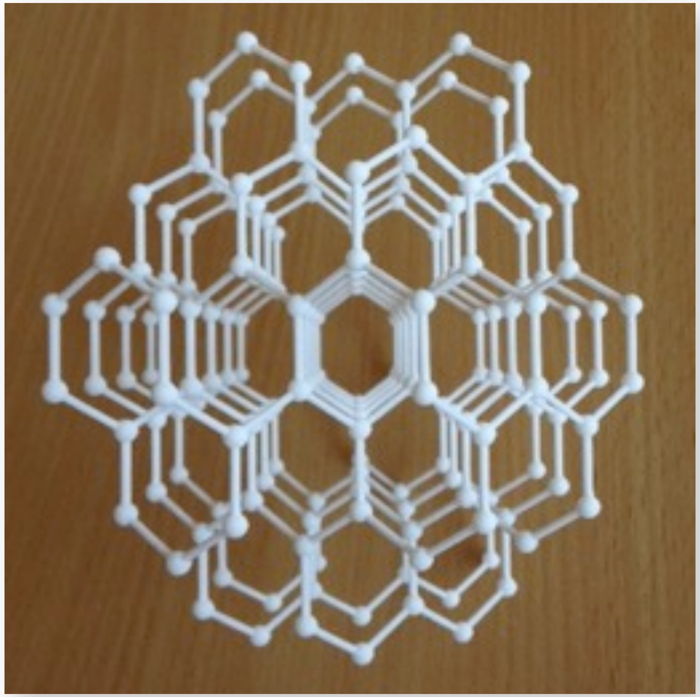


kagome lattice — medial lattice → / ← premedial lattice — honeycomb lattice

Medial and premedial lattices

medial lattice
of triangles

hyperkagome → hyperhoneycomb

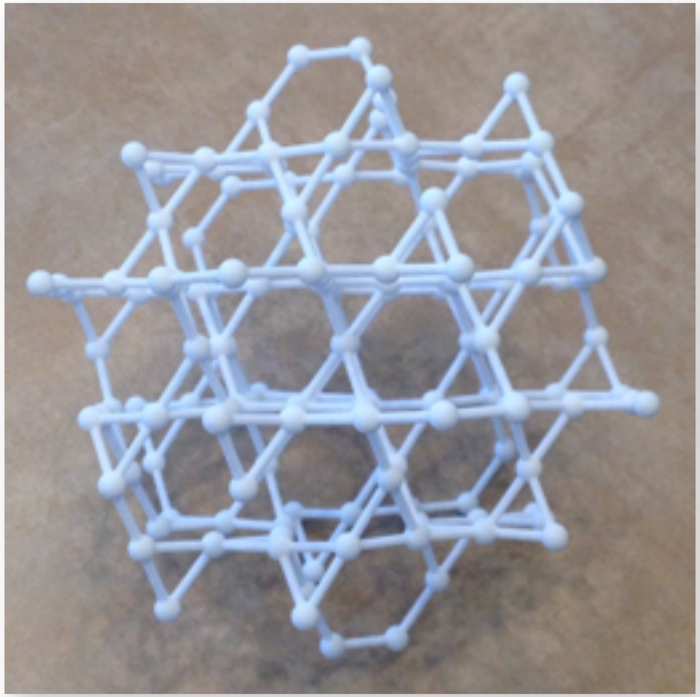


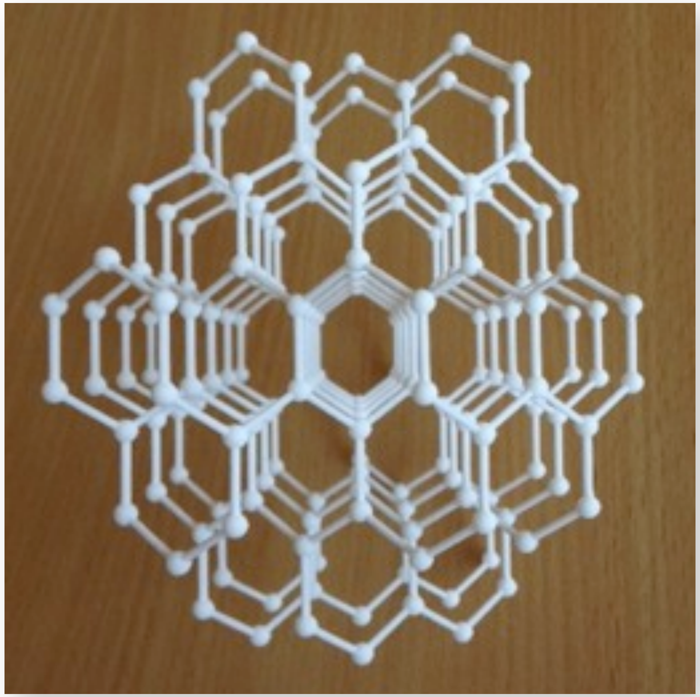
Medial and premedial lattices

hyperkagome

medial lattice
of triangles

hyperhoneycomb





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medial lattice of triangles

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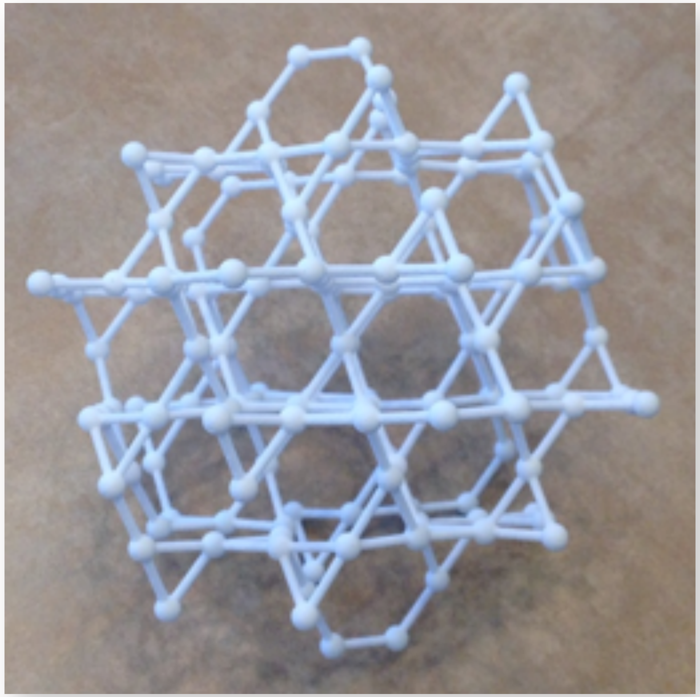

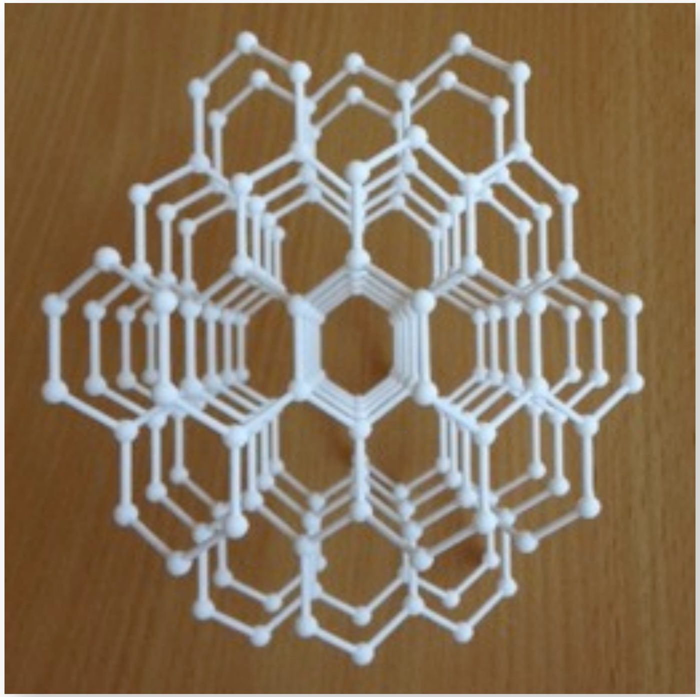

The hyperkagome is **chiral**.

Medial and premedial lattices

medial lattice
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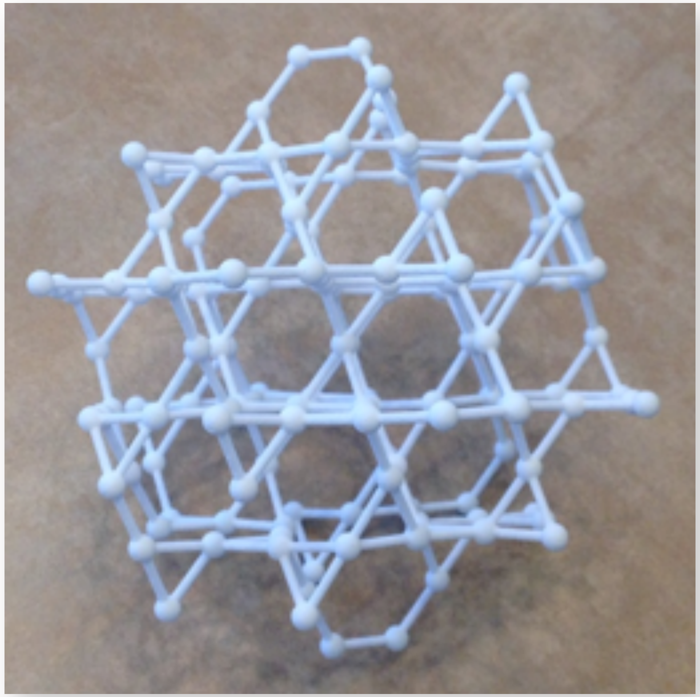

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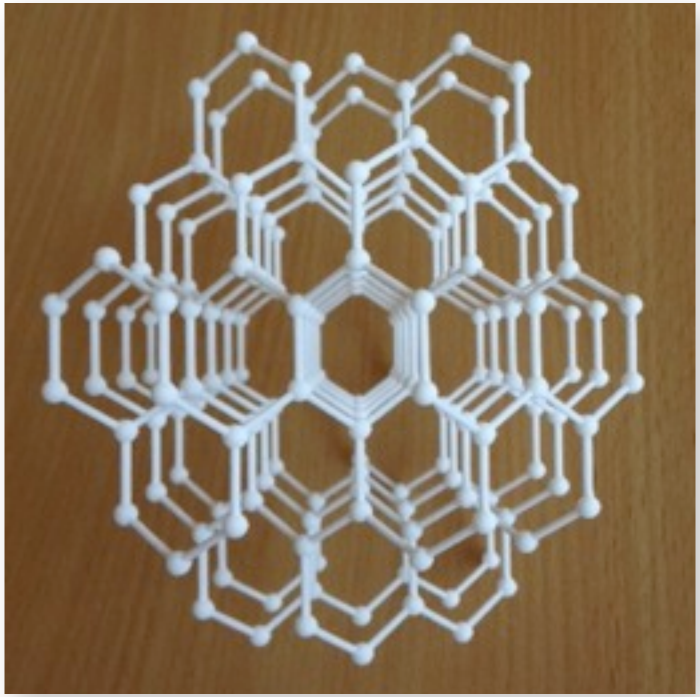

The hyperhoneycomb is **not chiral!**

Medial and premedial lattices

medial lattice
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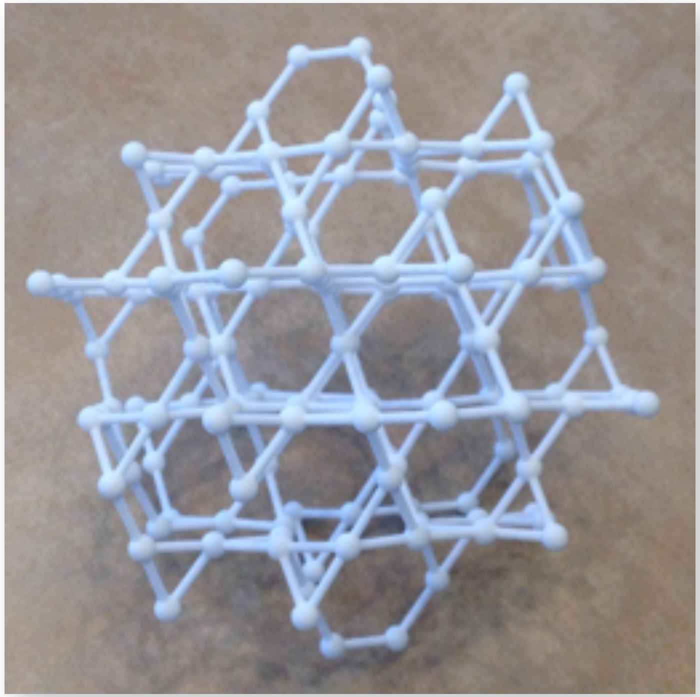
hyperkagome → hyperhoneycomb



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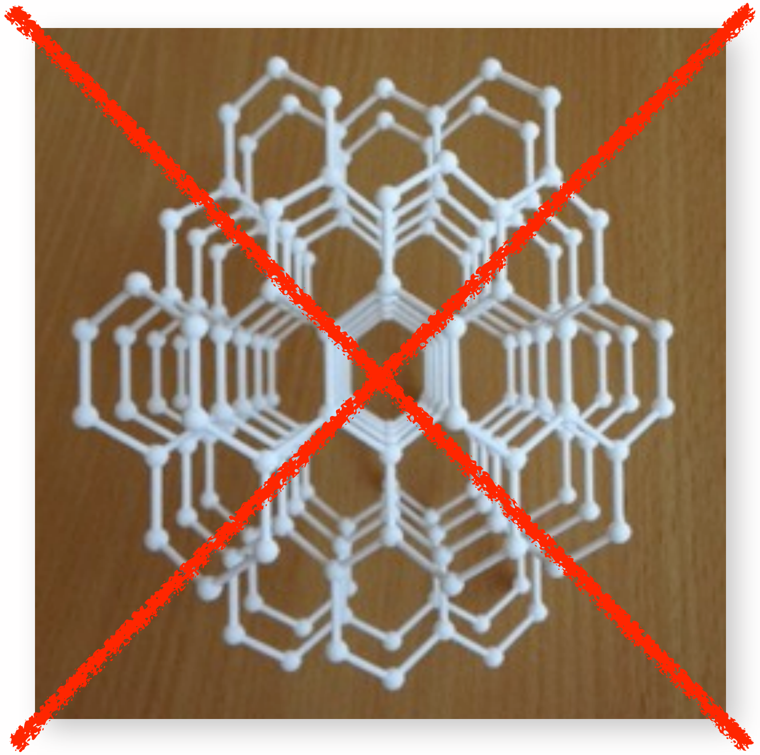

