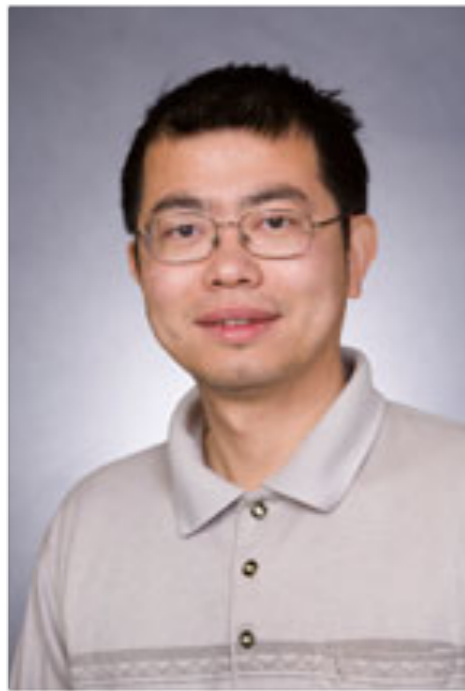


Strongly Interacting Electrons in Low Dimensions
Princeton Center for Theoretical Sciences
September 12, 2011

Gamma Matrix Generalizations of the Kitaev Model

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Hsiang-Hsuan Hung

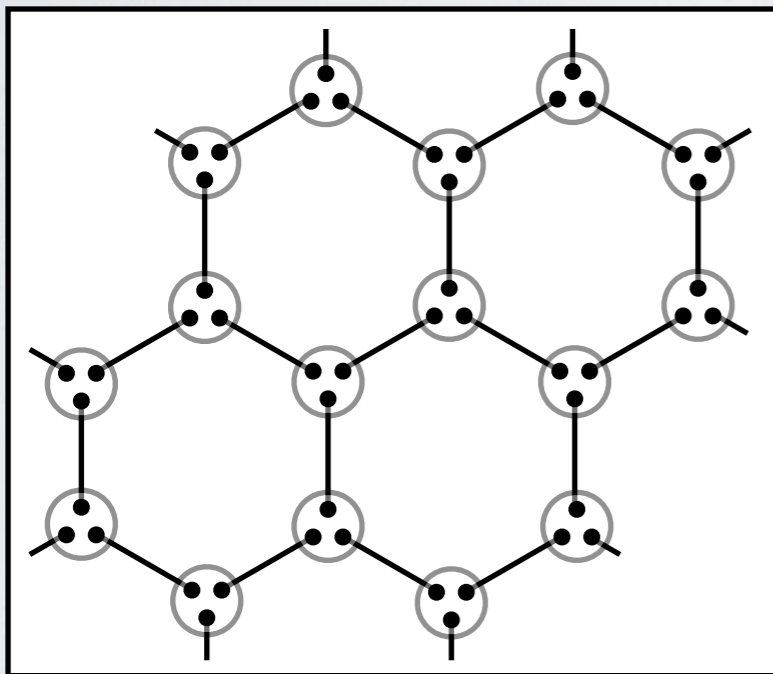


Zhoushen Huang



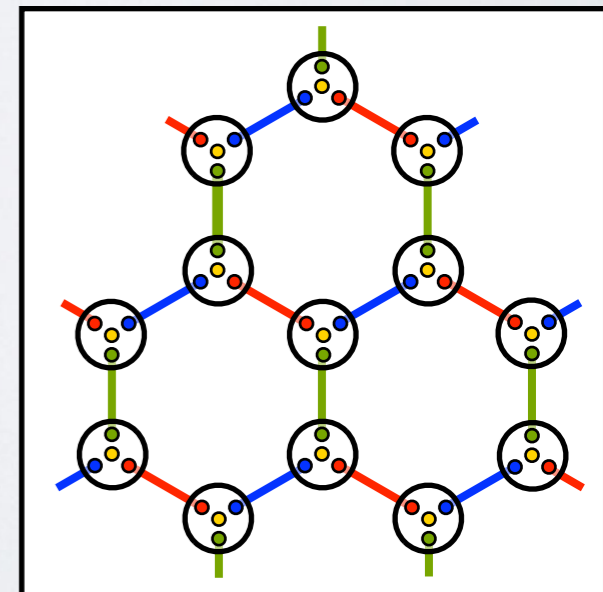
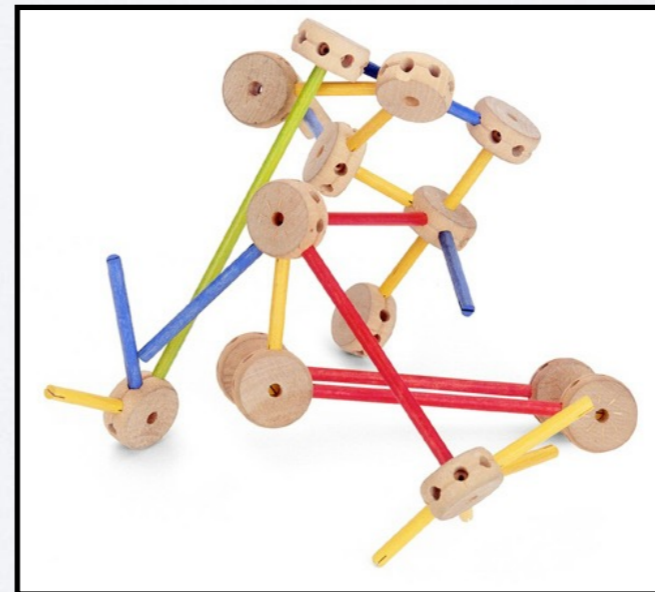
Why I like these models

1) They remind me of Tinker Toys from my childhood.



2) Geometric pictures and ridiculous Hamiltonians remind me of AKLT models from when I was a postdoc.

3) Many species of Majorana fermions = excuse for figures with pretty colors.



Seminar BINGO!

To play, simply print out this bingo sheet and attend a departmental seminar.

Mark over each square that occurs throughout the course of the lecture.

The first one to form a straight line (or all four corners) must yell out

BINGO!! to win!



