Spin liquids and (Majorana) metals

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CRC 1238
Control and Dynamics of Quantum Materials

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Spin liquids

In **frustrated magnets**, the suppression of magnetic ordering can lead to the **formation of spin liquids**.

The **local moments** in spin liquid ground states are **highly correlated** but **still fluctuate strongly** down to zero temperature.

Herbertsmithite

Volborthite

hyperkagome $Na_4Ir_3O_8$

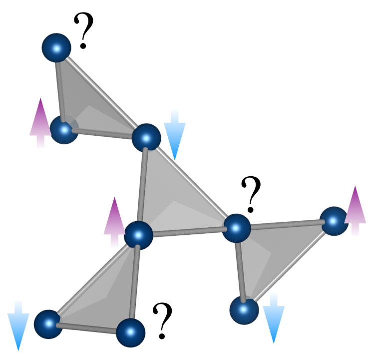
Spin liquids

Herbertsmithite

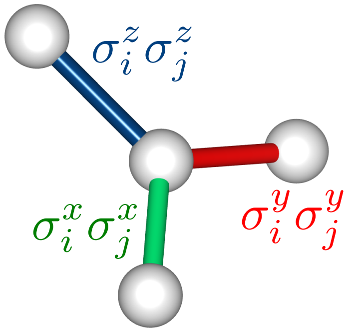
Volborthite

hyperkagome $Na_4Ir_3O_8$

What features are we looking for in these materials?



geometric frustration



exchange frustration

Spin liquids & fractionalization

Quantum spin liquids are macroscopically entangled quantum states, where the original **spins fractionalize** into novel, emergent degrees of freedom that carry a fractional quantum number – **partons + gauge field**.

> Spin liquids can be **dichotomous states**, where an electronic Mott **insulator** harbors emergent itinerant degrees of freedom that form a **metal**.

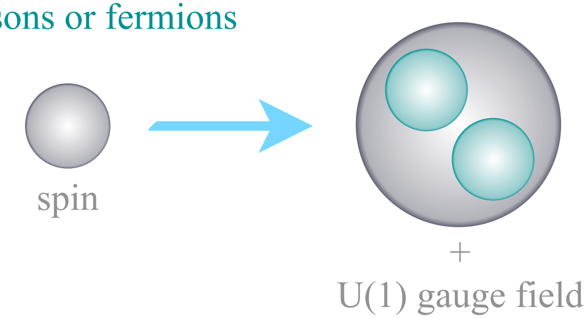
auxiliary fermions (or bosons)

$c_1^\dagger c_1 + c_2^\dagger c_2 = 2S$

bosons or fermions

$$S^\gamma = \frac{1}{2} c_\alpha^\dagger \sigma_{\alpha,\beta}^\gamma c_\beta$$

Pauli matrices

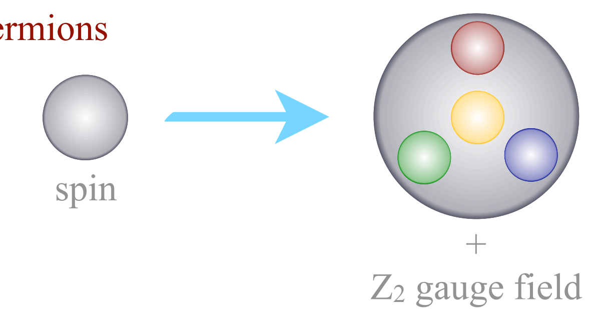


spinon metal w/ spinon Fermi surface

Majorana fermions

Majorana fermions

$$S^\gamma = i a^\gamma c$$



Majorana metal w/ Majorana Fermi surface

this talk

Part I – fractionalization

Majorana metals and quantum spin liquids in **3D Kitaev models**.

Majorana fermions

Majorana fermions

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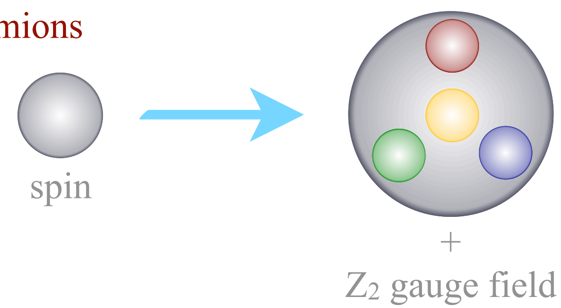
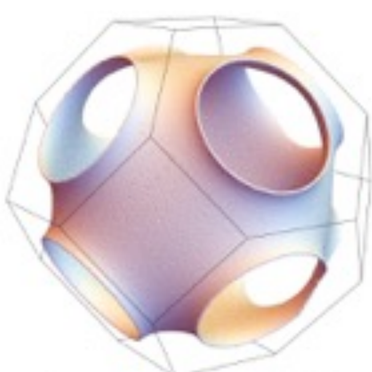


Majorana metal
w/ Majorana
Fermi surface

Part II – "doubling"

Spiral spin liquids and metals in **classical spin systems**.



classical spin system / spin spirals

$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

free fermion system / metal

Majorana metals

PRB **93**, 085101 (2016)
PRL **115**, 177205 (2015)
PRL **114**, 157202 (2015)
PRB **89**, 235102 (2014)

Kitaev models

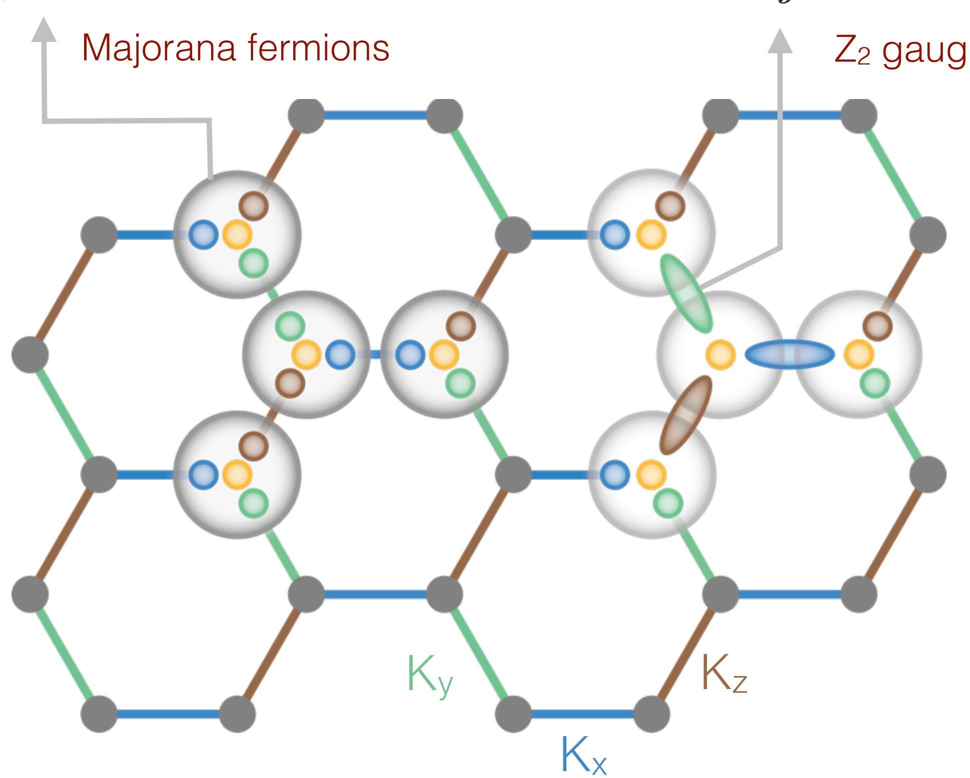
$$H_{\text{Kitaev}} = \sum_{\gamma-\text{bonds}} K_\gamma \; S_i^\gamma S_j^\gamma$$

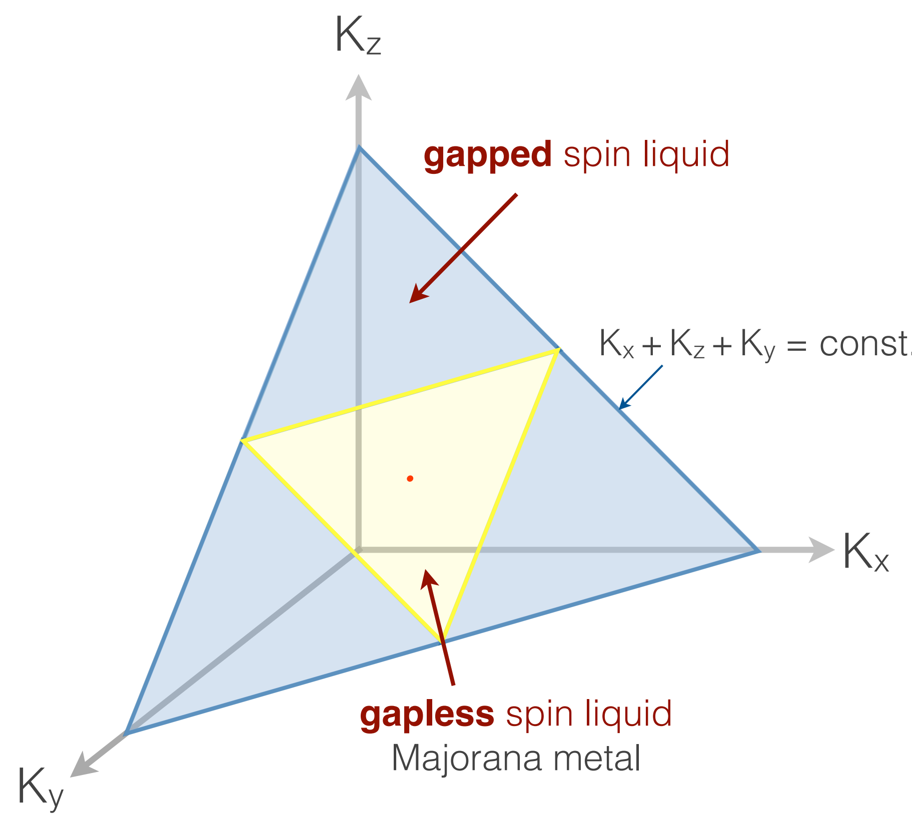
relevant to various *5d*[5] and *4d*[5] "Kitaev materials"
including Na_2IrO_3, Li_2IrO_3, $RuCl_3$, ...
mini review in arXiv:1701.07056

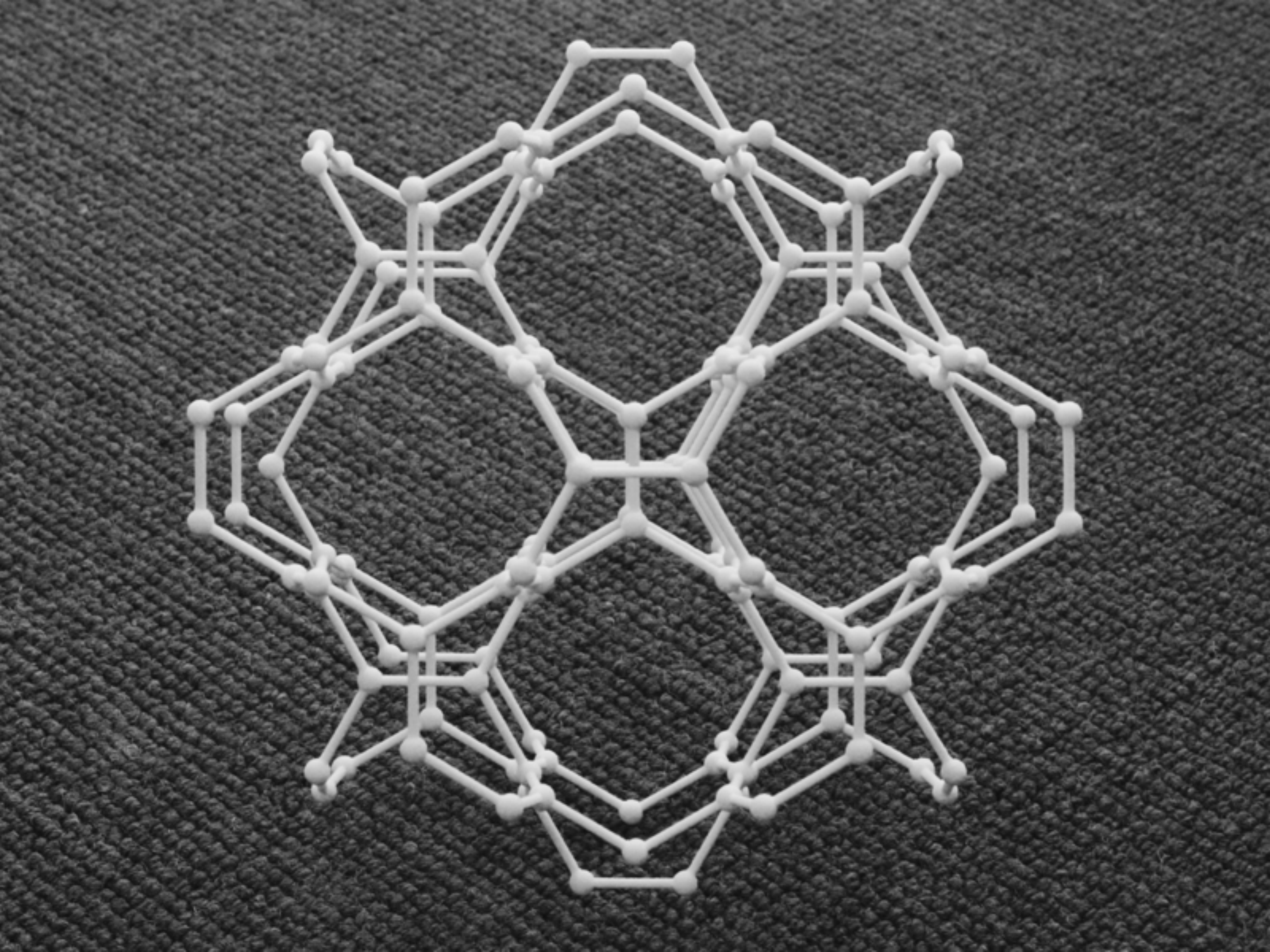
$$S^\gamma = i a^\gamma c \qquad \hat{u}_{jk} = i a_j^\gamma a_k^\gamma$$

