Classification of gapless Z_2 spin liquids in three-dimensional Kitaev models

HVI – New states of matter and their excitations
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PRB 89, 235102 (2014)
PRL 114, 157202 (2015)
arXiv:1506.01379

Collaborators

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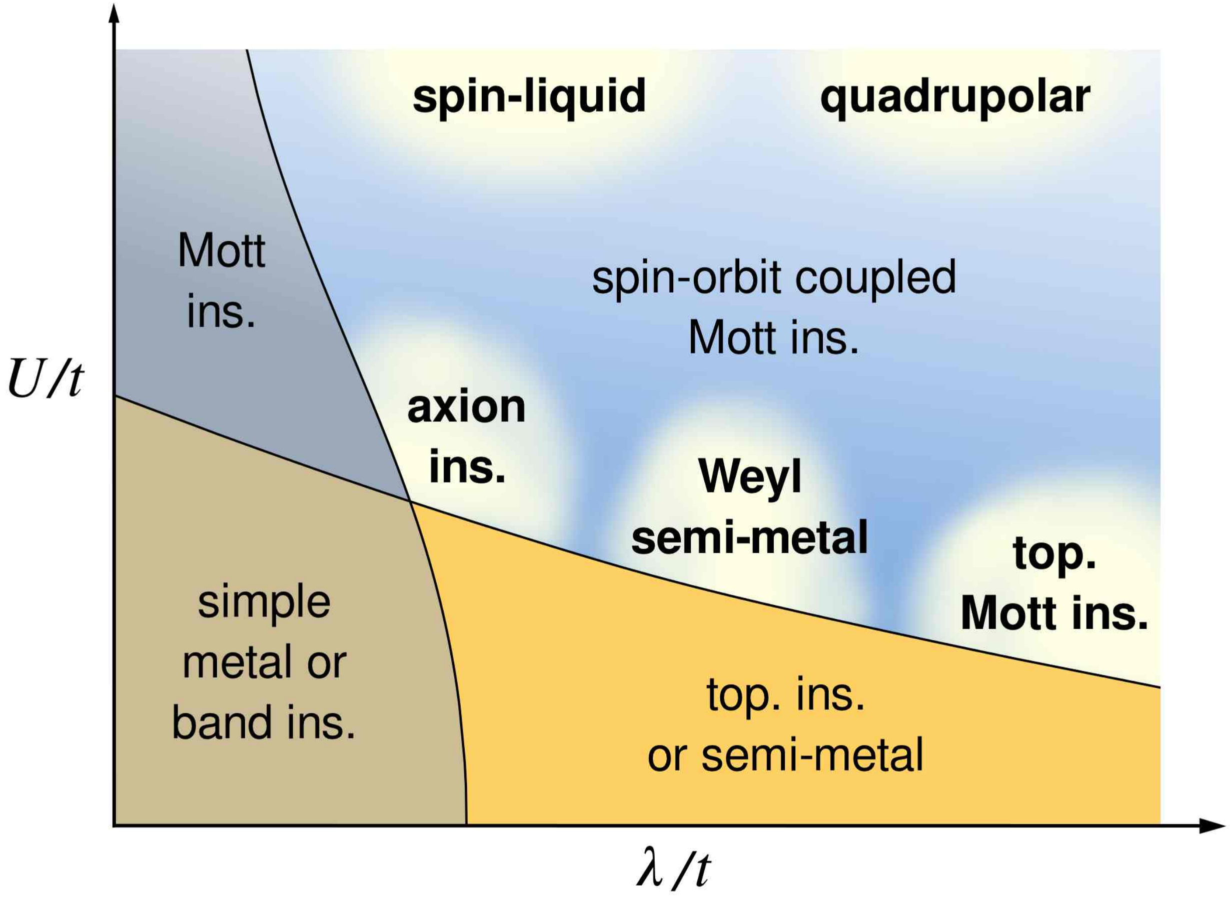
poster on Weyl Spin Liquids

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**.