SEMINAR B I N G O

Speaker bashes previous work	Repeated use of "um..."	Speaker sucks up to host professor	Host Professor falls asleep	Speaker wastes 5 minutes explaining outline
Laptop malfunction	Work ties in to Cancer/HIV or War on Terror	"...et al."	You're the only one in your lab that bothered to show up	Blatant typo
Entire slide filled with equations	"The data <i>clearly</i> shows..."	FREE Speaker runs out of time	Use of Powerpoint template with blue background	References Advisor (past or present)
There's a Grad Student wearing same clothes as yesterday	Bitter Post-doc asks question	"That's an interesting question"	"Beyond the scope of this work"	Master's student bobs head fighting sleep
Speaker forgets to thank collaborators	Cell phone goes off	You've no idea what's going on	"Future work will..."	Results conveniently show improvement

JORGE CHAM © 2007

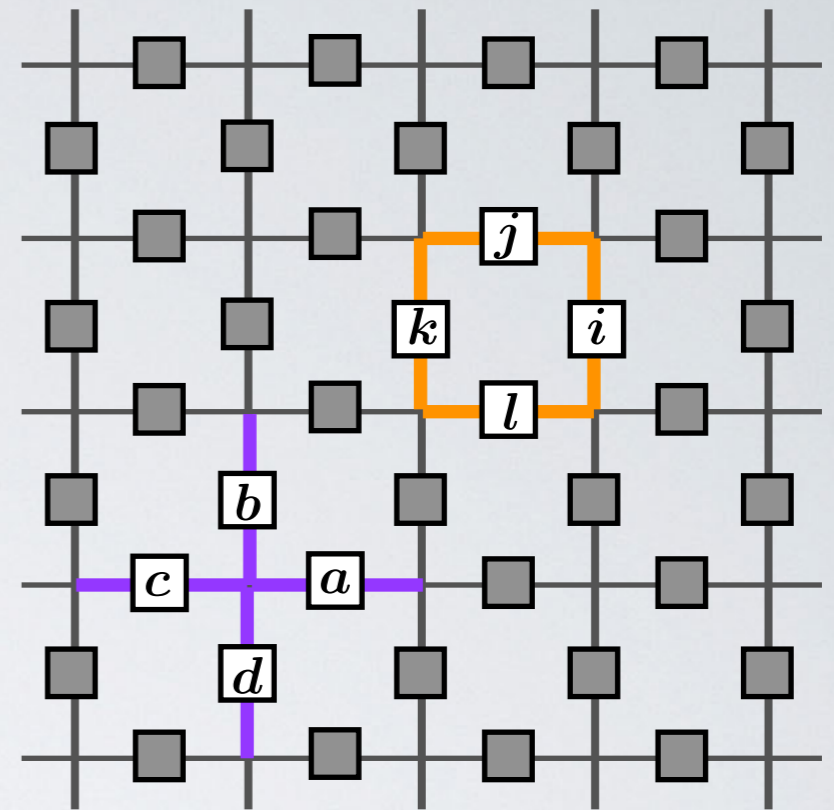
Kitaev toric code (2003):

$$\mathcal{H} = -J_E \sum_{\square} \sigma_a^z \sigma_b^z \sigma_c^z \sigma_d^z - J_M \sum_{\square} \sigma_i^x \sigma_j^x \sigma_k^x \sigma_l^x$$

+
□

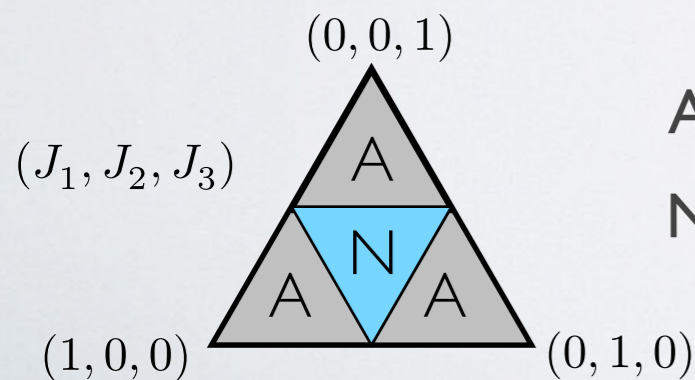
electric charges
magnetic vortices

Topologically degenerate ground state (4x on torus) with gap to electric (e) and magnetic (m) excitations that have nontrivial mutual statistics and form composite (e-m) fermions.

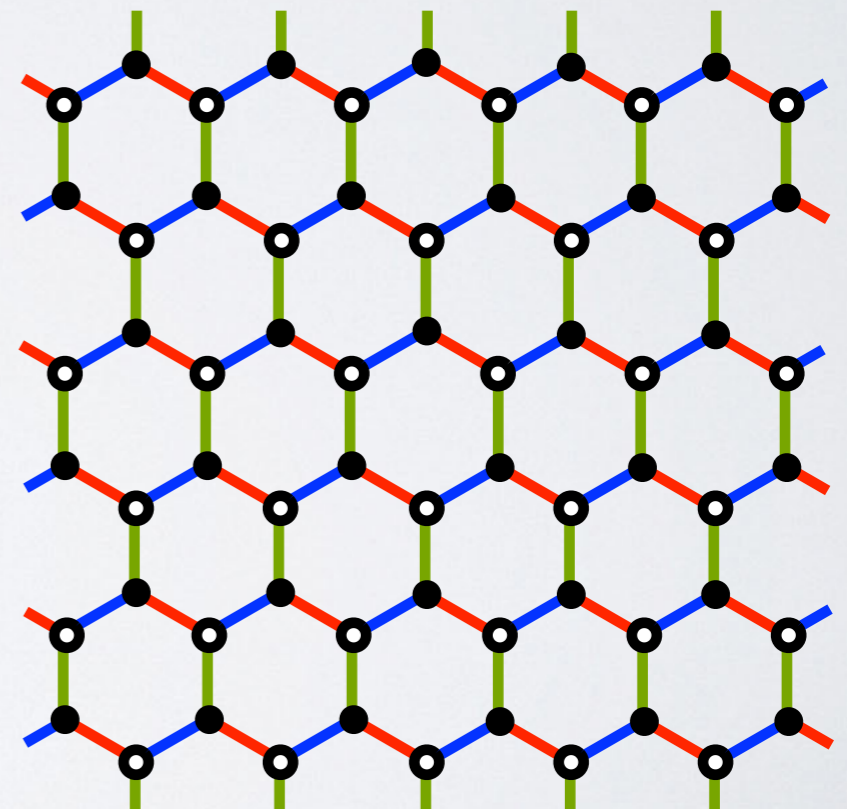


Kitaev honeycomb model (2006):