Majorana fermions

Z_2 gauge field







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)

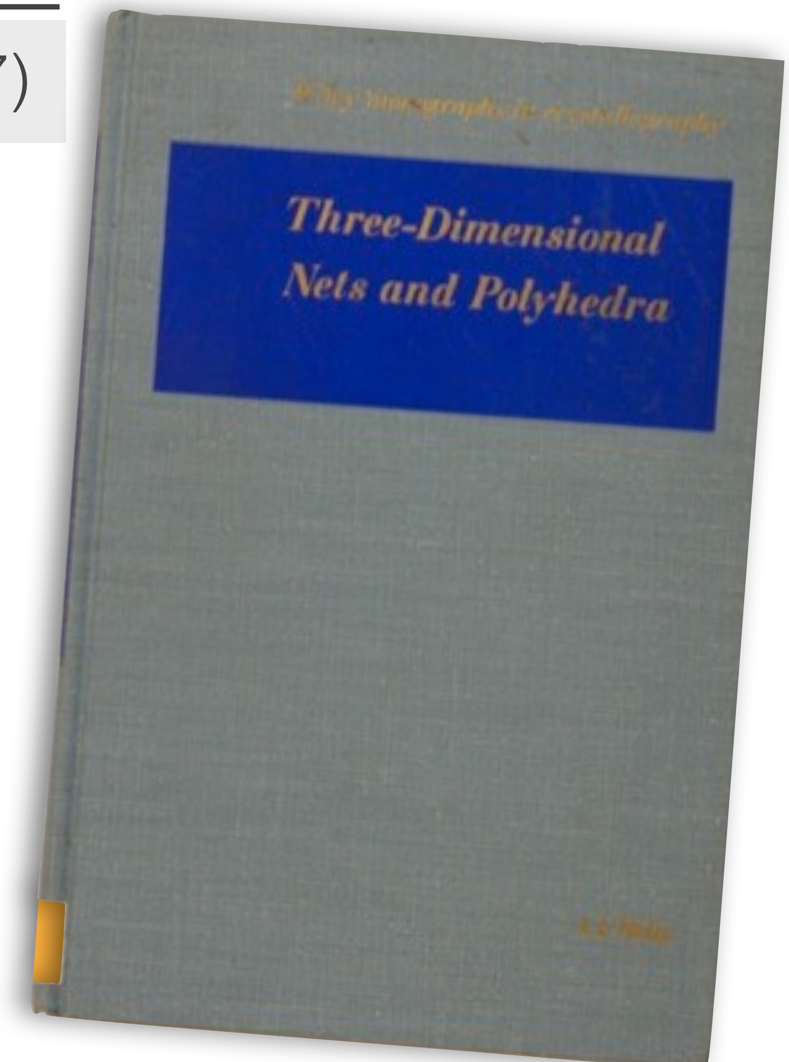
platonic solids

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			

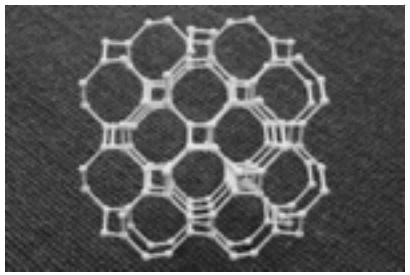


A.F.Wells, 1977

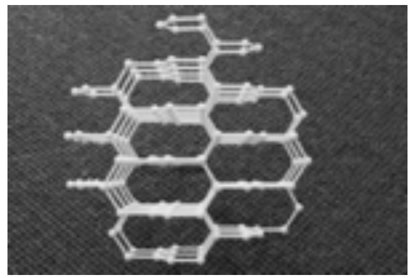
Tricoordinated lattices

Classification by elementary loop length (polygonality)

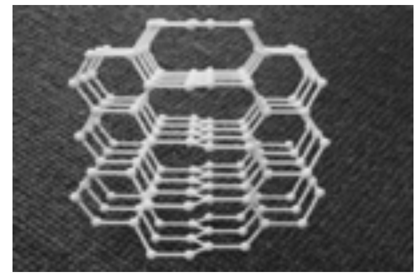
(10,3)



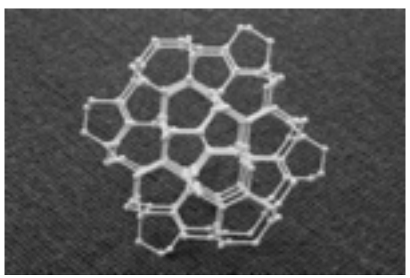
hyperoctagon

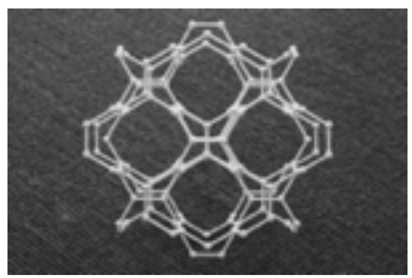


hyperhoneycomb

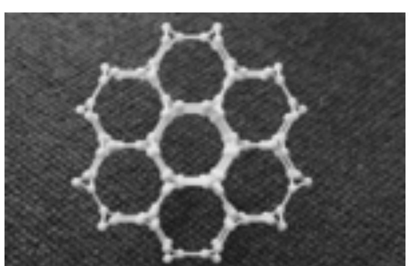


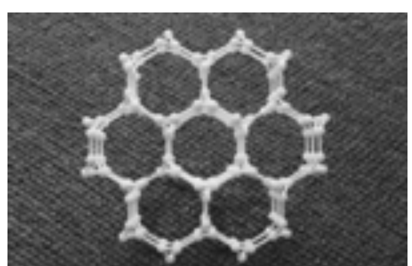
(9,3)

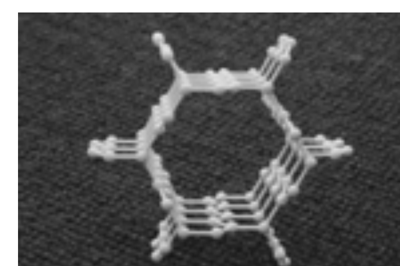




(8,3)







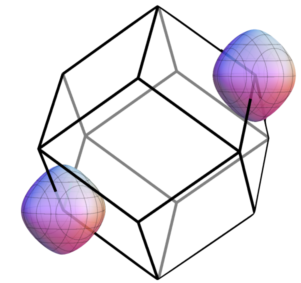
Tricoordinated lattices

		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	✓		

Majorana metals

PRB **93**, 085101 (2016)

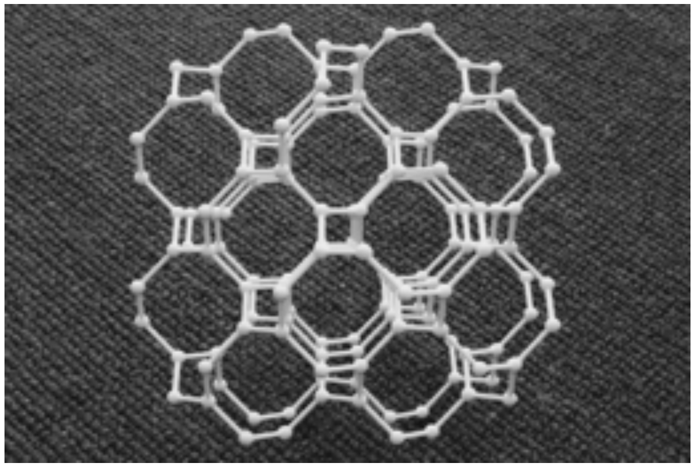
		Majorana metal	TR breaking
3D lattices	(10,3)a	Fermi surface	Fermi surface
	(10,3)b	nodal line	Weyl nodes
	(10,3)c	nodal line	Fermi surface
	(9,3)a	Weyl nodes	Weyl nodes
	(8,3)a	Fermi surface	Fermi surface
	(8,3)b	Weyl nodes	Weyl nodes
	(8,3)c	nodal line	Weyl nodes
	(8,3)n	gapped	gapped
2D	(6,3)	Dirac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

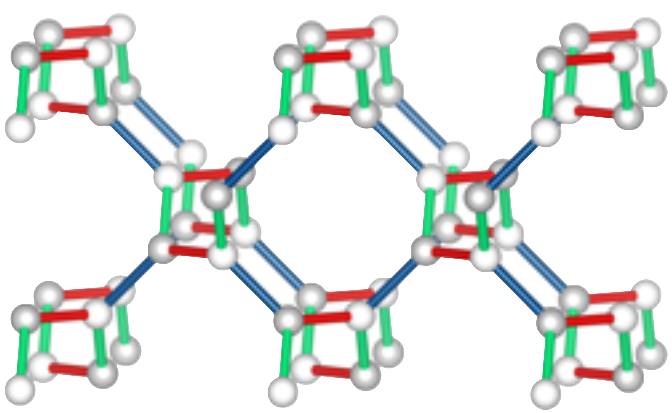


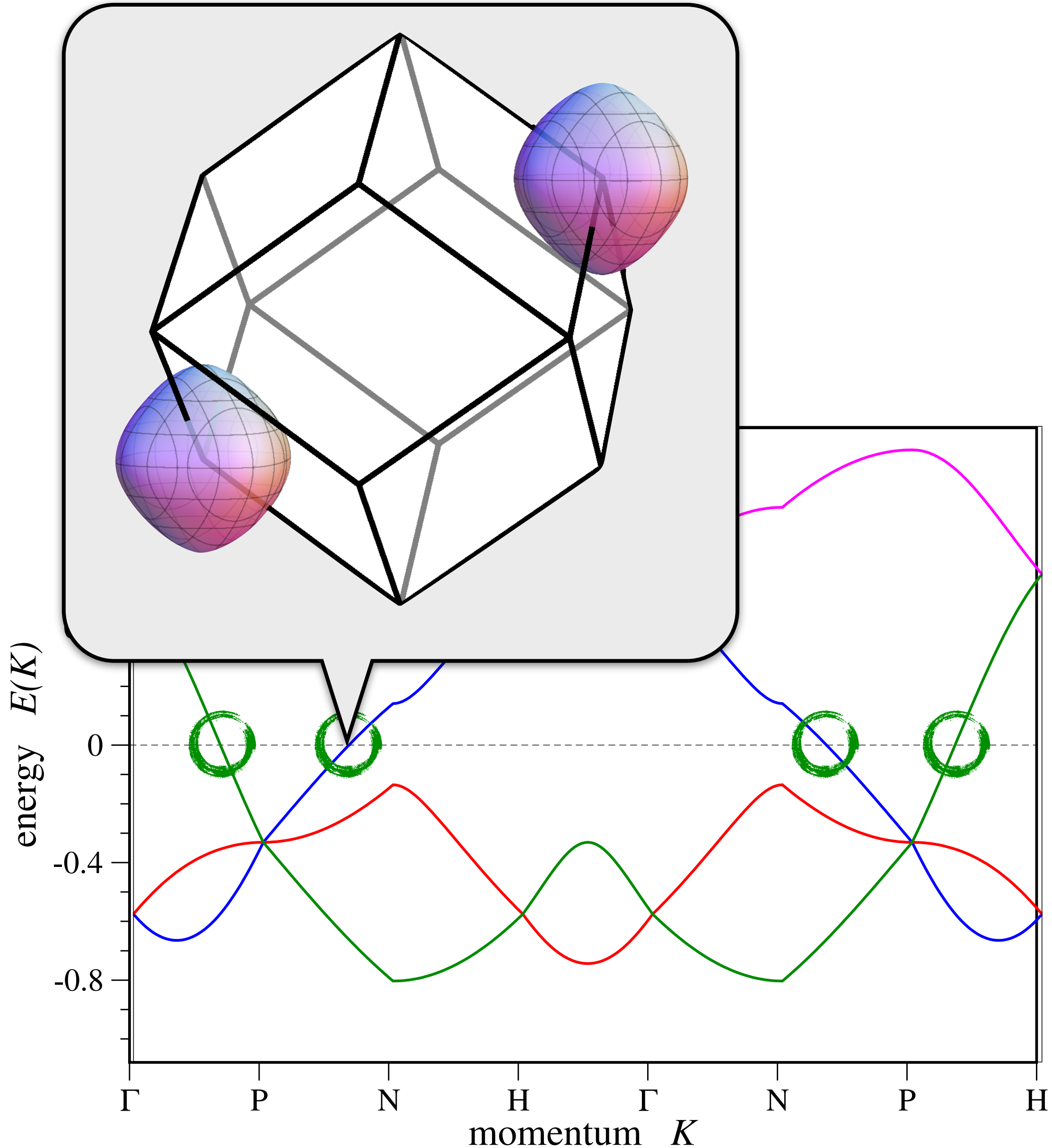
Majorana Fermi surfaces

Majorana Fermi surface

(10,3)a – hyperoctagon







Peierls instability of Fermi surface

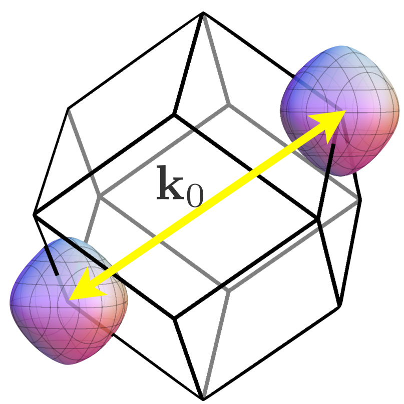
PRL **115**, 177205 (2015)

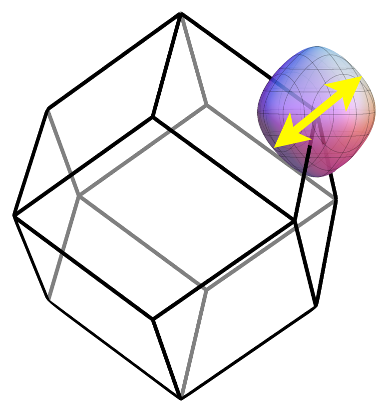
Fermi surface instabilities arise from additional spin interactions (e.g. a Heisenberg term), which introduce interactions between the Majorana fermions.

