Spin-Peierls Instabilities of three-dimensional Kitaev Spin Liquids

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arXiv:1506.01379
PRL 114, 157202 (2015)
PRB 89, 235102 (2014)

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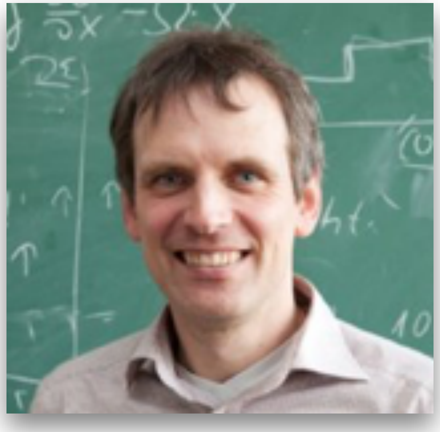
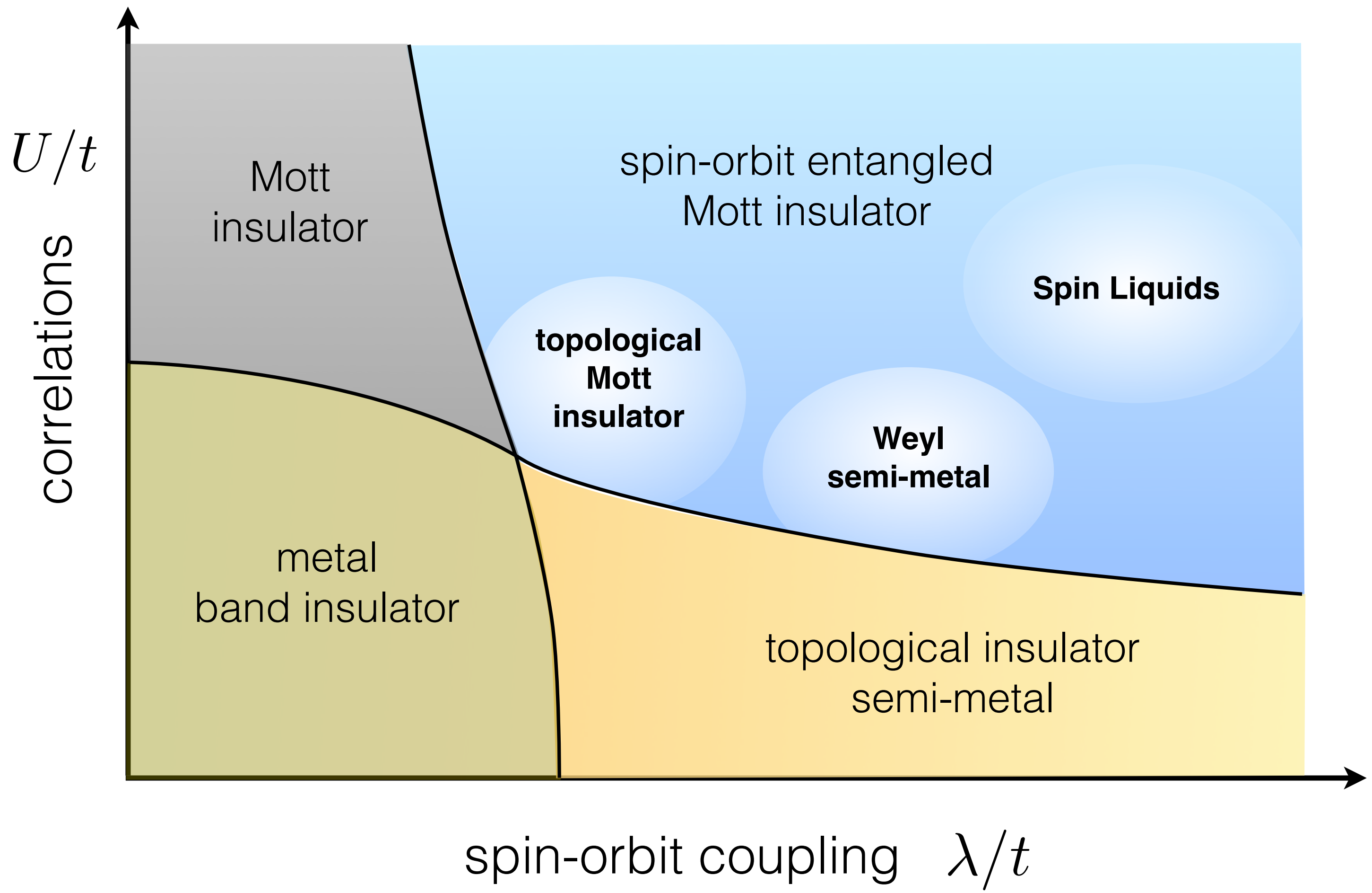


5d transition metal oxides

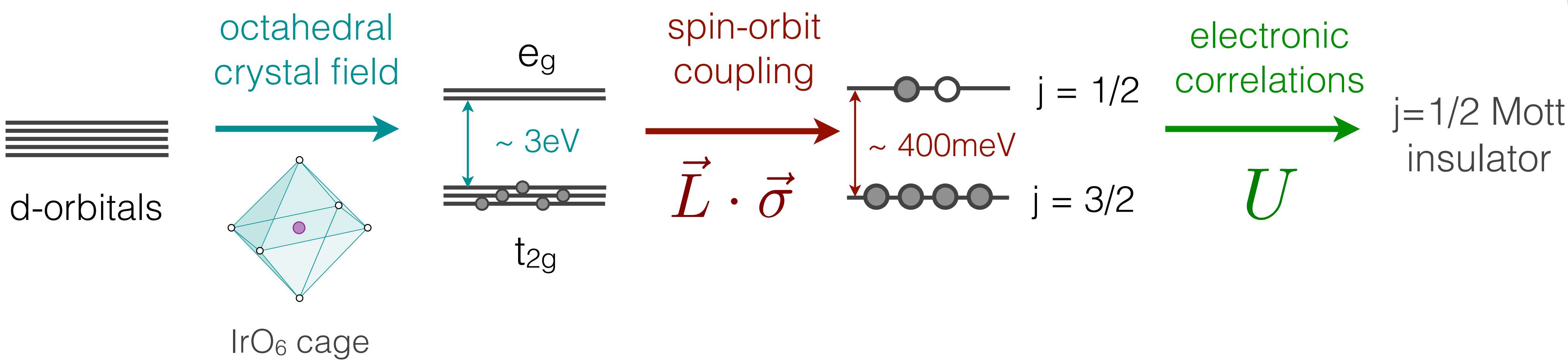
Largely *accidental* degeneracy of electronic correlations, spin-orbit entanglement, and crystal field effects results in a **broad variety of metallic and insulating states**.



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?**

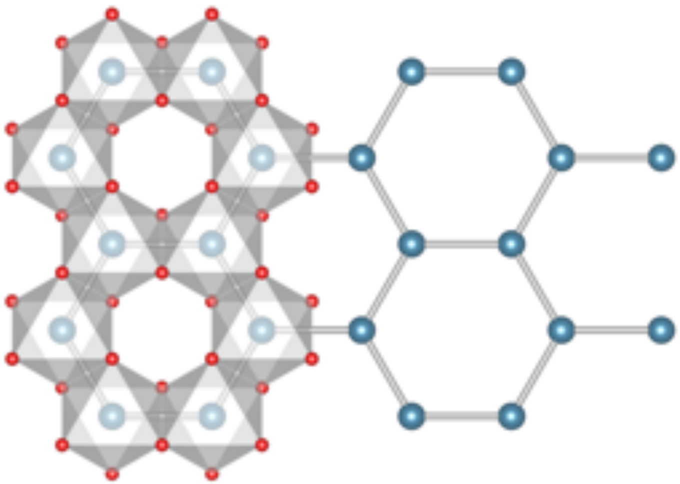
B.J. Kim et al. PRL 101, 076402 (2008)
B.J. Kim et al. Science 323, 1329 (2009)