$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x + J_2 \sum_{\langle ij \rangle} \sigma_i^y \sigma_j^y + J_3 \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z$$



A : gapped abelian phases
 N : gapless nonabelian phase



Majorana fermions

Self-conjugate (“real”) fermions : $\theta = \theta^\dagger$

Many species : $\{\theta^a, \theta^b\} = 2\delta^{ab}$

2 Majorana = 1 Dirac : $c = \frac{1}{2}(\theta_1 + i\theta_2)$ $c^\dagger = \frac{1}{2}(\theta_1 - i\theta_2)$

$2N$ Majoranas $\Rightarrow 2^N$ states

$$\begin{array}{c} \swarrow \quad \searrow \\ \{c, c^\dagger\} = 1 \end{array}$$

$S = 1/2$ algebra represented with Majoranas

Four Majorana species : θ^a ($a = 0, 1, 2, 3$)

$$\sigma^x = i\theta^0\theta^1 = -i\theta^2\theta^3$$

Pauli matrices : $\sigma^\alpha = i\theta^0\theta^\alpha$ ($\alpha = 1, 2, 3$)

$$\sigma^y = i\theta^0\theta^2 = +i\theta^1\theta^3$$

Constraint : $\theta^0\theta^1\theta^2\theta^3 = 1$

$$\sigma^z = i\theta^0\theta^3 = -i\theta^1\theta^2$$

Projector onto constraint sector : $P = \frac{1}{2}(1 + \theta^0\theta^1\theta^2\theta^3)$

2D Toric Code

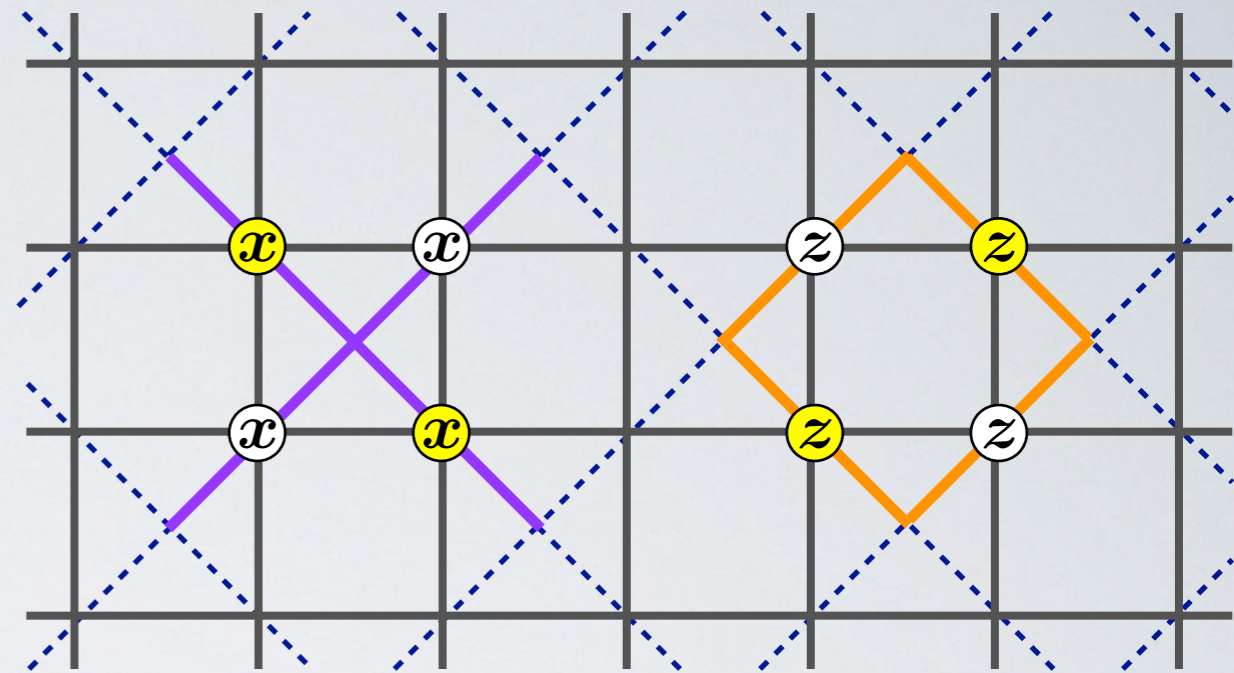
Apply unitary transformation $U = e^{i\frac{\pi}{4}\sigma^y}$

to all NW/SE links: $\begin{Bmatrix} \sigma^x \\ \sigma^z \end{Bmatrix} \longrightarrow \begin{Bmatrix} -\sigma^z \\ \sigma^x \end{Bmatrix}$

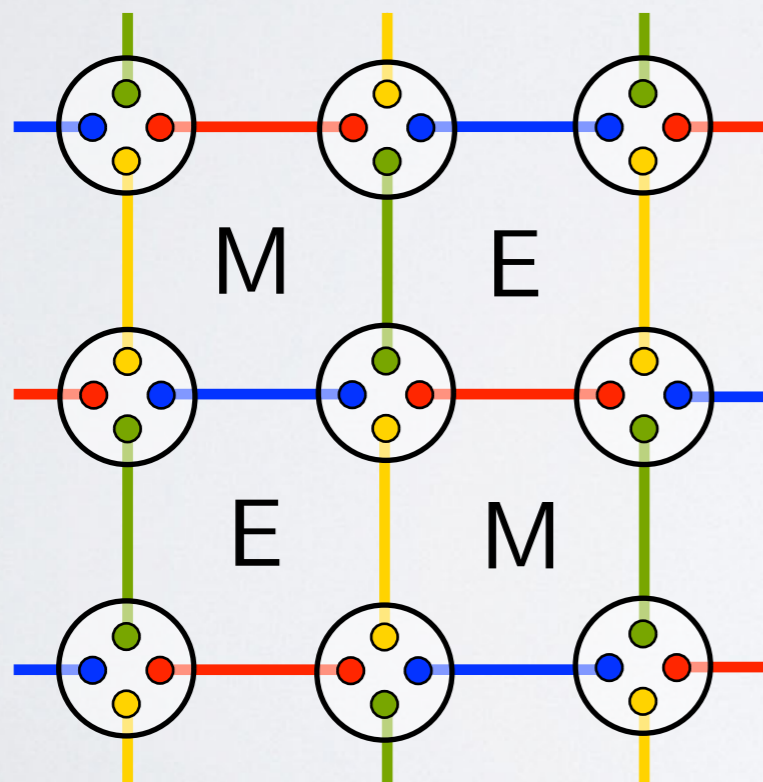
This yields Wen's model (rotated by $\pi/4$)