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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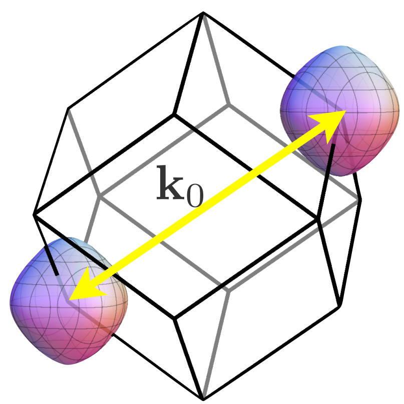
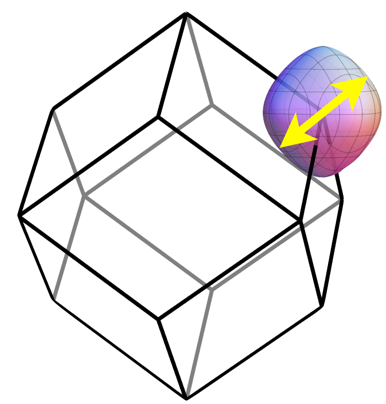




(complex) fermion

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.

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

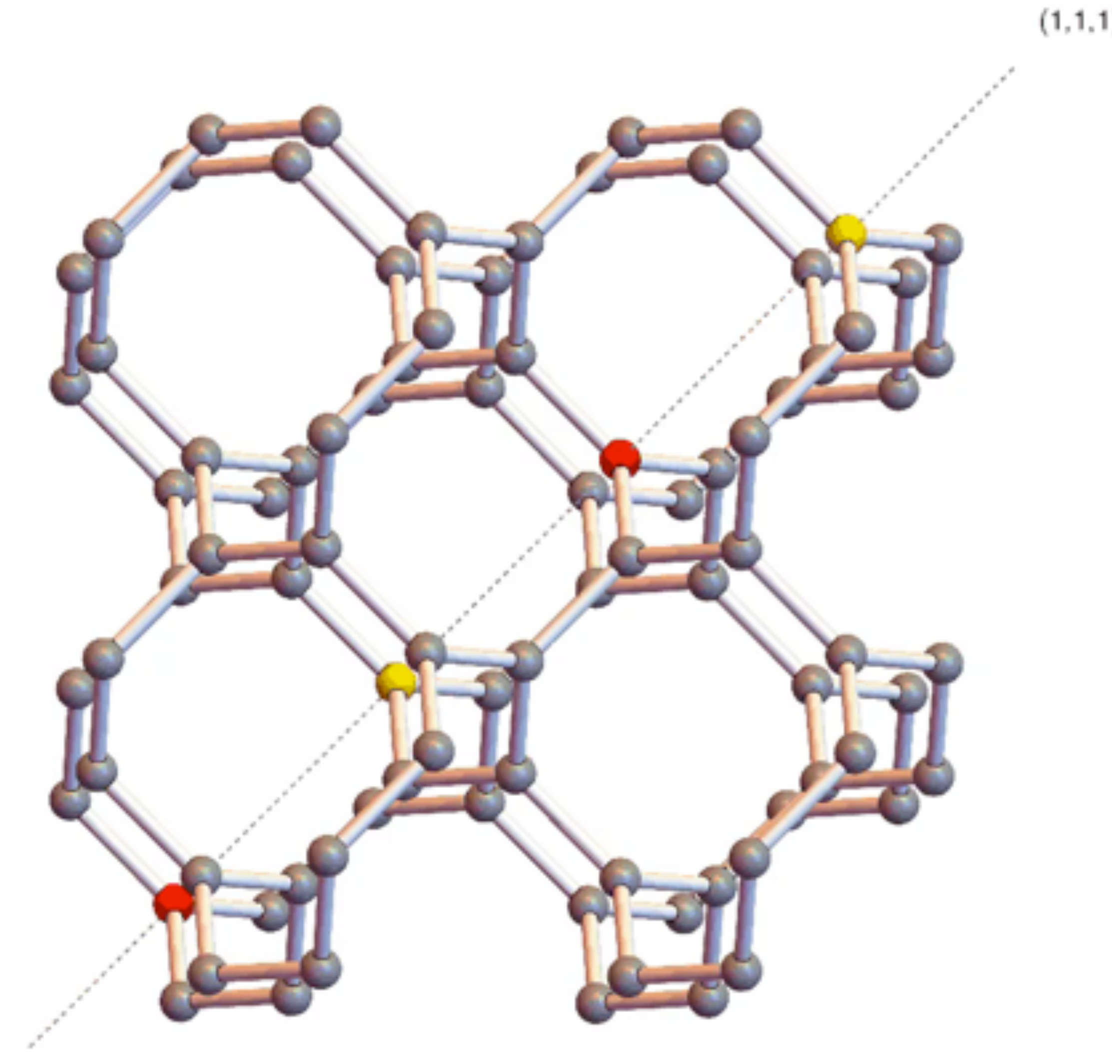
time-reversal symmetry

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

Peierls instability of Fermi surface

PRL **115**, 177205 (2015)

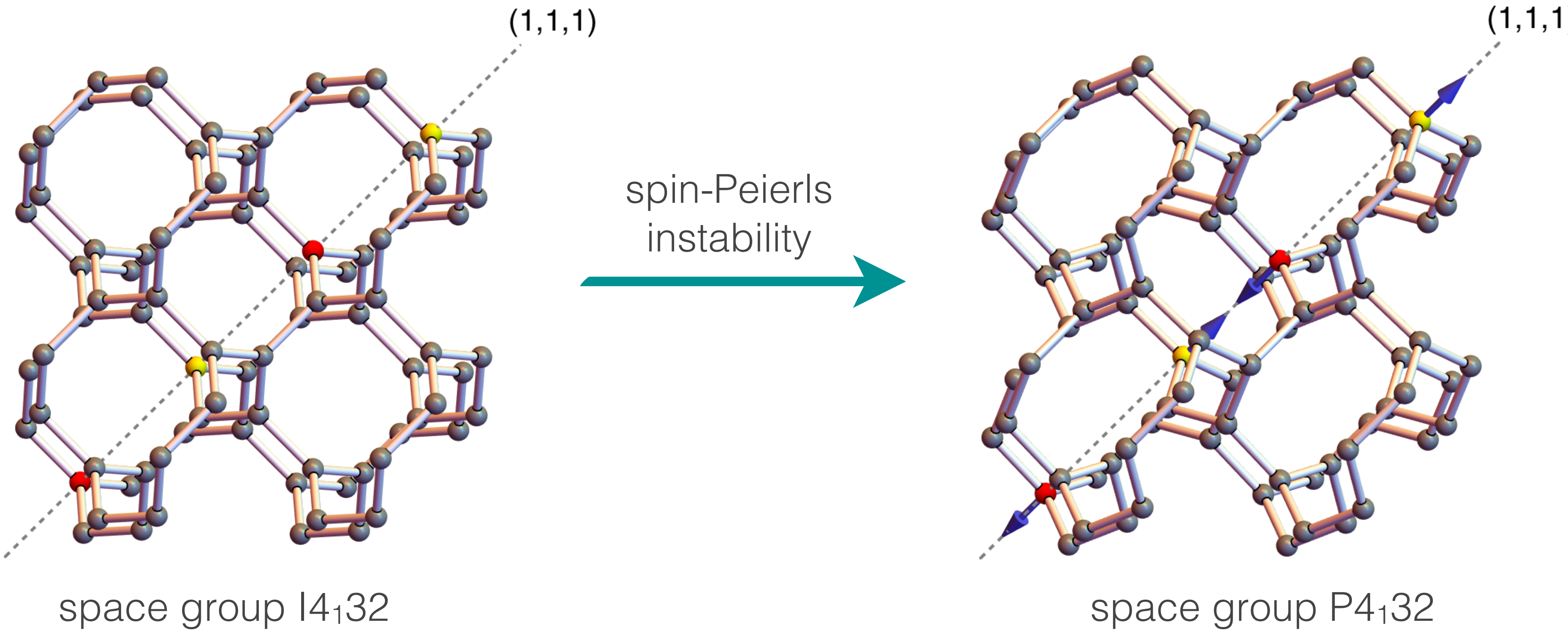
The **doubling of the unit cell** will generically be reflected in **shifts of the position of atoms**.



Peierls instability of Fermi surface

PRL **115**, 177205 (2015)

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



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

PRB **93**, 085101 (2016)

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3D lattices	(10,3)a	Fermi surface	Fermi surface
	(10,3)b	nodal line	Weyl nodes
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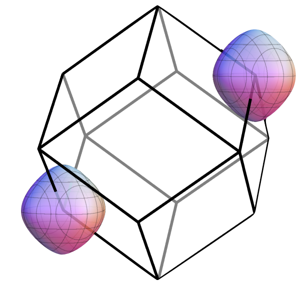
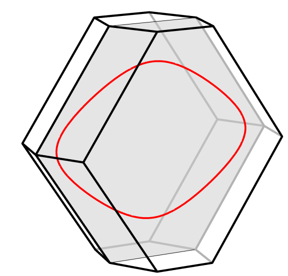


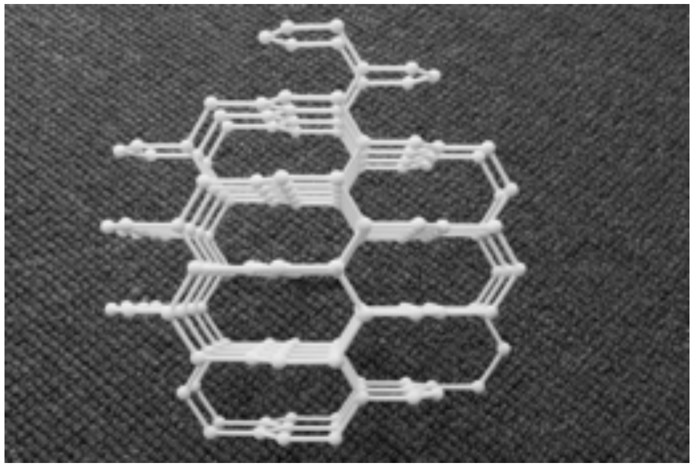
Majorana Fermi surfaces

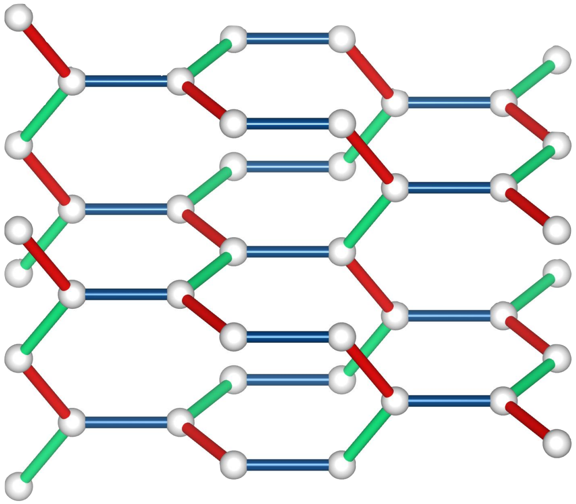


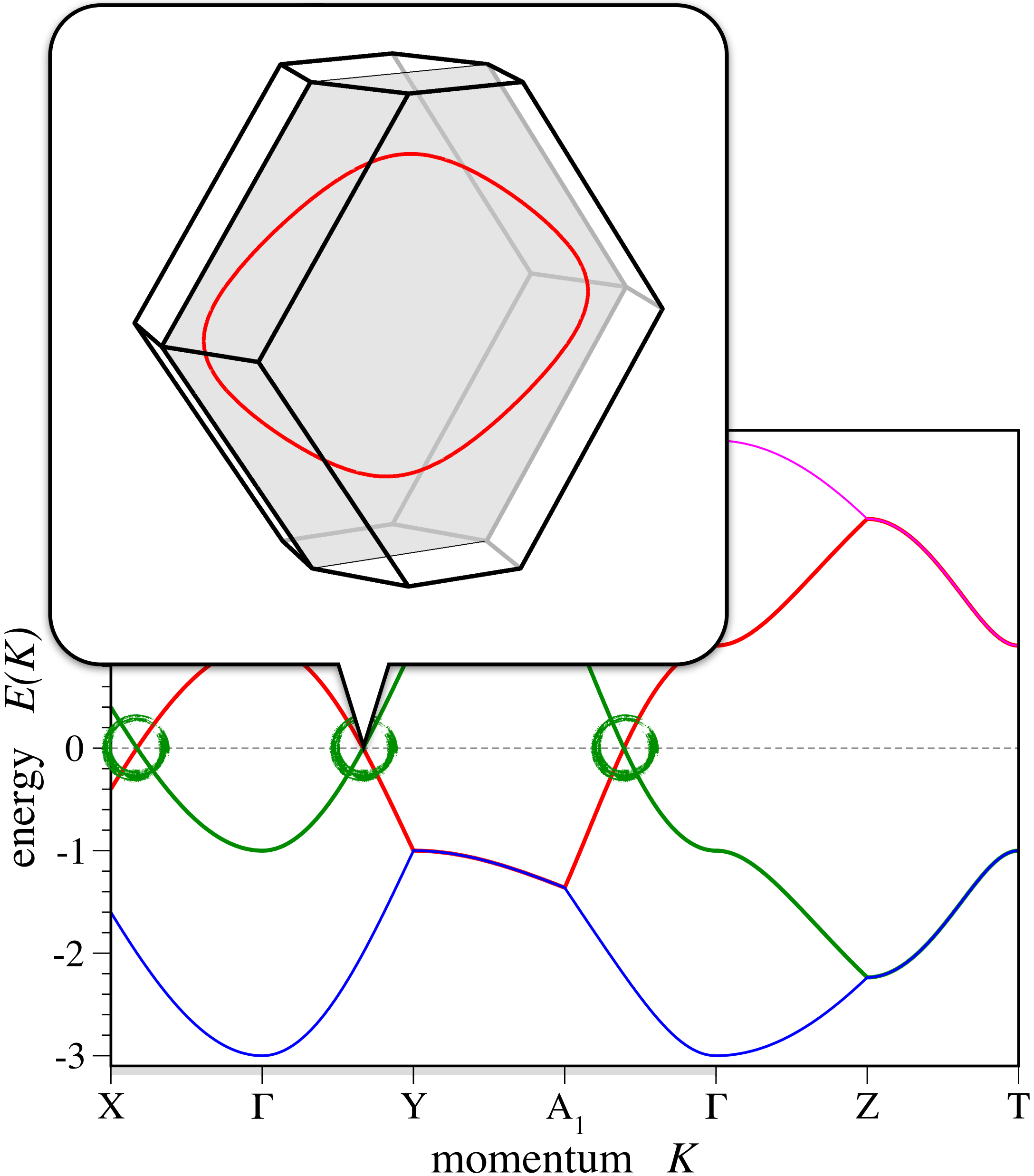
nodal lines

Majorana nodal lines

(10,3)b – hyperhoneycomb







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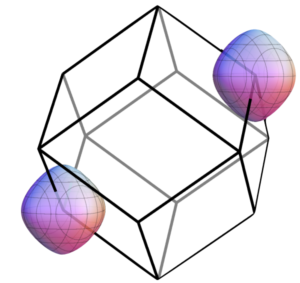
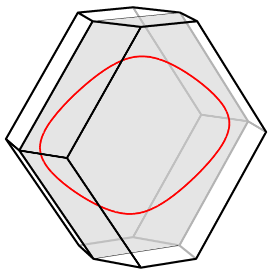
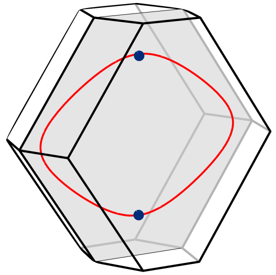