$(Na,Li)_2IrO_3$ 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

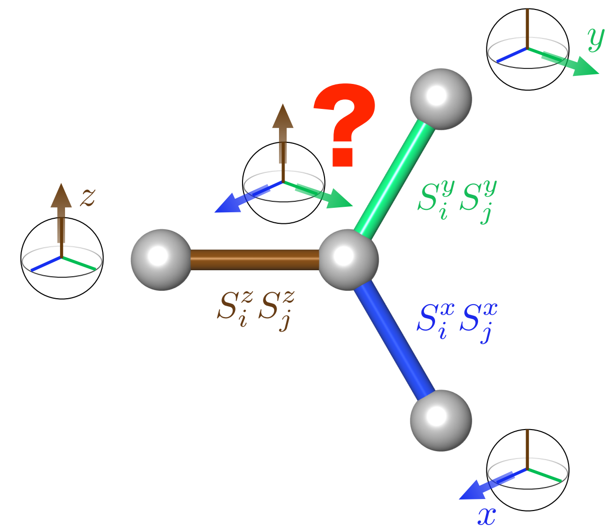


Na_2IrO_3

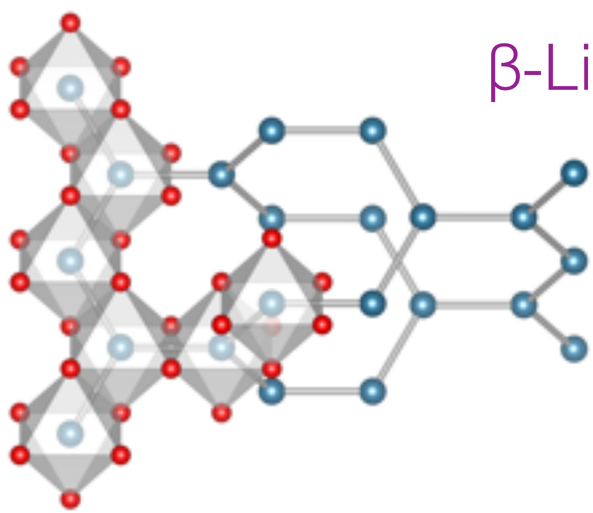
α-Li_2IrO_3

see also $RuCl_3$

Kitaev exchange

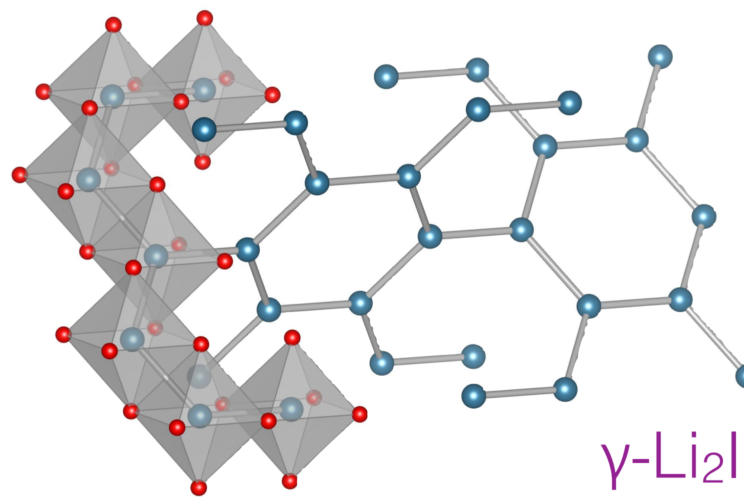


hyperhoneycomb



β-Li_2IrO_3

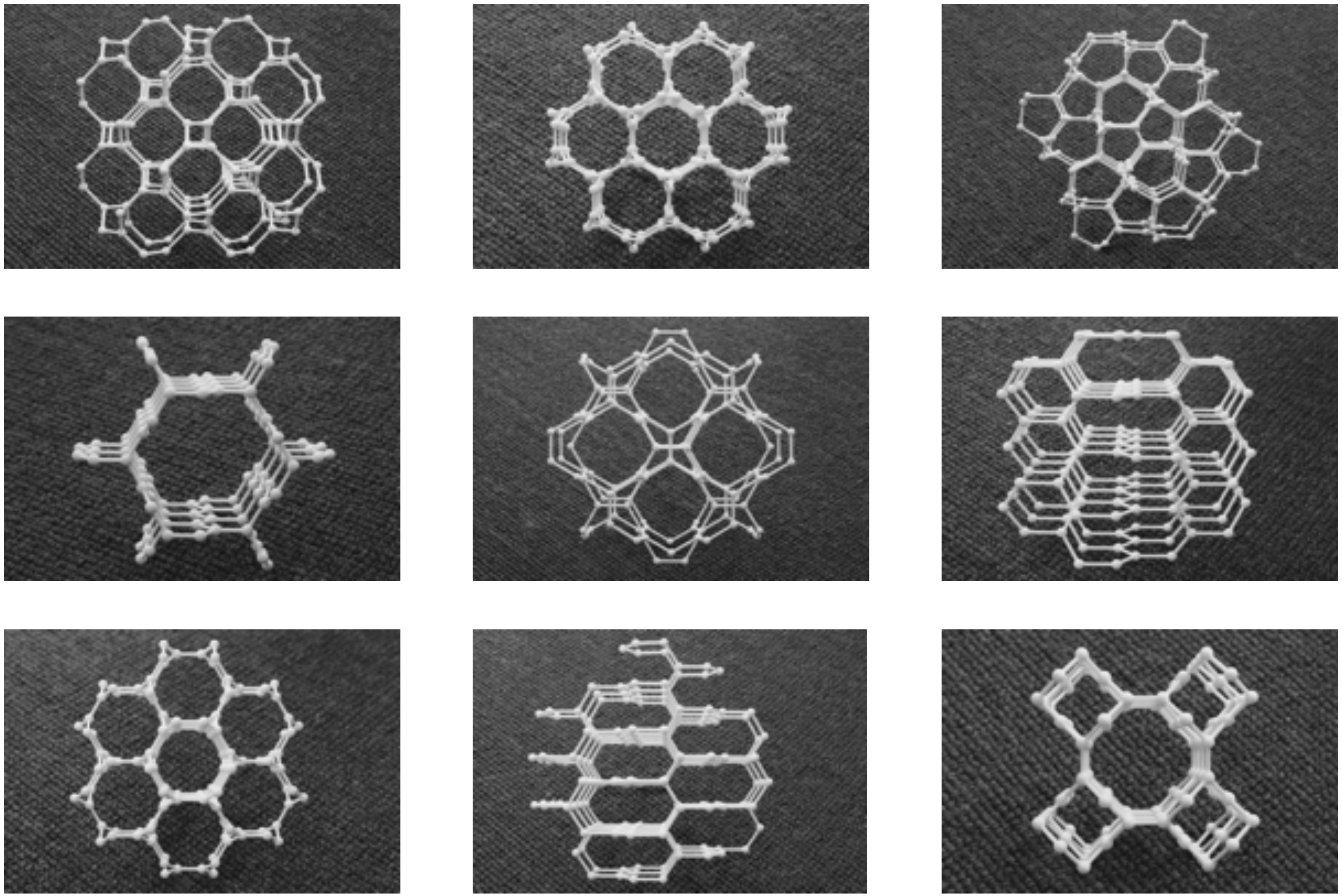
harmonic honeycomb



γ-Li_2IrO_3

Tricoordinated lattices in 3D

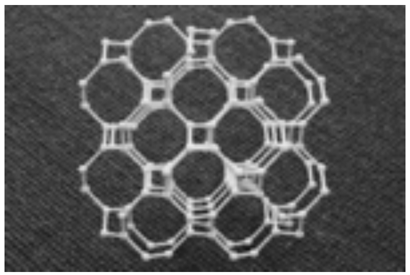
How many such lattices exist?



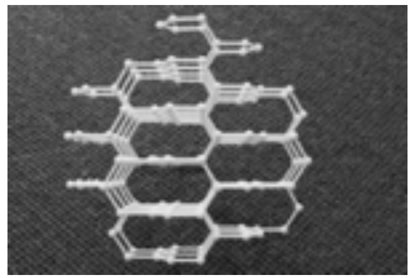
Tricoordinated lattices in 3D

Classification by elementary loop length (polygonality)

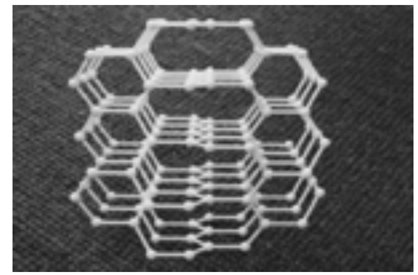
(10,3)



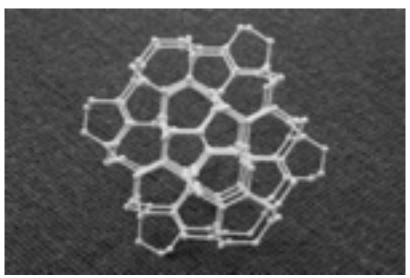
hyperoctagon

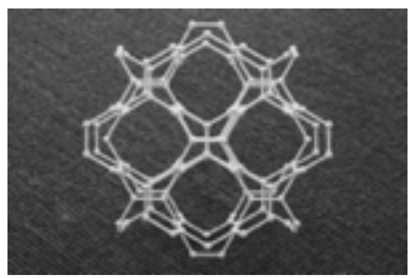


hyperhoneycomb

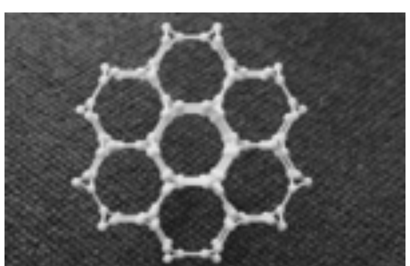


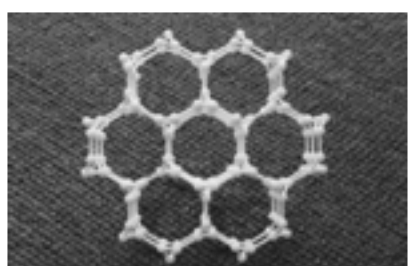
(9,3)

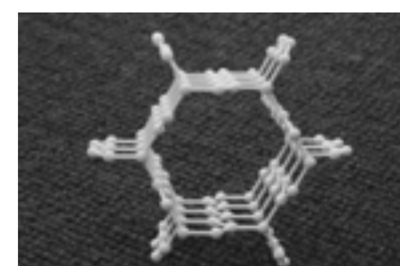




(8,3)







Lattice classifications

polygonality \ connectivity	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)

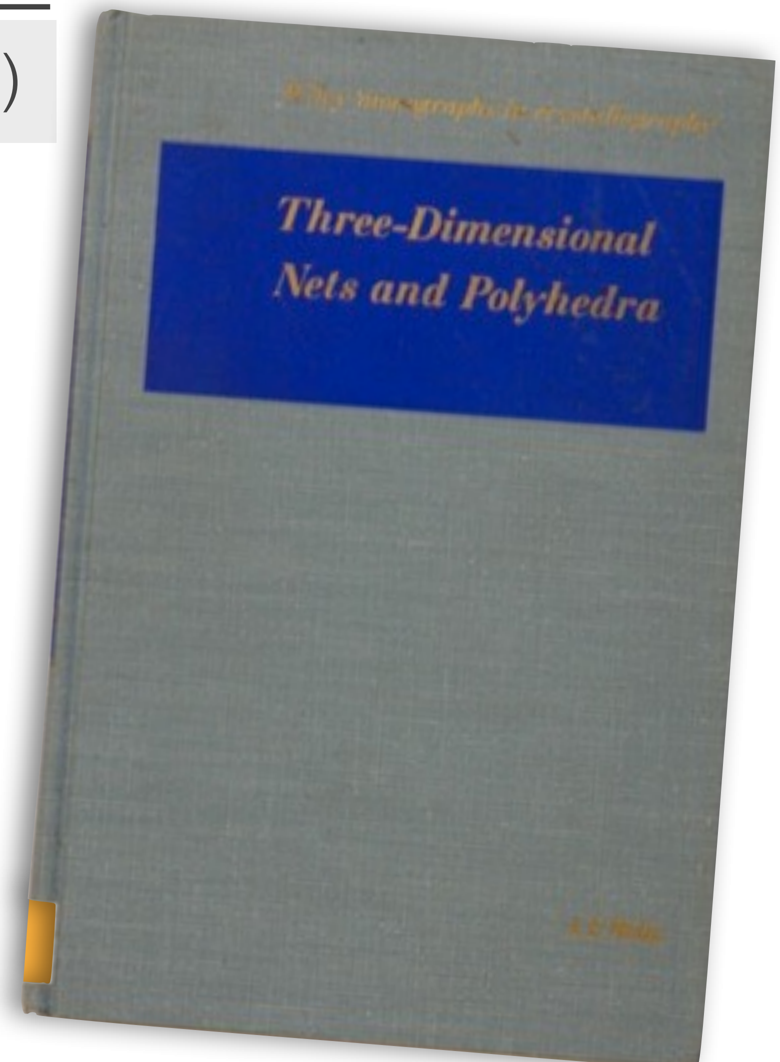
platonic solids

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			

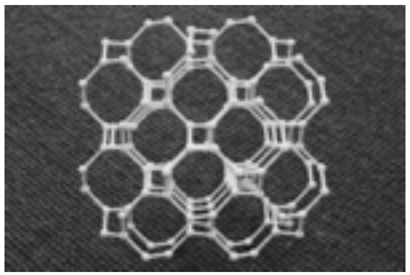


A.F.Wells, 1977

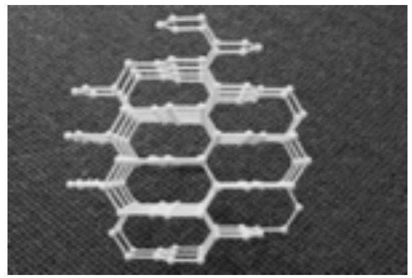
Tricoordinated lattices

Classification by elementary loop length (polygonality)