$$\mathcal{H} = -J_E \sum_{\square, E} \sigma_i^x \sigma_j^z \sigma_k^x \sigma_l^z - J_M \sum_{\square, M} \sigma_i^x \sigma_j^z \sigma_k^x \sigma_l^z$$

(Wen, 2003)



(construction due to A. Kitaev)



Define the \mathbb{Z}_2 gauge fields $u_{ij} = -i \theta_i^a \theta_j^a$ ($a = 0, 1, 2, 3$)
 $u_{ij} = \pm 1$

Magic : Sticks of same color never share a vertex means that the gauge fields u_{ij} commute!

$[u_{ij}, u_{kl}] = 0 \Rightarrow$ classical \mathbb{Z}_2 gauge theory.

$$\mathcal{H} = -J_E \sum_{\square, E} u_{ij} u_{jk} u_{kl} u_{li} - J_M \sum_{\square, M} u_{ij} u_{jk} u_{kl} u_{li}$$

$$\begin{aligned} \sigma^x &= i \theta^0 \theta^1 = -i \theta^2 \theta^3 & \sigma^y &= i \theta^0 \theta^2 = +i \theta^1 \theta^3 \\ \sigma^z &= i \theta^0 \theta^3 = -i \theta^1 \theta^2 \end{aligned}$$

Ground state : $\phi_p = u_{ij} u_{jk} u_{kl} u_{li} = +1$

Honeycomb Lattice Model

$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x + J_2 \sum_{\langle ij \rangle} \sigma_i^y \sigma_j^y + J_3 \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z$$

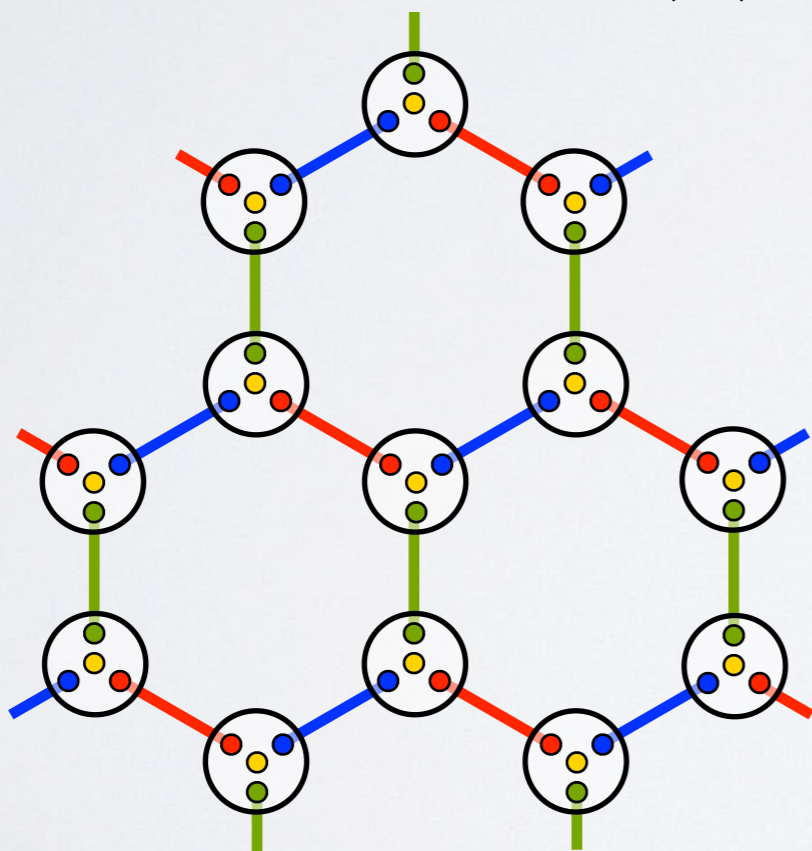
$$\sigma^x = i \theta^0 \theta^1 = -i \theta^2 \theta^3$$

$$\sigma^y = i \theta^0 \theta^2 = +i \theta^1 \theta^3$$

$$\sigma^z = i \theta^0 \theta^3 = -i \theta^1 \theta^2$$

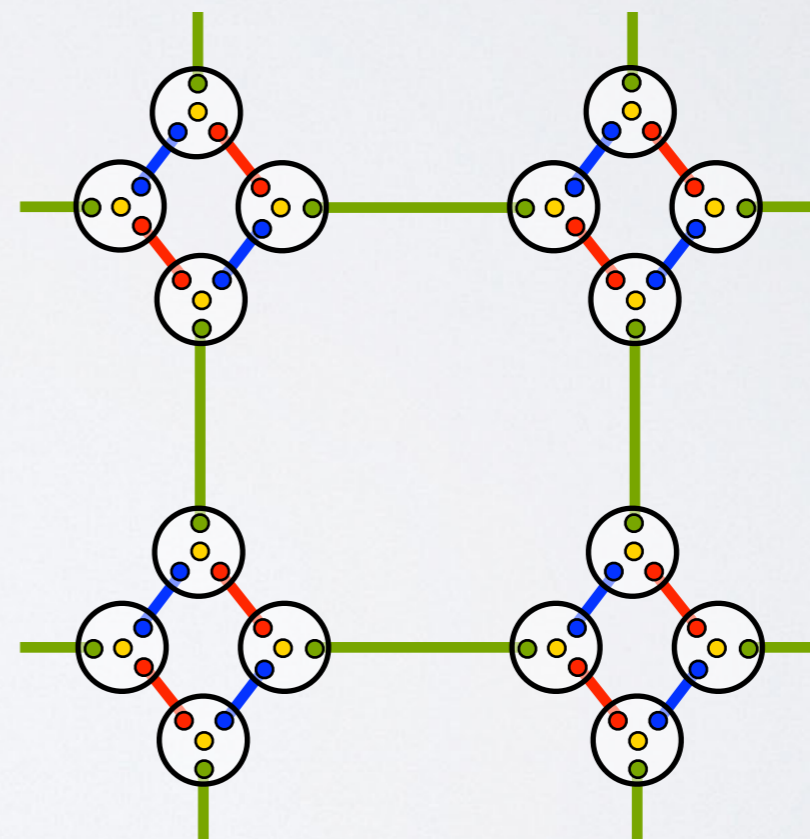
The honeycomb lattice is threefold coordinated. The magic stick rule still holds, but one Majorana species is free to hop in the presence of a static \mathbb{Z}_2 gauge field.