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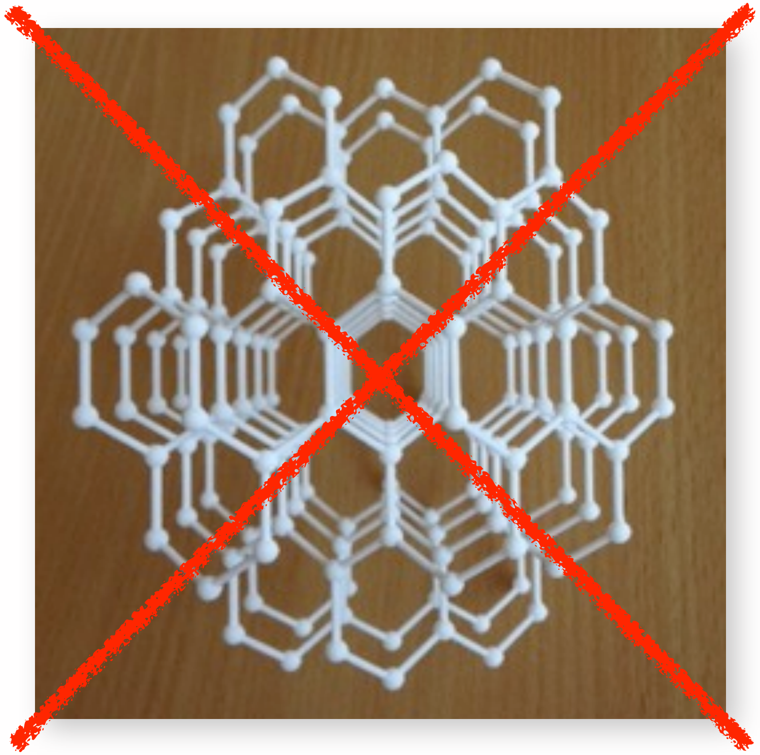
Medial and premedial lattices

medial lattice
of triangles

hyperkagome → hyperhoneycomb

square-octagon projection



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Medial and premedial lattices

medial lattice
of triangles

hyperkagome → hyperoctagon

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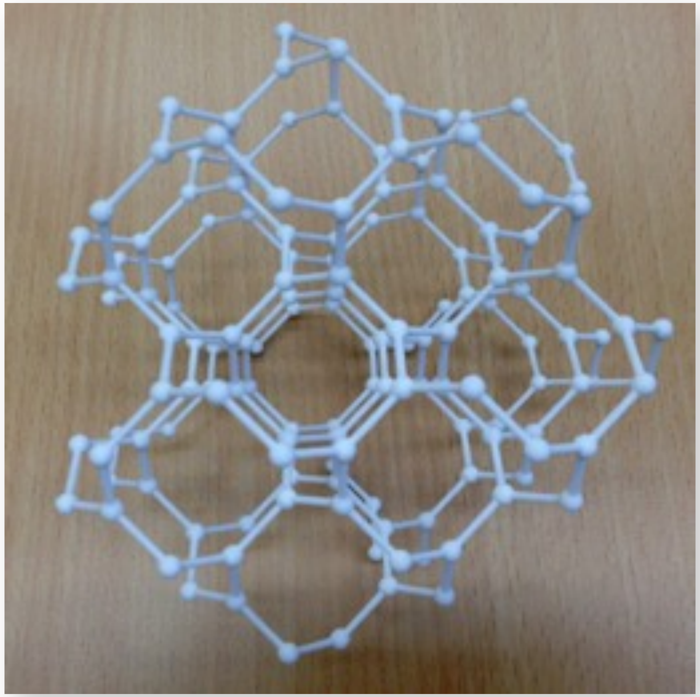
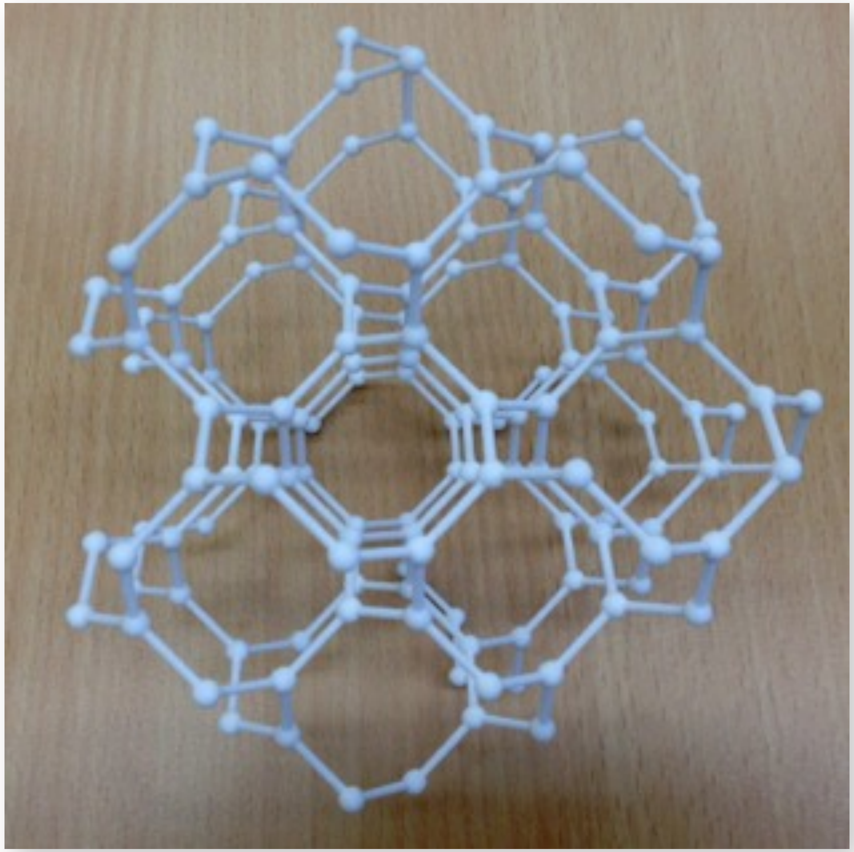


✓

square-octagon projection

The hyperoctagon lattice

γ-Li_2IrO_3



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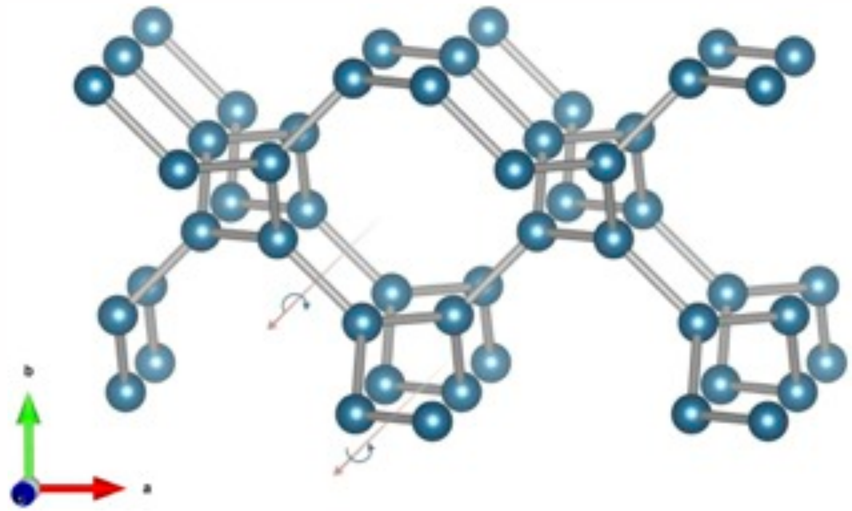
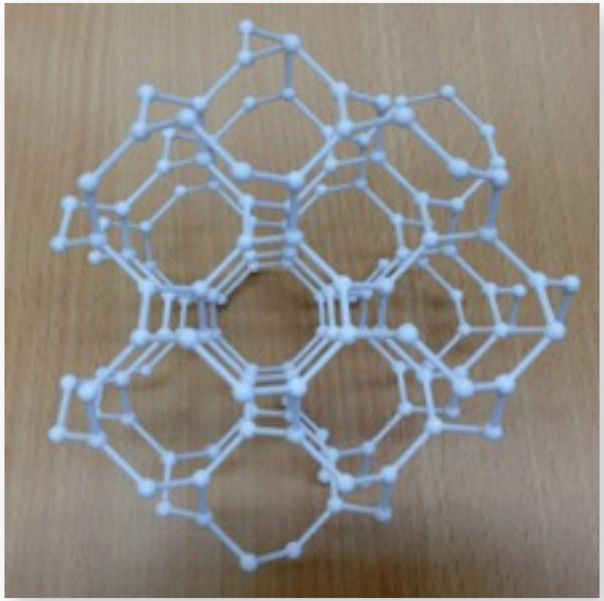


truly **3D tricoordinated** Ir lattice

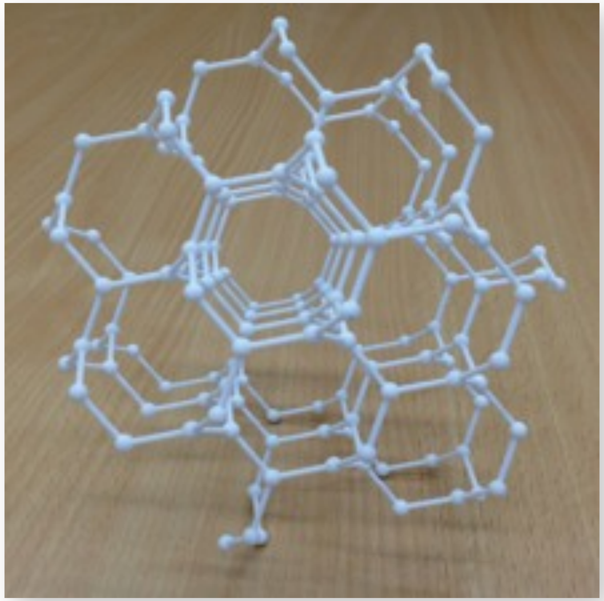
space group **$I4_132$** (no. 214)