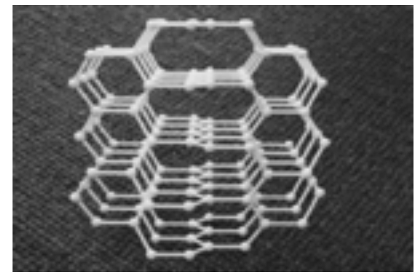
(10,3)



hyperoctagon



hyperhoneycomb



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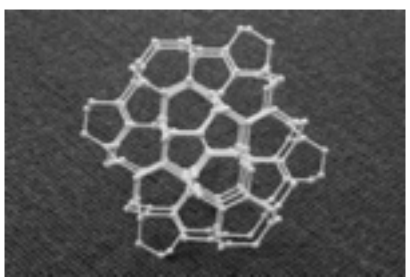
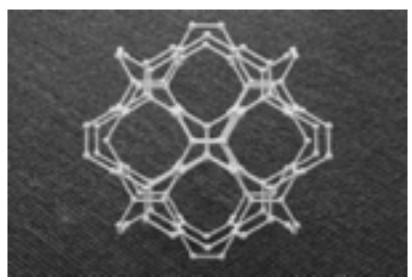
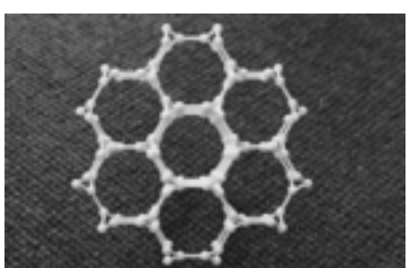
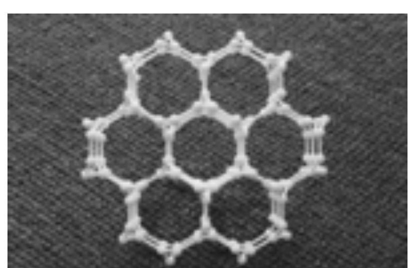
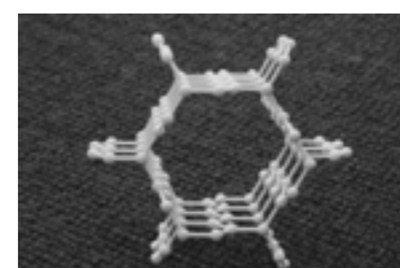




(8,3)





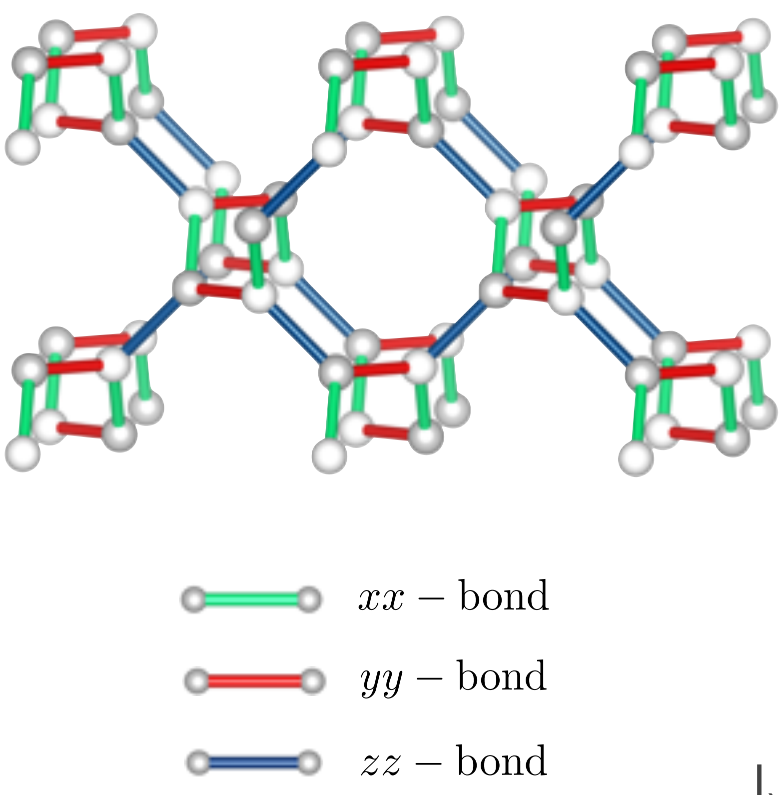


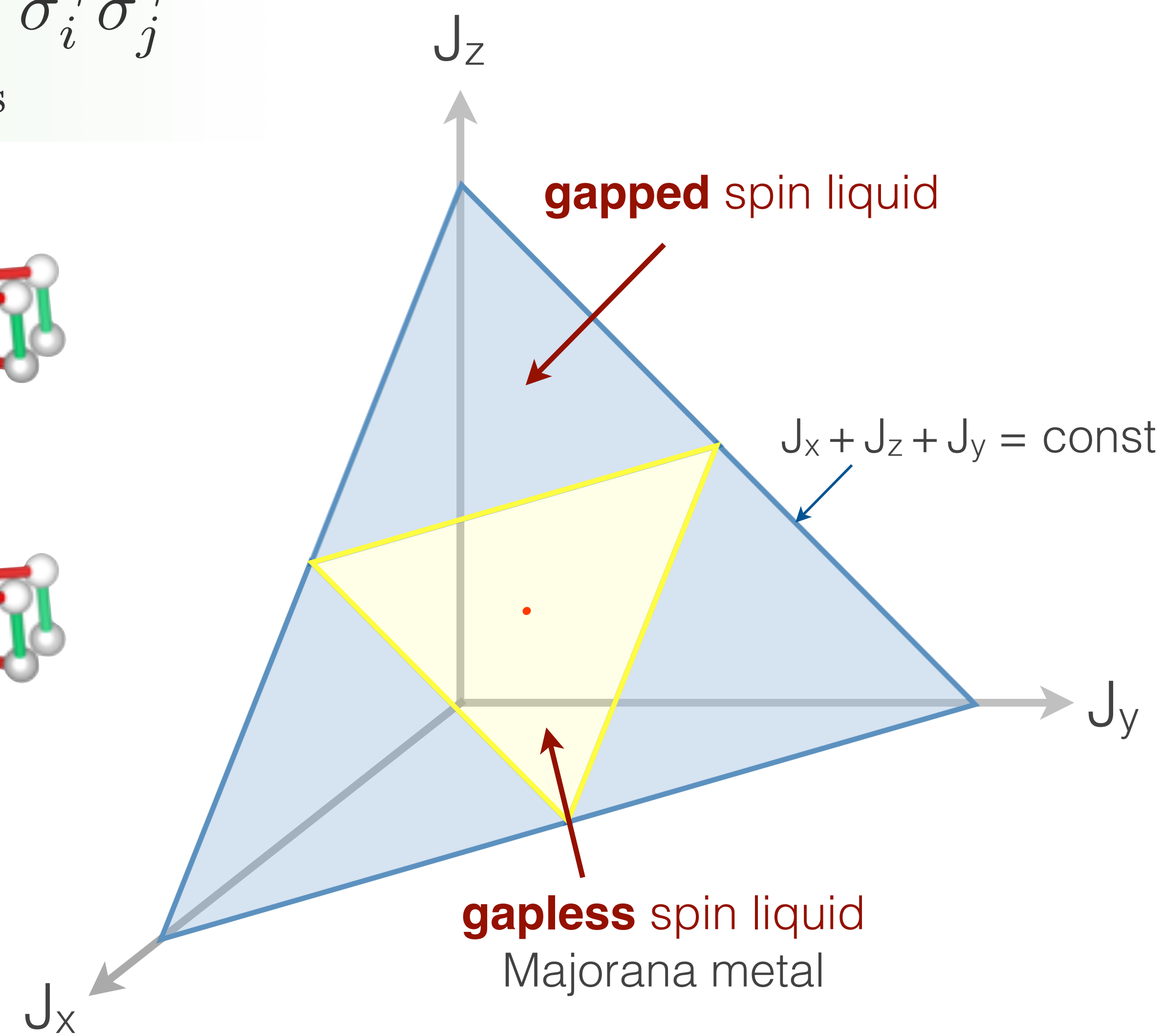
Tricoordinated lattices

		other names	Z	inversion	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	✓		

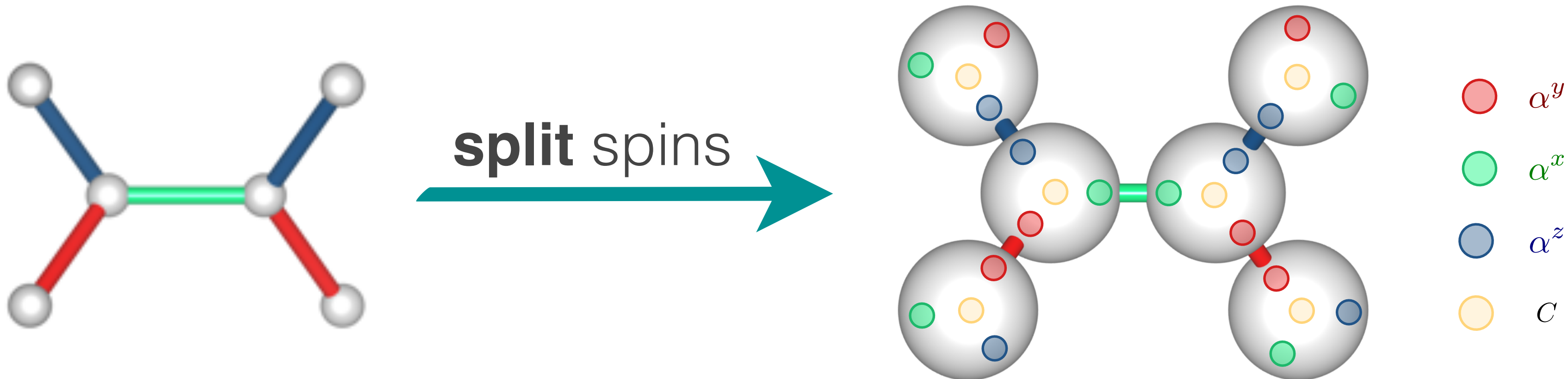
A family of 3D Kitaev models

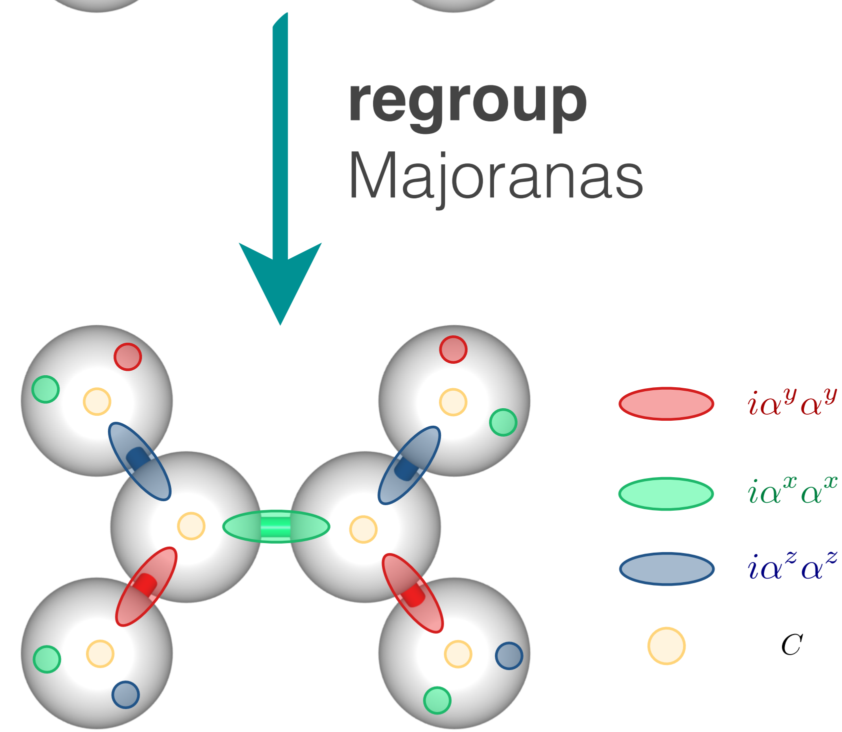
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma$$