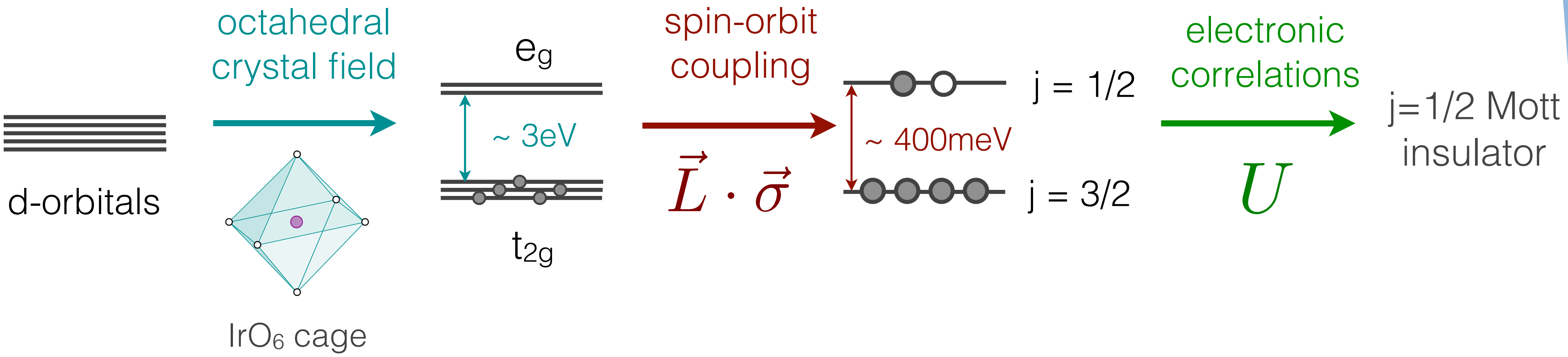


W. Witczak-Krempa, G. Chen, Y. B. Kim, and L. Balents, Annual Review of Condensed Matter Physics 5, 57 (2014).

j=1/2 Mott insulators

most common
Iridium valence

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



octahedral crystal field

spin-orbit coupling

electronic correlations

d-orbitals

IrO_6 cage

e_g

~ 3eV

t_{2g}

$\vec{L} \cdot \vec{\sigma}$

j = 1/2

~ 400meV

j = 3/2

U

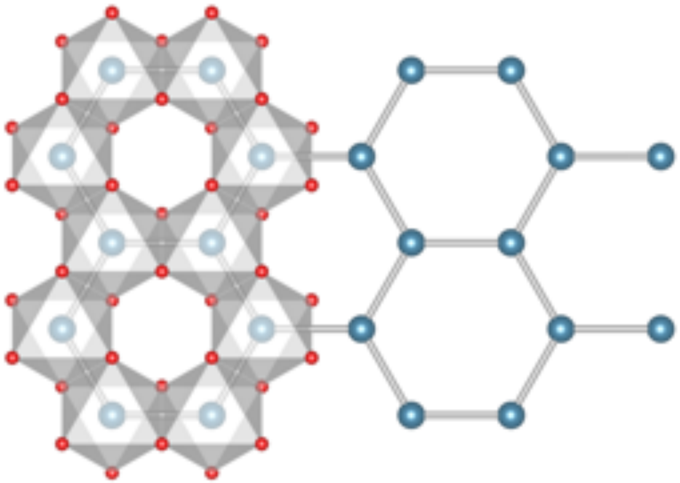
j=1/2 Mott insulator

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

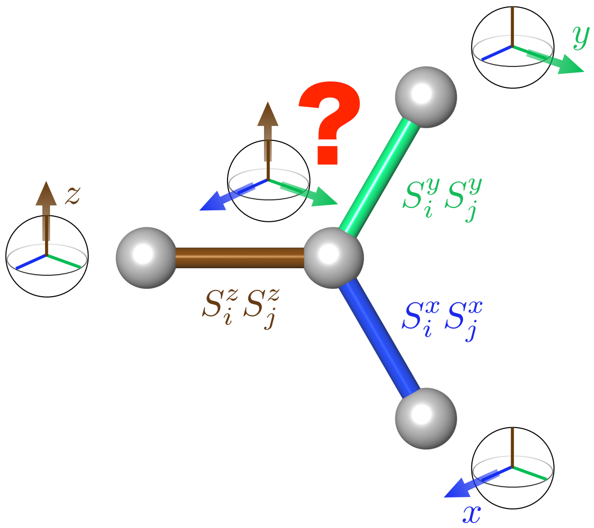


Na_2IrO_3

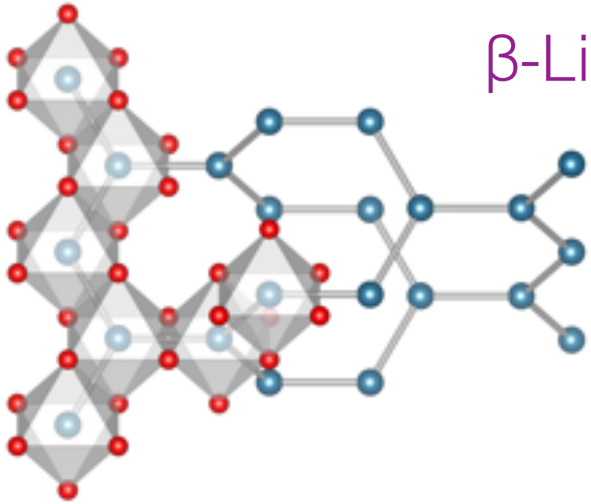
α-Li_2IrO_3

see also $RuCl_3$

Kitaev exchange

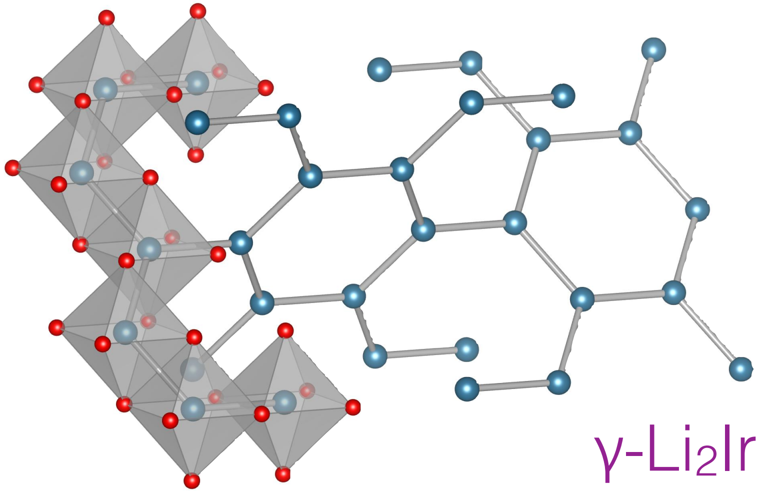


hyperhoneycomb



β-Li_2IrO_3

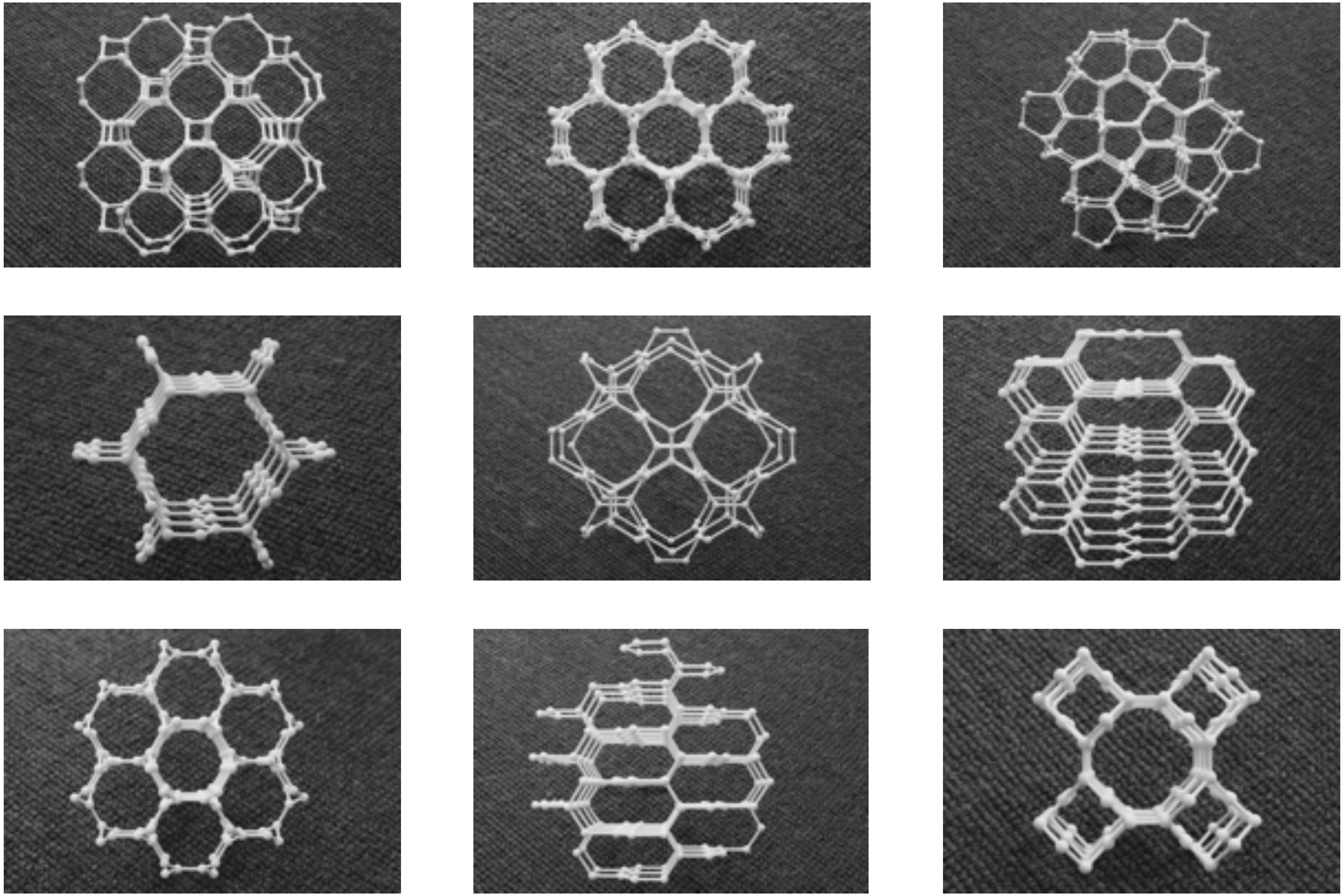
hyperhoneycomb H_1



γ-Li_2IrO_3

Tricoordinated lattices in 3D

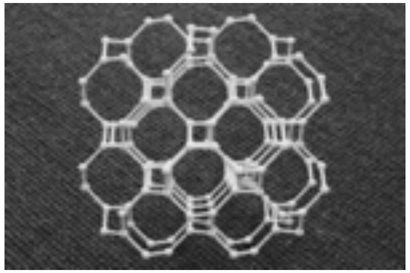
How many such lattices exist?



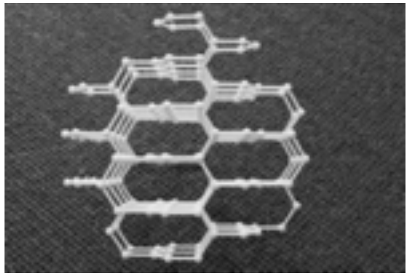
Tricoordinated lattices in 3D

Classification by elementary loop length (polygonality)

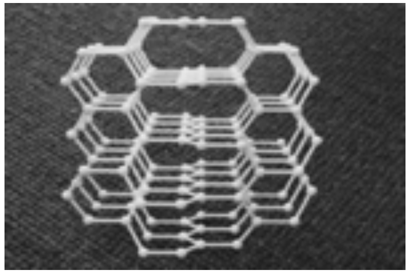
(10,3)



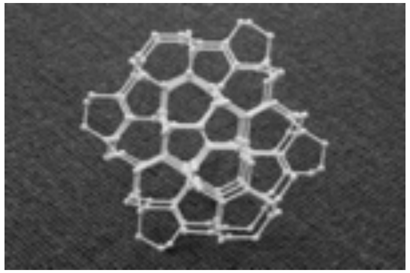
hyperoctagon

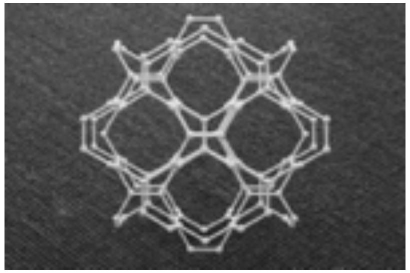


hyperhoneycomb

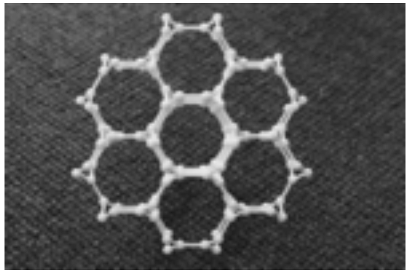


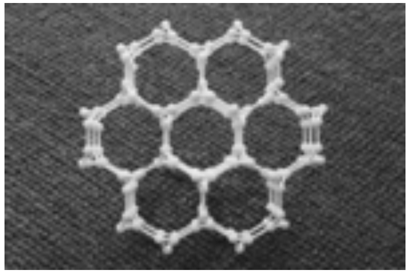
(9,3)

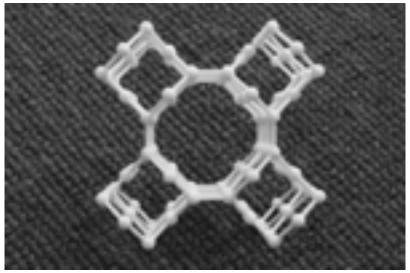


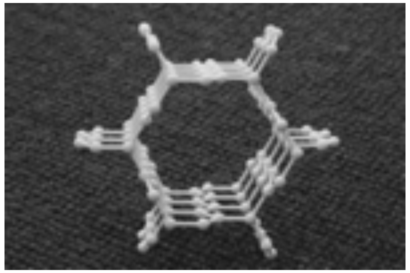


(8,3)









Lattice classifications

connectivity

polygonality

	3	4	5	6
3	(3,3) 	(3,4) 	(3,5) 	(3,6) **triangular**
4	(4,3) 	(4,4) **square**		
5	(5,3) 			
6	(6,3) **honeycomb**			

Schäfli symbol

(p,c)