Majorana Fermi surfaces



nodal lines



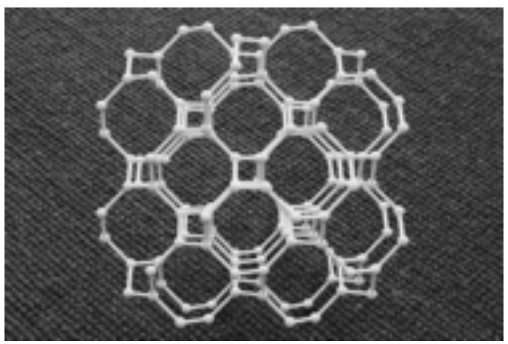
Weyl nodes

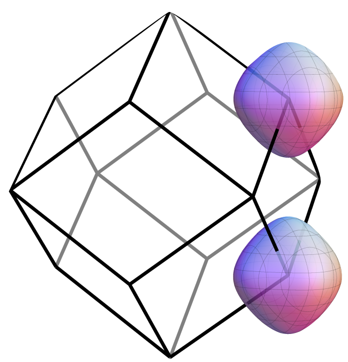
Breaking time-reversal symmetry

PRL **114**, 157202 (2015)

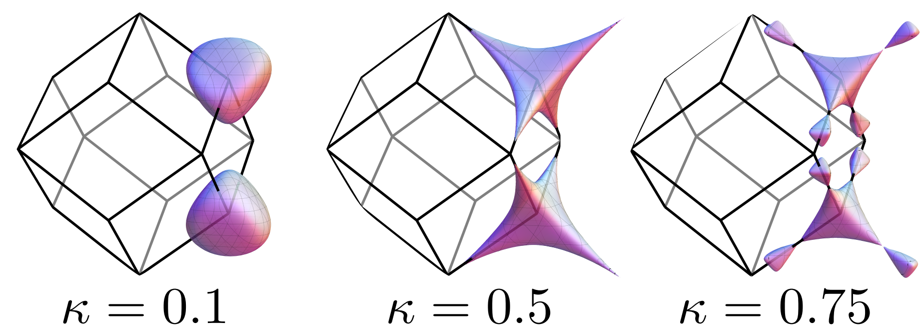
$$H_{\text{Kitaev}} = -J_K \sum_{\gamma-\text{bonds}} \sigma_i^{\gamma} \sigma_j^{\gamma} - \sum_j \vec{h} \cdot \vec{\sigma}_j$$

(10,3)a – hyperoctagon



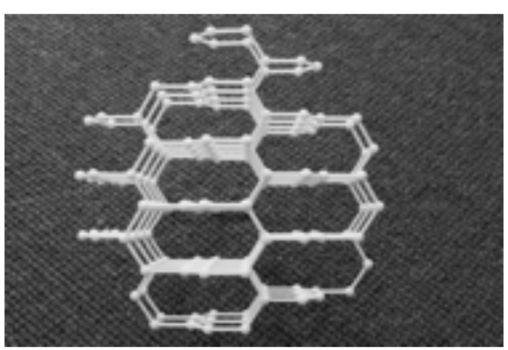


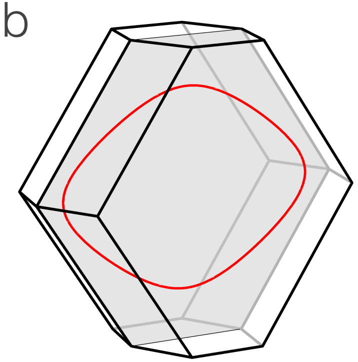
Fermi **surface**



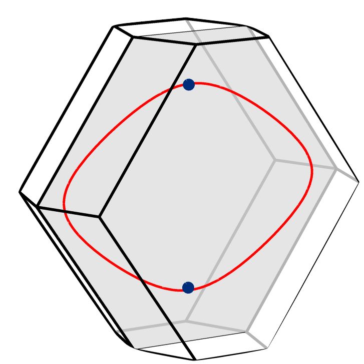
Fermi surface **deforms**

(10,3)b – hyperhoneycomb





Fermi **line**

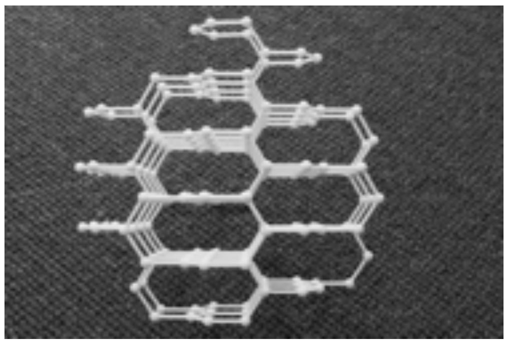


Fermi line **gaps out**, but two **Weyl nodes remain**

Weyl physics – energy spectrum

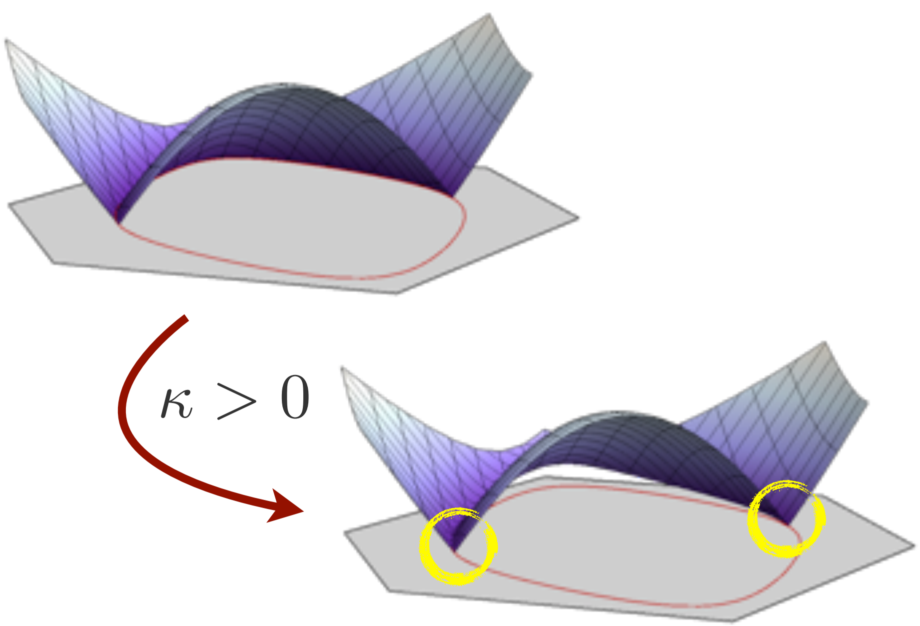
PRL **114**, 157202 (2015)

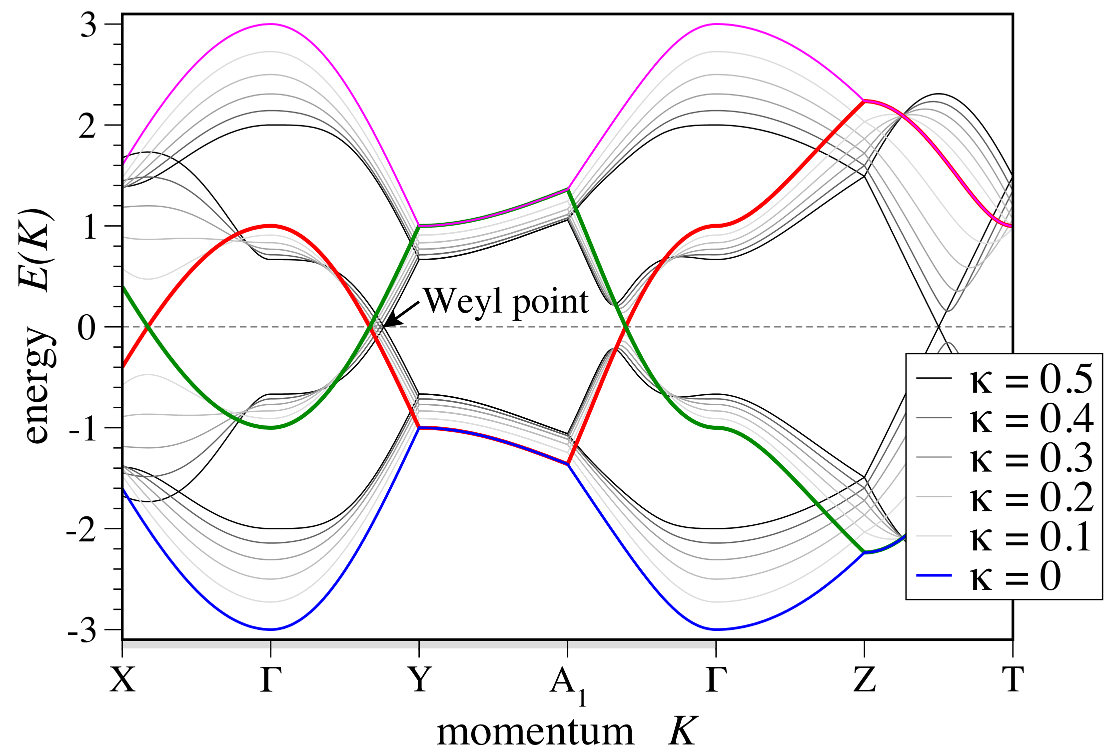
(10,3)b – hyperhoneycomb



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**

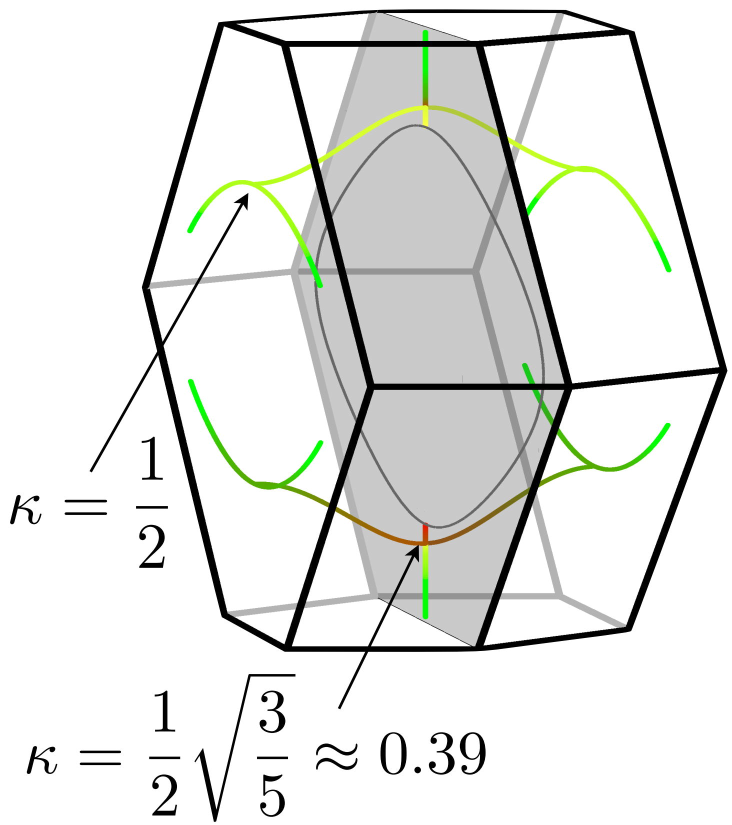




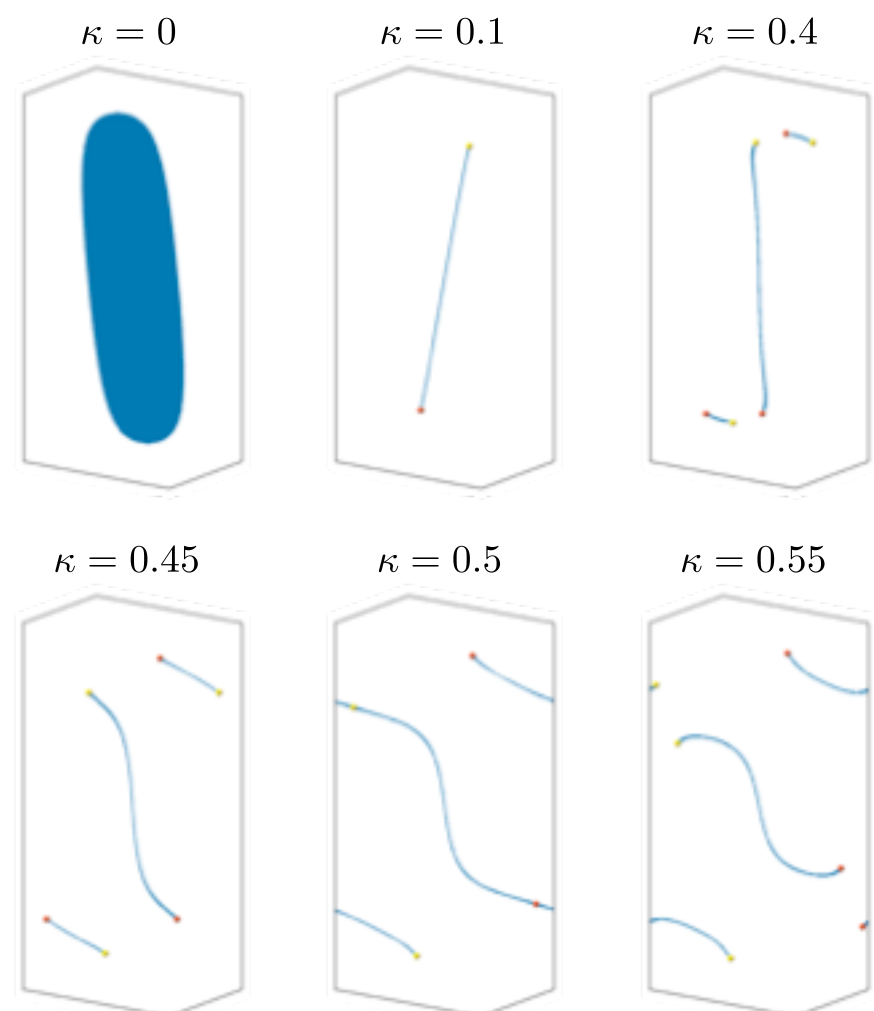
Weyl physics – surface states

PRL **114**, 157202 (2015)