Solving 3D Kitaev models – fractionalization

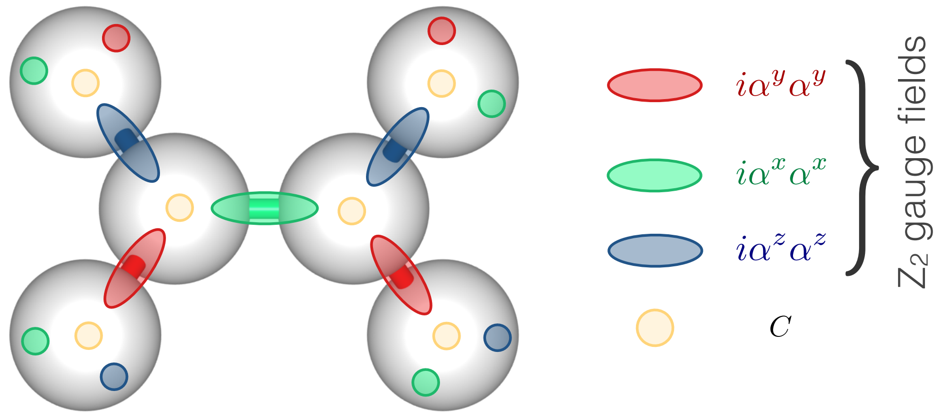


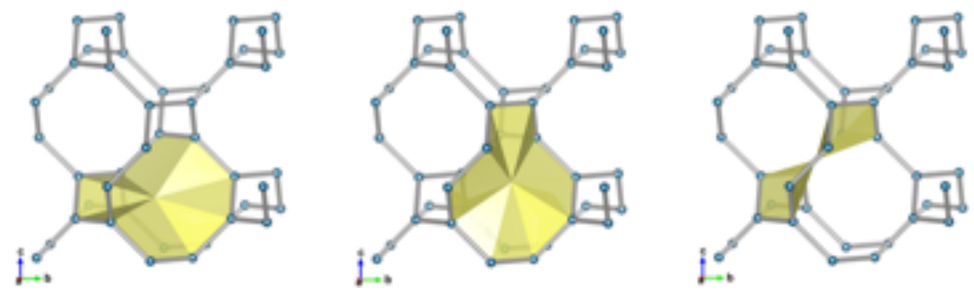


Step 1: Represent spins in terms of four **Majorana fermions** $\sigma^\alpha = i a^\alpha c$

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

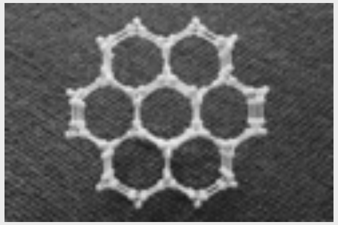




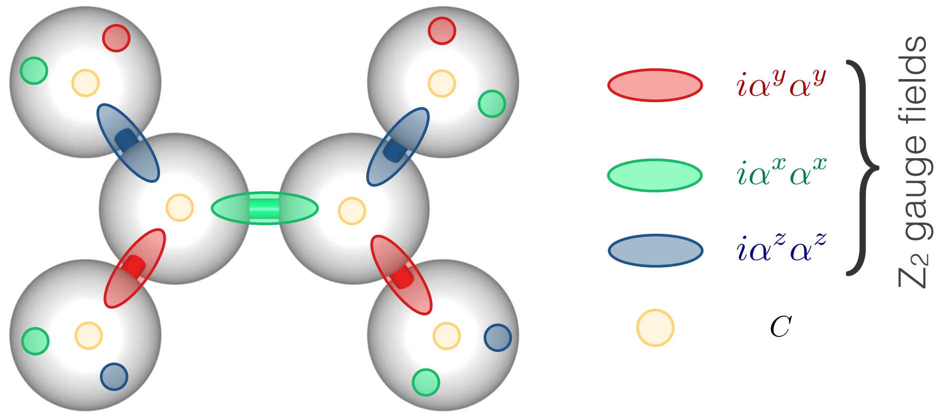
Z_2 gauge fields are constrained by minimal volumes.

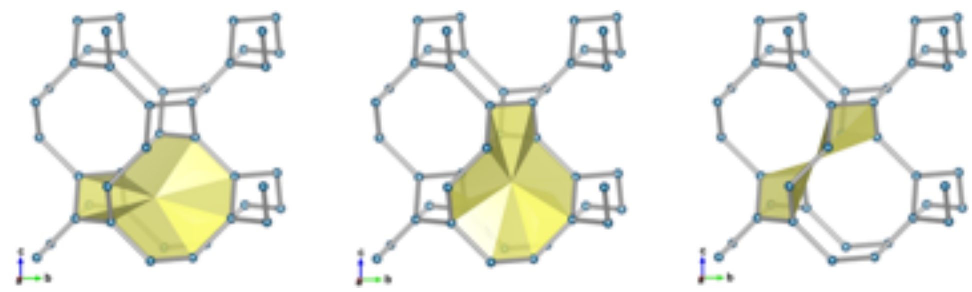
The emergent **Z_2 gauge field** are **static** degrees of freedom. Generically, one has to find its **gapped** ground-state configuration* via educated guesses, Monte Carlo sampling or for some lattices via **Lieb's theorem**.

There are only two lattices fulfilling Lieb's theorem, the two-dimensional **honeycomb lattice** and the three-dimensional **(8,3)b lattice**.



Solving 3D Kitaev models – the fine print





Z_2 gauge fields are constrained by minimal volumes.

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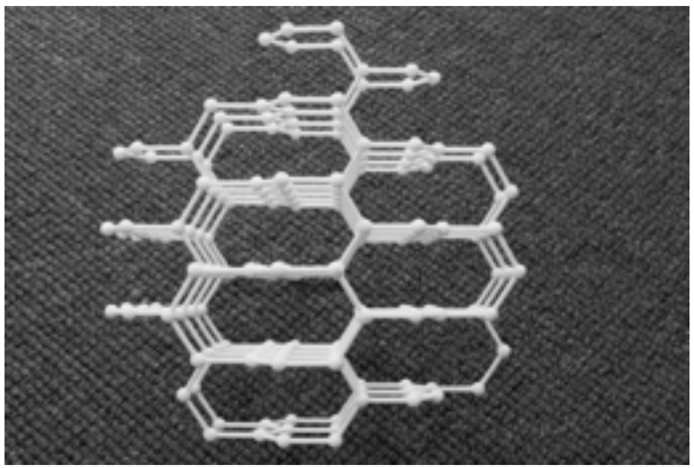
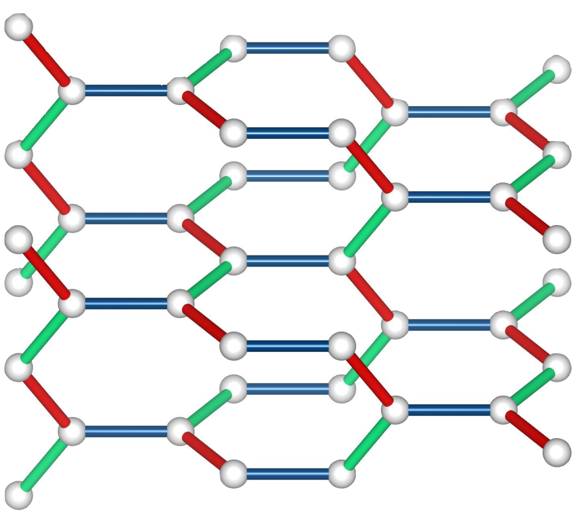
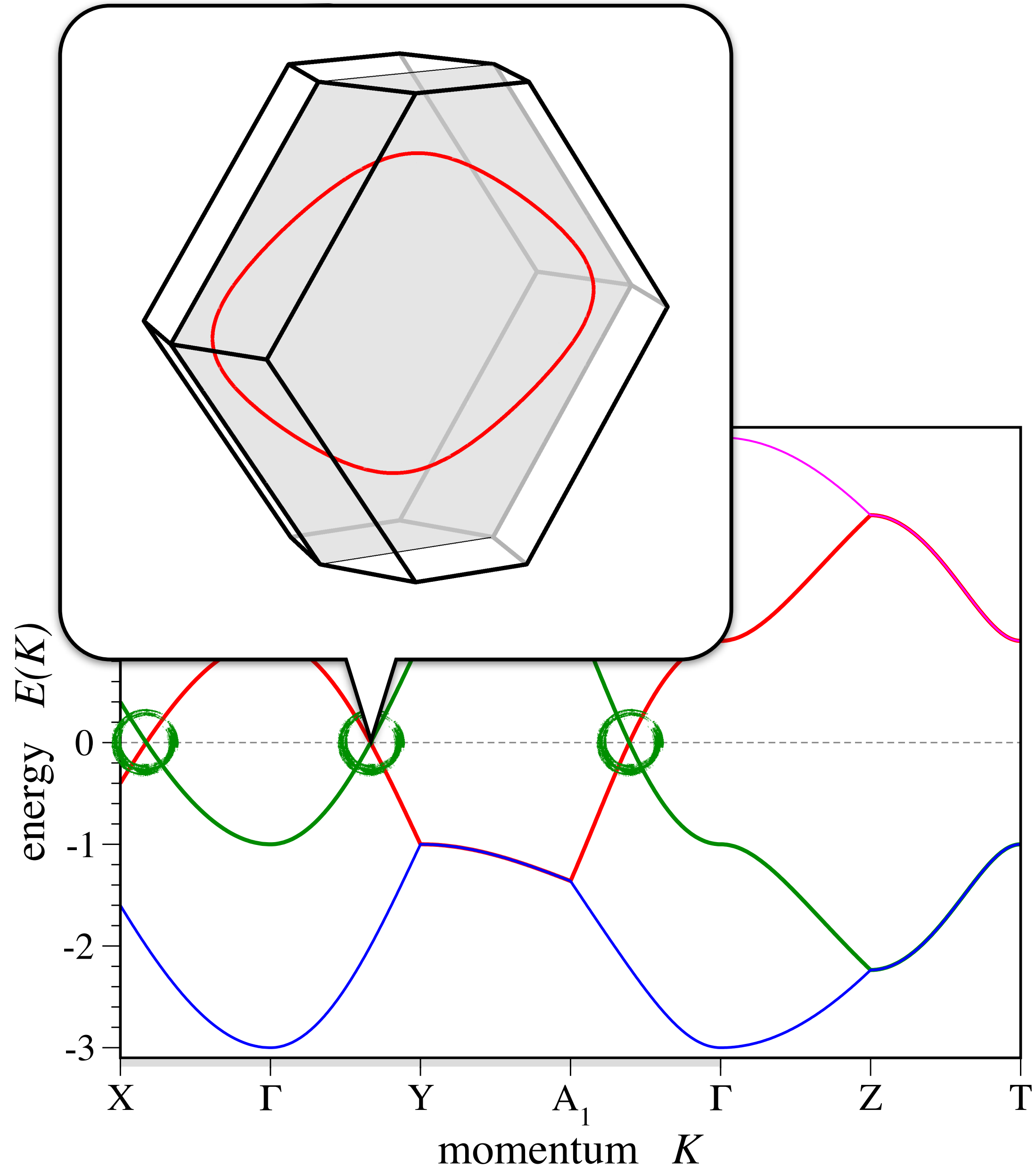
	(8,3)b	Weyl nodes	Weyl nodes	✓
	(8,3)c	nodal line	Weyl nodes	✗
	(8,3)n	gapped	gapped	✗
2D	(6,3)	Dirac nodes	gapped	✗