🟥 platonic solids

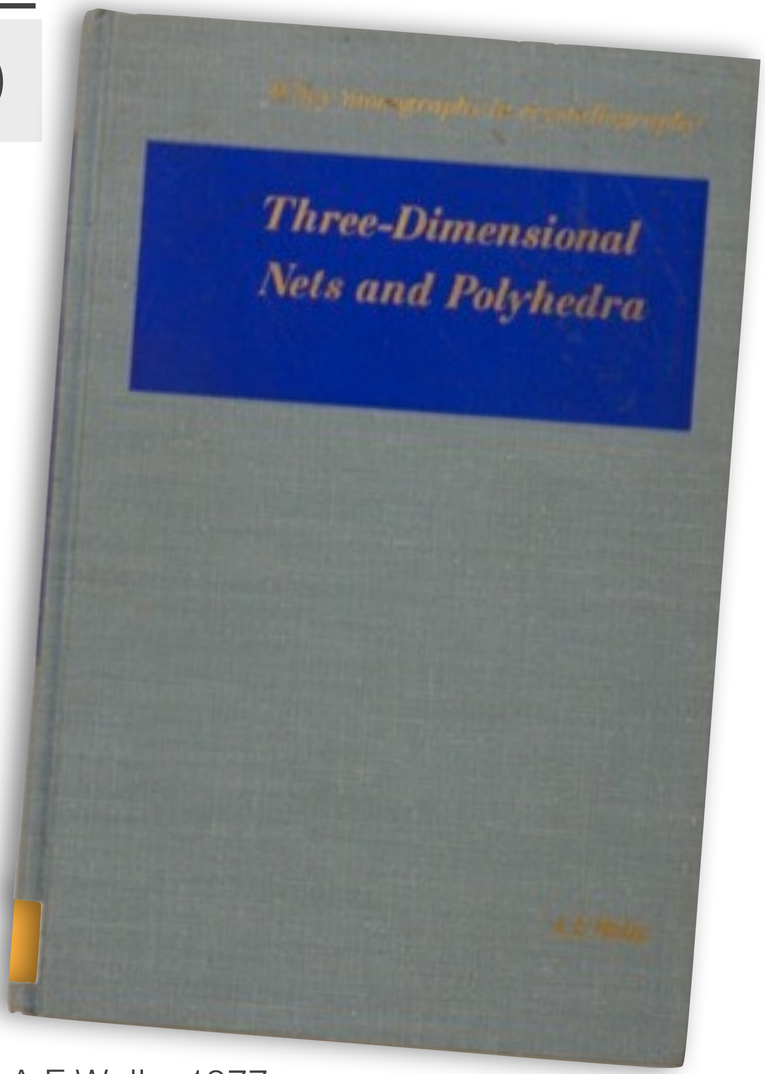
🟦 2d lattices

Tricoordinated lattices

connectivity

polygonality

	3	4	5	6	7
3	(3,3)	(3,4)	(3,5)	(3,6)	(3,7)
4	(4,3)	(4,4)	(4,5)		
5	(5,3)	(5,4)			
6	(6,3)	(6,4)	other 3D lattices		
7	(7,3)	**0** crystals + 4 nets			
8	(8,3)	**4** crystals + 11 nets			
9	(9,3)	**2** crystals + 1 net			
10	(10,3)	**3** crystals + 4 nets			

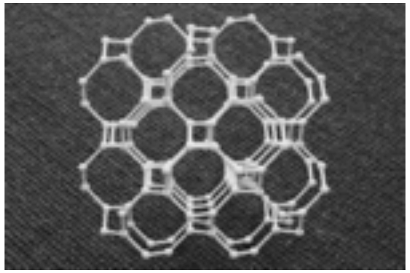


A.F.Wells, 1977

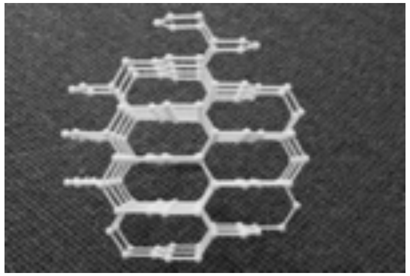
Tricoordinated lattices

Classification by elementary loop length (polygonality)

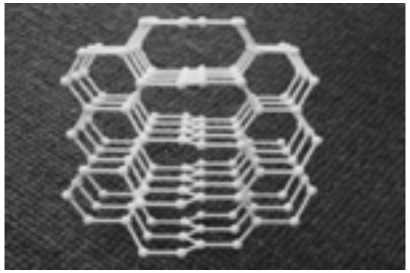
(10,3)



hyperoctagon



hyperhoneycomb



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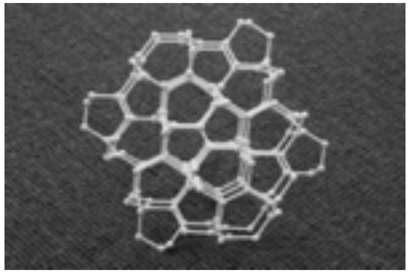
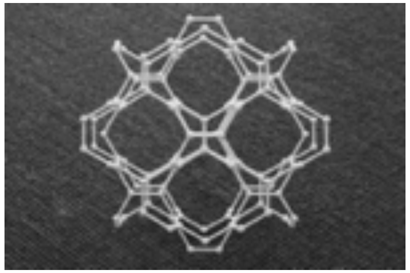
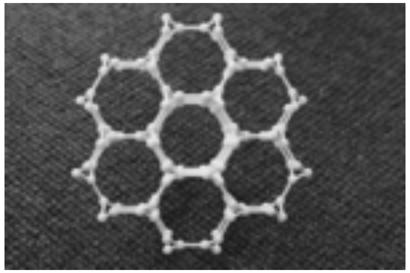
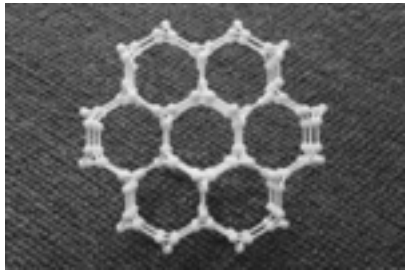
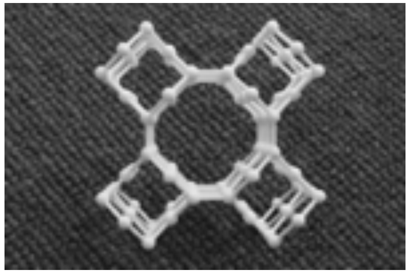


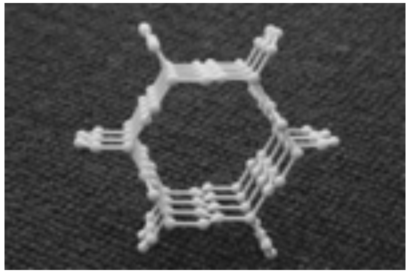


(8,3)