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



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



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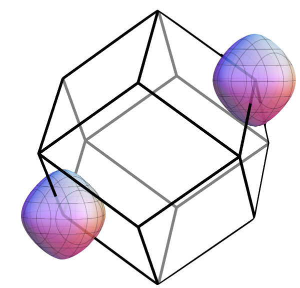
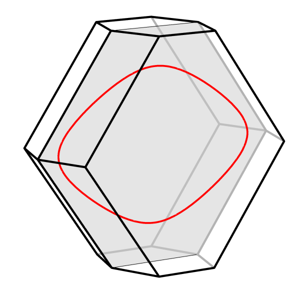
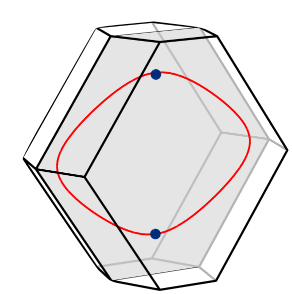
	(8,3)c	nodal line	Weyl nodes
	(8,3)n	gapped	gapped
2D	(6,3)	Dirac nodes	gapped



Majorana Fermi surfaces



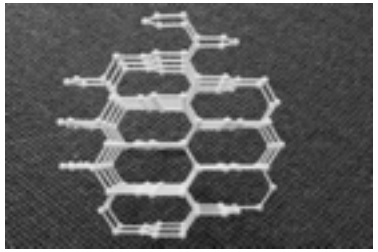
nodal lines



Weyl nodes

Three scenarios for Weyl physics

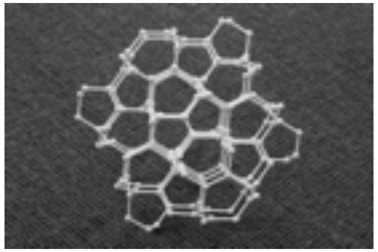
(10,3)b – hyperhoneycomb



explicit breaking of time-reversal symmetry

symmetry class D

(9,3)a

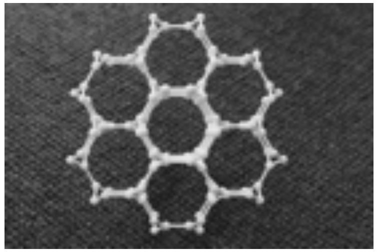


spontaneous breaking of time-reversal symmetry

symmetry class D

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

(8,3)b



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

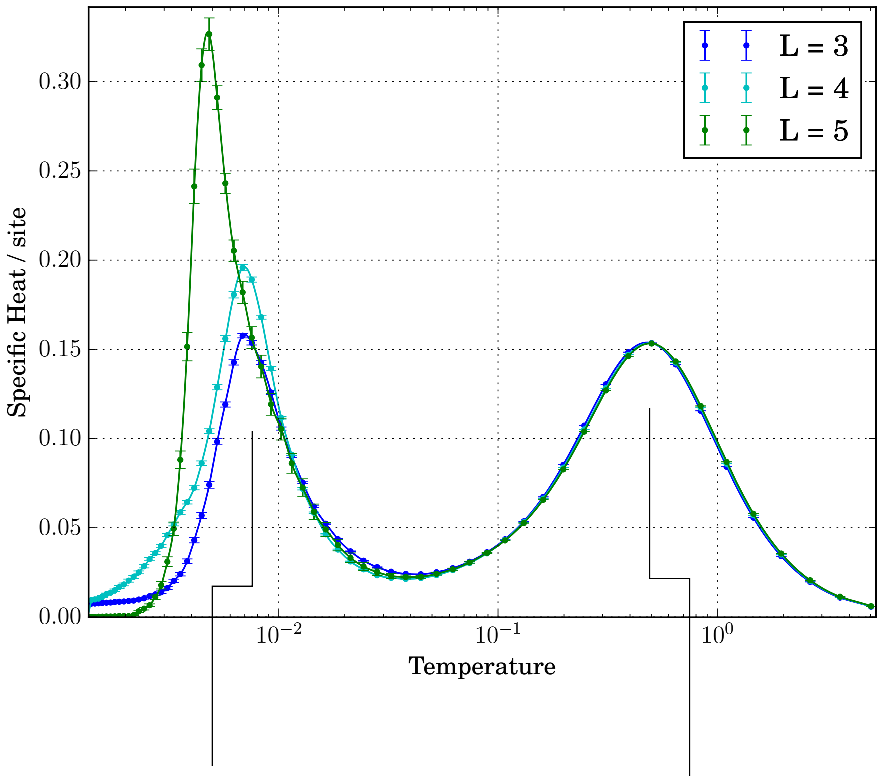
symmetry class BDI

symmetry scenario
beyond electronic systems

Z_2 gauge physics

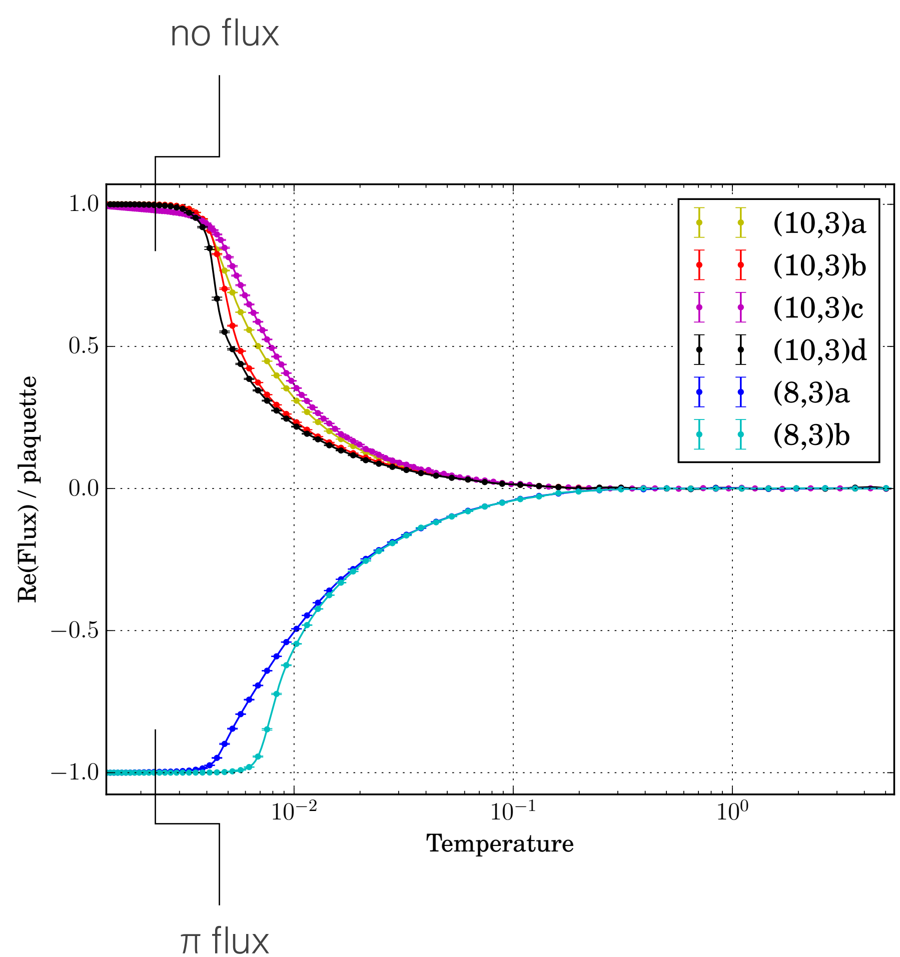
In three spatial dimensions, the spin fractionalization of the Kitaev model has a distinct (experimental) signature – the underlying **Z_2 gauge theory** generically exhibits a **finite-temperature phase transition**.

see also Motome group, PRL (2014)

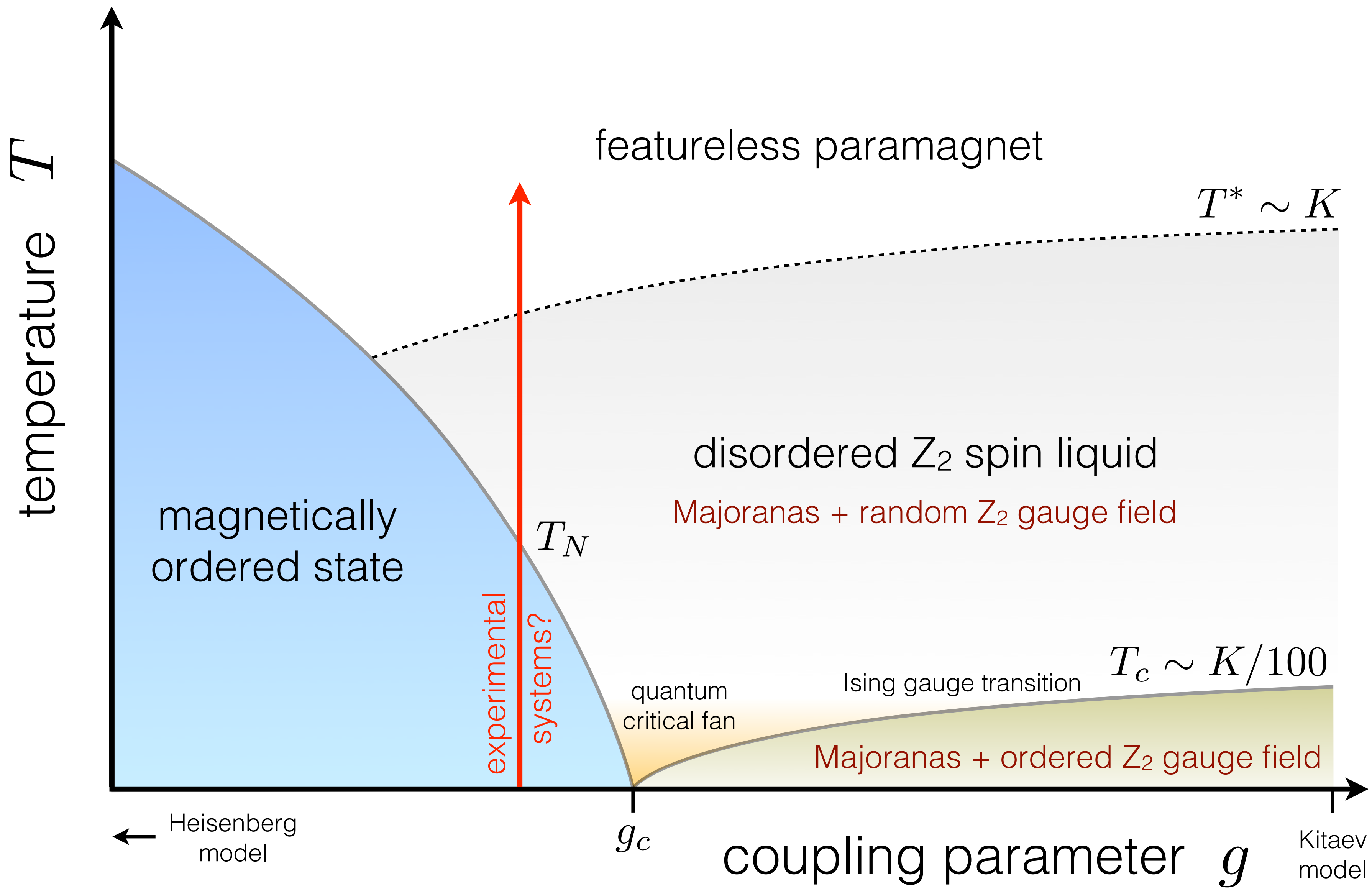


Z_2 ordering transition
(inverted Ising transition)

thermal crossover
(fractionalization)



Going beyond the Kitaev model ...