Majorana Fermi lines

(10,3)b – hyperhoneycomb







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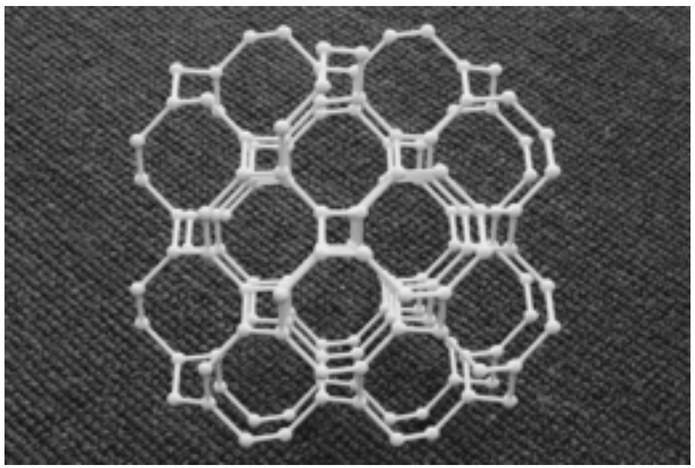
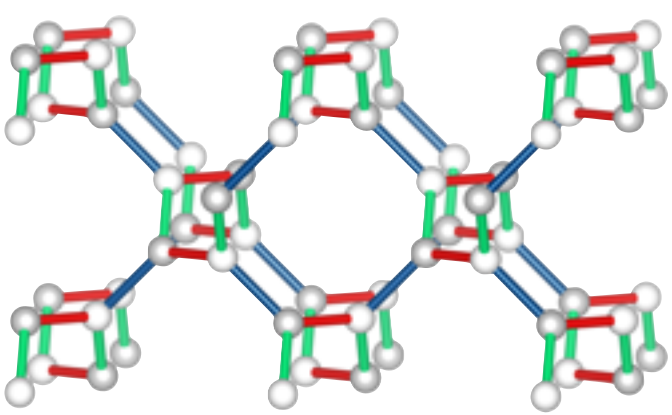
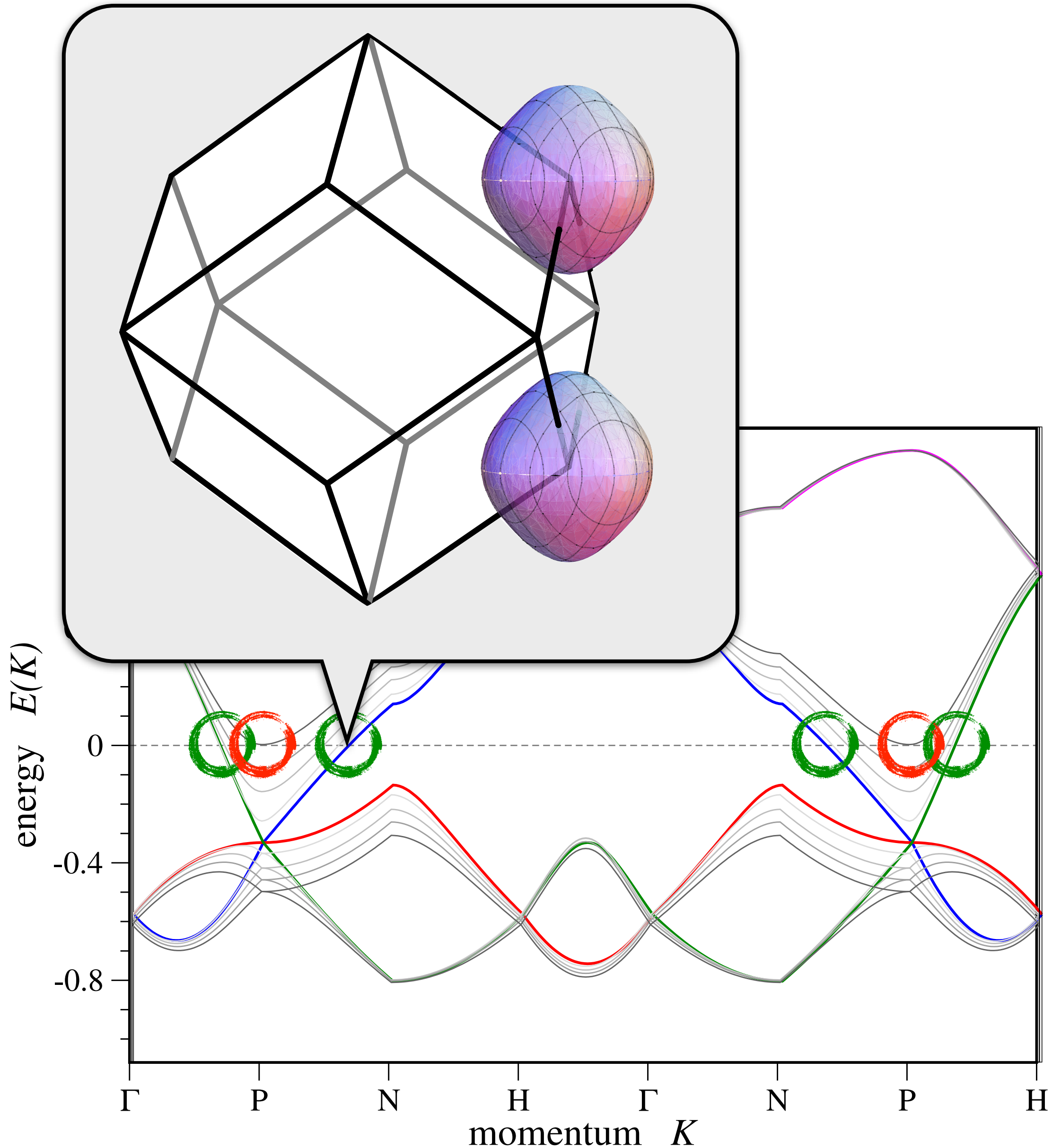
	(10,3)c	nodal line	Fermi surface	✗
	(9,3)a	Weyl nodes	Weyl nodes	✗
	(8,3)a	Fermi surface	Fermi surface	✓
	(8,3)b	Weyl nodes	Weyl nodes	✓
	(8,3)c	nodal line	Weyl nodes	✗
	(8,3)n	gapped	gapped	✗
2D	(6,3)	Dirac nodes	gapped	✗

Majorana Fermi surface

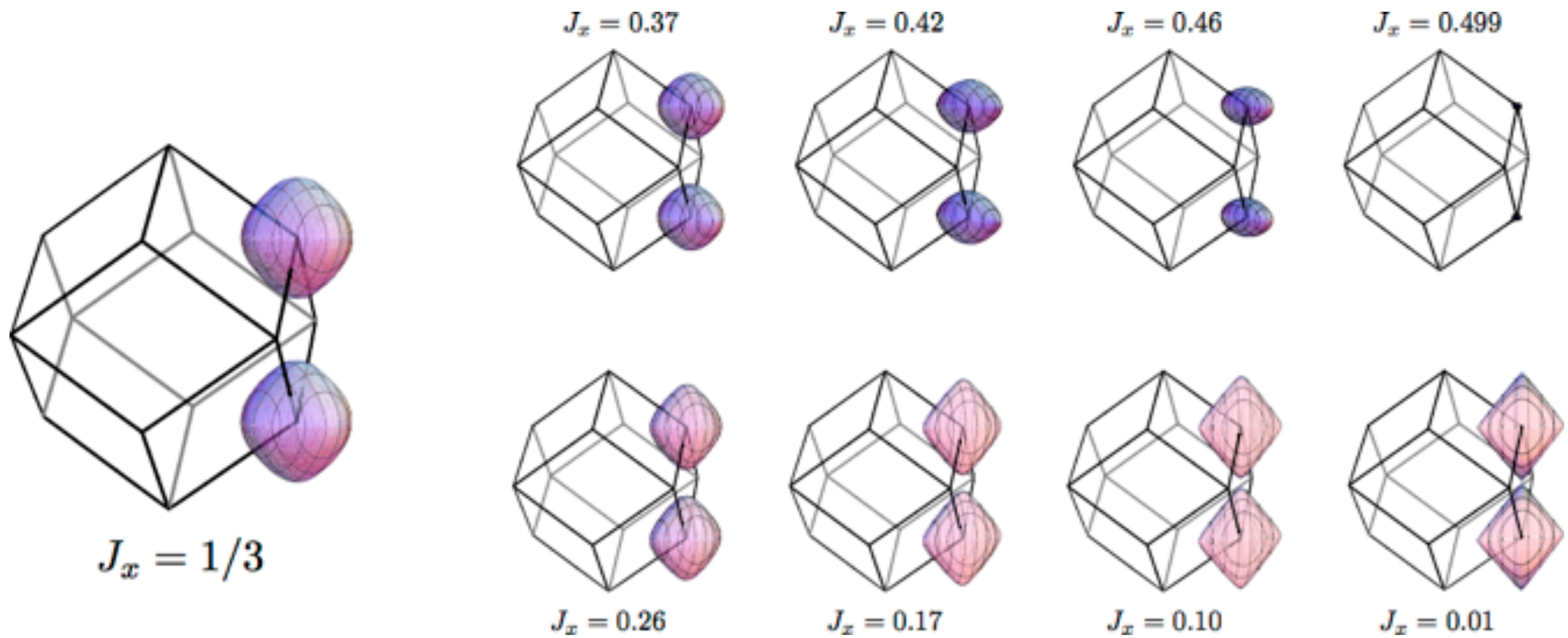
(10,3)a – hyperoctagon







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**.

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

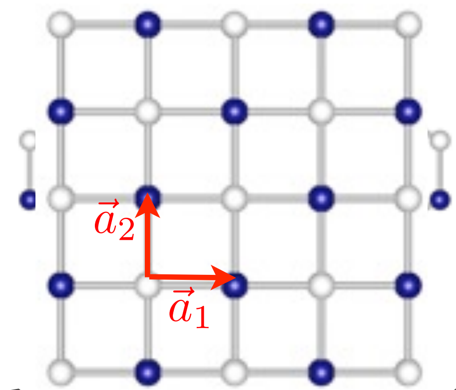
U(1) spin liquid	$C(T) \propto T \ln(1/T)$	γ = C/T diverges
Z_2 spin liquid with spinon Fermi surface	$C(T) \propto T$	γ = C/T constant
Z_2 spin liquid with spinon Fermi line	$C(T) \propto T^2$	γ = C/T vanishes

Why is the Fermi surface stable?

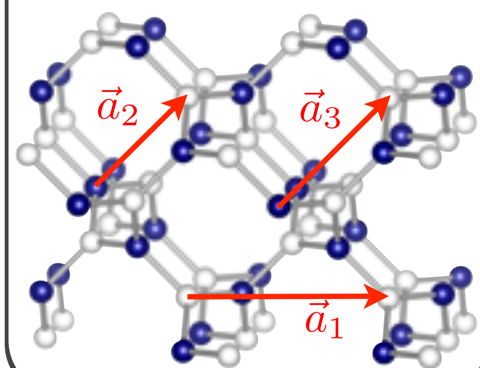
Symmetry relations

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

square 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.