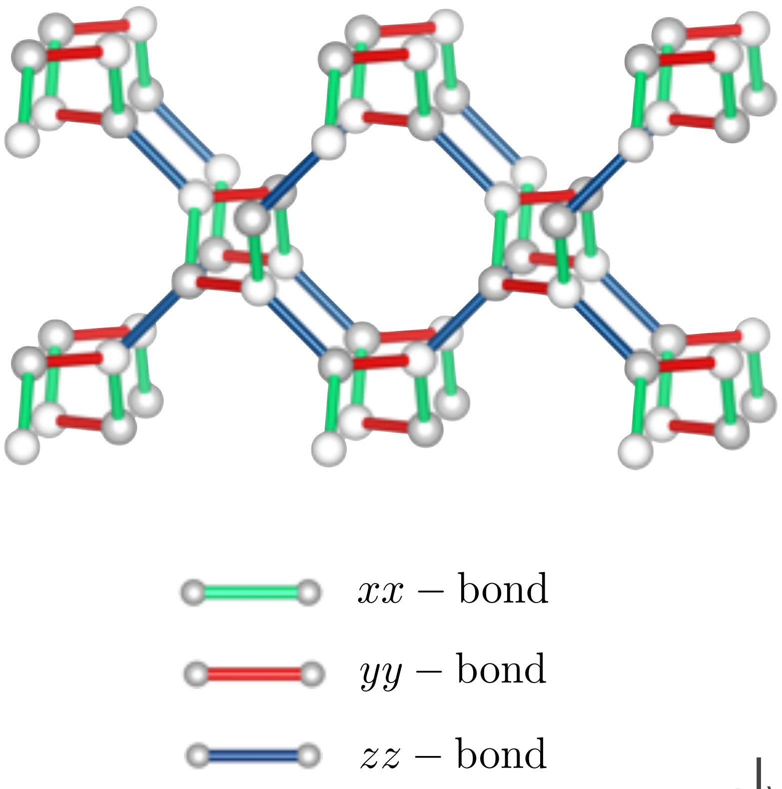


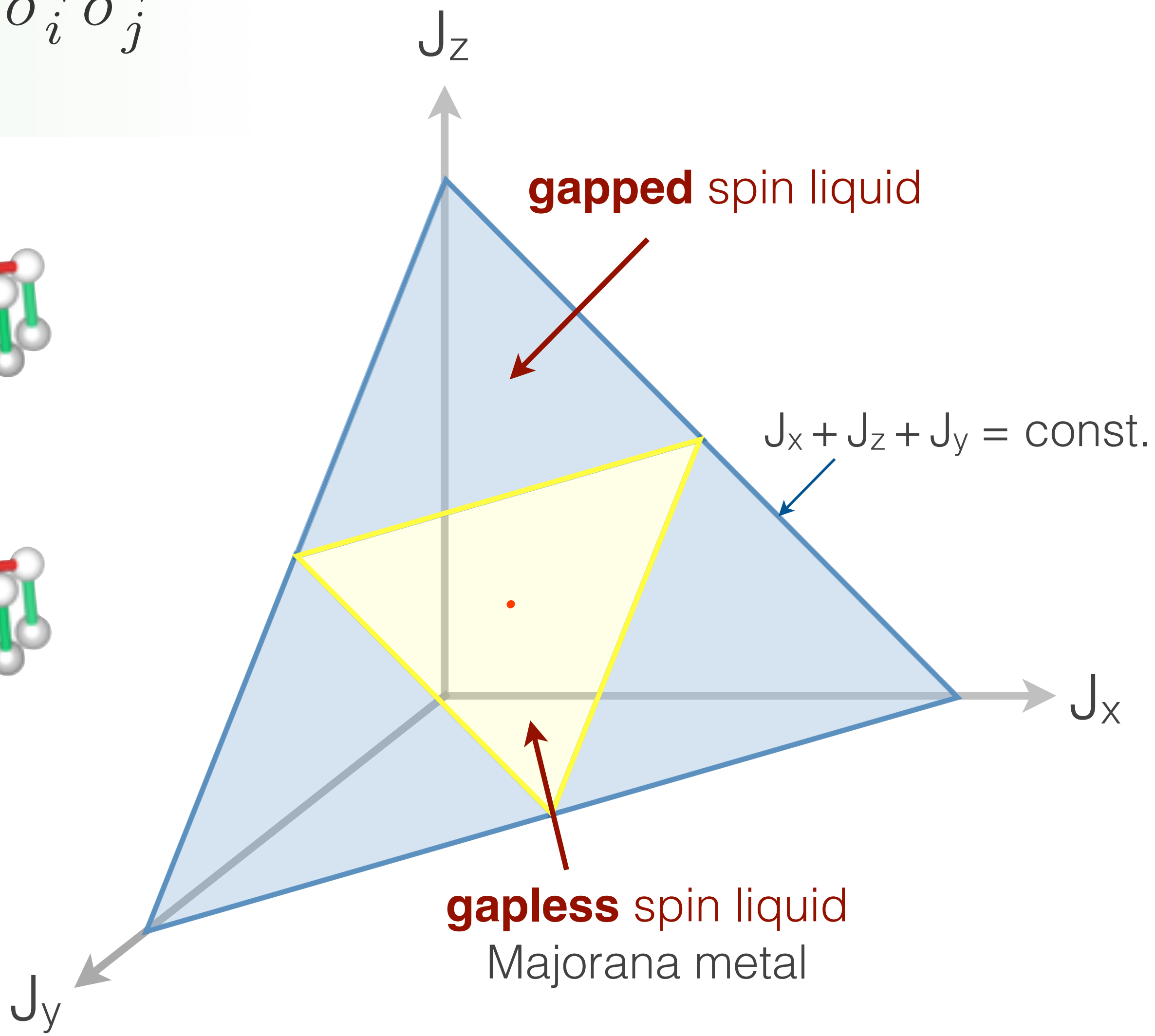
Tricoordinated lattices

		other names	Z	inversion	Lieb	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	✓	✓		

A family of 3D Kitaev models

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



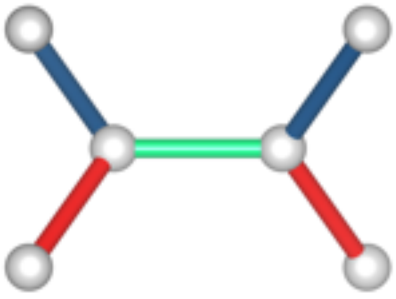


gapped spin liquid

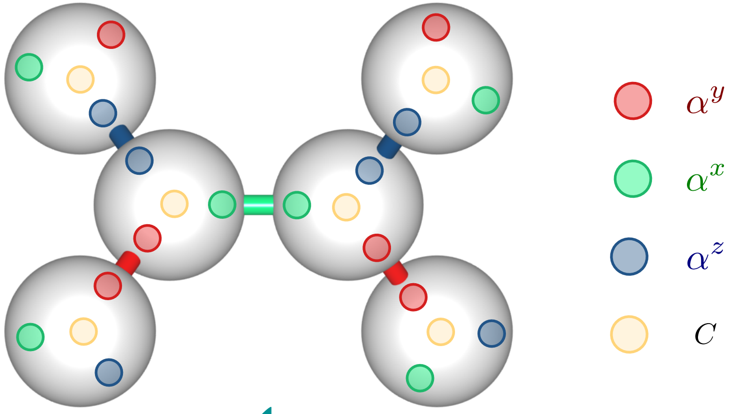
$J_x + J_z + J_y = \text{const.}$

gapless spin liquid
Majorana metal

Solving 3D Kitaev models – fractionalization



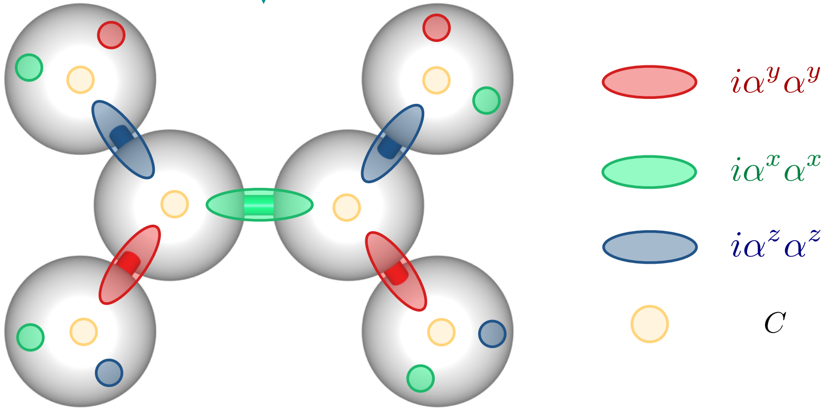
split spins



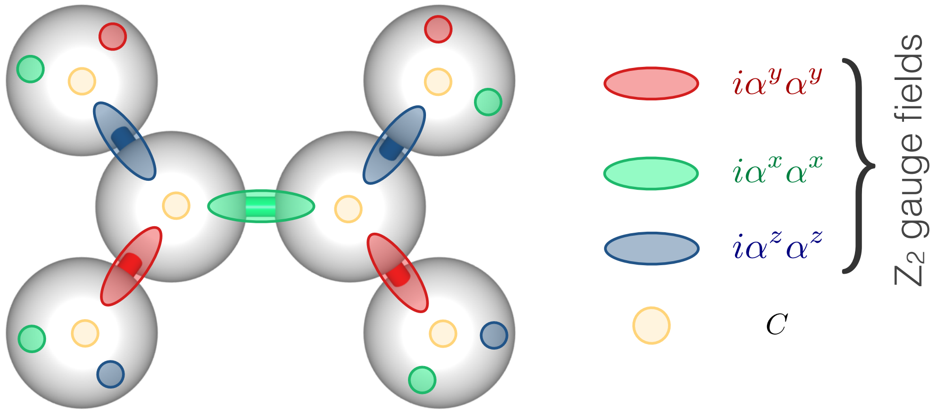
regroup
Majoranas

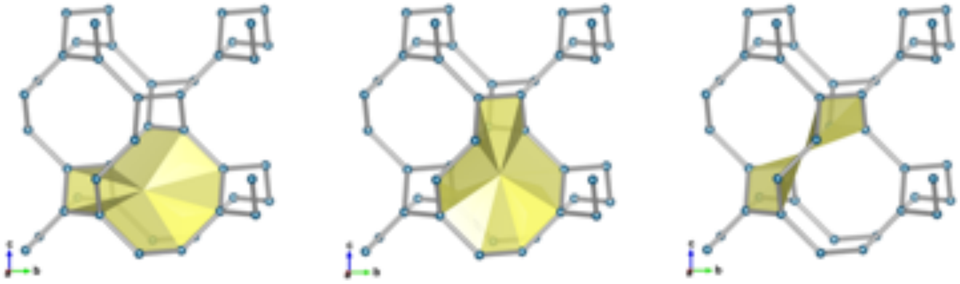
Step 1: Represent spins in terms of four **Majorana fermions** $\sigma^\alpha = i a^\alpha c$

Step 2: Bond operators $\hat{u}_{jk} = i a_j^\alpha a_k^\alpha$ realize an emergent **Z$_2$ gauge field**



Solving 3D Kitaev models – the fine print





Z_2 gauge fields are constrained by minimal volumes.

The emergent **Z_2 gauge field** 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**.

*For 3D Kitaev models the gauge fields freeze out at a *finite-temperature* Ising transition. Nasu, Udagawa, Motome PRL (2015)

The emergent **Majorana fermions** are **itinerant** degrees of freedom. Generically, they form a **gapless** collective state – a **Majorana metal**.

Majorana metals

		Majorana metal	TR breaking	Peierls instability
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	✗