possibly third crystalline form of Li_2IrO_3

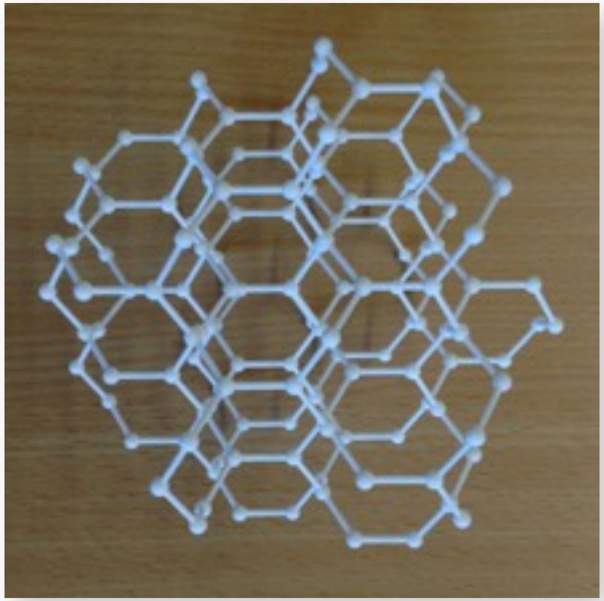
Hyperoctagon – space group symmetries



four-fold skew symmetry



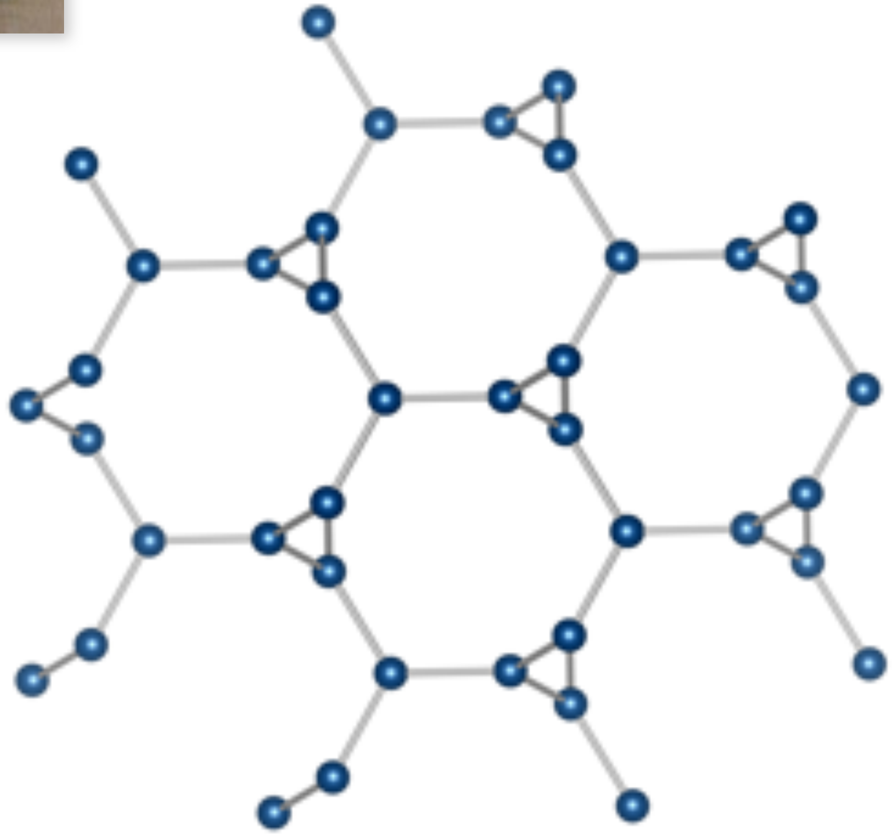
three-fold symmetry



two-fold symmetry

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

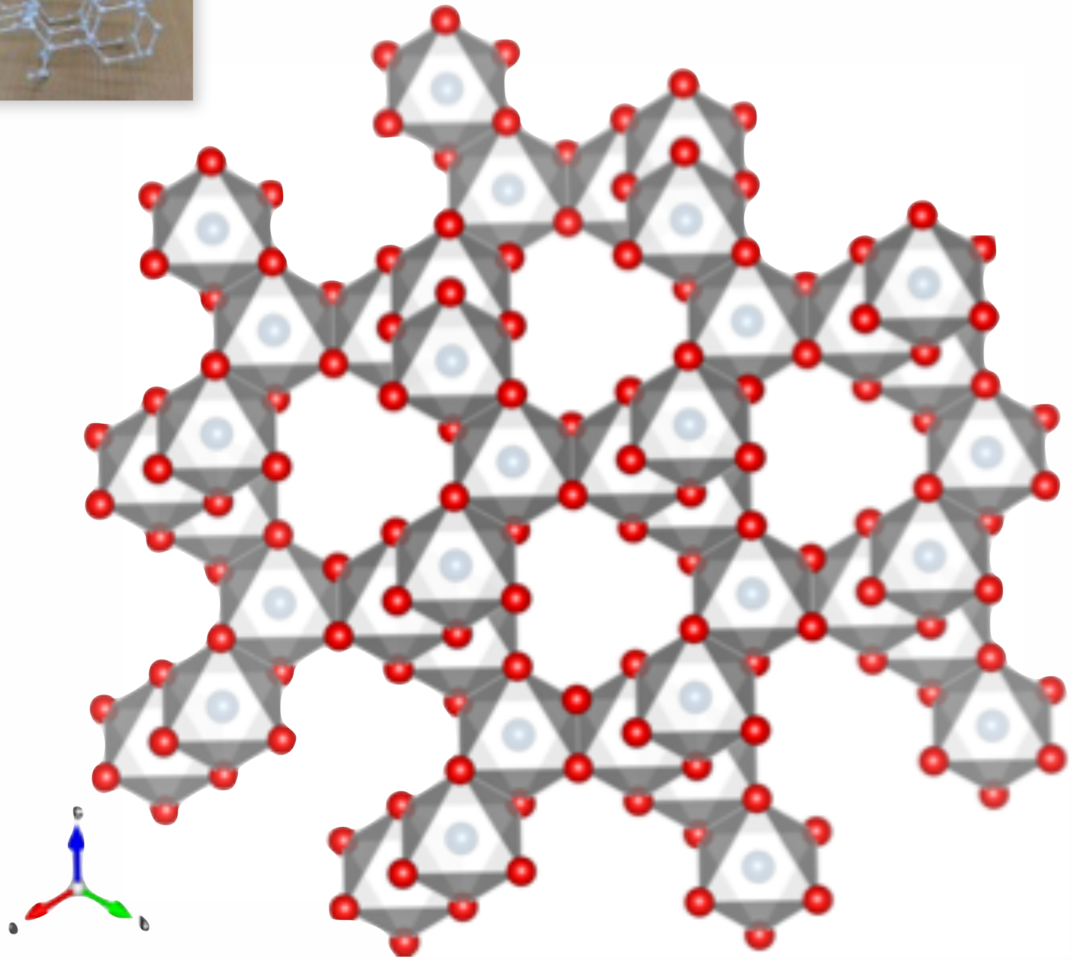
Hyperoctagon materials



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

bond-sharing IrO_6 **oxygen cages**

Hyperoctagon materials



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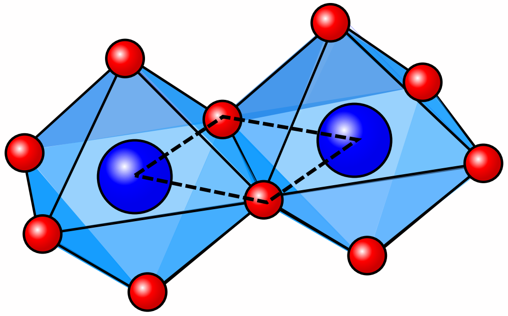
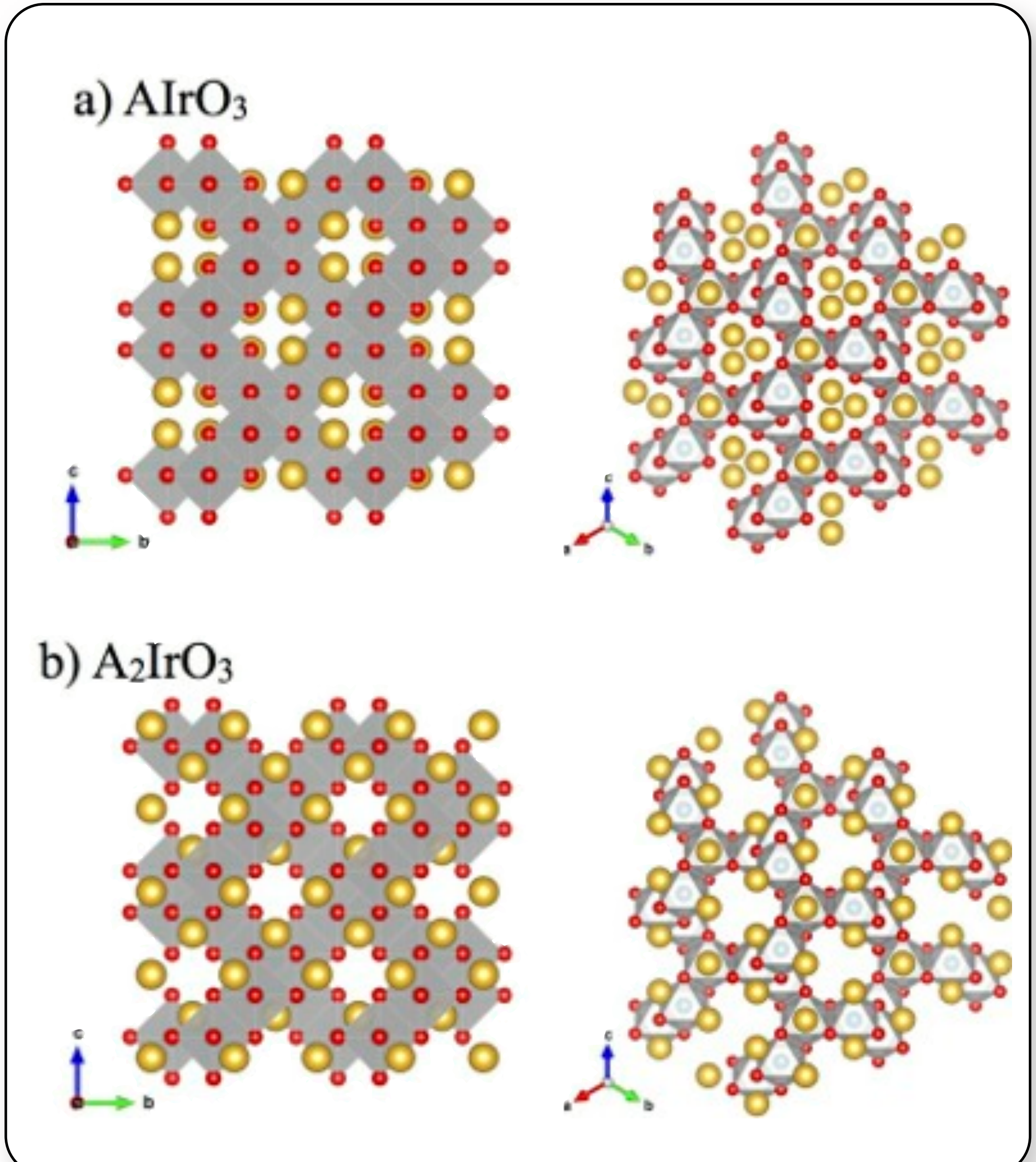


Hyperoctagon materials



space group **I4$_1$32** (no. 214)

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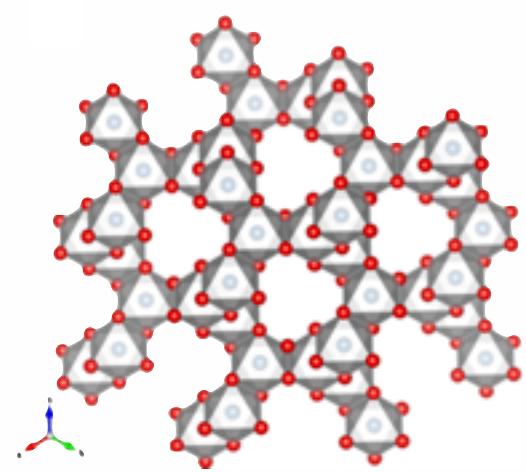


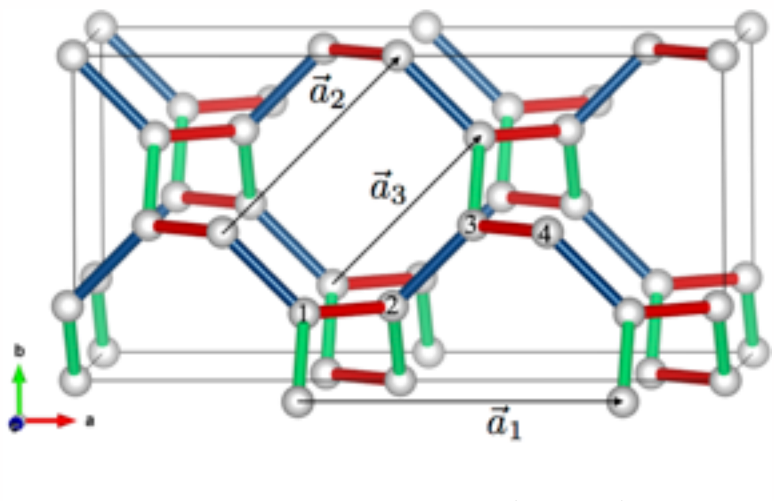
chemical **valences**

$A^{2+}(IrO_3)^{2-}$

$(A_2)^{2+}(IrO_3)^{2-}$

A three-dimensional Kitaev model

$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma S_i^\gamma S_j^\gamma$$



xx − bond

yy − bond

zz − bond

A three-dimensional Kitaev model

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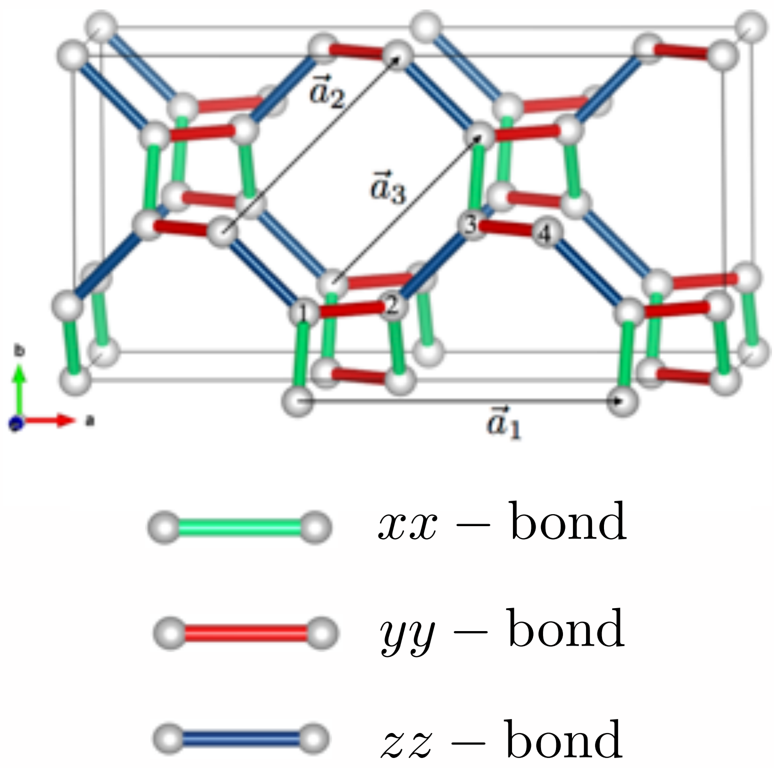
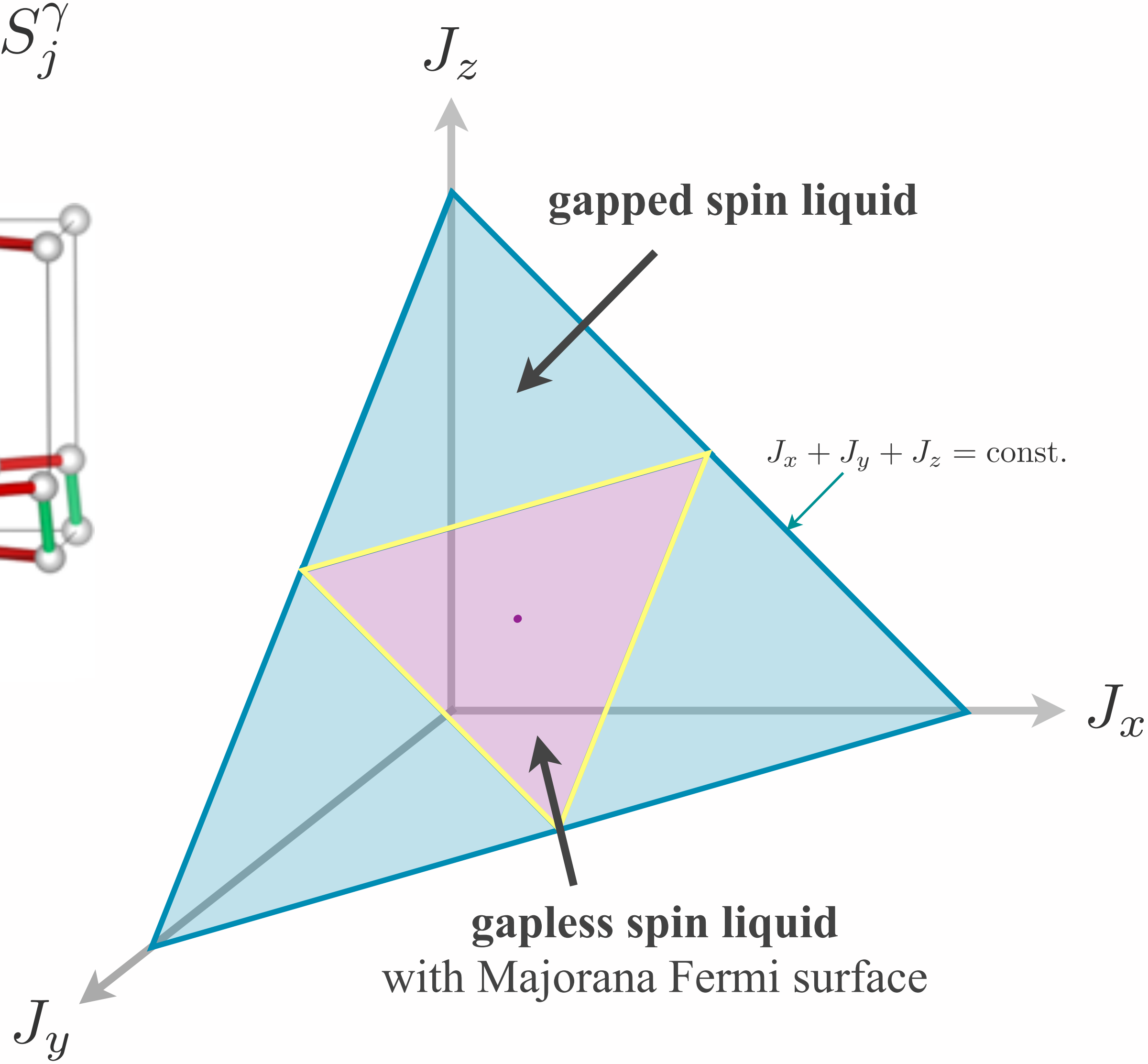
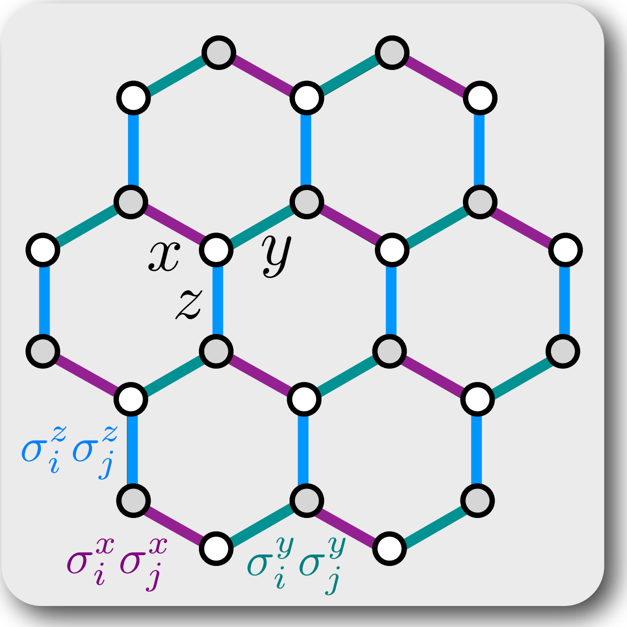