Spiral spin liquids

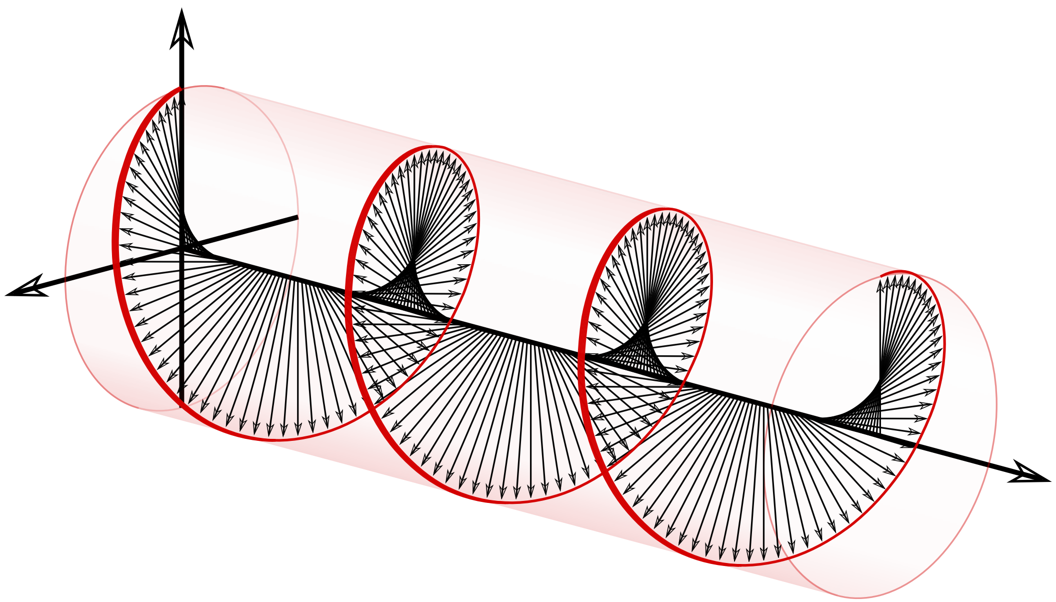
J. Attig & ST, arXiv:1705.04073

Spin spirals

Coplanar spirals typically arise in the presence of **competing interactions**

Elementary ingredient for

- multiferroics
- spin textures/multi-q states
  - skyrmion lattices
  - Z_2 vortex lattices
- spiral spin liquids



Description in terms of a single wavevector

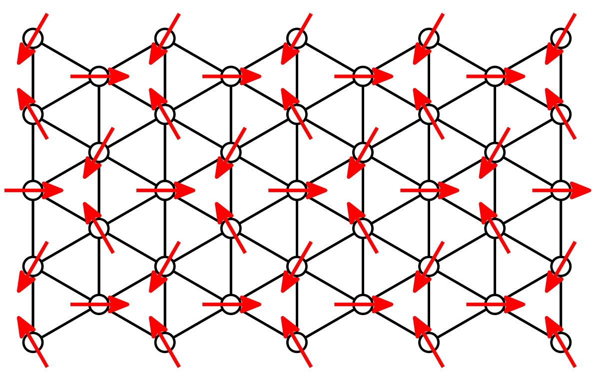
$$\vec{S}(\vec{r}) = \mathrm{Re}\left(\left(\vec{S}_1 + i\vec{S}_2\right) e^{i\vec{q}\vec{r}}\right)$$

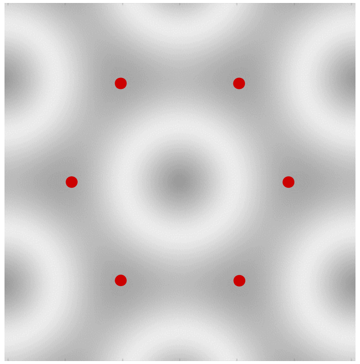
Spin spirals

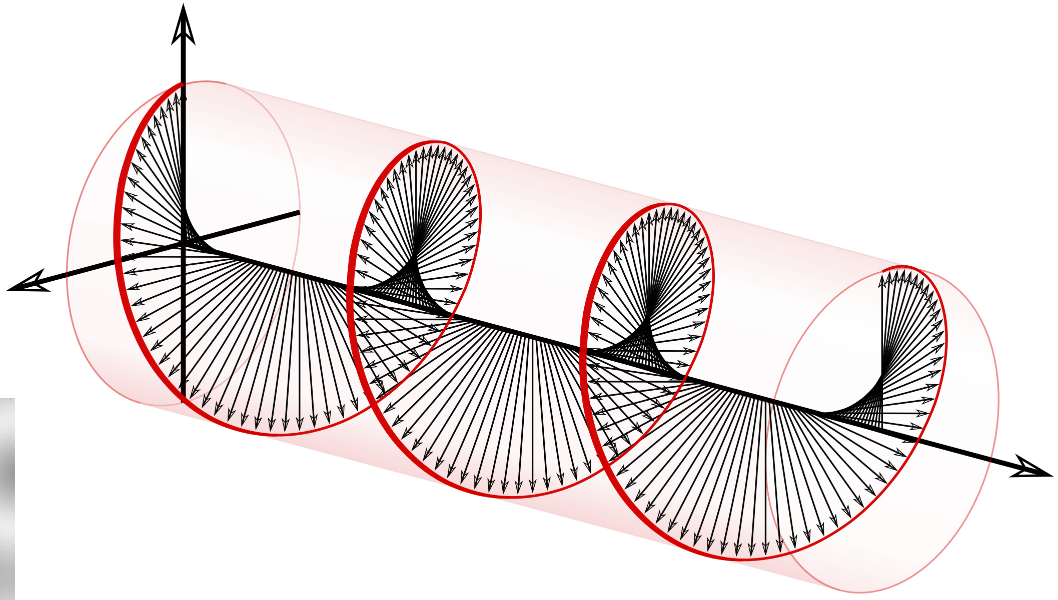
Coplanar spirals typically arise in the presence of **competing interactions**

Familiar example

- **120º order** of Heisenberg AFM on triangular lattice





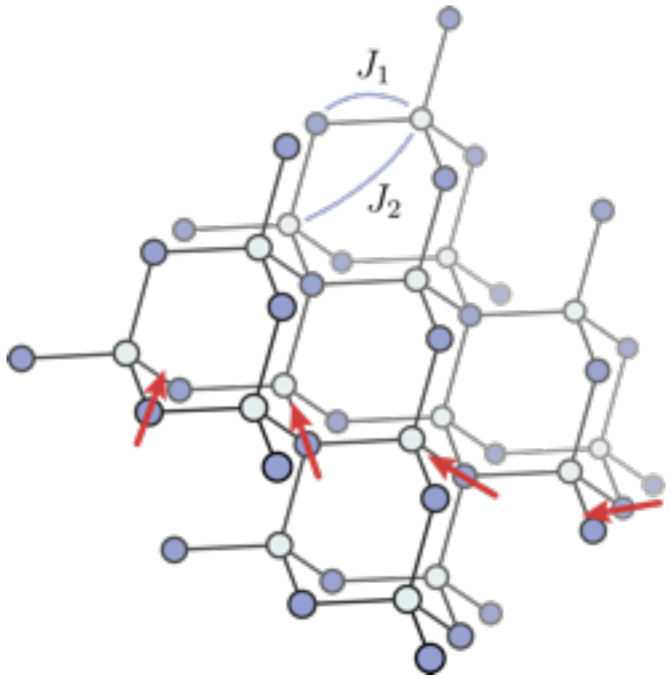


$$\vec{S}(\vec{r}) = \mathrm{Re}\left(\left(\vec{S}_1 + i\vec{S}_2\right) e^{i\vec{q}\vec{r}}\right)$$

$$\vec{q} = \left(\pm\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}}\right)$$

Spin spirals

Frustrated diamond lattice antiferromagnets

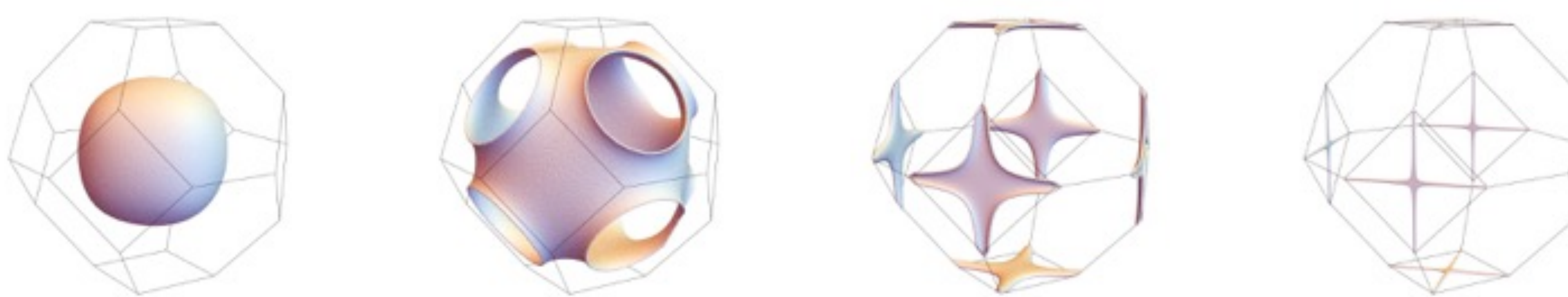


A-site spinels

$MnSc_2S_4$	S=5/2
$FeSc_2S_4$	S=2
$CoAl_2O_4$	S=3/2
$NiRh_2O_4$	S=1

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \vec{S}_j$$

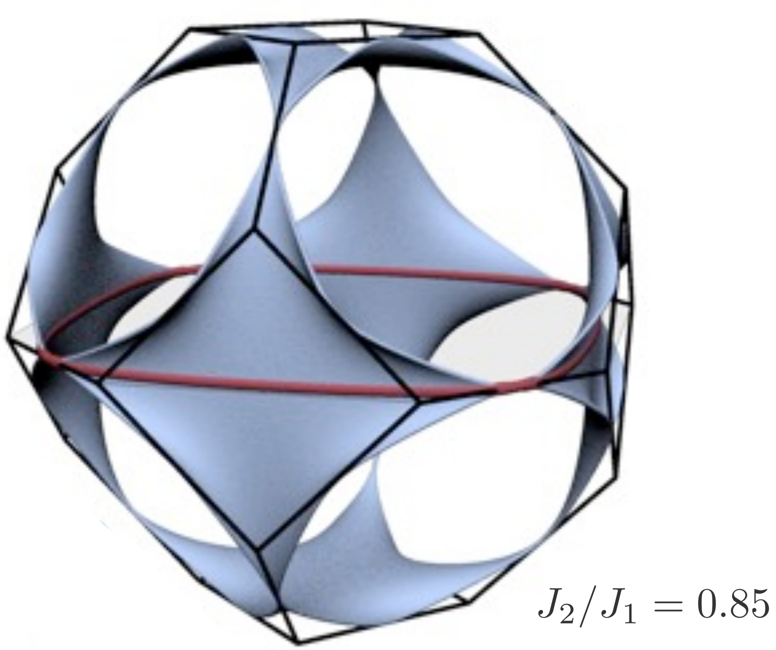
degenerate coplanar spirals form **spin spiral surfaces** in *k*-space

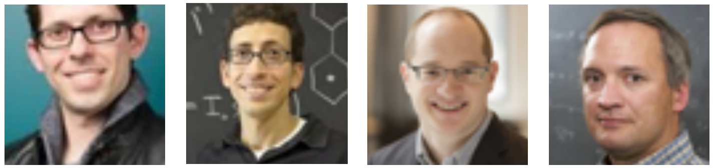


$J_2/J_1 = 0.2$ $J_2/J_1 = 0.4$ $J_2/J_1 = 3$ $J_2/J_1 = 100$

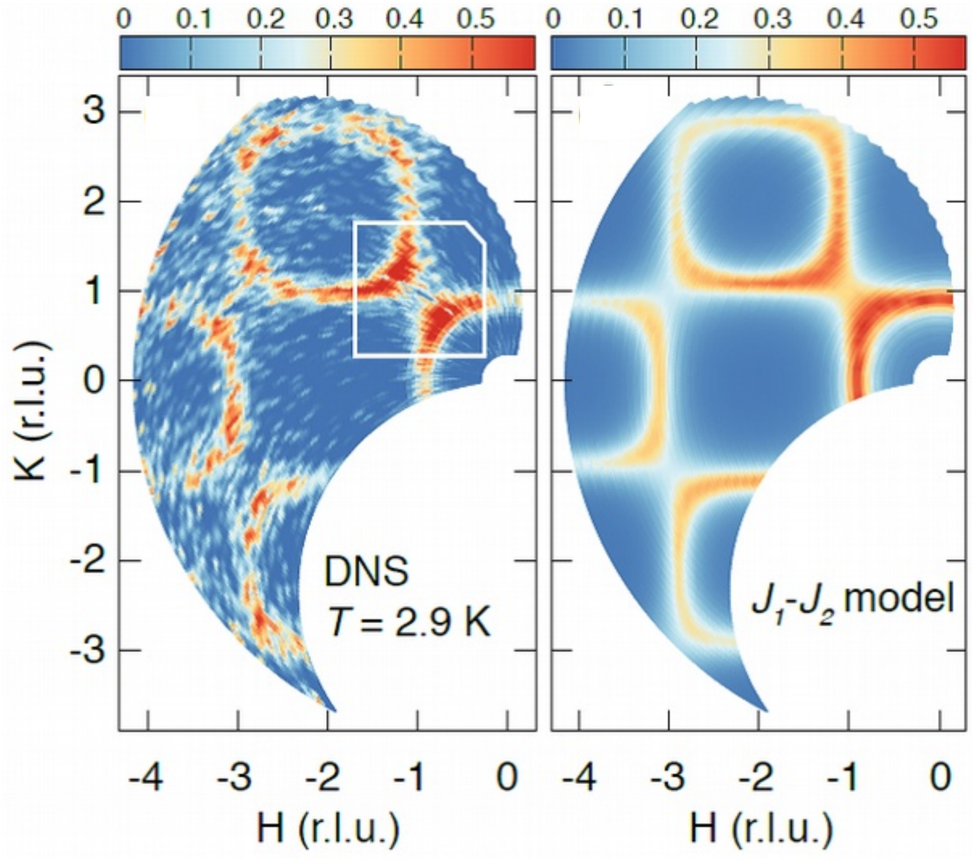
Spin spirals

Experimental observation of spin spiral surface in inelastic neutron scattering of $MnSc_2S_4$.





Nature Phys. **3**, 487 (2007)

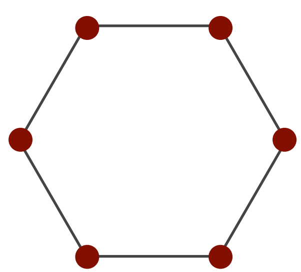


Nature Phys. **13**, 157 (2017)

Spin spiral manifolds

Spiral manifolds are extremely reminiscent of **Fermi surfaces**

triangular lattice

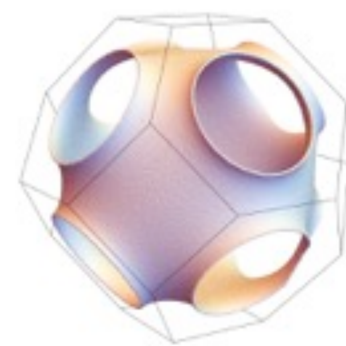


Dirac points

FCC lattice

nodal lines

diamond lattice



Fermi surface

But:

Spiral manifolds describe ground state of classical spin system, while Fermi surfaces are features in the middle of the energy spectrum of an electronic quantum system.