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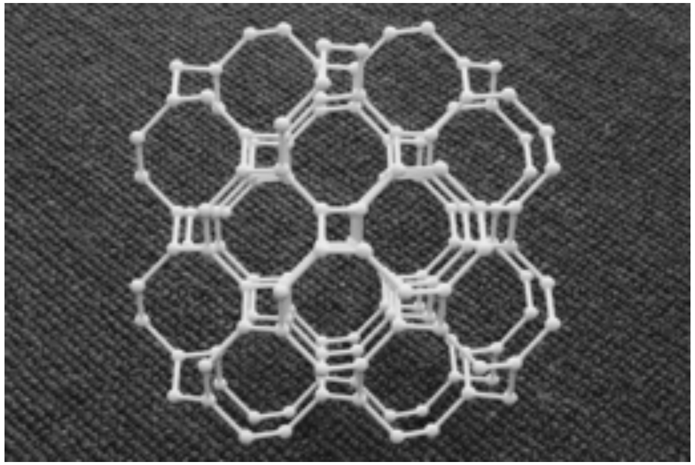
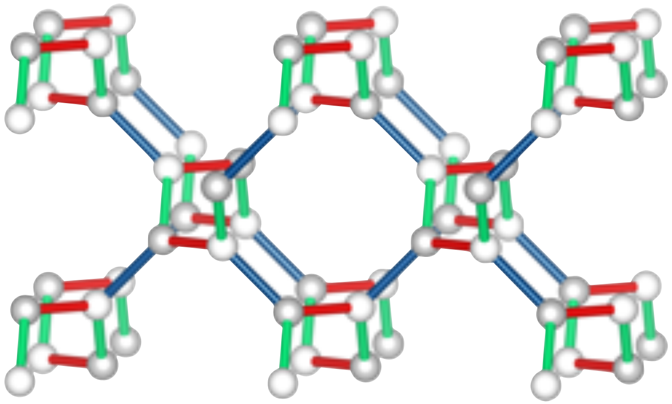
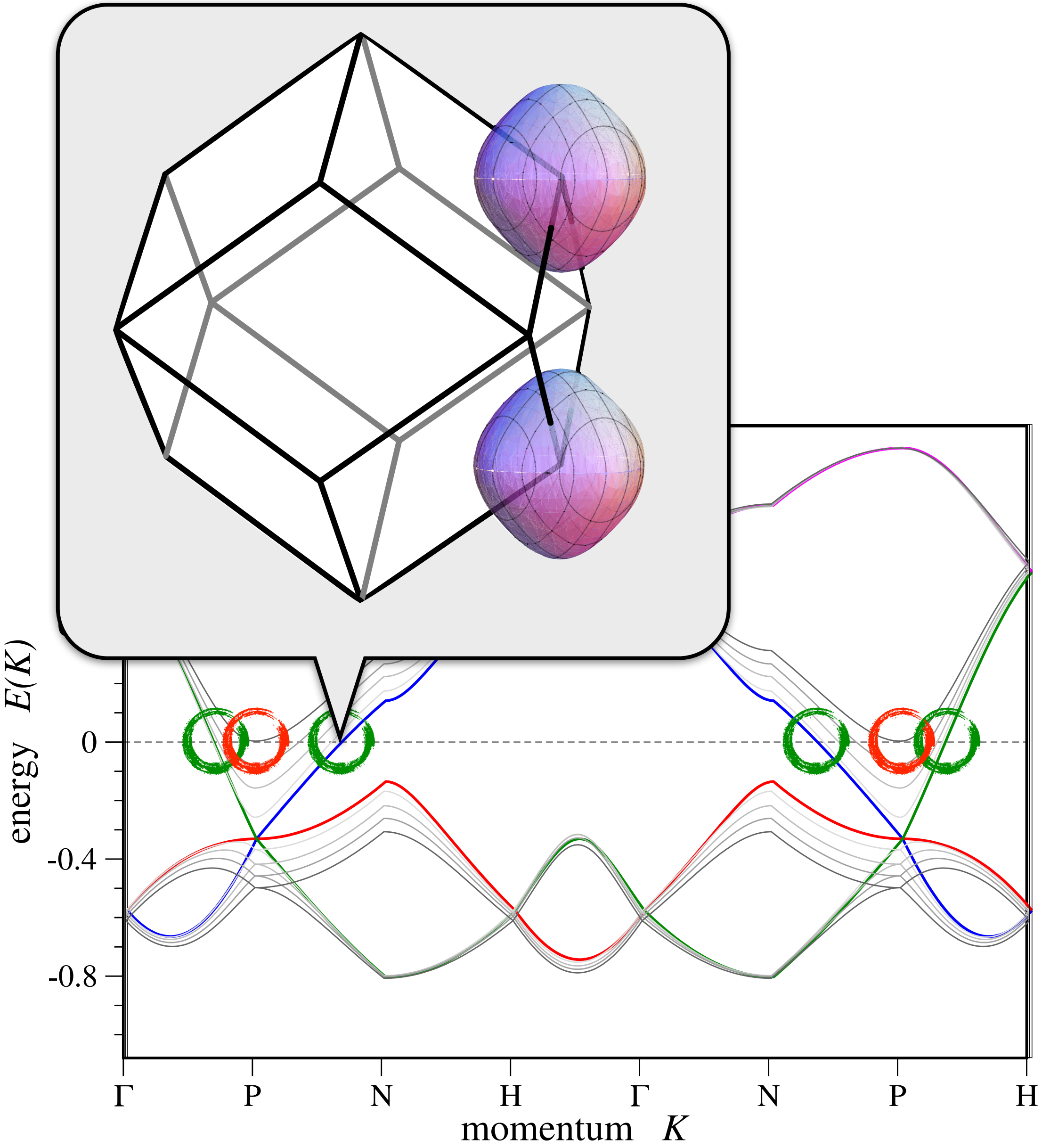
	(8,3)c	nodal line	Weyl nodes	✗
	(8,3)n	gapped	gapped	✗
2D	(6,3)	Dirac nodes	gapped	✗

Majorana Fermi surface

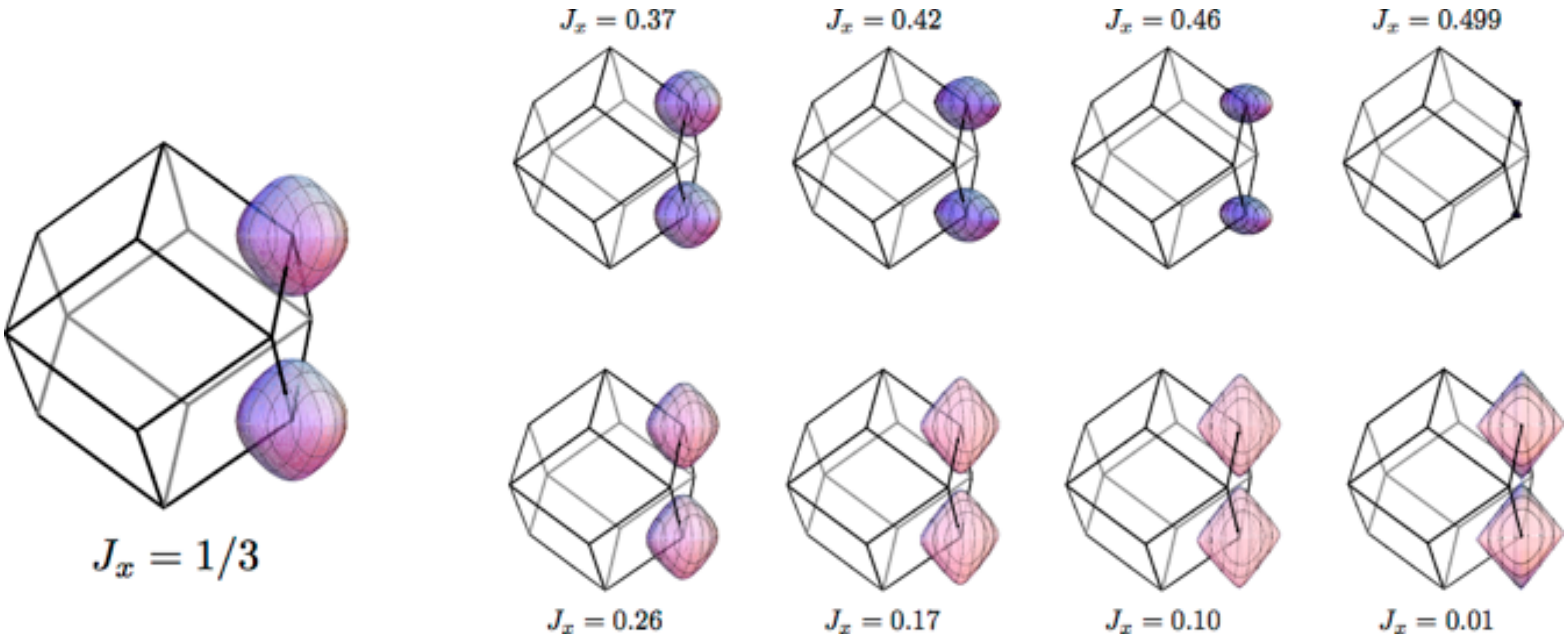
(10,3)a – hyperoctagon







Majorana Fermi surface



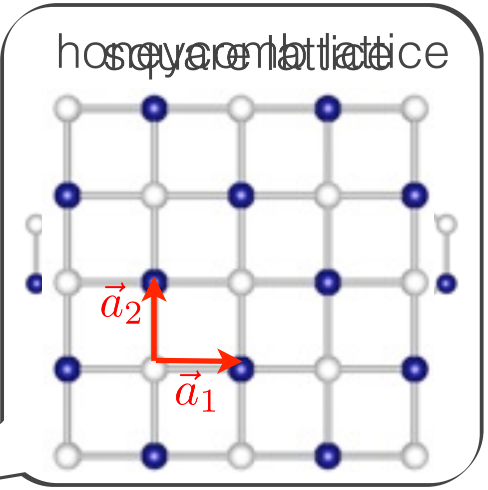
The hyperoctagon Kitaev model exhibits a full **two-dimensional Majorana Fermi surface**.

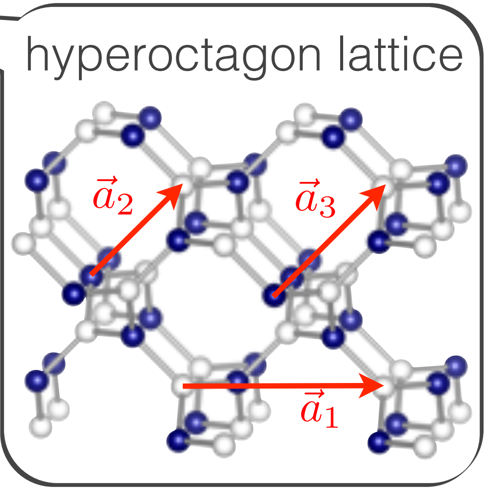
Recasting our result in the language of spin liquids, what we have found is the first **exactly solvable microscopic model** of a spin liquid with a **spinon Fermi surface**.

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	$\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k} + \mathbf{k}_0)$





$\mathbf{k}_0$ 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

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

complex-valued function

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

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

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

complex matrix

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

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

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

generic band Hamiltonian with TR symmetry

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

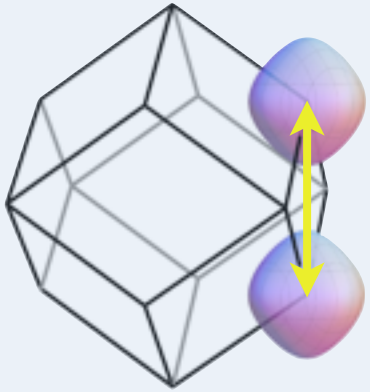
Peierls instability of Fermi surface

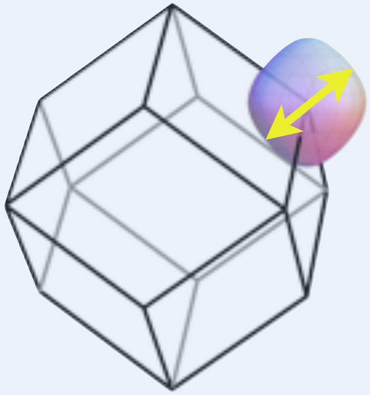
Fermi surface instabilities arise from additional spin interactions (e.g. a Heisenberg term), which introduce interactions between the Majorana fermions.