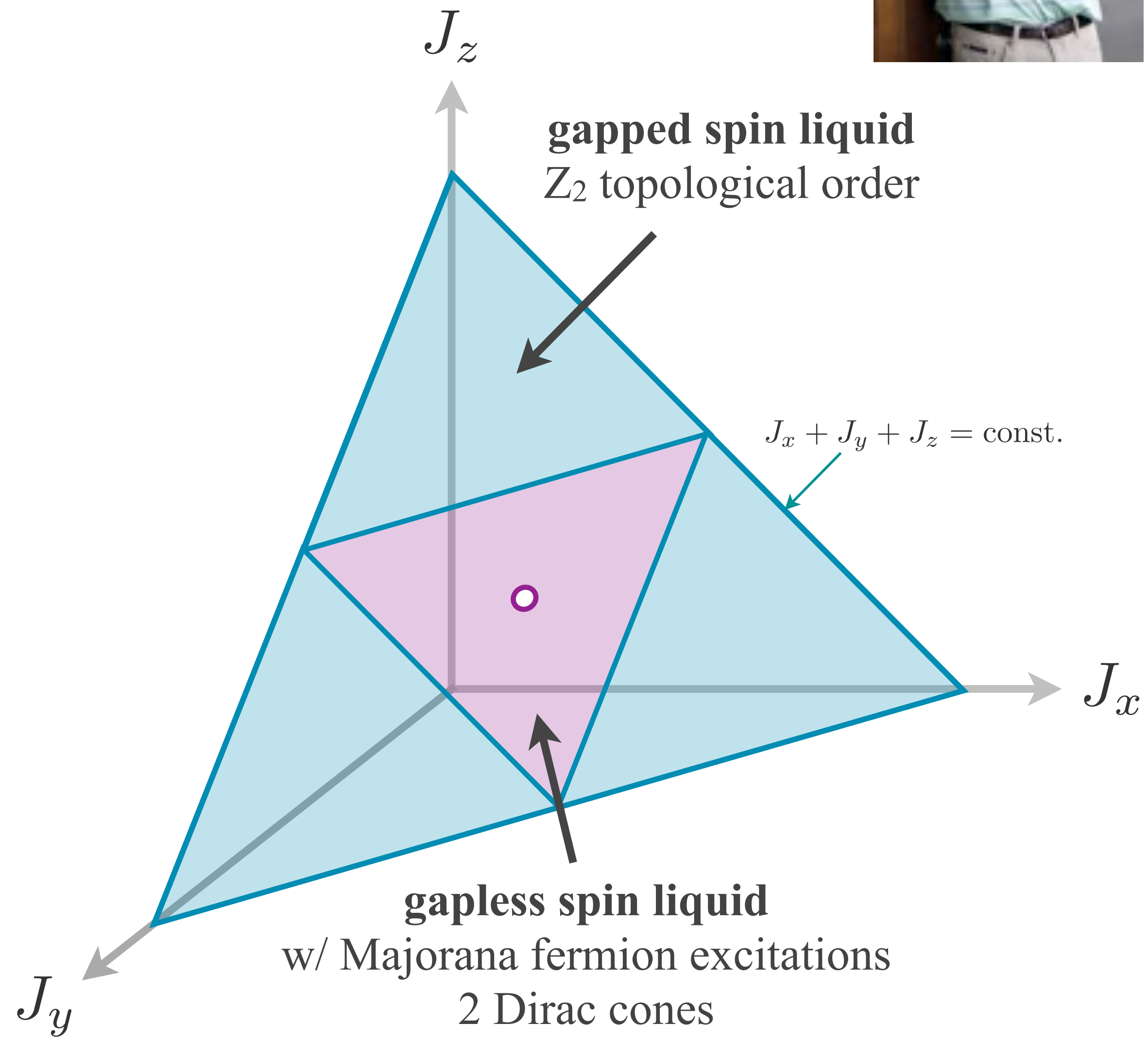


The 2D Kitaev model



$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma \sigma_i^\gamma \sigma_j^\gamma$$

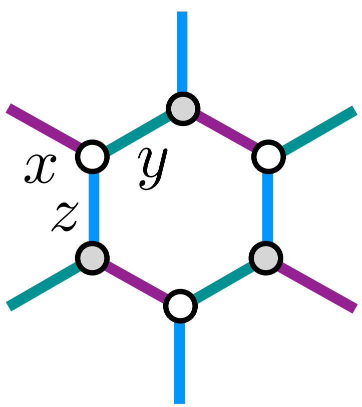
Rare combination of a model of fundamental conceptual importance and an *exact* analytical solution.

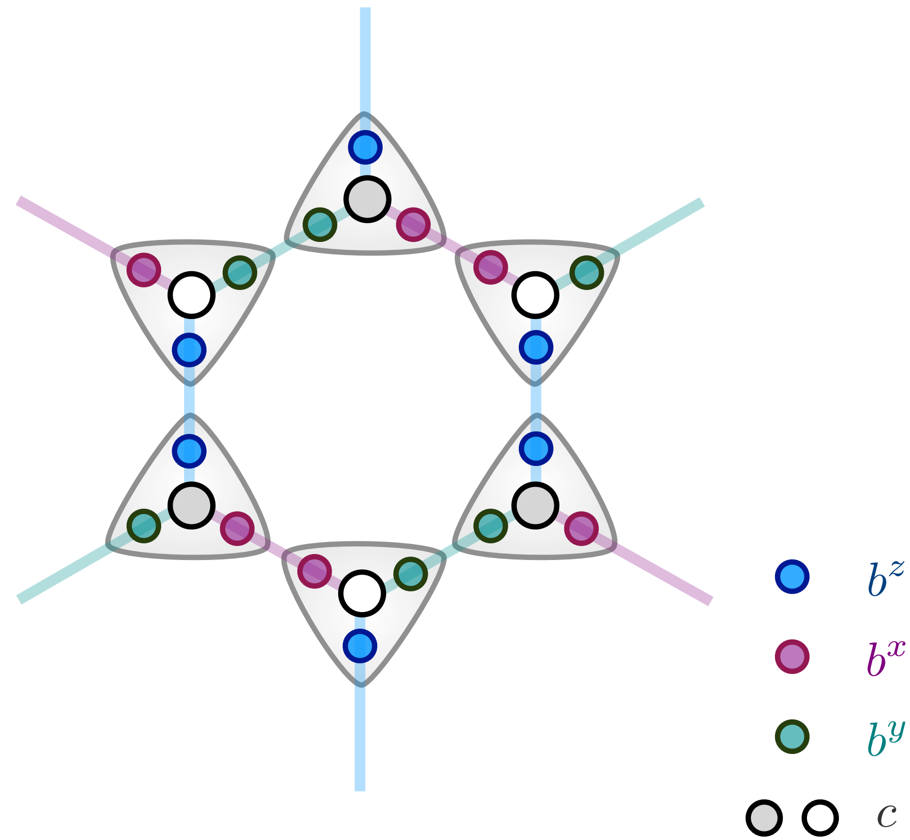


A. Kitaev, Ann. Phys. **321**, 2 (2006)

Solving the 2D Kitaev model

Step 1: **Majorana fermionization**





fermions $a_\uparrow \; a_\uparrow^\dagger \; a_\downarrow \; a_\downarrow^\dagger$

Majorana fermions

$$b^x = a_\uparrow + a_\downarrow^\dagger \qquad \sigma^y = i\, b^y c$$

$$b^y = -i\left(a_\uparrow - a_\downarrow^\dagger\right) \qquad \sigma^x = i\, b^x c$$

$$b^z = a_\downarrow + a_\uparrow^\dagger \qquad \sigma^z = i\, b^z c$$

$$c = -i\left(a_\downarrow - a_\uparrow^\dagger\right)$$

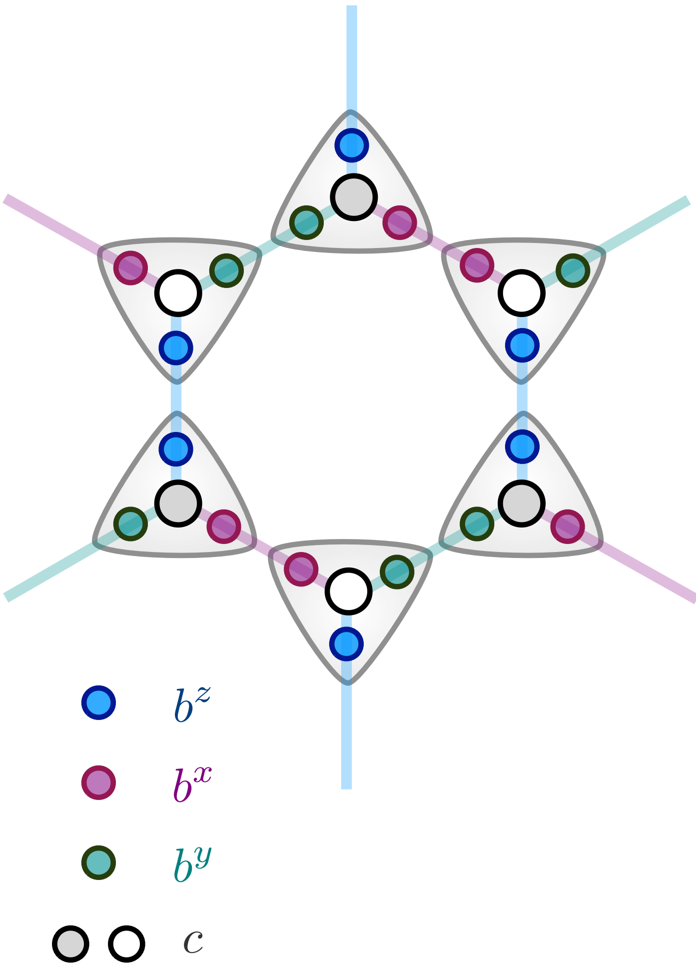
$$\underbrace{D = -i\,\sigma^x\sigma^y\sigma^z}_{\text{gauge operator}} = b^x b^y b^z c$$

$$[D, \sigma^\gamma] = 0$$

physical subspace $D = 1$

Solving the 2D Kitaev model

Step 2: **Introduce Z2 gauge fields**



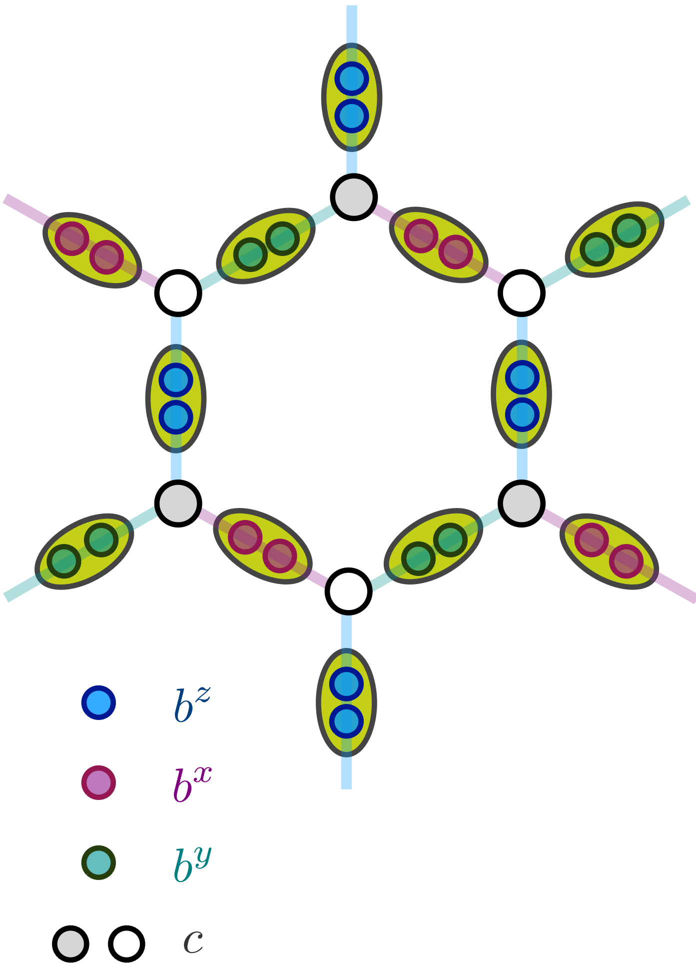
In the language of Majorana fermions, we now have