Spin spiral manifolds

Luttinger-Tisza

spin spirals in a nutshell

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij}\, \vec{S}_i \vec{S}_j$$

Fourier transform of spin model

$$= \sum_{\vec{k}} \sum_{A,B} S^A_{\vec{k}}\, \mathbf{M}_{A,B}(\vec{k})\, S^B_{-\vec{k}}$$

diagonalize matrix

$$\mathbf{M}_{A,B}(\vec{k}) = \sum_{\vec{r}^A_{B,j}} J_{\vec{r}_j}\, e^{-i\vec{k}\cdot\vec{r}_j}$$

find **minimal** eigenvalues

$$\lambda_j(\vec{k})$$

free fermions in a nutshell

$$\mathcal{H} = \sum_{\langle i,j \rangle} t_{ij}\, c_i^\dagger c_j$$

Fourier transform of spin model

$$= \sum_{\vec{k}} \sum_{A,B} c^\dagger_{A,\vec{k}}\, \mathbf{H}_{A,B}(\vec{k})\, c_{B,\vec{k}}$$

diagonalize matrix

$$\mathbf{H}_{A,B}(\vec{k}) = \sum_{\vec{r}^A_{B,j}} t_{\vec{r}_j}\, e^{-i\vec{k}\cdot\vec{r}_j}$$

find **zero** eigenvalues

$$\epsilon_j(\vec{k})$$

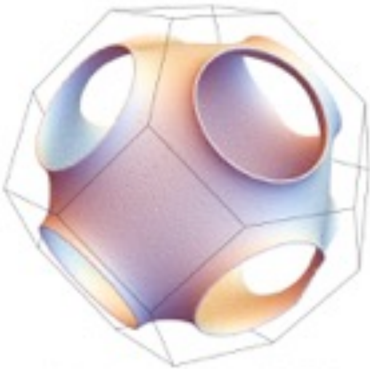
Spin spiral manifolds

spin spirals in a nutshell

$\mathbf{M}_{A,B}(\vec{k})$

with **minimal** eigenvalues

$\lambda_j(\vec{k})$



make ansatz

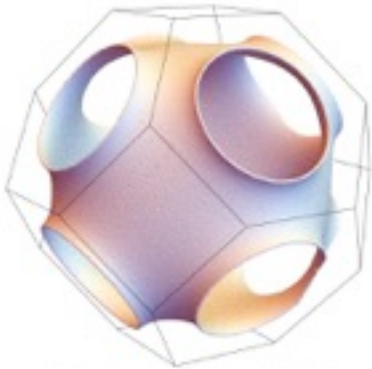
$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

free fermions in a nutshell

$\mathbf{H}_{A,B}(\vec{k})$

with **zero** eigenvalues

$\epsilon_j(\vec{k})$



$\mathbf{H}(\vec{k})^2$ has eigenvalues $\epsilon_j(\vec{k})^2$

zero eigenvalues of $\mathbf{H}(\vec{k})$

are minimal eigenvalues of $\mathbf{H}(\vec{k})^2$

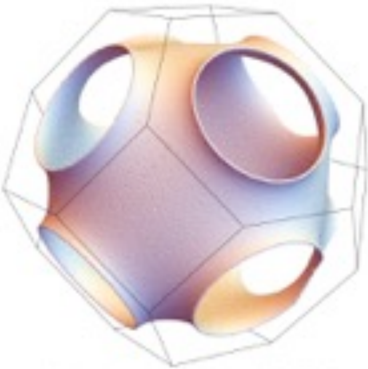
Mapping classical to quantum

spin spirals in a nutshell

$$\mathbf{M}_{A,B}(\vec{k})$$

with **minimal** eigenvalues

$$\lambda_j(\vec{k})$$



$$\mathbf{H}(\vec{k})^2$$

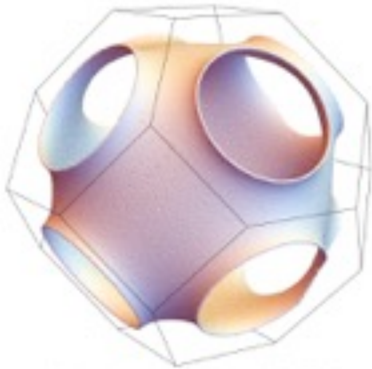
$$\sqrt{\mathbf{M}(\vec{k})}$$

free fermions in a nutshell

$$\mathbf{H}_{A,B}(\vec{k})$$

with **zero** eigenvalues

$$\epsilon_j(\vec{k})$$



$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

mapping of a classical to quantum system
(of same spatial dimensionality)
via a 1:1 matrix correspondence

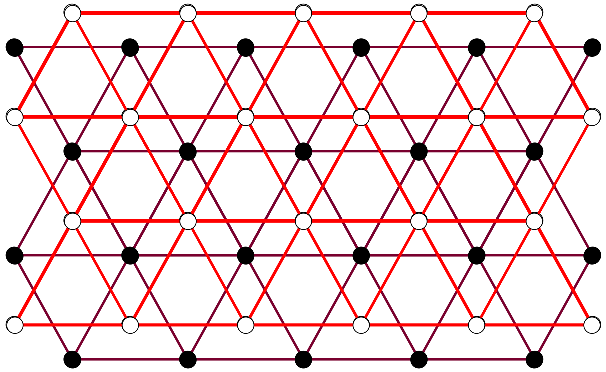
→ reminiscent of "topological mechanics"

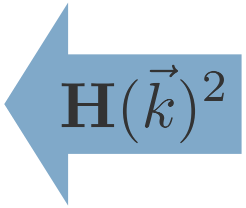
Mapping classical to quantum

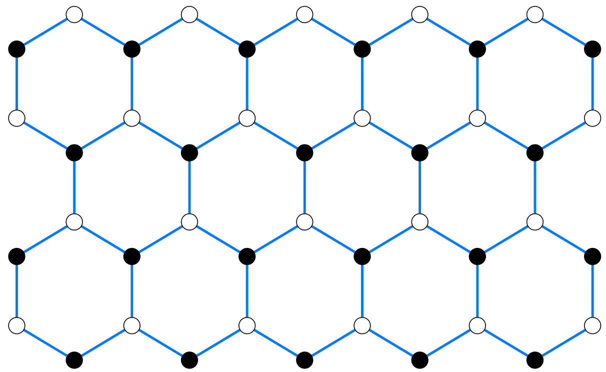
$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

What does **"squaring"** of quantum system mean?

Explicit **lattice construction**.







coplanar spirals on triangular lattice

$$\vec{q} = \left(\pm\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}} \right)$$

free fermions on honeycomb lattice

$$\vec{q} = \left(\pm\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}} \right)$$

Mapping classical to quantum

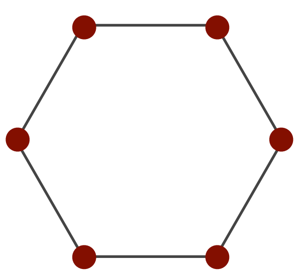
$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

What does **“squaring”** of quantum system mean?

Explicit **lattice construction**.

spin spirals
triangular lattice

120º order



Dirac points

free fermions
honeycomb lattice

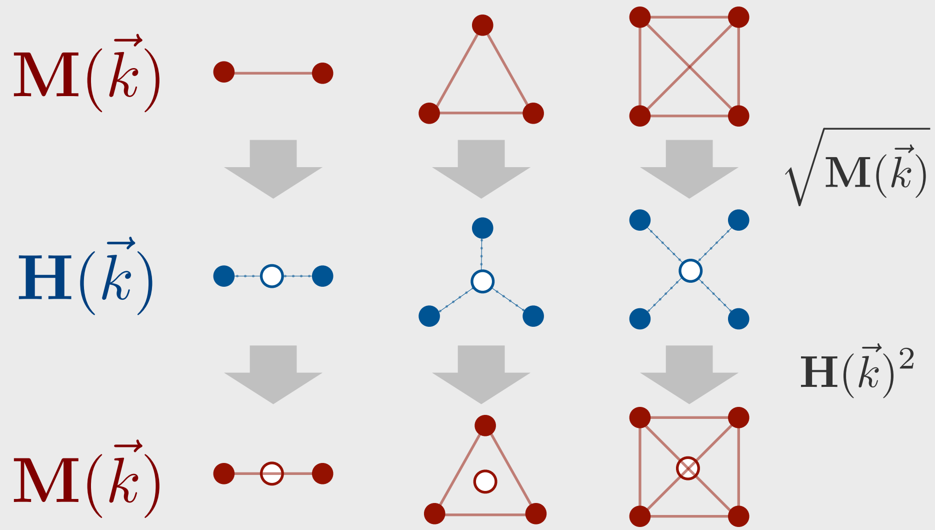
spin spirals
FCC lattice

degenerate spirals

nodal lines

free fermions
diamond lattice

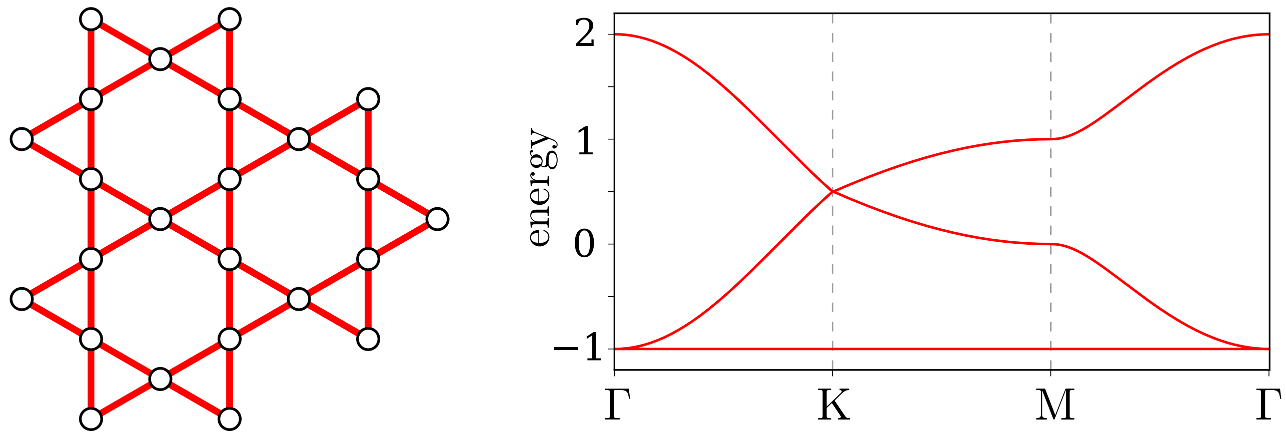
general lattice construction



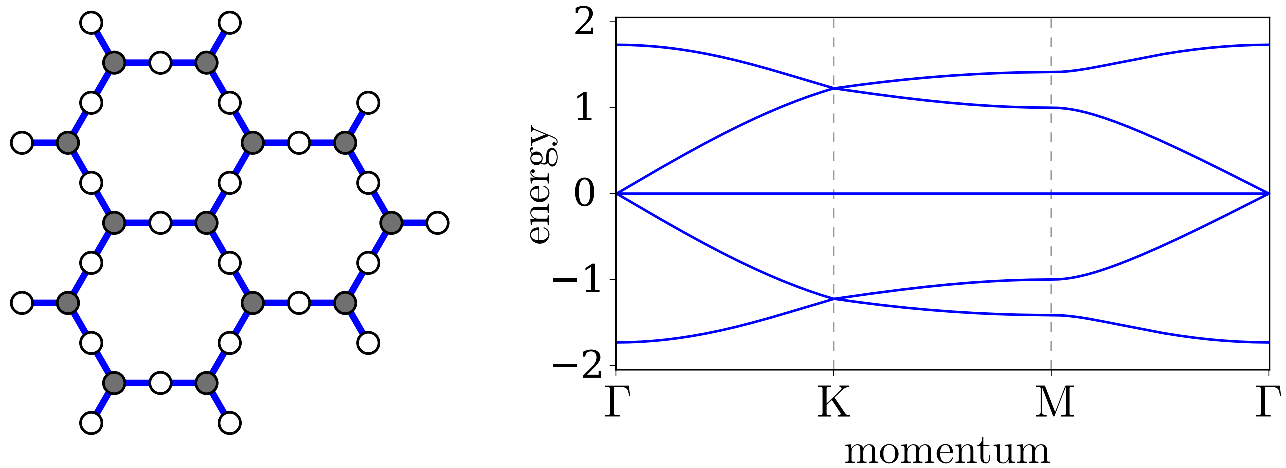
Examples

Spectra of the **kagome** and **extended honeycomb** lattice.

spins



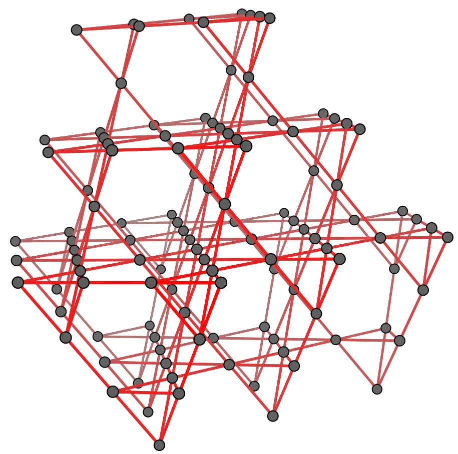
fermions

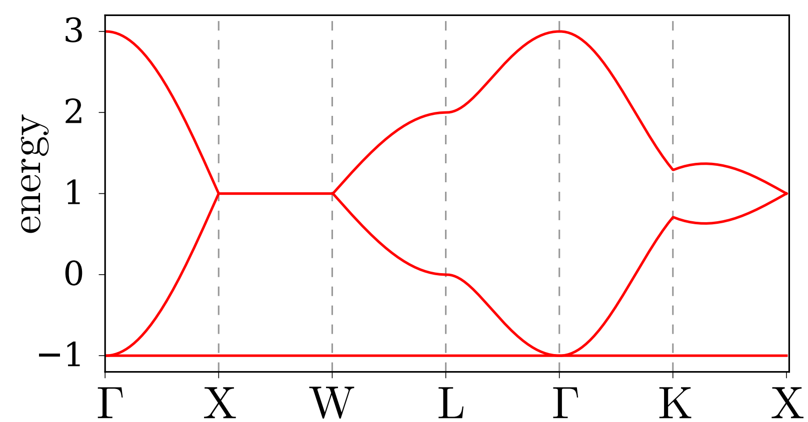


Examples

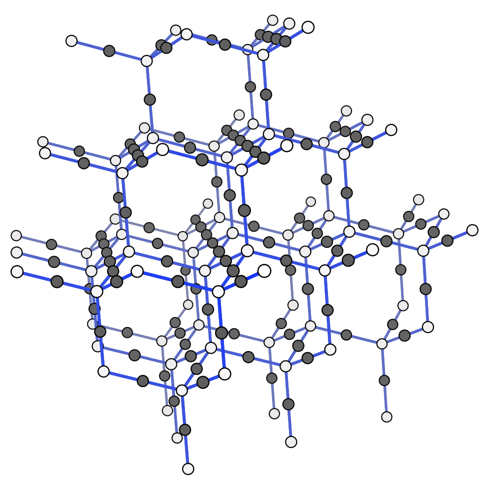
Spectra of the **pyrochlore** and **extended diamond** lattice.