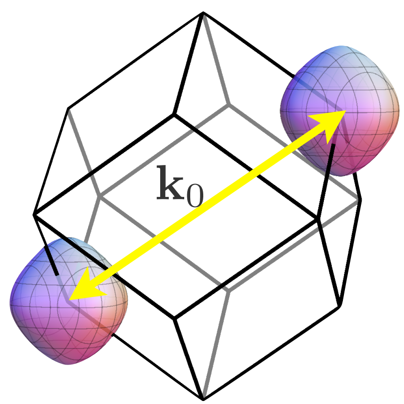
Peierls instability of Fermi surface

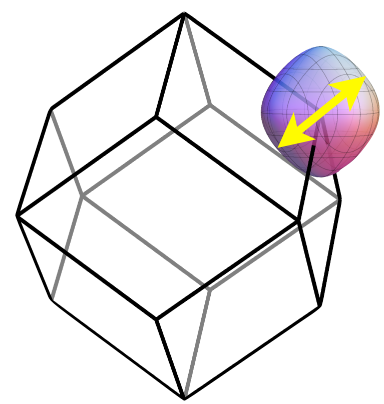
Fermi surface instabilities arise from additional spin interactions (e.g. a Heisenberg term), which introduce interactions between the Majorana fermions.

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

$$\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}+\mathbf{k}_0}$$

$$E_{\mathbf{k}_0/2+\mathbf{k}} = E_{\mathbf{k}_0/2-\mathbf{k}}$$

time-reversal symmetry

$$c_j(\mathbf{R}) \xrightarrow{\mathcal{T}} (-1)^j e^{i\mathbf{k}_0\cdot\mathbf{R}} c_j(\mathbf{R})$$

time-reversal symmetry

$$f^\dagger_{\mathbf{k}_0/2+\mathbf{k}} \xrightarrow{\mathcal{T}} f^\dagger_{\mathbf{k}_0/2-\mathbf{k}}$$

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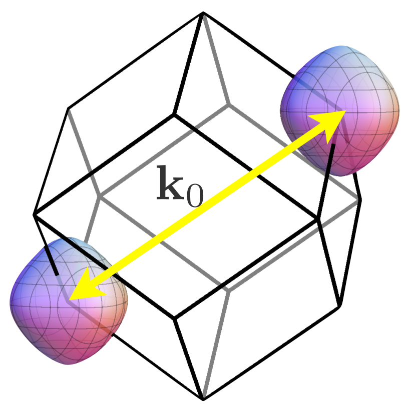
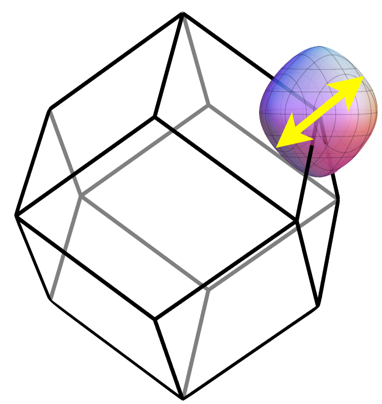
perfect nesting
between the two surfaces





(complex) fermion

conventional
BCS instability

Pairing terms

$$f^\dagger_{\mathbf{k}_0/2+\mathbf{k}} f^\dagger_{\mathbf{k}_0/2-\mathbf{k}}$$

carry **finite momentum** $\mathbf{k}_0$
and can only arise if translational symmetry is spontaneously broken.

$$E_{\mathbf{k}_0/2+\mathbf{k}} = E_{\mathbf{k}_0/2-\mathbf{k}}$$

time-reversal symmetry

$$f^\dagger_{\mathbf{k}_0/2+\mathbf{k}} \xrightarrow{\mathcal{T}} f^\dagger_{\mathbf{k}_0/2-\mathbf{k}}$$

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.

Generic form of the induced interactions between Majorana fermions

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

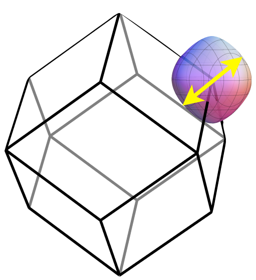
Recast the Majorana Hamiltonian in terms of complex fermions (at low energies)

$$H_{\text{eff}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} f^\dagger_{\mathbf{k}} f_{\mathbf{k}} + \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} V^1_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}\, f^\dagger_{\mathbf{k}_1} f^\dagger_{\mathbf{k}_2} f_{\mathbf{k}_3} f_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3} + \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} V^2_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}\, f^\dagger_{\mathbf{k}_1} f^\dagger_{\mathbf{k}_2} f^\dagger_{\mathbf{k}_3} f^\dagger_{-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3} + h.c.$$

$f^\dagger_{\mathbf{k}} f^\dagger_{-\mathbf{k}}$

$f^\dagger_{\mathbf{k}_1} f^\dagger_{\mathbf{k}_2} f^\dagger_{\mathbf{k}_3} f_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3}$

high-energy



spinless fermions ⟶ p-wave superconductivity

$$T_c = E_{0,\alpha}\, e^{-c_\alpha J/U} \quad \text{for} \quad U \ll J$$

$$H_{\text{BCS}} = \sum_k \epsilon_k f^\dagger_{\mathbf{k}} f_{\mathbf{k}} + \sum_{k_x>0} \Delta_{\mathbf{k}}\, f^\dagger_{\mathbf{k}_0/2+\mathbf{k}} f^\dagger_{\mathbf{k}_0/2-\mathbf{k}} + h.c.$$

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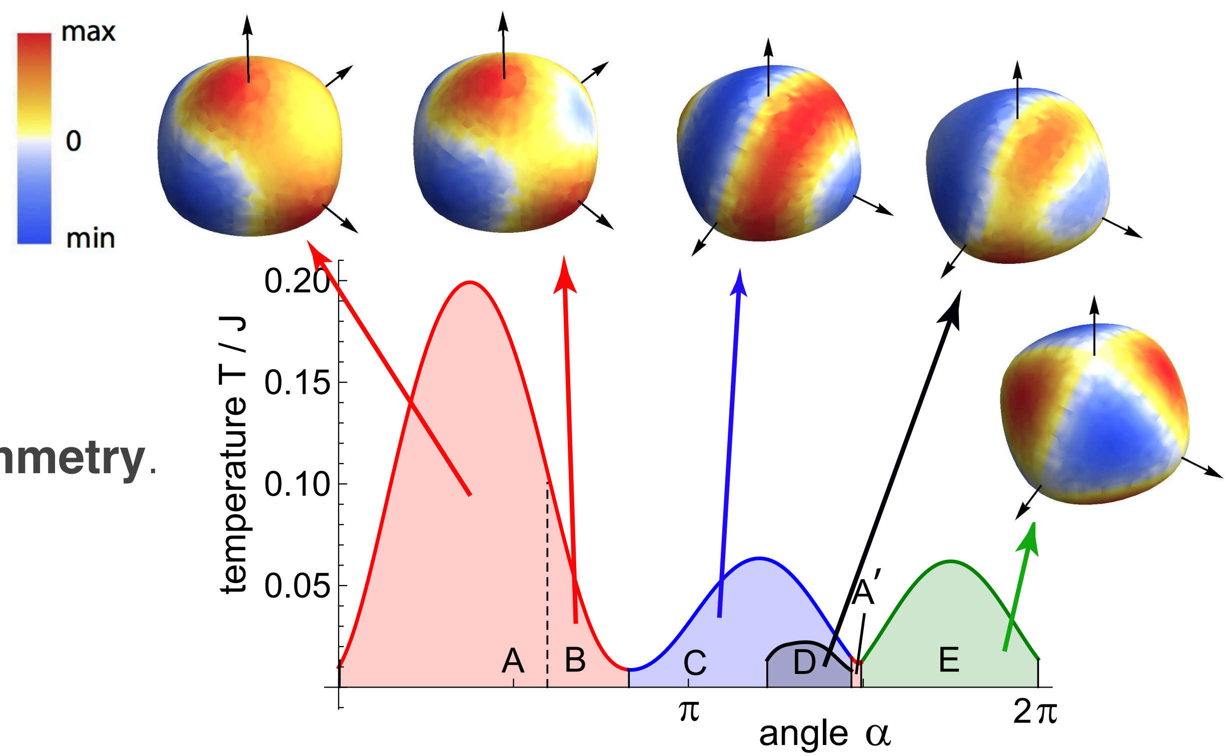
$$\Delta \sim \langle f^{\dagger}_{\mathbf{k}_0+\mathbf{q}} f^{\dagger}_{\mathbf{k}_0-\mathbf{q}} \rangle$$

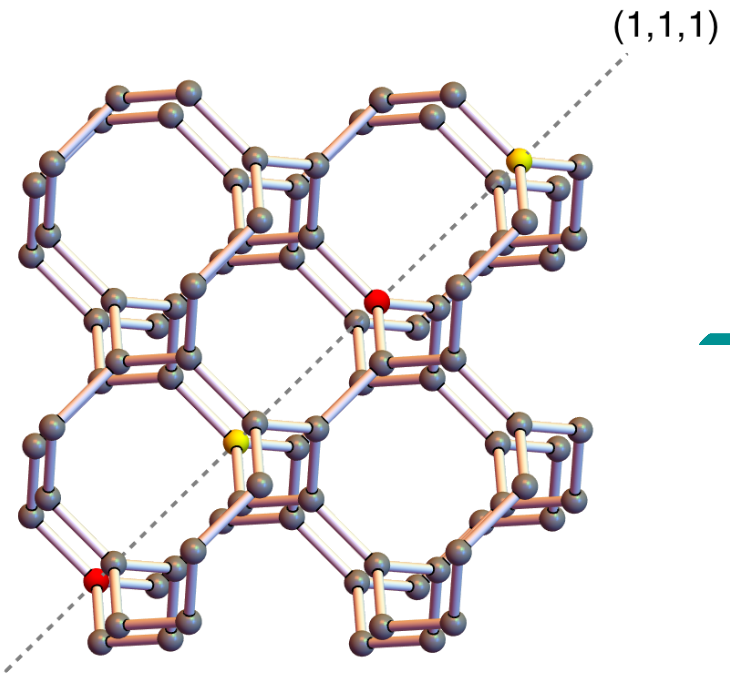


All phases **break translational symmetry**.

Phases A – D break additional **(rotational) lattice symmetries**.