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} u_{ij} i \theta_i^0 \theta_j^0 \quad (u_{ij} = \pm 1)$$



honeycomb lattice

(Kitaev 2006)



square-octagon lattice

(Yang et al. 2007 , Baskaran et al. 2009 , Kells et al. 2010)

Counting spin, fermion and gauge freedoms

Consider N sites on a torus

Spins : 2^N degrees of freedom

N Majoranas (θ_i^0) : $2^{N/2}$ DOF ($\frac{1}{2}N$ Dirac fermions)

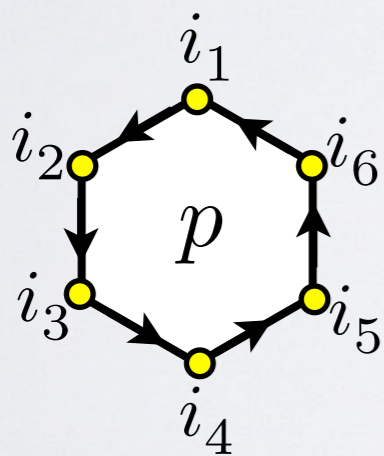
$\frac{3}{2}N$ \mathbb{Z}_2 gauge fields (u_{ij}) : $2^{3N/2}$ DOF

4 Majoranas per site

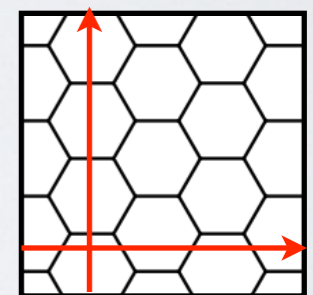
$$4^N = \overbrace{(\sqrt{2}^4)^N} \text{ DOF}$$

too many!

Count *gauge-invariant* freedoms : $\frac{1}{2}N$ hexagon fluxes ϕ_p ; 1 constraint $\prod_p \phi_p = 1$



2 Wilson cycles $W_{H/V} = \prod_{H/V} u_{ij}$



$\Rightarrow \frac{1}{2}N + 1$ independent flux variables

$$\phi_p = u_{i_1 i_2} u_{i_2 i_3} u_{i_3 i_4} u_{i_4 i_5} u_{i_5 i_6} u_{i_6 i_1}$$

Projection onto the constraint sector :

$$\Lambda_i = \theta_i^0 \theta_i^1 \theta_i^2 \theta_i^3, \quad P_i = \frac{1}{2} + \frac{1}{2} \Lambda_i$$

Suppose $u_{ij}|\psi\rangle = +|\psi\rangle$. Then $u_{ij}\Lambda_i|\psi\rangle = -\Lambda_i|\psi\rangle$ but $[P_i, \phi_p] = 0$, so

the effect of projection $|\Psi\rangle \rightarrow \left(\prod_i P_i\right)|\Psi\rangle$ is to sum over all gauge configurations

consistent with a given flux assignment : $|\Psi_0\rangle = \sum_g R_g |\psi_0(u)\rangle \otimes |\phi(u)\rangle$
sum over gauge configurations \nearrow g \uparrow fermion WF gauge field WF
gauge transformation

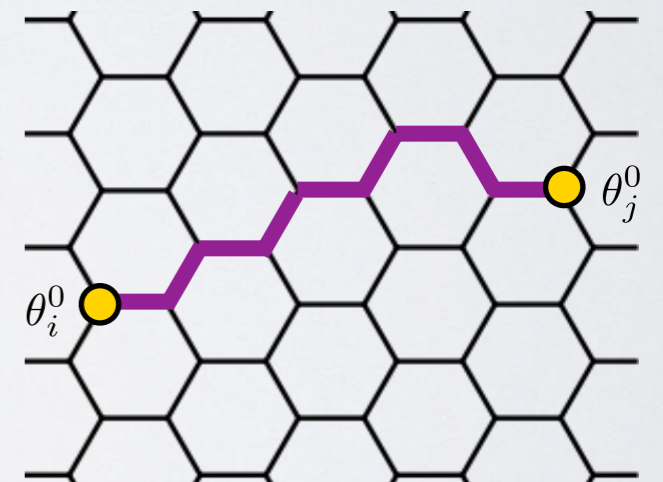
Starting from some $|\Psi_0\rangle$ we can build the Hilbert space

multiplying by products of even numbers of Majoranas θ_i^0 .

\mathcal{H} preserves (Dirac) fermion number modulo 2.