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





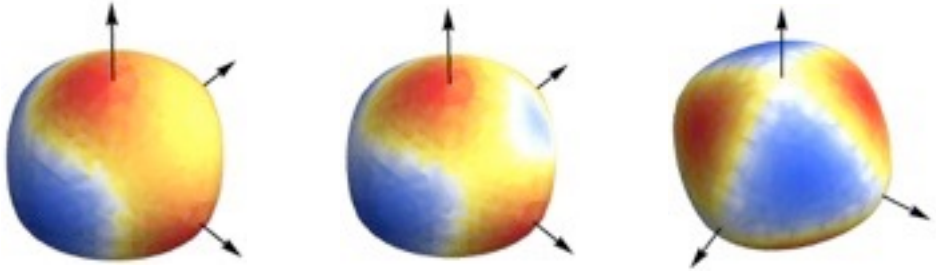
(complex) fermion

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, arXiv:1506.01379

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

Majorana metals

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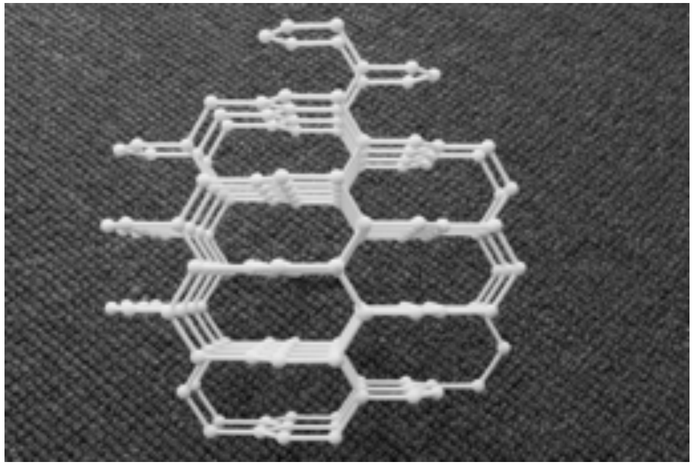
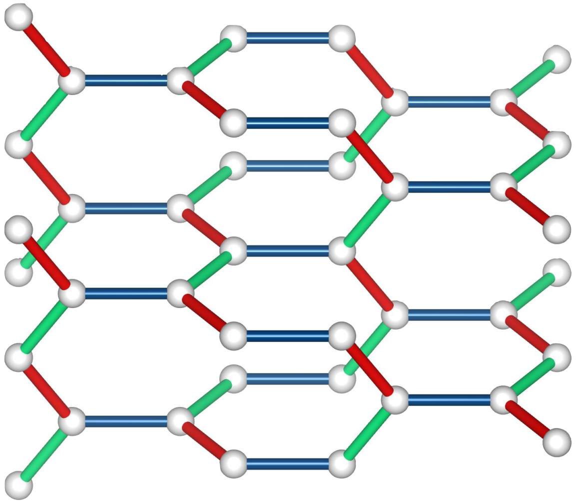
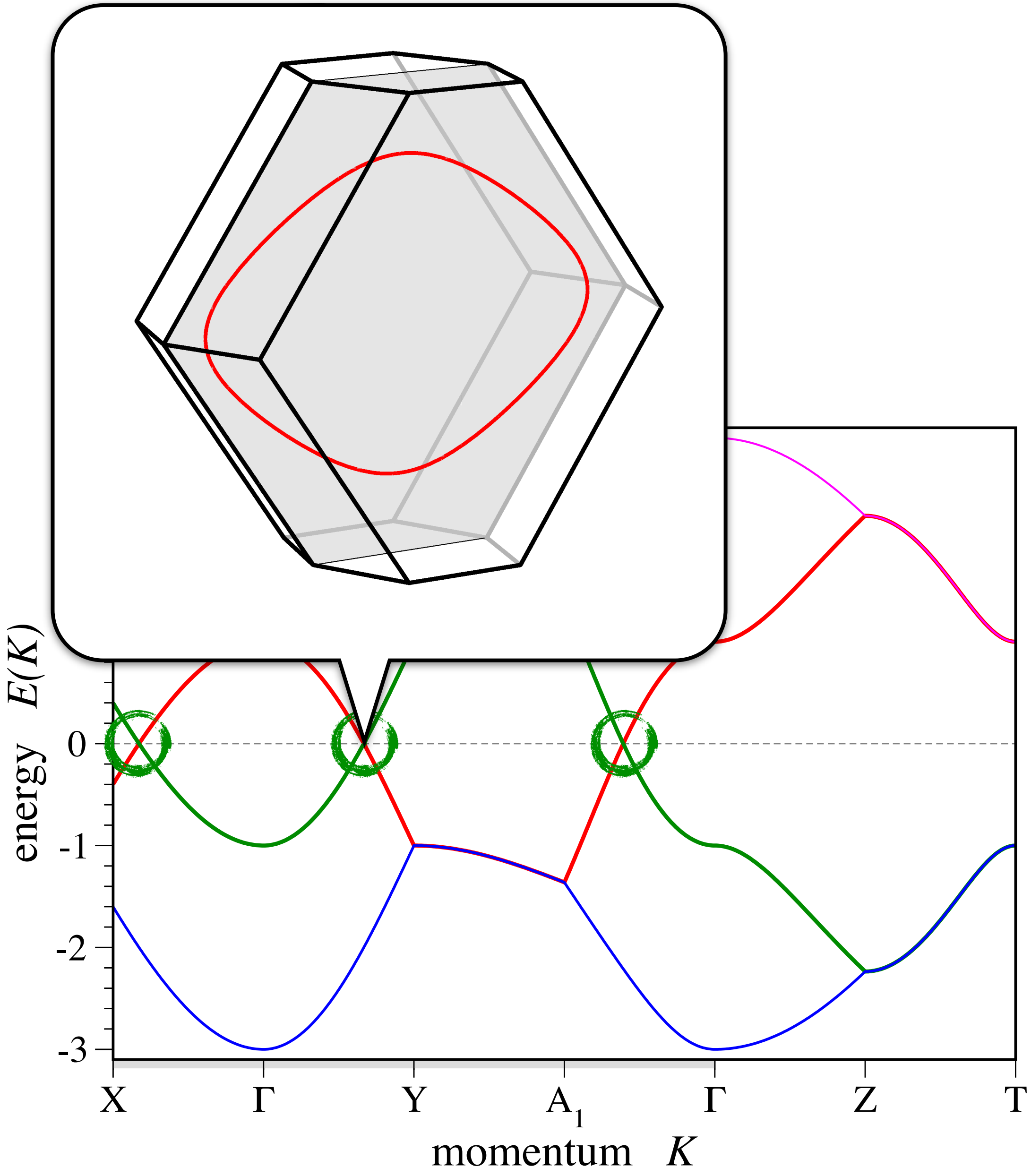
Majorana Fermi lines

(10,3)b – hyperhoneycomb







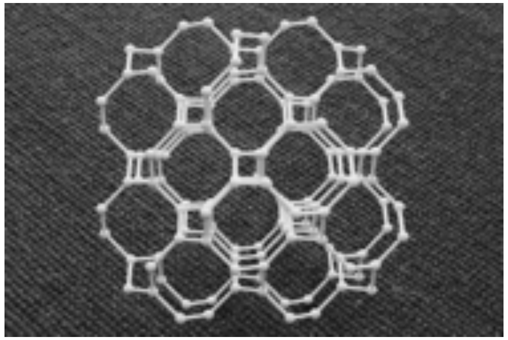
Majorana metals

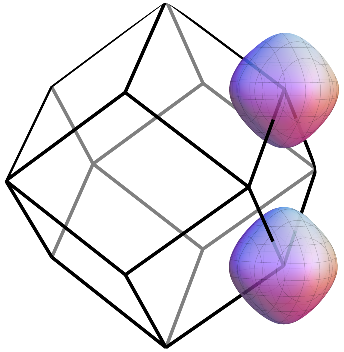
		Majorana metal	TR breaking	Peierls instability
3D lattices	(10,3)a	Fermi surface	Fermi surface	✓
	(10,3)b	nodal line	Weyl nodes	✗
	(10,3)c	nodal line	Fermi surface	✗
	(9,3)a	Weyl nodes	Weyl nodes	✗
	(8,3)a	Fermi surface	Fermi surface	✓
	(8,3)b	Weyl nodes	Weyl nodes	✓
	(8,3)c	nodal line	Weyl nodes	✗
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

Breaking time-reversal symmetry

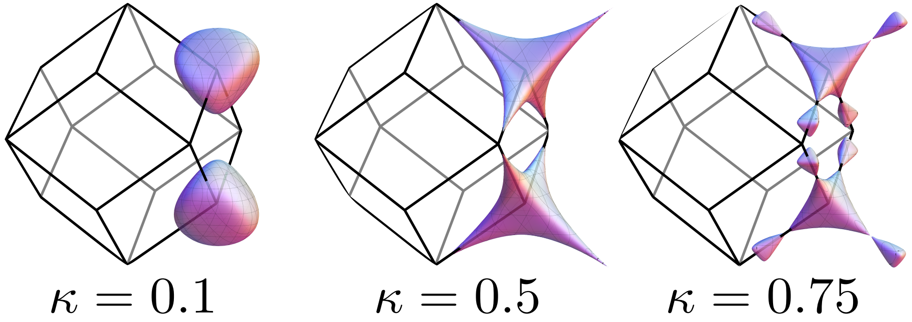
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma - \sum_j \vec{h} \cdot \vec{\sigma}_j$$