$$\sigma_j^\gamma \sigma_k^\gamma = \left(i\, b_j^\gamma c_j\right)\left(i\, b_k^\gamma c_k\right) = -i\, u_{jk} c_j c_k$$

$$u_{jk} = i\, b_j^\gamma b_k^\gamma$$

Solving the 2D Kitaev model

Step 3: **Free Majorana Hamiltonian**



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$$u_{jk} = i\, b_j^\gamma b_k^\gamma$$

which immediately allows us to write the Hamiltonian as

$$\mathcal{H} = \frac{i}{4} \sum_{\langle jk \rangle} A_{jk} c_j c_k$$

$$A_{jk} = 2 J_\gamma u_{jk}$$

Hamiltonian is skew-symmetric, because

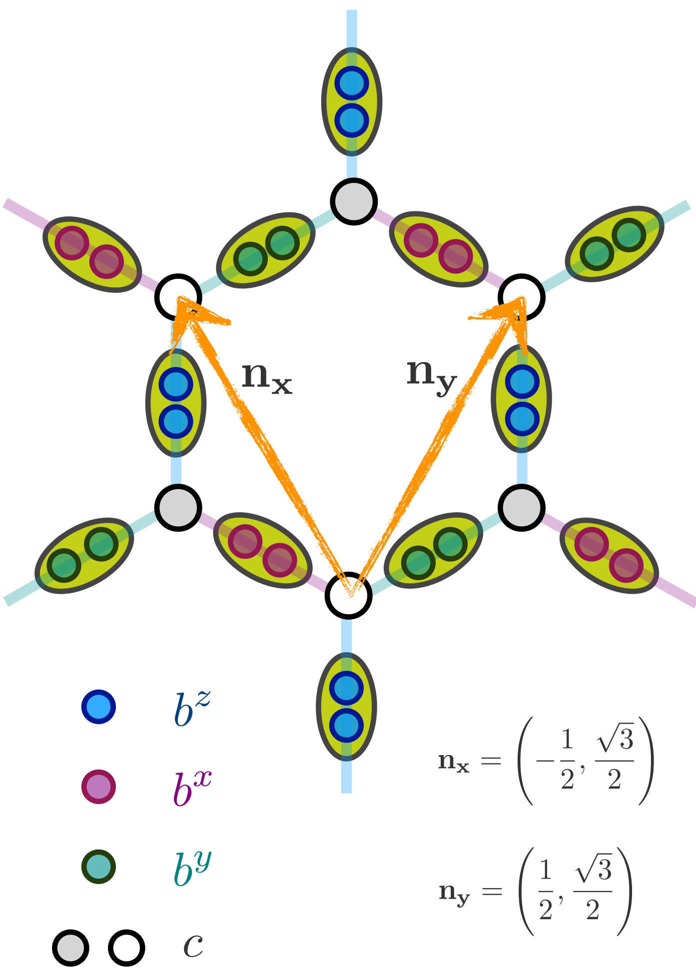
$$u_{jk} = -u_{kj} \longrightarrow A_{jk} = -A_{kj}$$

Finally, there is a gauge choice to be made

u_{jk} has eigenvalues ± 1

Solving the 2D Kitaev model

Step 4: **Diagonalization of Hamiltonian**



$$\mathbf{n_x} = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$

$$\mathbf{n_y} = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$

The Hamiltonian has turned into a free (Majorana) fermion problem

$$\mathcal{H} = \frac{i}{4} \sum_{\langle jk \rangle} A_{jk} c_j c_k$$

which can readily be diagonalized by Fourier transformation

$$\mathcal{H}(\mathbf{q}) = \frac{i}{2} A(\mathbf{q}) = \begin{pmatrix} 0 & i f(\mathbf{q}) \\ -i f^*(\mathbf{q}) & 0 \end{pmatrix}$$

$$f(\mathbf{q}) = J_x e^{i\mathbf{q}\cdot\mathbf{n_x}} + J_y e^{i\mathbf{q}\cdot\mathbf{n_y}} + J_z$$

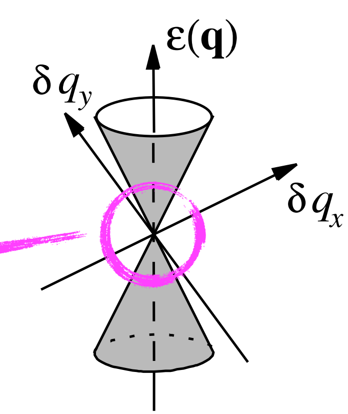
thus yielding a gapless energy spectrum of the form

$$\epsilon(\mathbf{q}) = \pm |f(\mathbf{q})|$$

Dirac cones

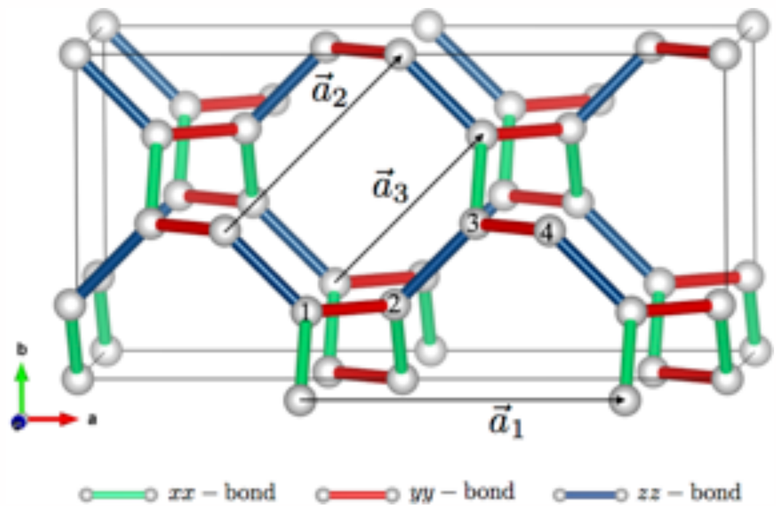
$$\mathbf{q}_1^* = \left(\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}}\right)$$

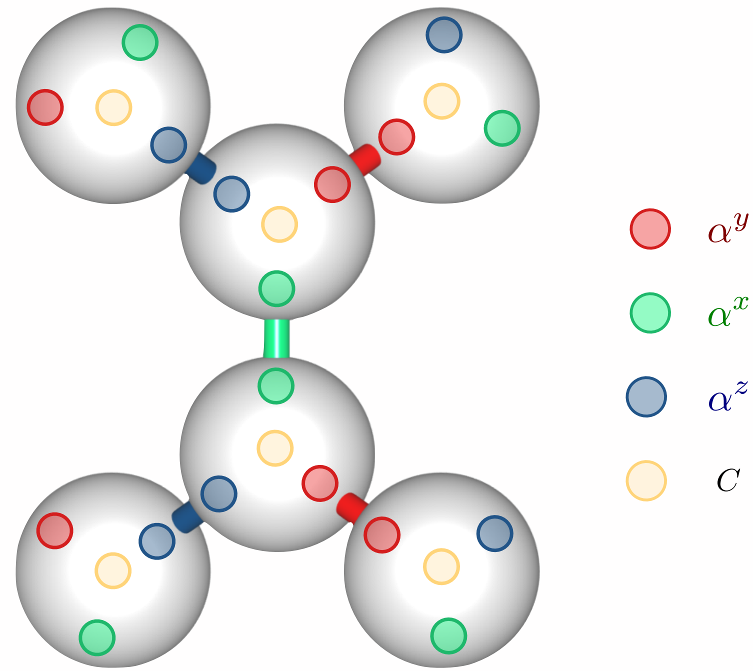
$$\mathbf{q}_2^* = \left(-\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}}\right)$$



Let's redo this for the 3D model

Step 1: **Majorana fermionization**





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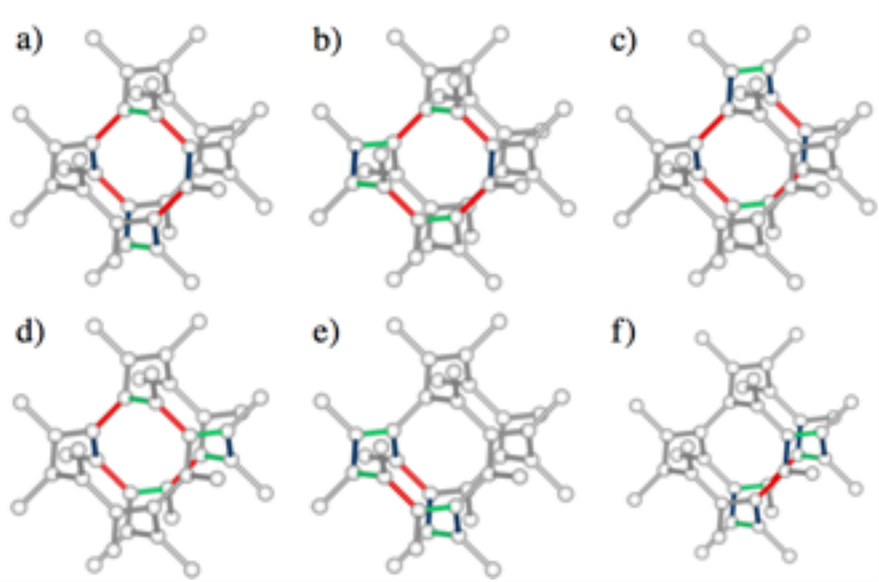
physical subspace $D = 1$

Loops and conserved quantities

Six distinct loops in the hyperoctagon lattice

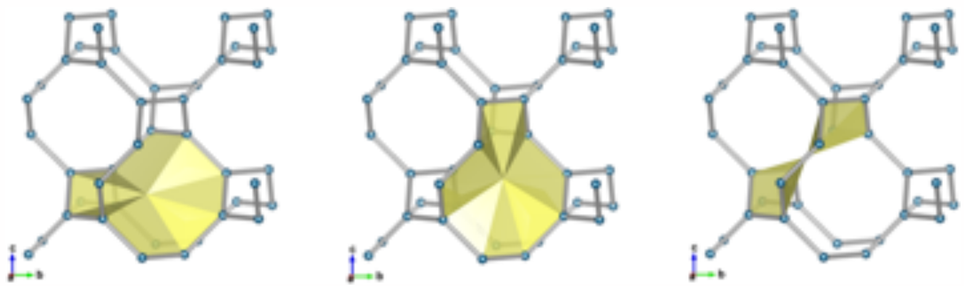


Two distinct loop operators for each loop

$$W_l = \prod_{\langle i,j \rangle, \gamma} \sigma_i^\gamma \sigma_j^\gamma \qquad \tilde{W}_l = \prod_{i \in l} \sigma_i^{\gamma_i}$$

$$W_l = -\tilde{W}_l$$

Loop operators are **not** all linearly **independent.**

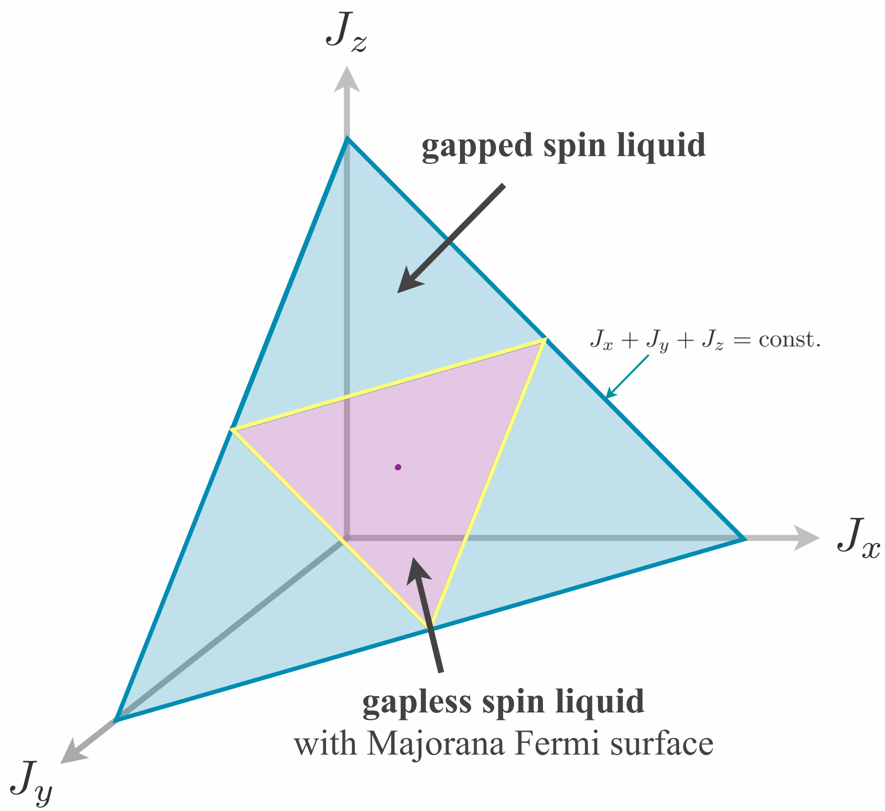


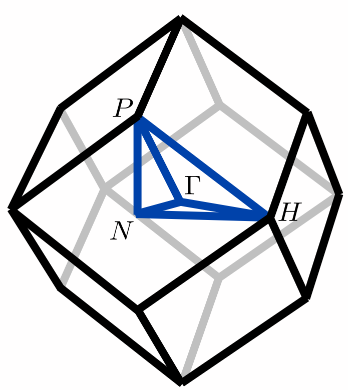
Three loops form the smallest **closed volume.**