So everything works out to give :

$$2^{\frac{N}{2}+1} [\text{gauge DOF}] \times 2^{\frac{N}{2}-1} [\text{Majorana DOF}] = 2^N [\text{spin DOF}]$$



Majorana fermions in a static \mathbb{Z}_2 gauge field

Hamiltonian : $\mathcal{H} = \frac{i}{4} \sum_{i,j} A_{ij} \theta_i \theta_j$ with $A_{ij} = 2J_{ij} u_{ij}$

Problem : must find optimal gauge configuration $\{\phi_p\}$, W_H , W_V

Solution : (1) numerical search, (2) Lieb's theorem (1994)

Time-reversal $\mathcal{T} = \mathcal{R} \mathcal{K}$ $\mathcal{R} =$ charge conjugation operator $\mathcal{R}^\dagger = \mathcal{R}^{-1} = -\mathcal{R}$
 $\mathcal{K} =$ complex conjugation operator

Choosing $\{\theta^0, \theta^2\}$ real, $\{\theta^1, \theta^3\}$ imaginary, with $\mathcal{R} = i \sigma^y = \theta^2 \theta^0$, one has

$$\mathcal{T} \theta^a \mathcal{T}^{-1} = -\theta^a \quad , \quad \mathcal{T} \sigma^\mu \mathcal{T}^{-1} = -\sigma^\mu$$

Time-reversal properties of \mathbb{Z}_2 gauge fields and fluxes :

$$\mathcal{T} u_{ij} \mathcal{T}^{-1} = -u_{ij} \quad , \quad \mathcal{T} \phi_p \mathcal{T}^{-1} = (-1)^{N_p} \phi_p$$

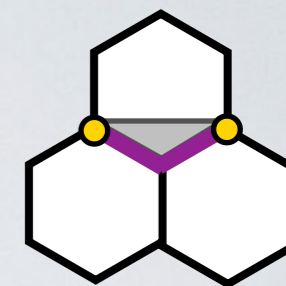
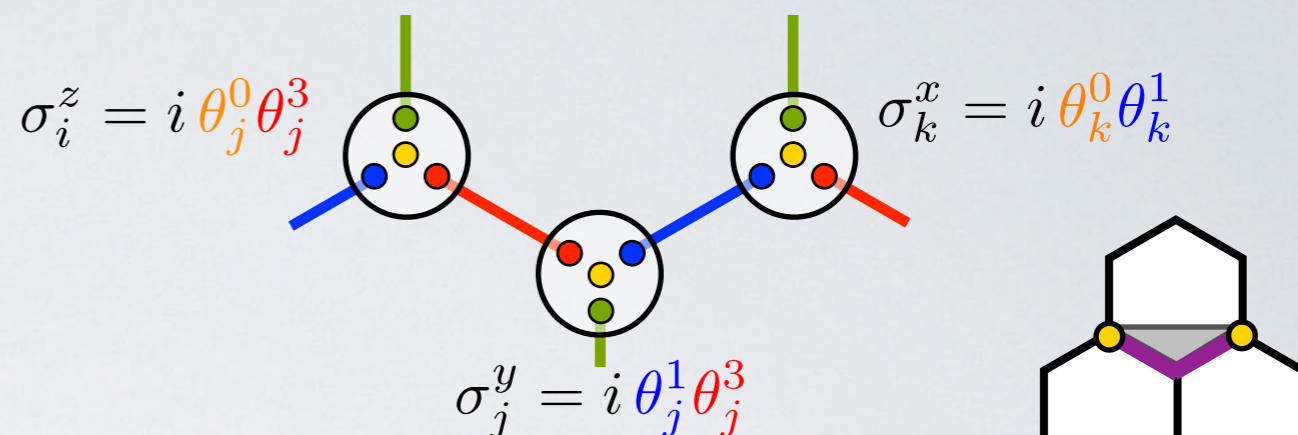
$N_p = \#$ sites on perimeter of p

even-membered rings \rightarrow flux is even under \mathcal{T}
odd-membered rings \rightarrow flux is odd under \mathcal{T}

Time-reversal broken states : two routes

1) Add explicit T breaking terms :

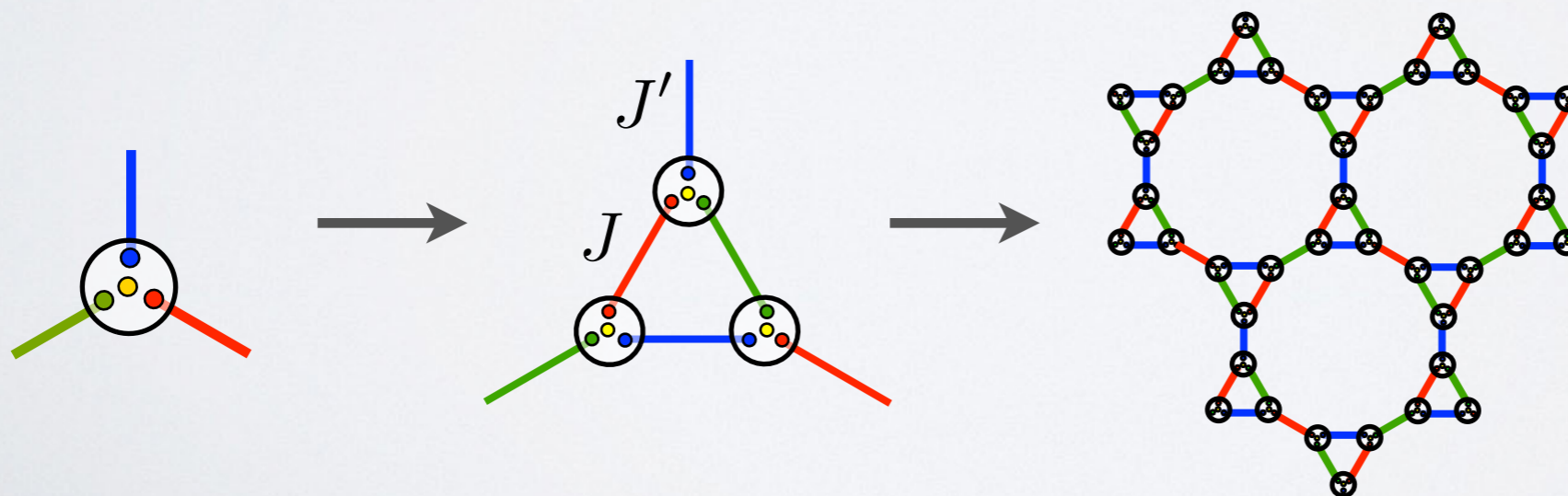
$$\sigma_i^z \sigma_j^y \sigma_k^x = i \theta_i^0 \theta_k^0 u_{ij} u_{jk}$$