(10,3)a – hyperoctagon



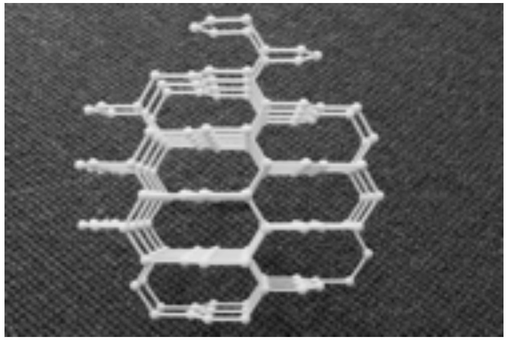


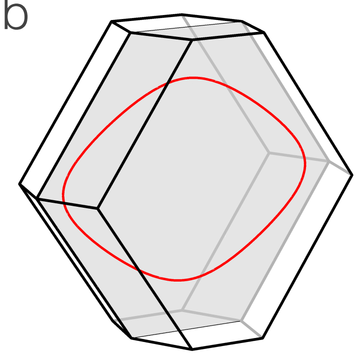
Fermi **surface**



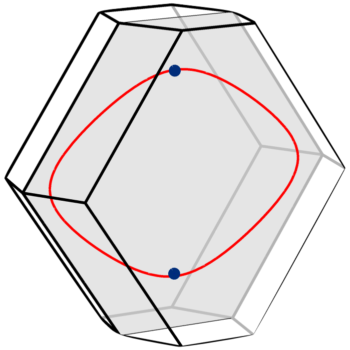
Fermi surface **deforms**

(10,3)b – hyperhoneycomb





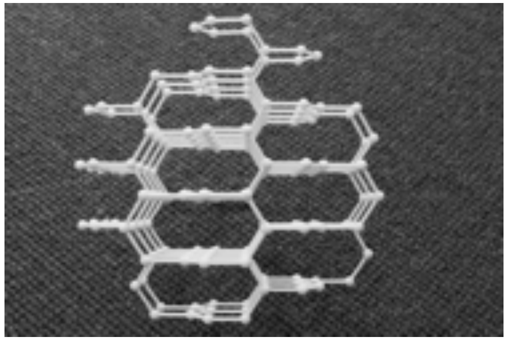
Fermi **line**



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

Weyl physics – energy spectrum

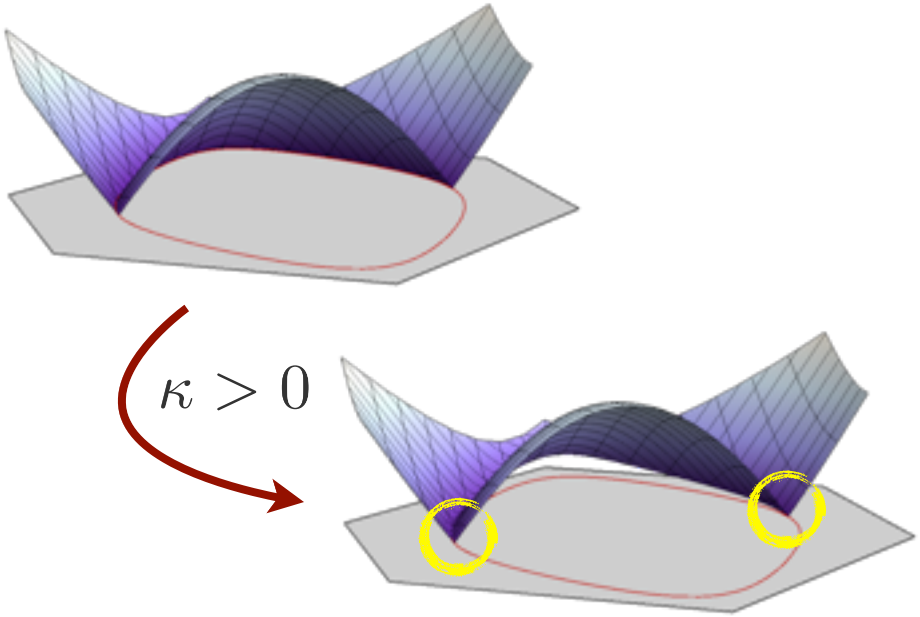
(10,3)b – hyperhoneycomb

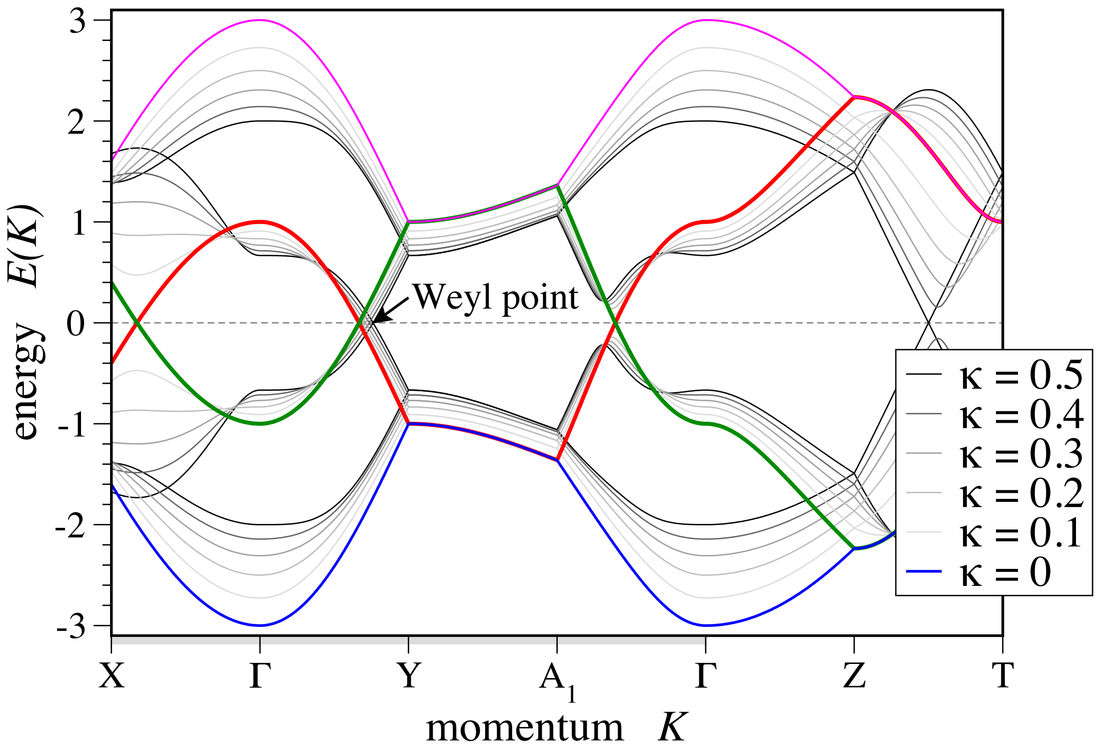


Touching of two bands in 3D is generically **linear**

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

Weyl nodes



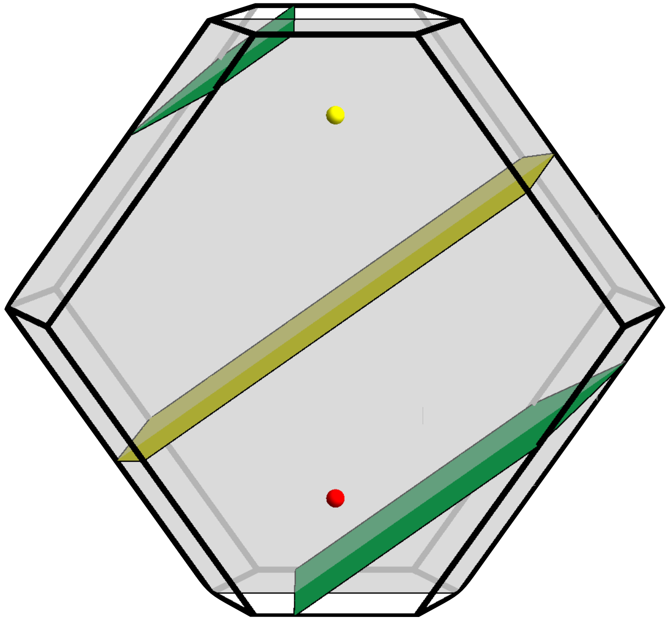


Weyl physics – Chern numbers

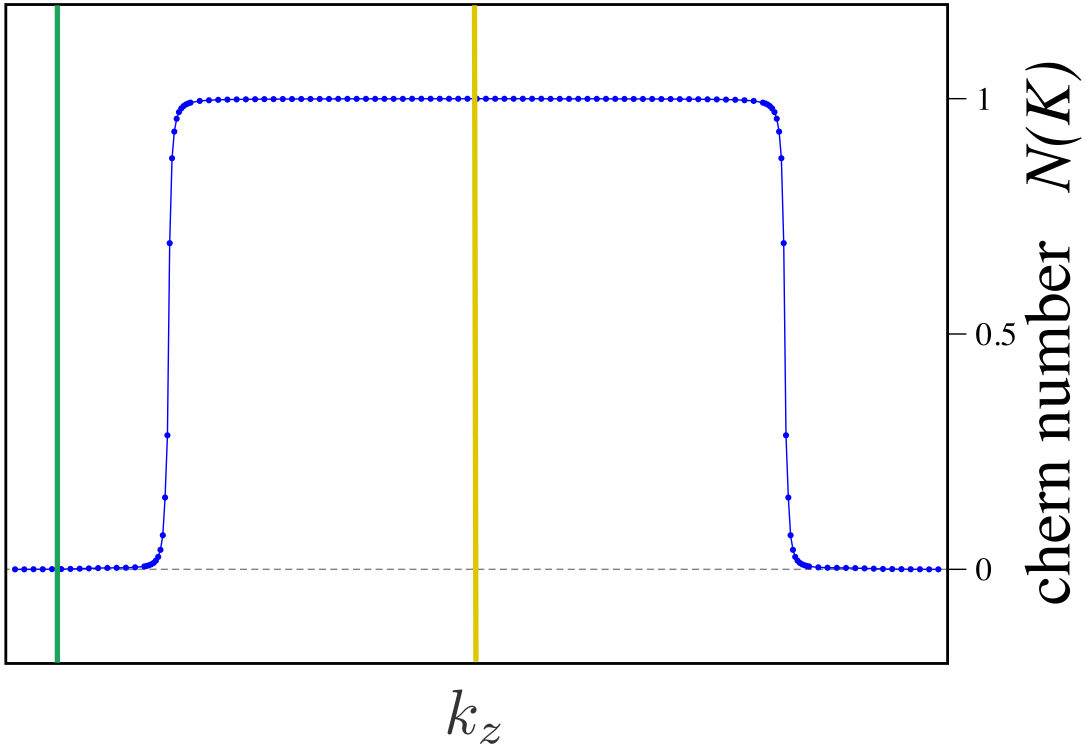
Weyl nodes are **sources or sinks of Berry flux**