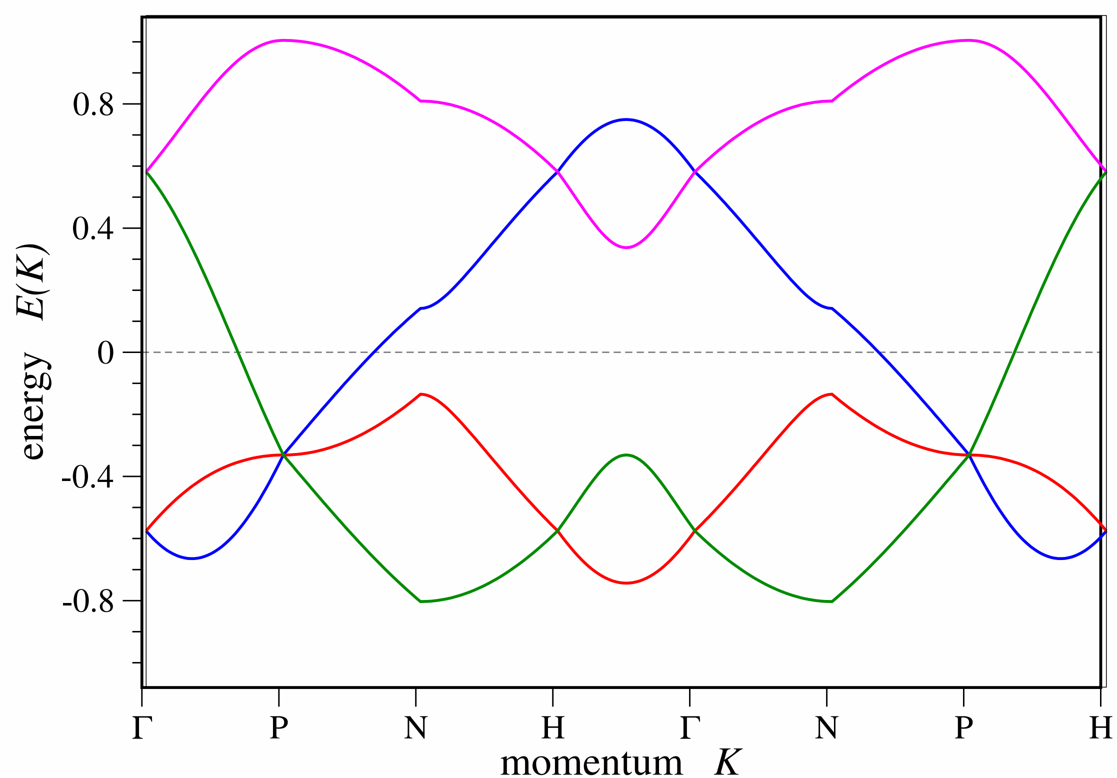
$$W_{l_a} W_{l_b} W_{l_c} = 1$$

The **groundstate** resides in the **flux-free** sector.

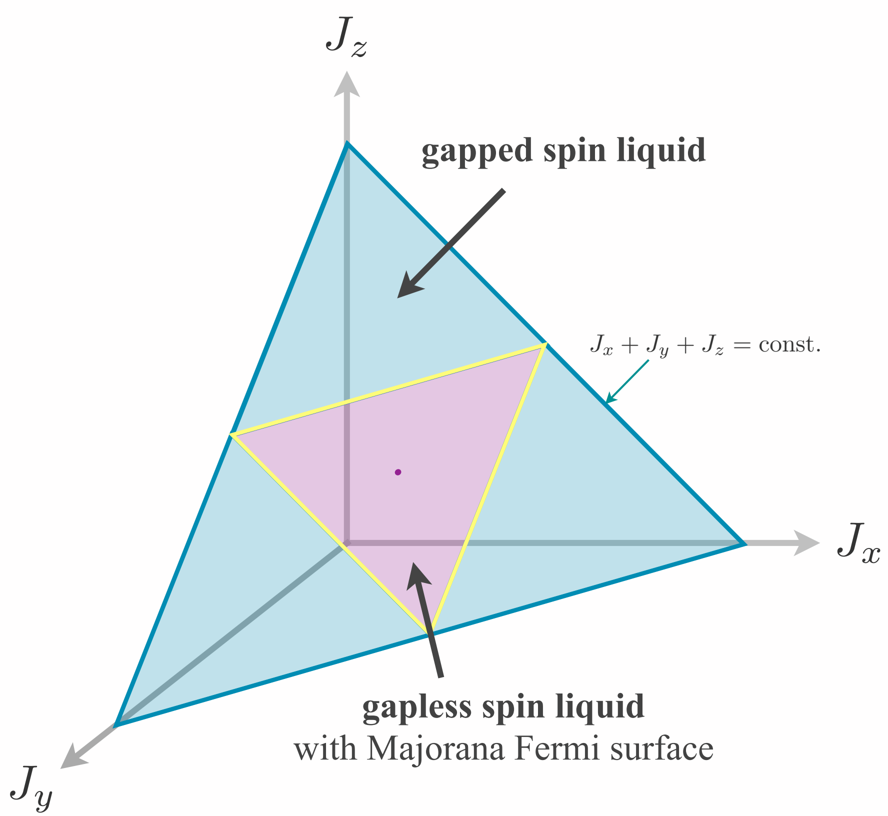
Majorana Fermi surface

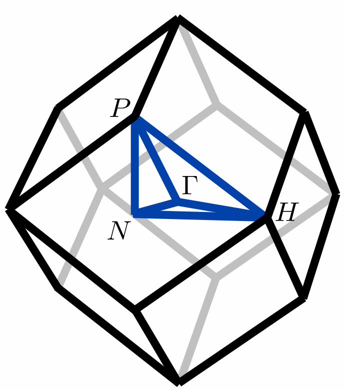


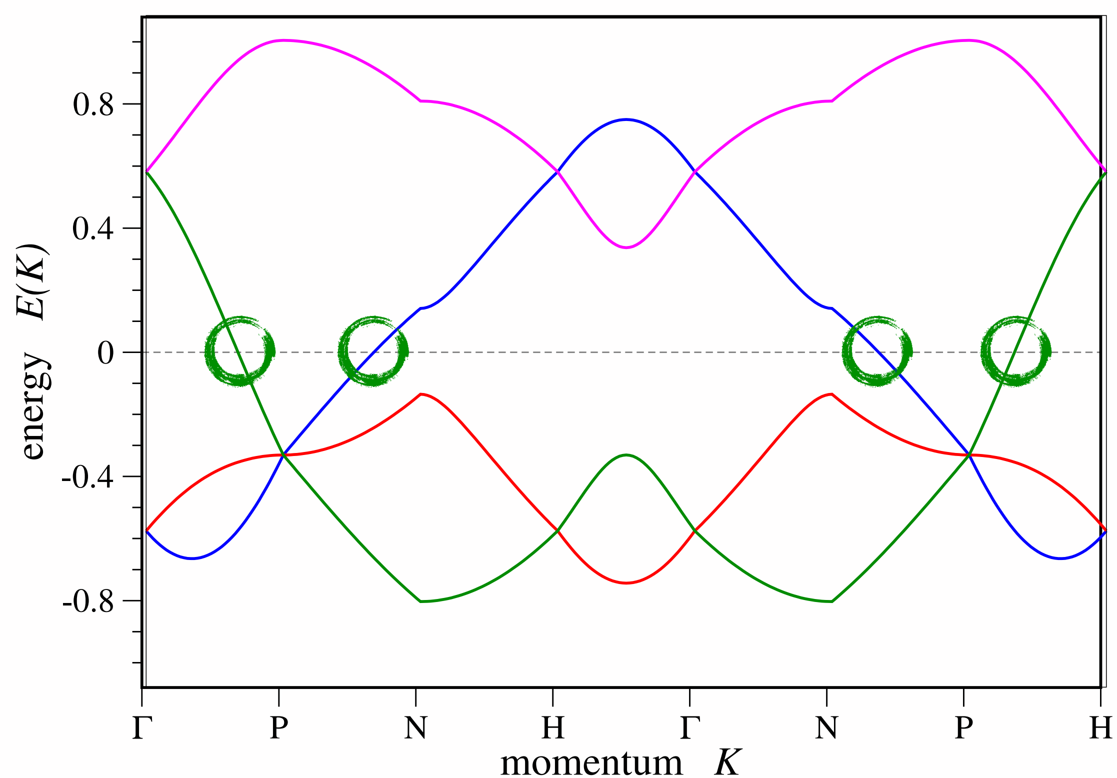




Majorana Fermi surface







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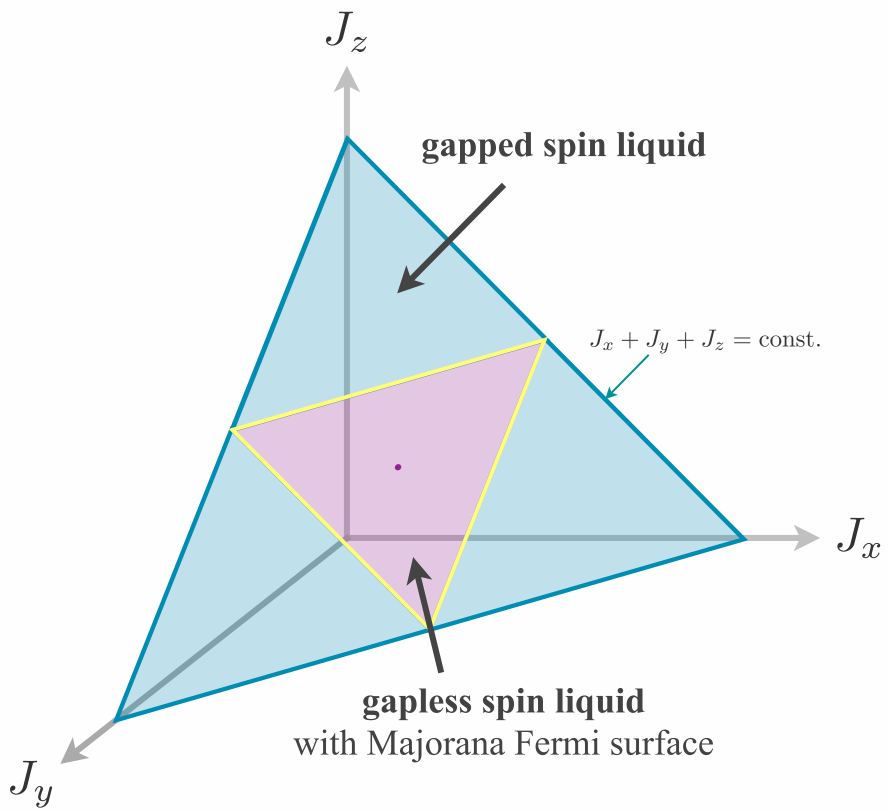