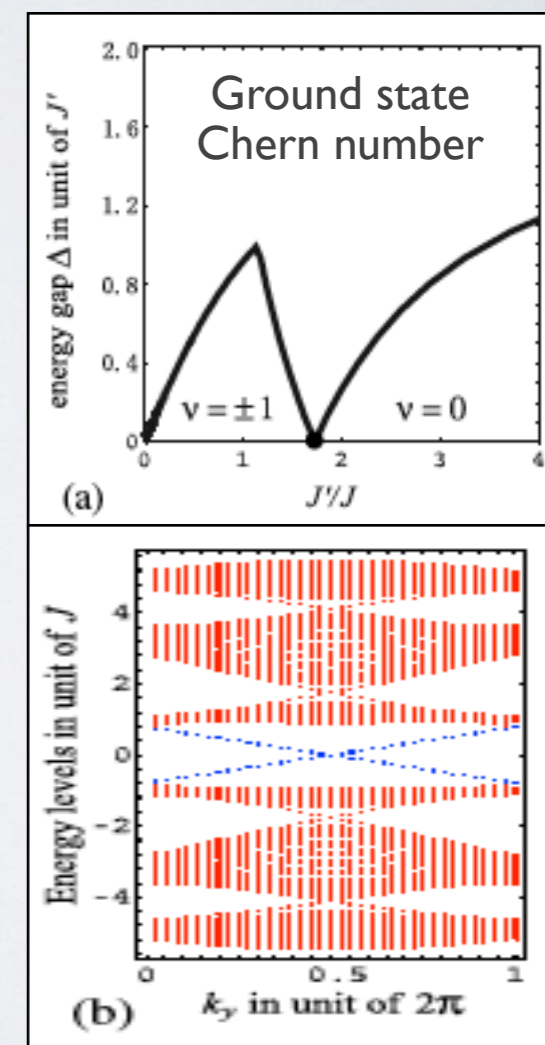
This yields next-neighbor hopping in the \mathbb{Z}_2 gauge field background.
Still noninteracting fermions! (Kitaev 2006)

2) Lattices with odd-membered loops

Spontaneous breaking of time-reversal when $\mathcal{THT}^{-1} = \mathcal{H}$

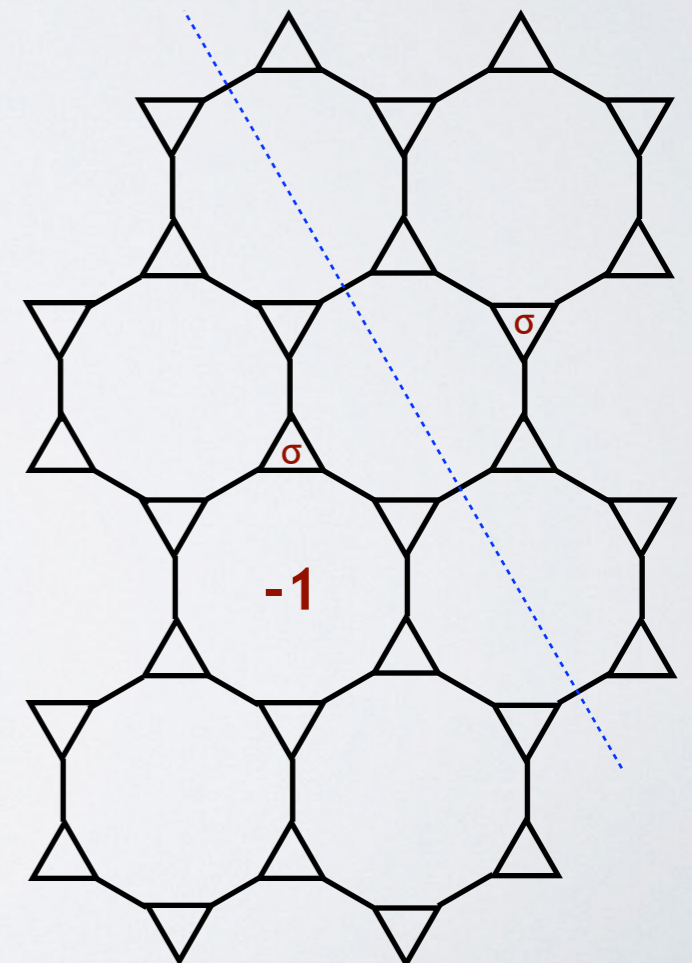
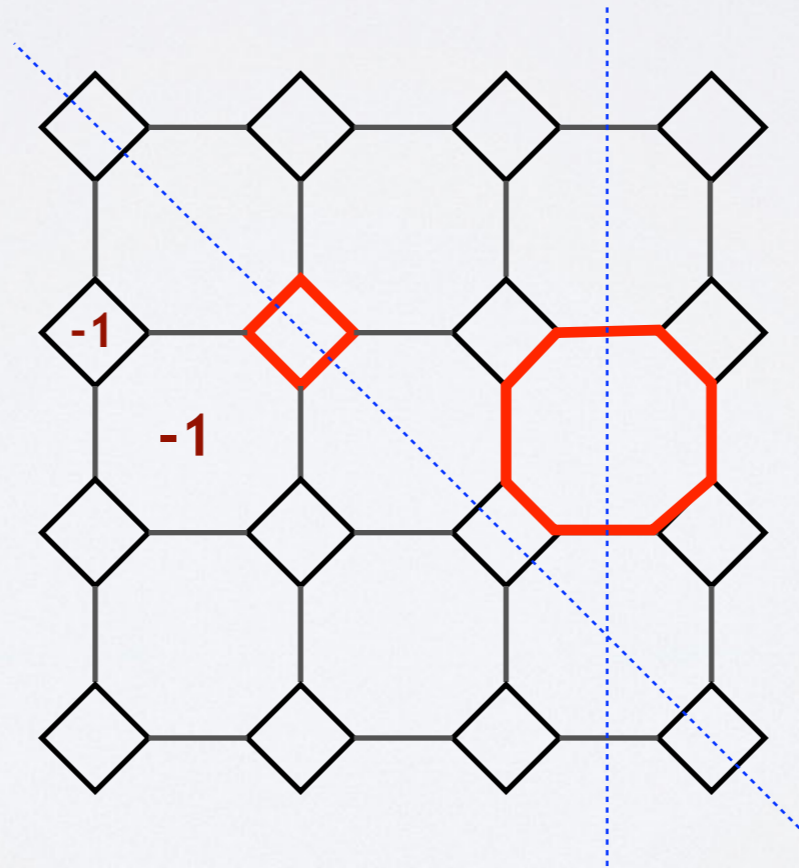
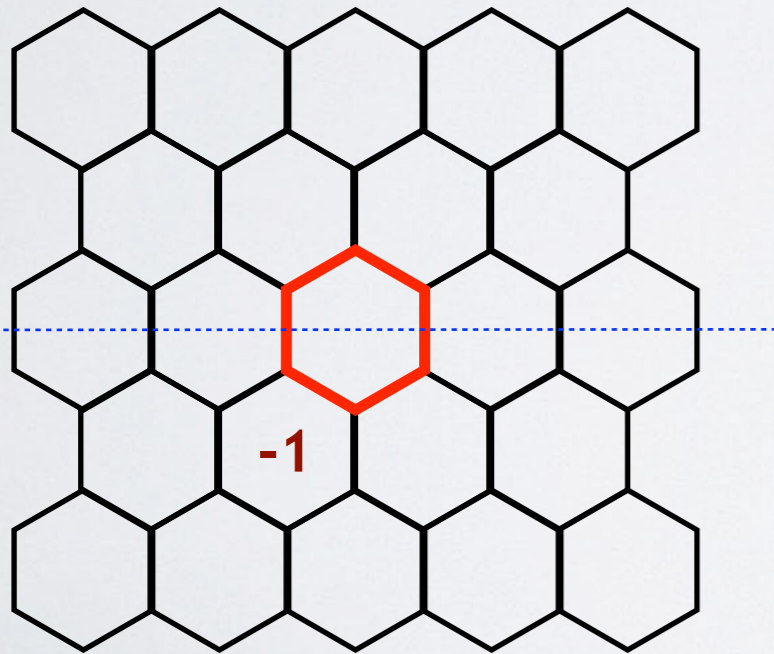