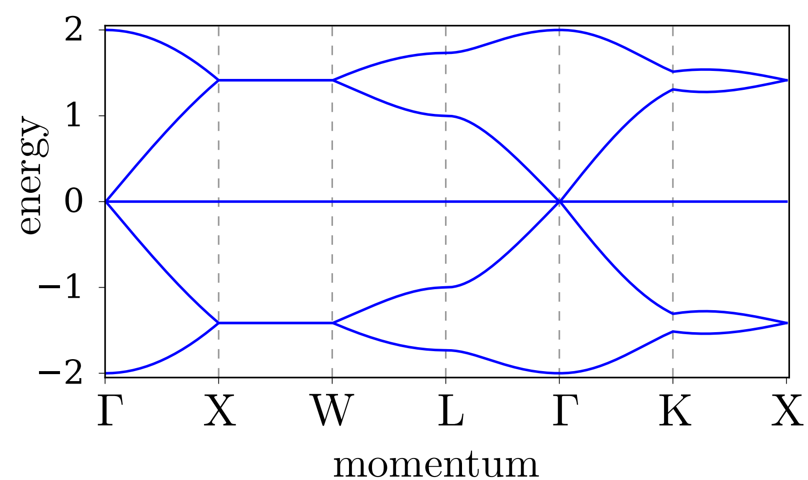
spins





fermions

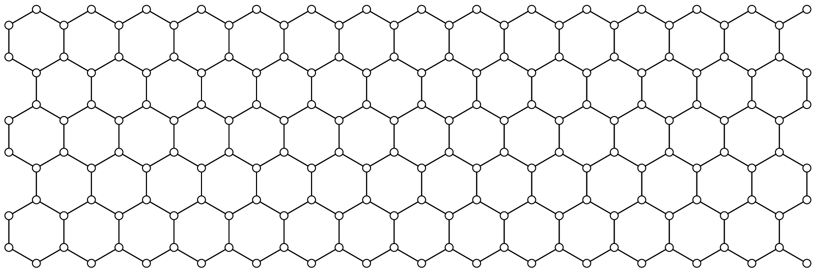




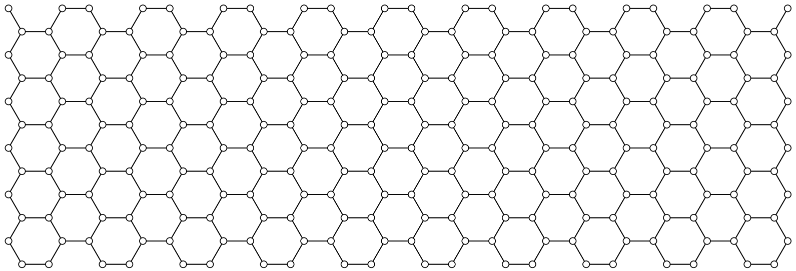
Topological spin spirals?

Are **topological band structures** in free fermion systems replicating themselves in classical spin systems?

Dirac nodes **edge states**

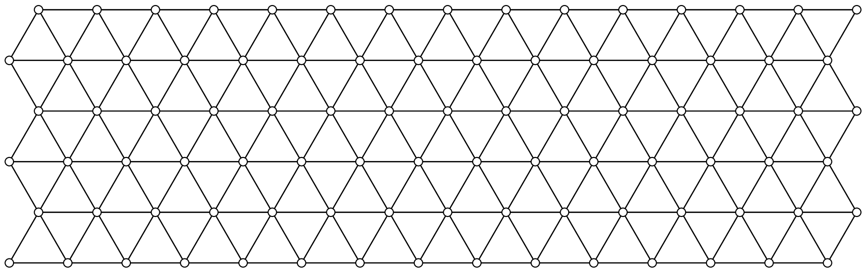


zig-zag edge

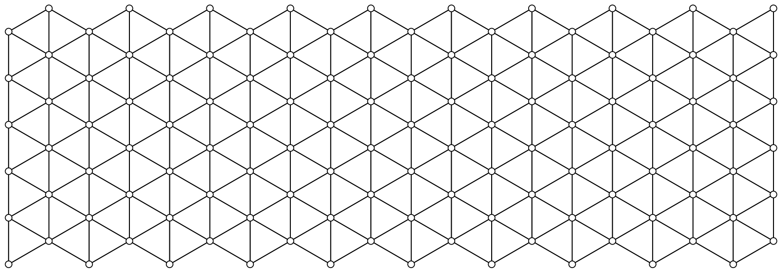


armchair edge

120º order **edge states**?



“zig-zag” edge

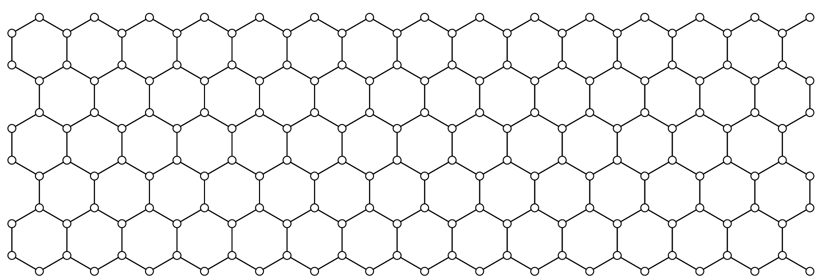


“armchair” edge

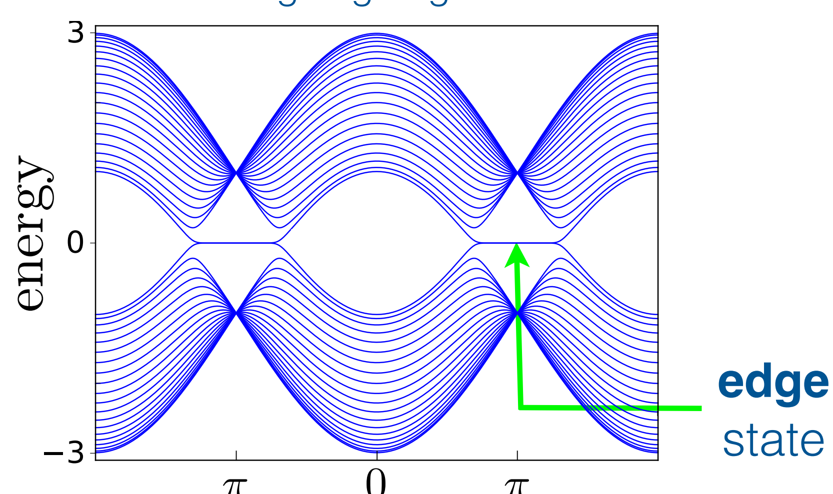
Topological spin spirals?

Are **topological band structures** in free fermion systems replicating themselves in classical spin systems?

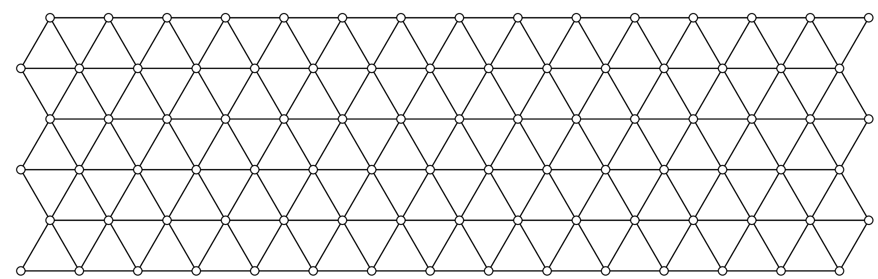
Dirac nodes **edge states**



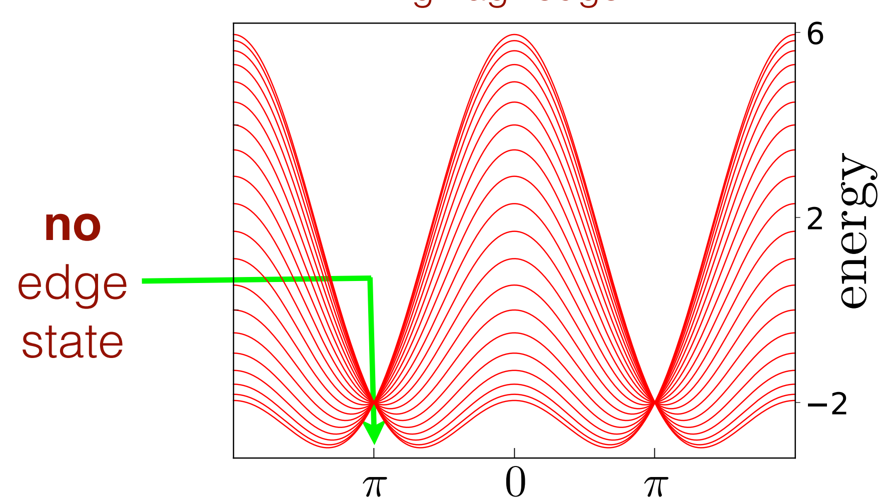
zig-zag edge



120^o order **edge states**?



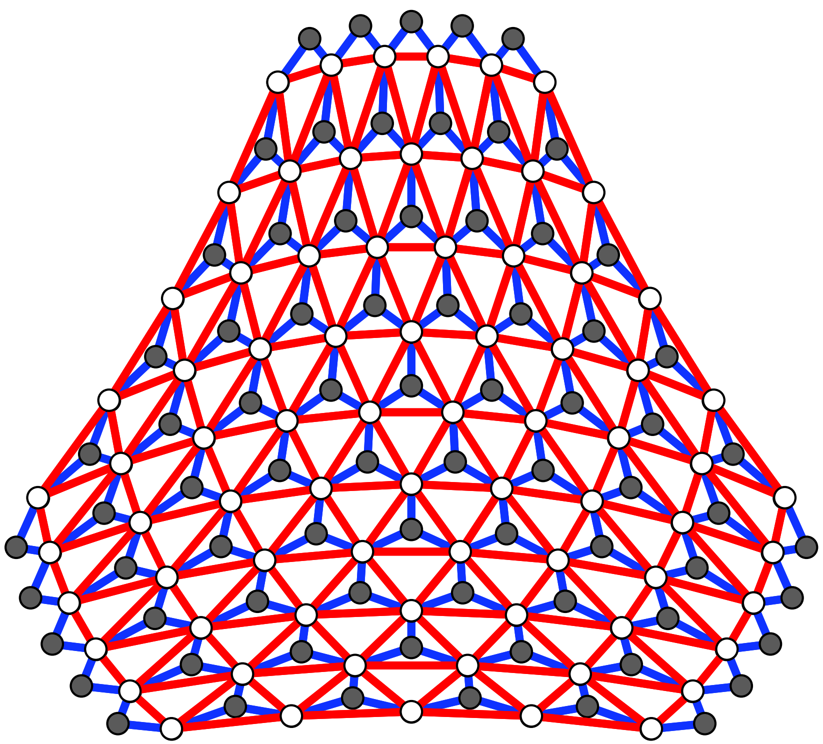
“zig-zag” edge



Topological spin spirals?

Are **topological band structures** in free fermion systems replicating themselves in classical spin systems?

triaxial strain for fermions



pseudomagnetic field
Landau level formation

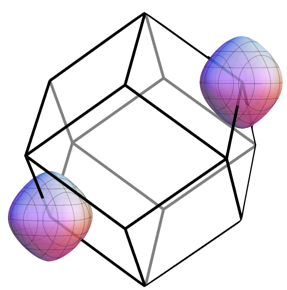
triaxial strain for spins

ground state with **topological features?**
→ future work ...

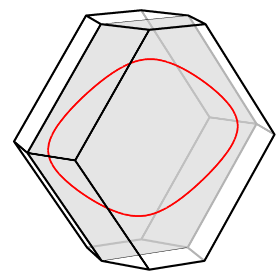
Summary

Spin liquids can be **dichotomous states**, where an electronic Mott **insulator** harbors emergent itinerant degrees of freedom that form a **metal**.

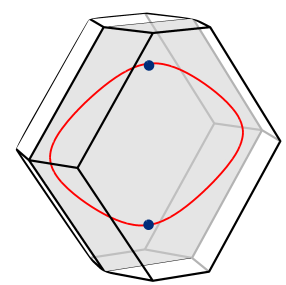
Majorana metals and quantum spin liquids in **3D Kitaev models**.



Majorana Fermi surfaces



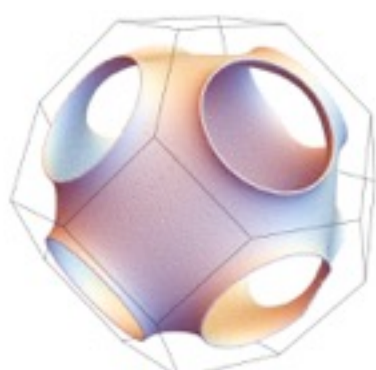
nodal lines



Weyl nodes

PRB **93**, 085101 (2016) PRL **115**, 177205 (2015) PRL **114**, 157202 (2015) PRB **89**, 235102 (2014)

Spiral spin liquids and metals in **classical spin systems**.



classical spin system / spin spirals

$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

free fermion system / metal

arXiv:1705.04073

Thanks!

@SimonTrebst