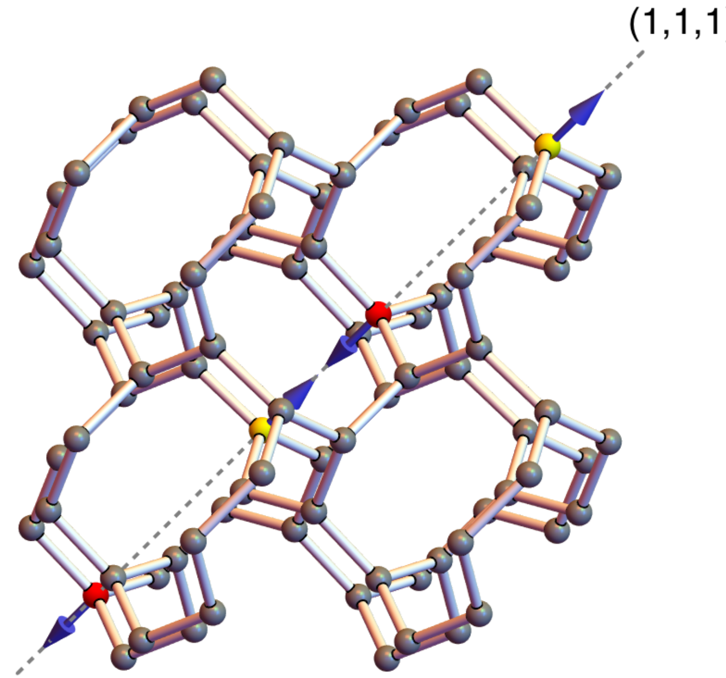
Peierls instability of Fermi surface

The **doubling of the unit cell** will generically be reflected in **shifts of the position of atoms** and in **valence bond correlations**.



space group $I4_132$

spin-Peierls instability



space group $P4_132$

valence bond correlations along $\mathbf{v} = (1/2, 1/2, 1/2)$

$$\langle\, \mathbf{S}(\mathbf{r}_0 + n\mathbf{v})\, \mathbf{S}(\mathbf{r}_0 + (n+1)\mathbf{v})\,\rangle \sim (-1)^n \Delta$$

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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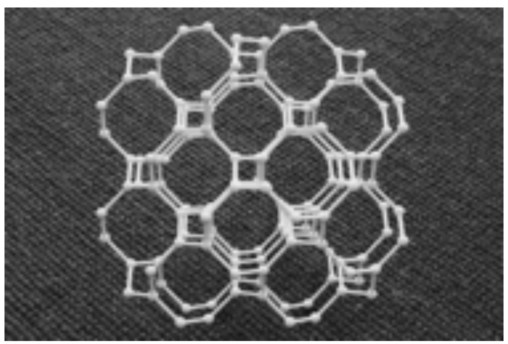
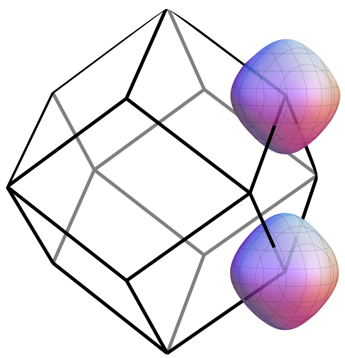
	(8,3)a	Fermi surface	Fermi surface	✓
	(8,3)b	Weyl nodes	Weyl nodes	✓
	(8,3)c	nodal line	Weyl nodes	✗
	(8,3)n	gapped	gapped	✗
2D	(6,3)	Dirac nodes	gapped	✗

Breaking time-reversal symmetry

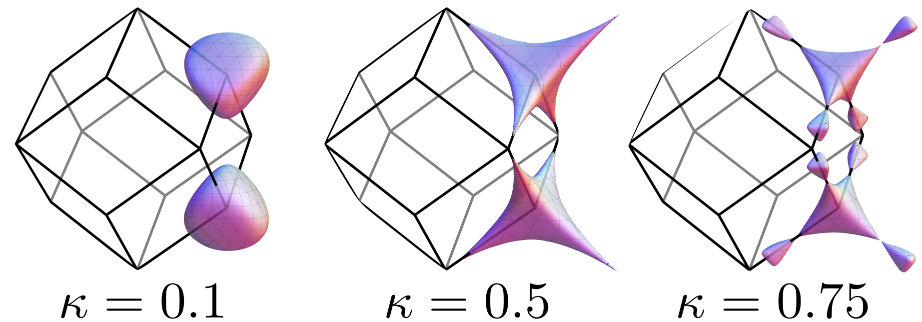
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma - \sum_j \vec{h} \cdot \vec{\sigma}_j$$