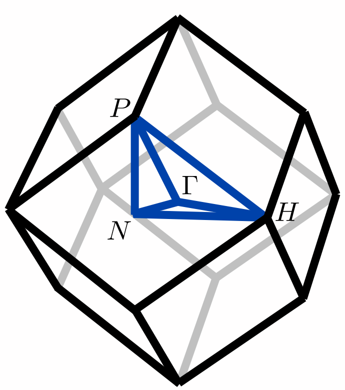

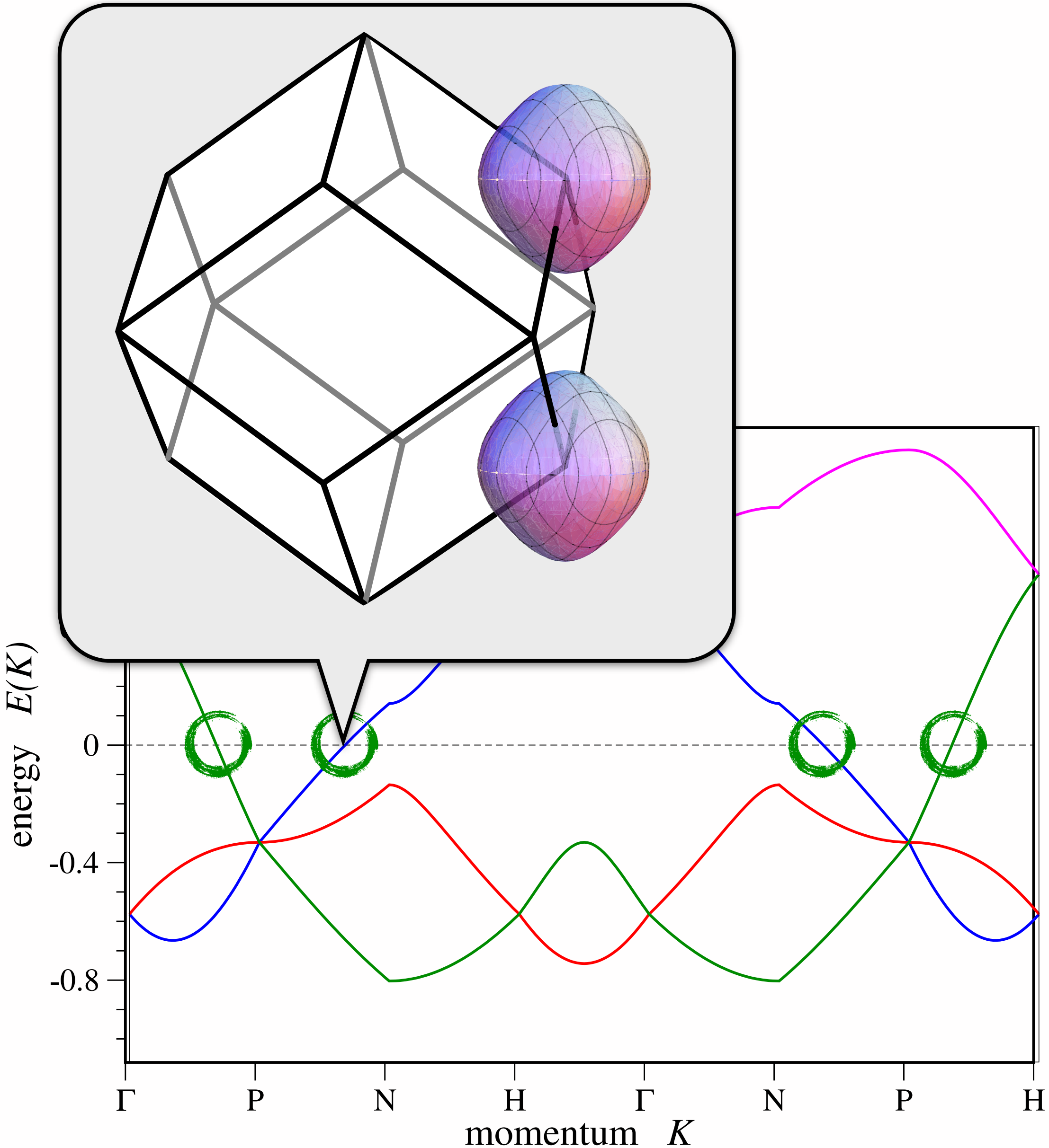

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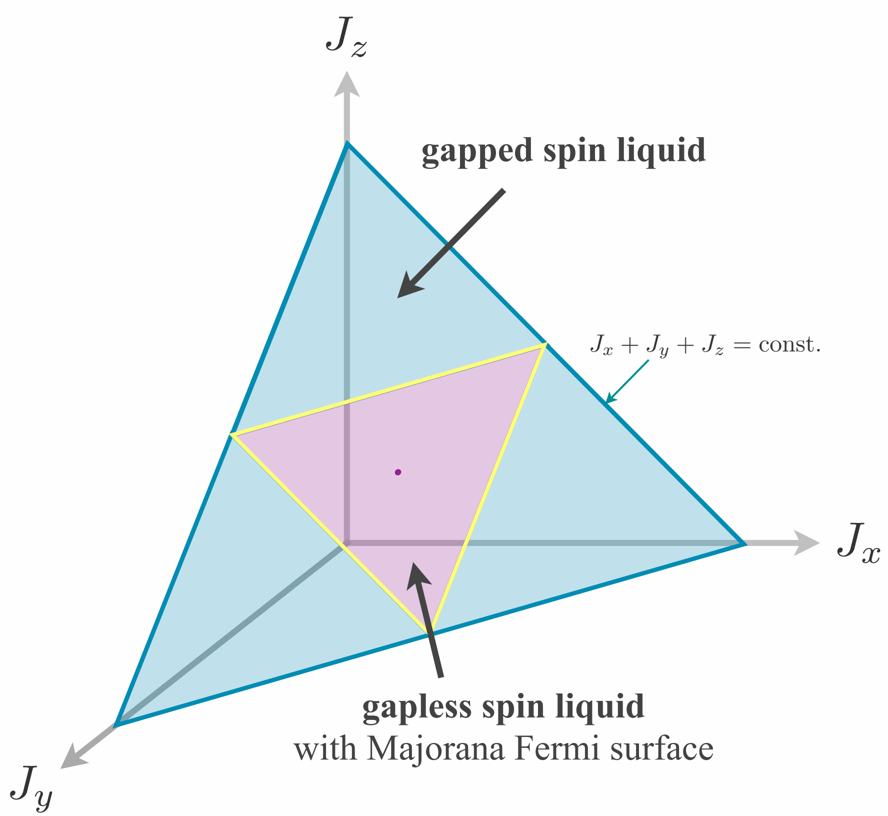

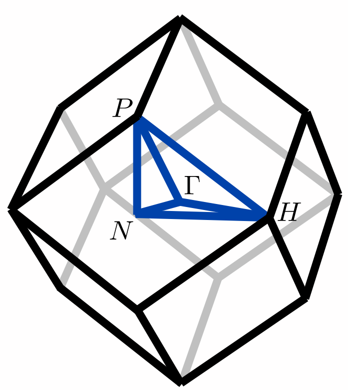

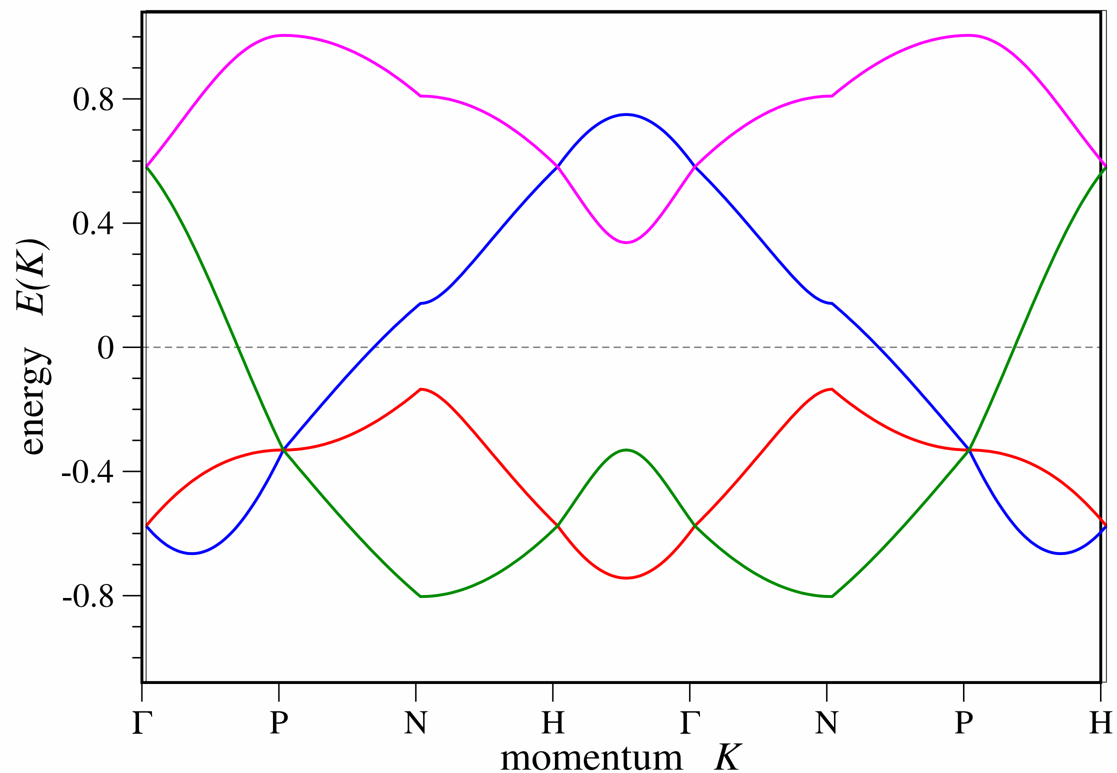

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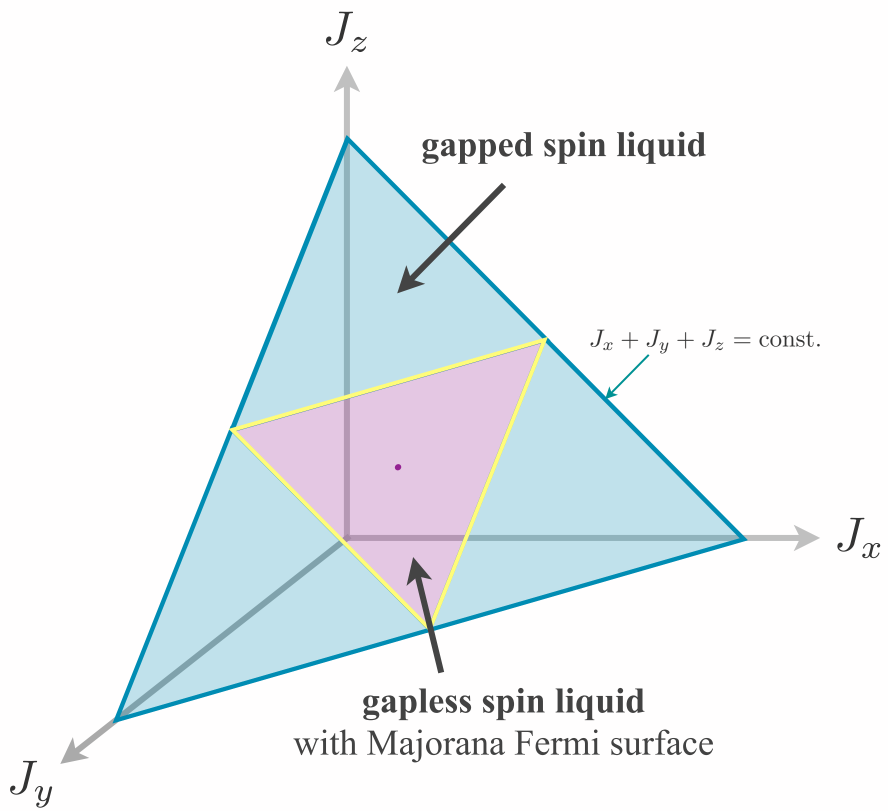

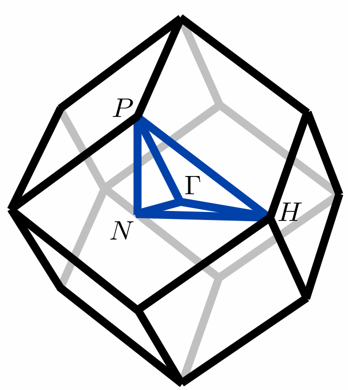

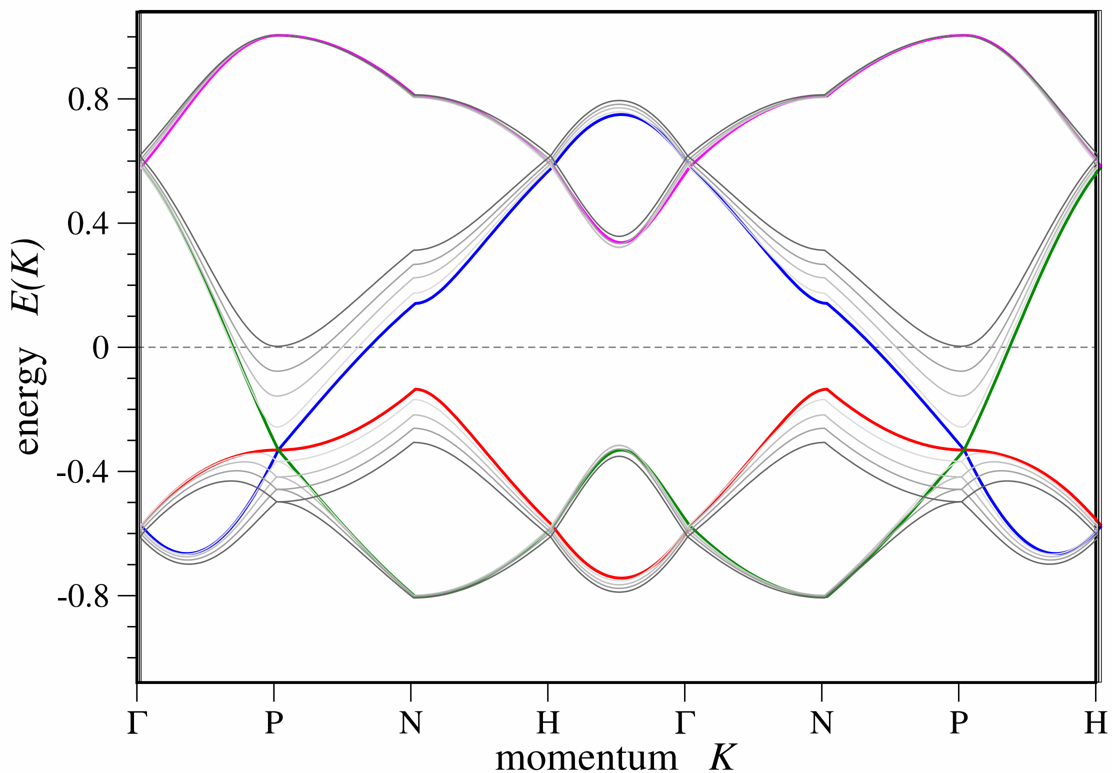

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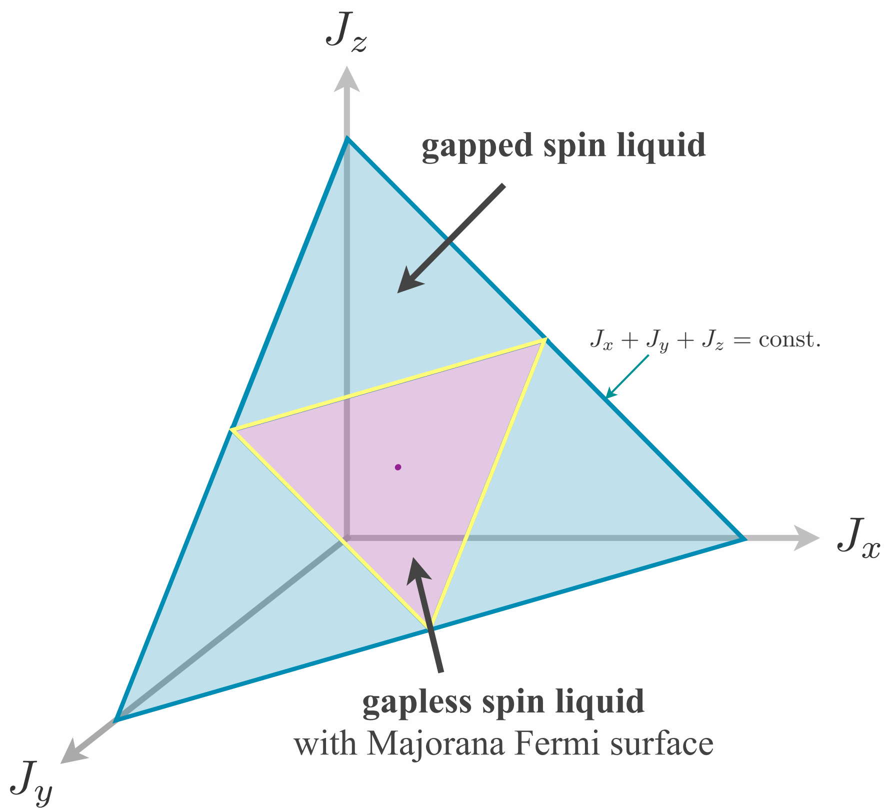