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

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



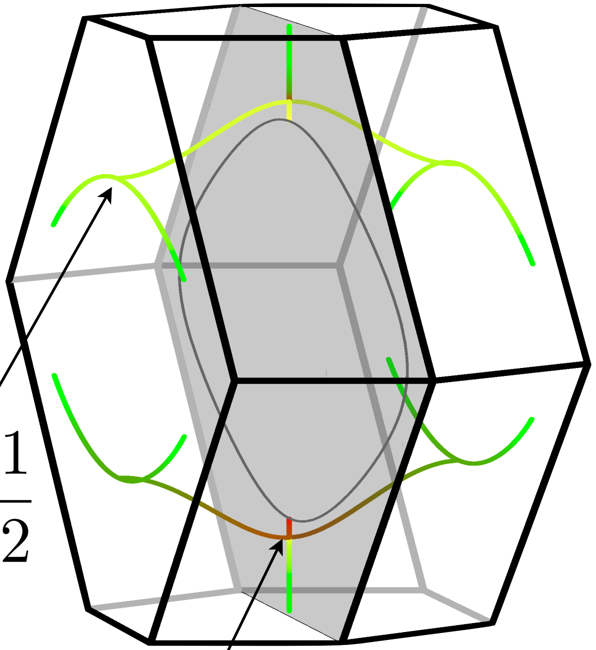
$\kappa = 0.05$



Weyl physics – surface states

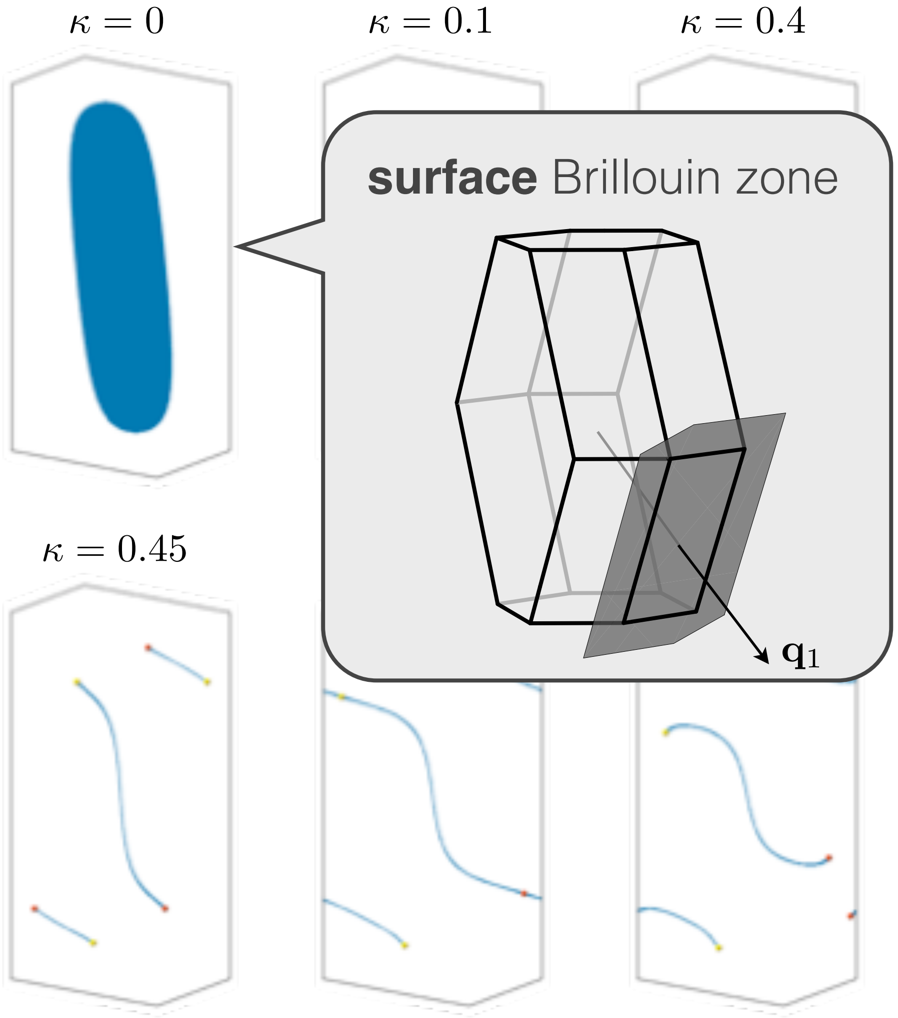
evolution of **Weyl nodes**
in the **bulk**

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

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

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

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

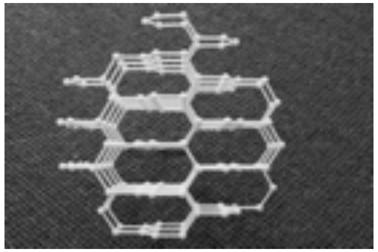
see also T. Meng and L. Balents, Phys. Rev. B 86, 054504 (2012).

Majorana metals

		Majorana metal	TR breaking	Lieb theorem
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	✓

Three scenarios for Weyl physics

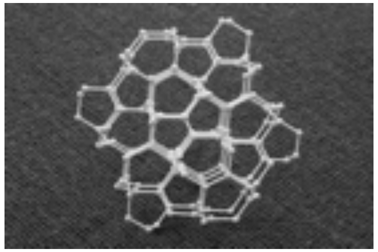
(10,3)b – hyperhoneycomb



explicit breaking of time-reversal symmetry

symmetry class D

(9,3)a

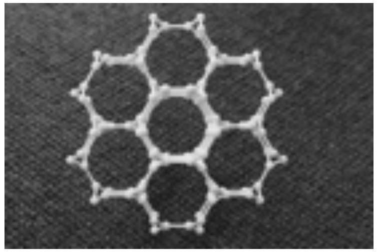


spontaneous breaking of time-reversal symmetry

symmetry class D

finite-temperature transition
possibly interesting (beyond Ising, LGW)

(8,3)b



no breaking of time-reversal symmetry
(nor inversion symmetry)

symmetry class BDI

symmetry scenario
beyond electronic systems

Summary

PRB 89, 235102 (2014)
PRL 114, 157202 (2015)
arXiv:1506.01379
(stay tuned for more)

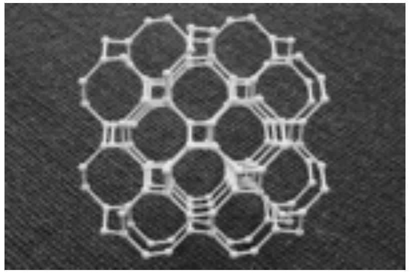
Kitaev models are paradigmatic examples for **spin fractionalization**.

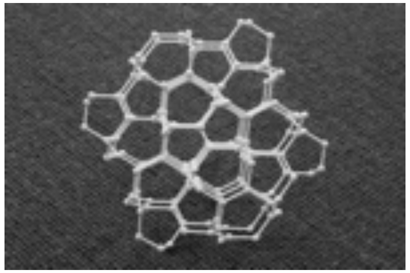
spin-1/2 $\sigma_j^\gamma = i\, b_j^\gamma c_j$ Majorana fermion + Z_2 gauge field

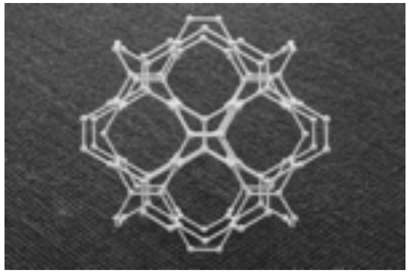
3D Kitaev models host a surprisingly rich variety of **gapless Z_2 spin liquids**.

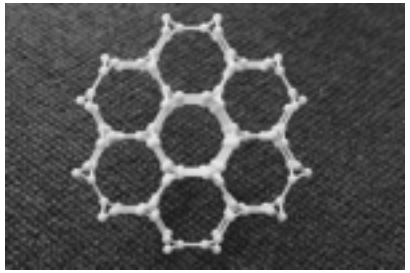
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma$$

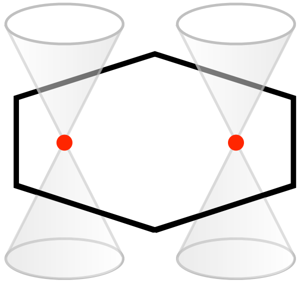
Analytical control of these models allows to provide first examples of tractable spin models with a **spinon Fermi surface** or a **Weyl spin liquid** ground state.



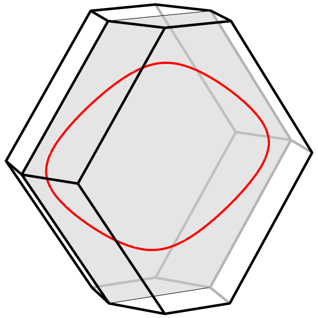




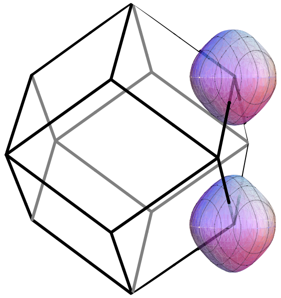




Dirac **points**



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



Fermi **surfaces**

Thanks!