(10,3)a – hyperoctagon



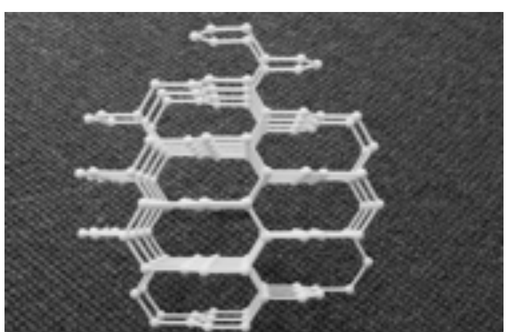


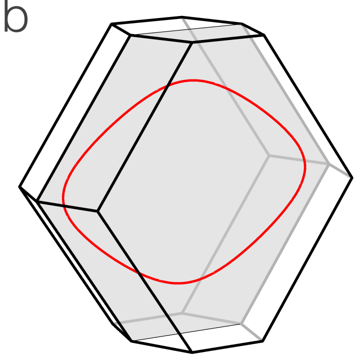
Fermi **surface**



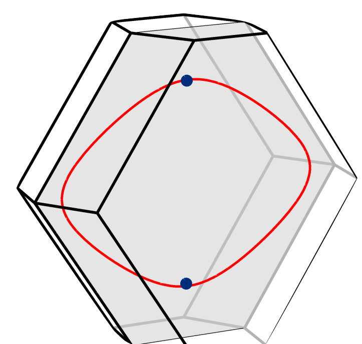
Fermi surface **deforms**

(10,3)b – hyperhoneycomb





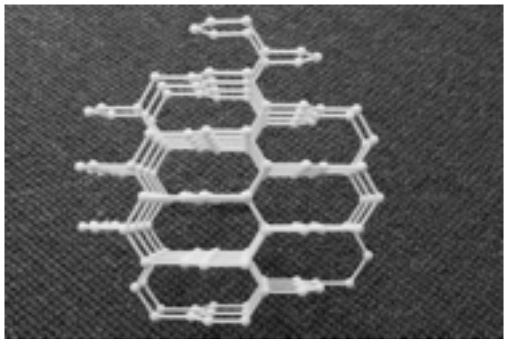
Fermi **line**



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

Weyl physics – energy spectrum

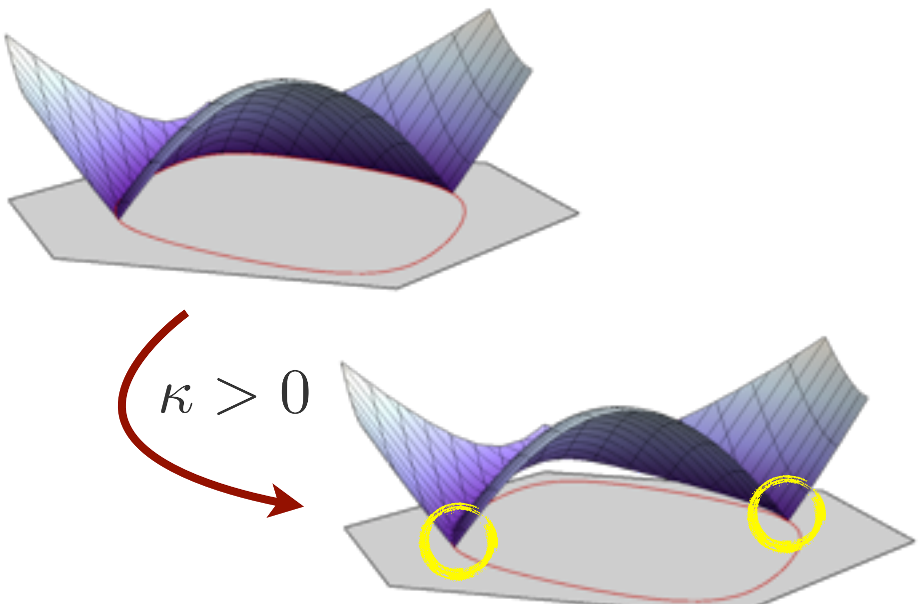
(10,3)b – hyperhoneycomb

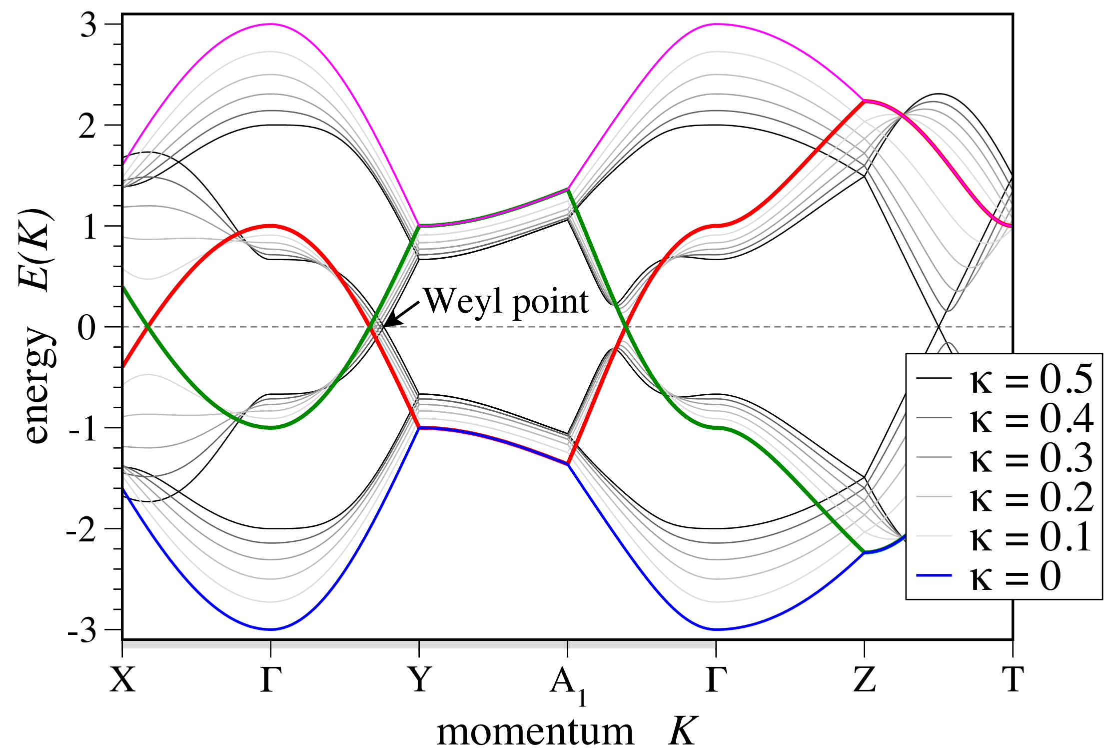


Touching of two bands in 3D is generically **linear**

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

Weyl nodes



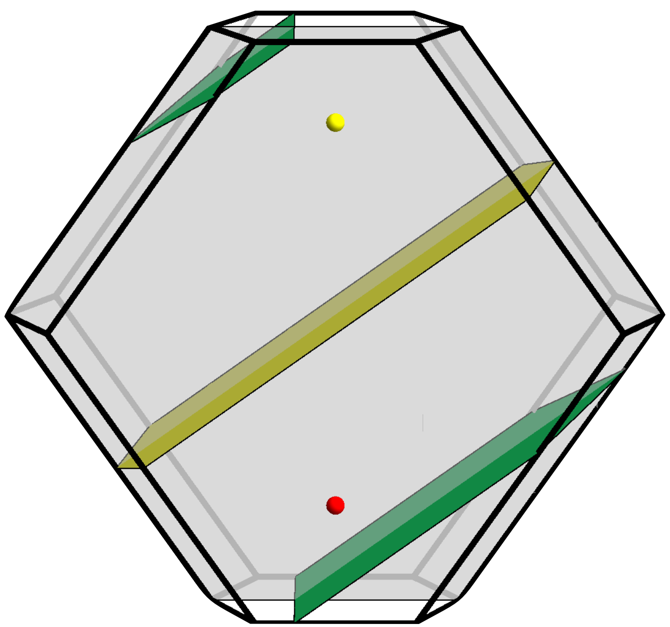


Weyl physics – Chern numbers

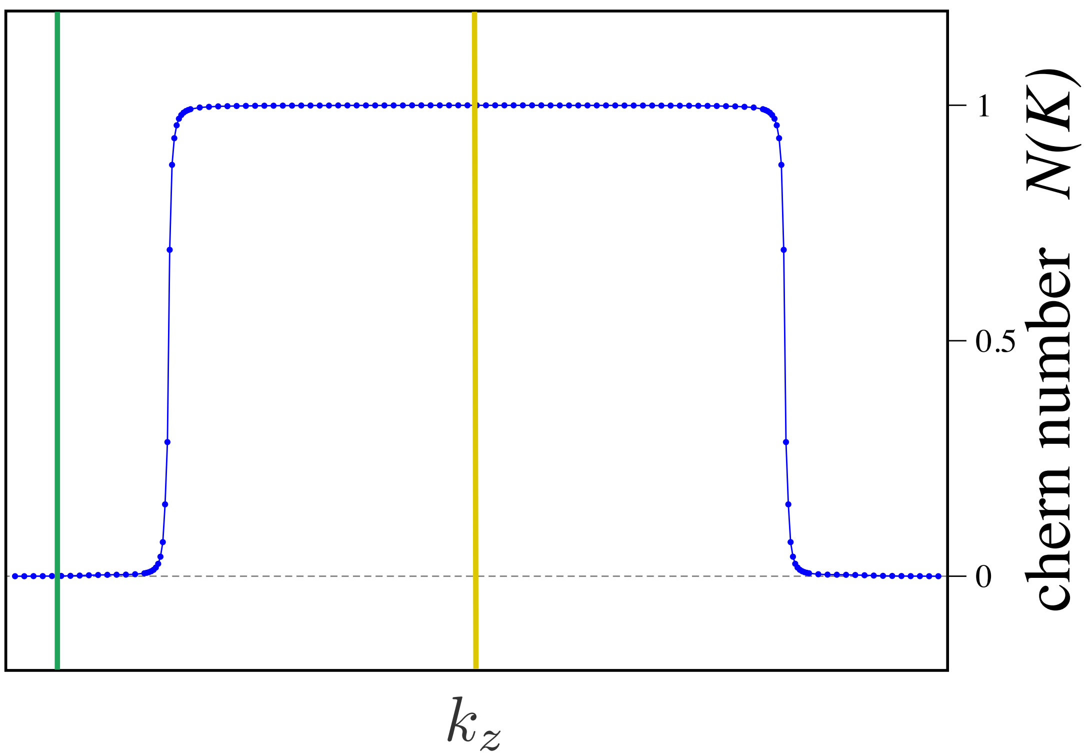
Weyl nodes are **sources or sinks of Berry flux**

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

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



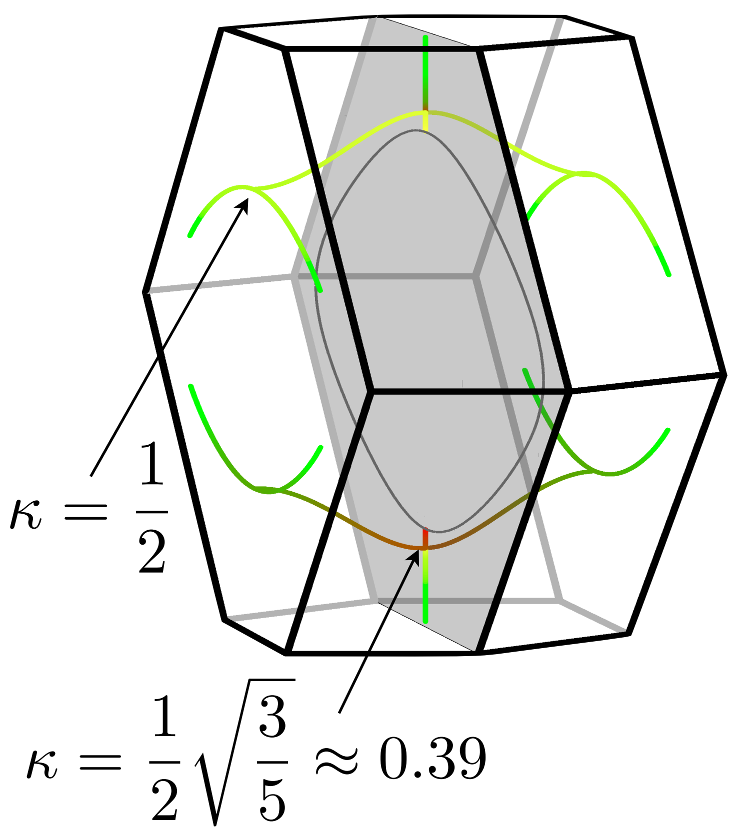
$\kappa = 0.05$

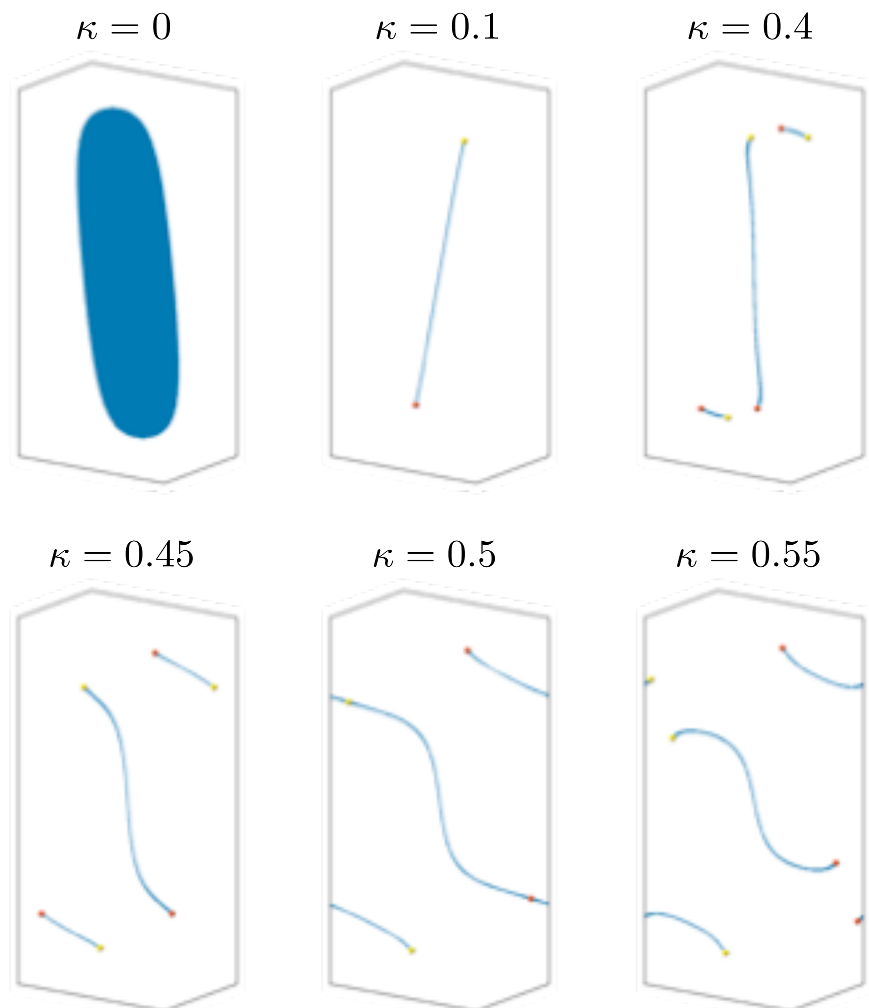


Weyl physics – surface states

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

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





Experimental signatures?

specific heat

Specific heat has bulk and surface contributions

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

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	✓
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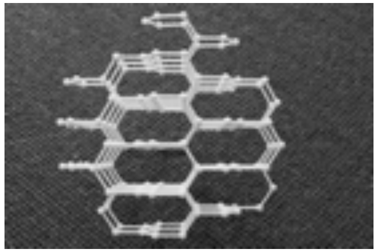
	(8,3)n	gapped	gapped	✗
2D	(6,3)	Dirac nodes	gapped	✓

Three scenarios for Weyl physics

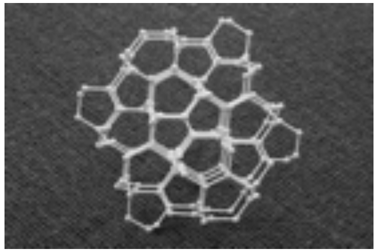
(10,3)b – hyperhoneycomb



explicit breaking of time-reversal symmetry

symmetry class D

(9,3)a

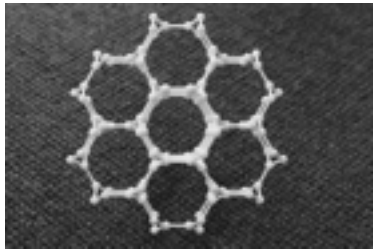


spontaneous breaking of time-reversal symmetry

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

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

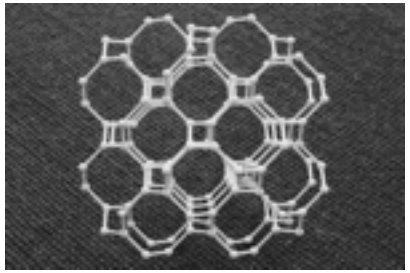
Kitaev models are paradigmatic examples for **spin fractionalization**.

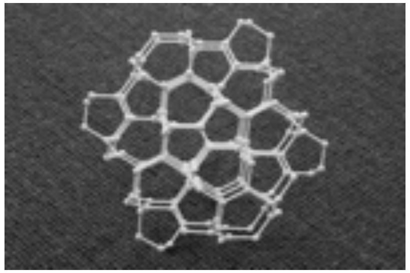
spin-1/2 $\sigma_j^\gamma = i\, b_j^\gamma c_j$ Majorana fermion + Z_2 gauge field

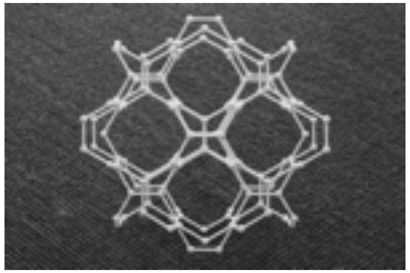
3D Kitaev models host a surprisingly rich variety of **gapless Z_2 spin liquids**.

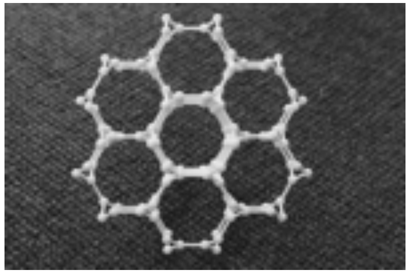
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^\gamma \sigma_j^\gamma$$

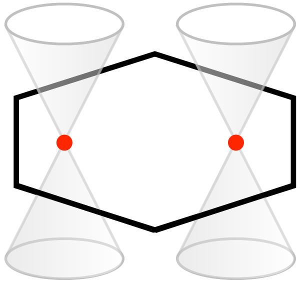
Analytical control of these models allows to provide first examples of tractable spin models with a **spinon Fermi surface** or a **Weyl spin liquid** ground state.



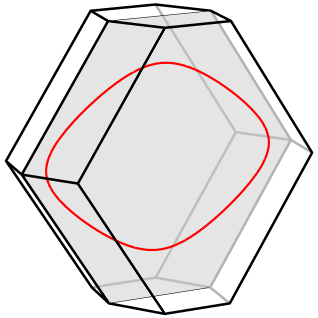




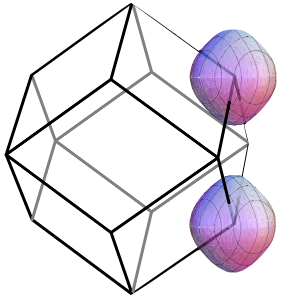




Dirac **points**



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



Fermi **surfaces**