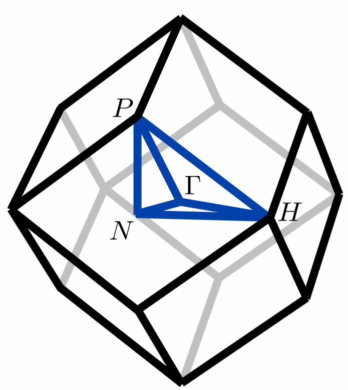

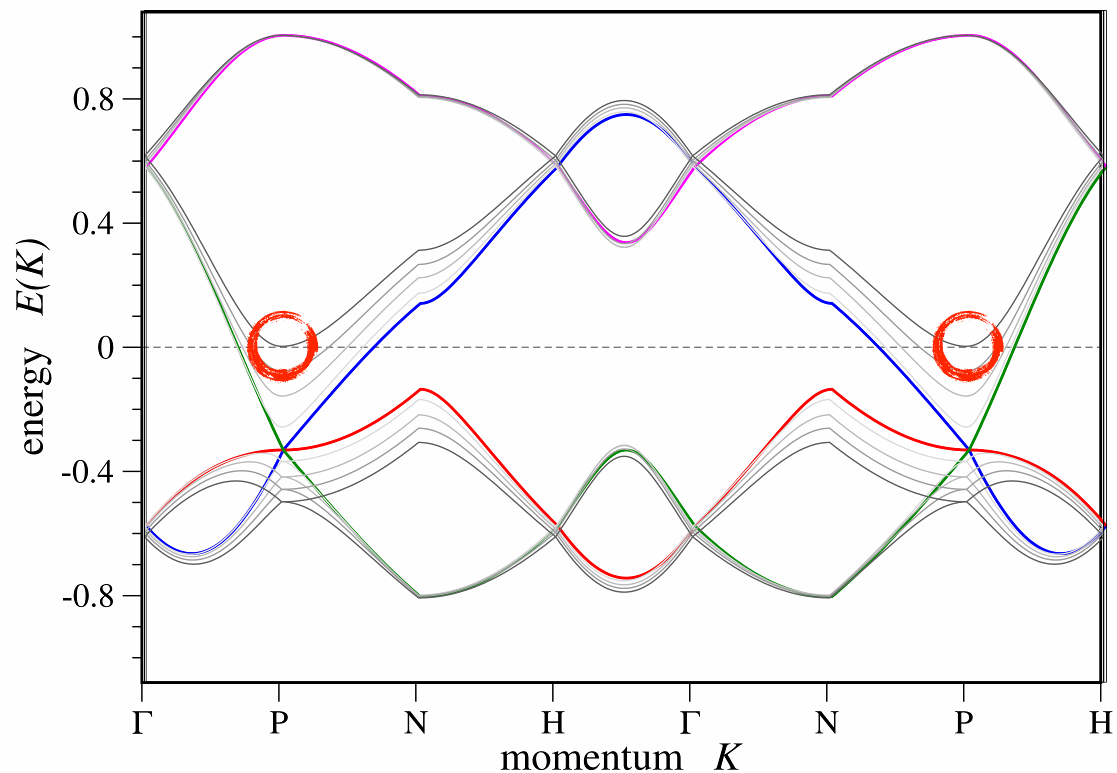

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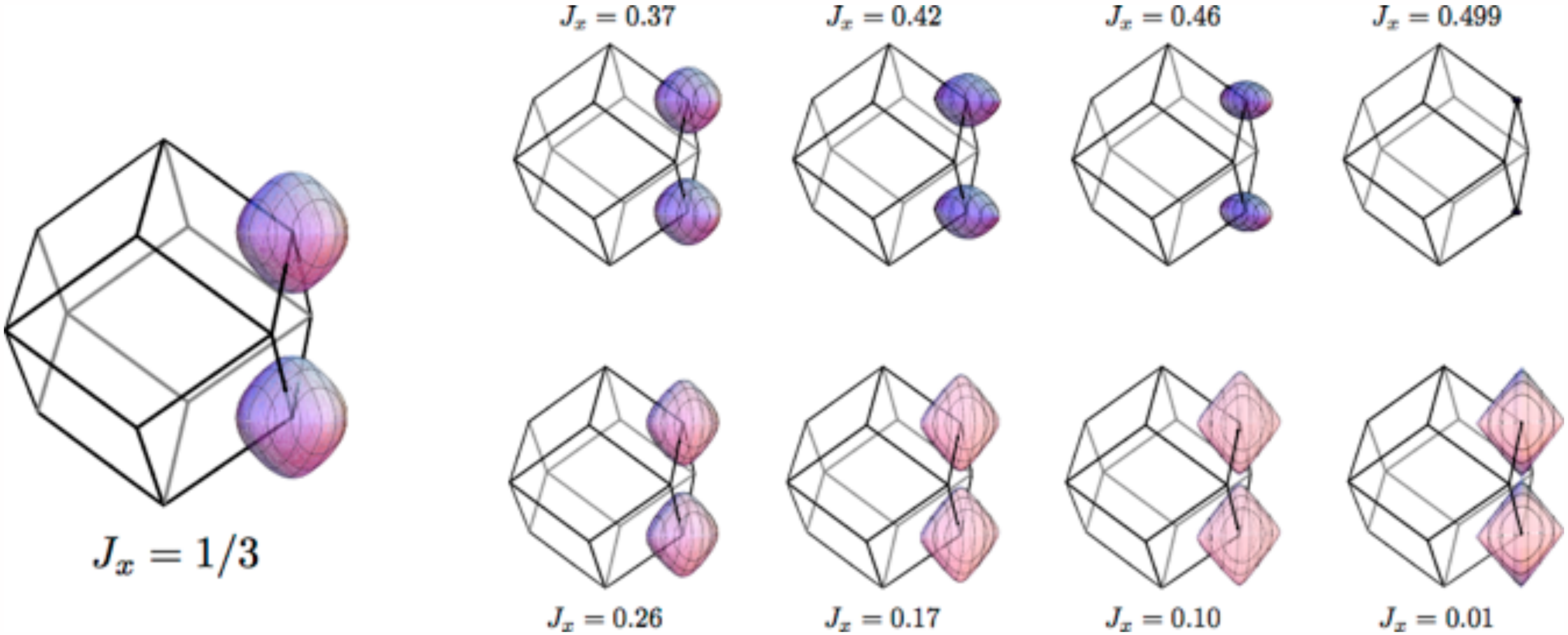
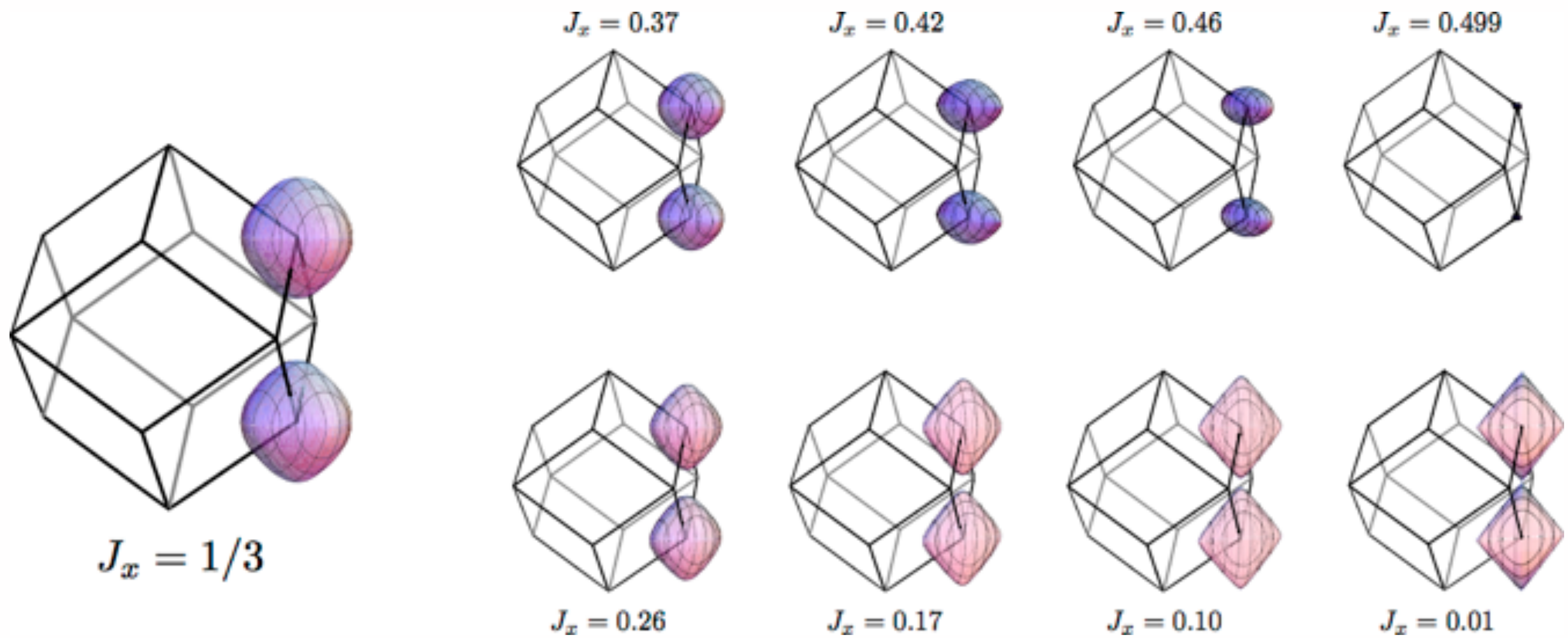


The hyperoctagon Kitaev model exhibits a full **two-dimensional Majorana Fermi surface**.

Majorana Fermi surface



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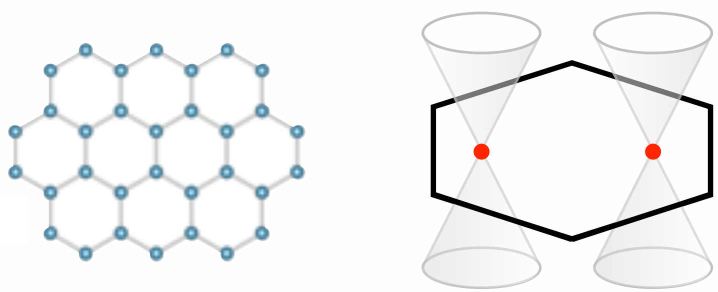
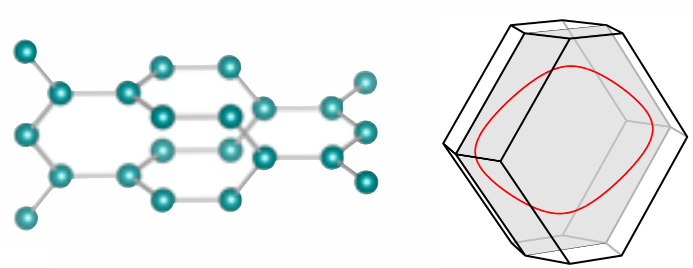
honeycomb – Fermi **points**



hyperhoneycomb – Fermi **lines**



Stability of the Fermi surface I

Some basic facts about **Majorana fermions**

$$c_j^\dagger(\mathbf{R}) = c_j(\mathbf{R}) \longrightarrow c_j^\dagger(\mathbf{k}) = c_j(-\mathbf{k})$$

Every energy state $E(\mathbf{k})$ has a 'particle-hole conjugate' partner

$$E(-\mathbf{k}) = -E(\mathbf{k})$$

For a **bipartite lattice** we further have

$$E(\mathbf{k}) = E(-\mathbf{k} - \mathbf{q}/2)$$

reciprocal lattice vector
of translation between sublattices

zero-energy modes
occur in pairs

honeycomb
hyperhoneycomb } $\mathbf{q} = 0 \longrightarrow E(\mathbf{k}) = -E(\mathbf{k})$

hyperoctagon $\mathbf{q} \neq 0 \longrightarrow E(\mathbf{k}) \neq -E(\mathbf{k})$

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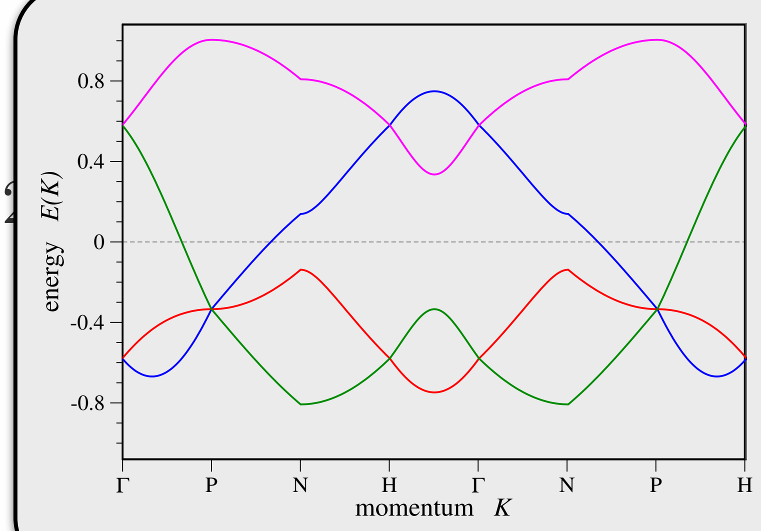


Stability of the Fermi surface I

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

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

→ 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.

Stability of the Fermi surface II

Time-reversal symmetry breaking

Classification of free (Majorana) fermion Hamiltonian in terms of **symmetry classes**

class *BDI* ⟶ class *D*

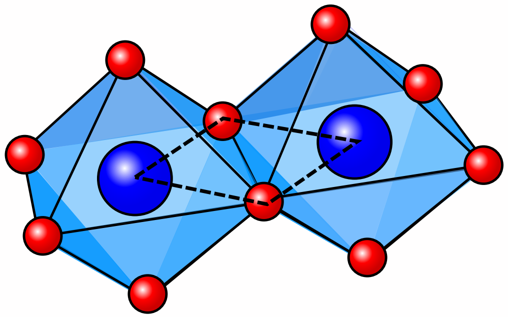
2D → $\mathbb{Z}$ classification
non-trivial Chern insulators
$\nu = \pm 1$
3D → no topological phases

S. Ryu: augment models to be in class *DIII* to get top. phases

Pairing instabilities

Natural candidate is **p-wave pairing**, since we have an effective description in **spinless fermions**.

What instabilities can be induced by an additional **Heisenberg** exchange?



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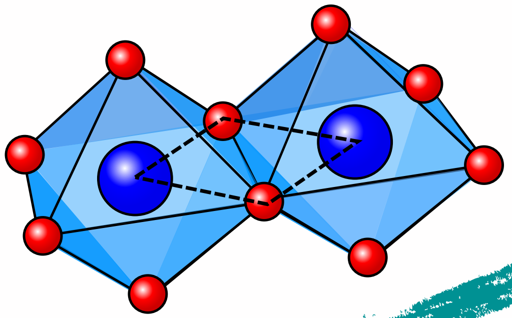

work in progress

Spin liquid with a spinon 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**.

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

Summary

Summary

- We have found an **exactly solvable SU(2) spin-1/2 model** hosting a gapless spin liquid with a **spinon Fermi surface**.
- The model is a **Kitaev model** on a 3D tri-coordinated lattice which we dubbed the **hyperoctagon lattice**
  (= the medial lattice of the hyperkagome lattice).

- Our original motivation to look into this is rooted in the physics of certain **spin-orbit entangled Iridates**
  (= really "heavy" 5d transition metal oxides).

arXiv:1401.7678