(Yao and Kivelson 2007)



Lieb's theorem (Lieb, 1994)

Consider a general single species Majorana Hamiltonian $\mathcal{H} = \frac{i}{4} A_{ij} \theta_i \theta_j$ on a lattice \mathcal{L} which has reflection planes which do not intersect any of the lattice sites. The \mathbb{Z}_2 gauge field on each link is $u_{ij} = \text{sgn}(A_{ij})$. We may assume $A = A^* = -A^t$. Then the lowest energy assignment of the plaquette fluxes is one which is reflection symmetric, and one in which each plaquette p bisected by a reflection plane has flux $\phi_p = -1$.



Diagonalization of lattice Majorana Hamiltonians

Assume a regular lattice with an even element basis :

$$\mathcal{H} = \frac{i}{4} \sum_{\mathbf{R}, \mathbf{R}'} A_{st}(\mathbf{R} - \mathbf{R}') \xi_s(\mathbf{R}) \xi_t(\mathbf{R}') = \frac{i}{4} \sum_{\mathbf{k}} A_{st}(\mathbf{k}) \xi_s(-\mathbf{k}) \xi_t(\mathbf{k})$$

where $A_{st}(\mathbf{k}) = -A_{ts}^*(\mathbf{k}) = -A_{ts}(-\mathbf{k}) = A_{st}^*(-\mathbf{k})$ and $\xi_s(\mathbf{k})^\dagger = \xi_s(-\mathbf{k})$.

The Hamiltonian may be reexpressed in terms of Dirac fermions:

$$\mathcal{H} = i \sum_{\mathbf{k}}' A_{st}(\mathbf{k}) \left(c_{\mathbf{k}s}^\dagger c_{\mathbf{k}t} - \frac{1}{2} \delta_{st} \right) + \frac{i}{4} \sum_{\mathbf{Q}} A_{st}(\mathbf{Q}) \xi_s(\mathbf{Q}) \xi_t(\mathbf{Q})$$

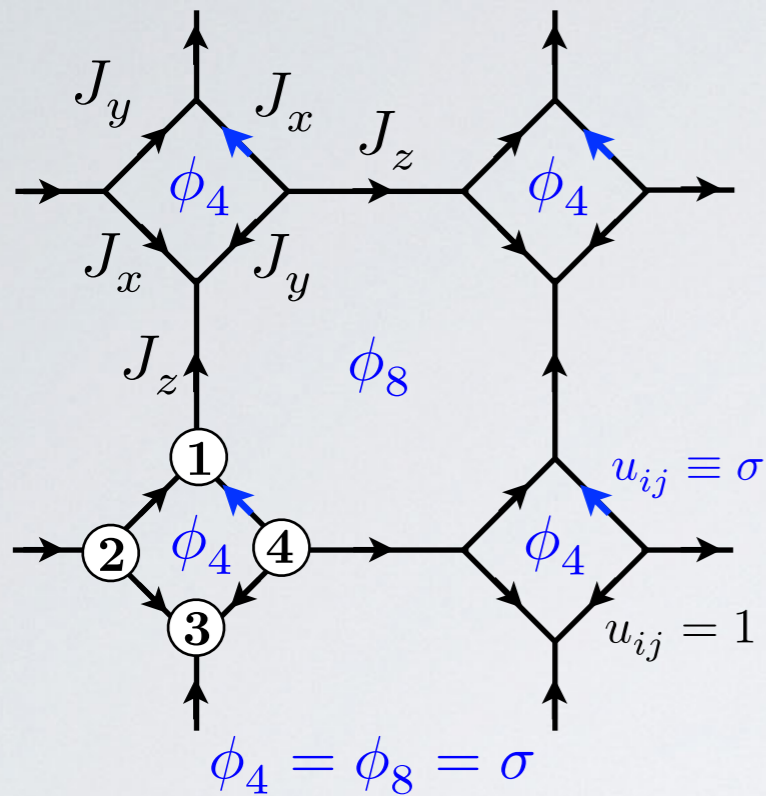
time reversal invariant momenta $\mathbf{Q} = \frac{1}{2}\mathbf{G}$

The spectrum of $iA(\mathbf{k})$ satisfies $\text{spec} \{ iA(\mathbf{k}) \} = -\text{spec} \{ iA(-\mathbf{k}) \}$

The spectrum consists of the positive eigenvalues of $iA_{st}(\mathbf{k})$ (plus half the zeros).

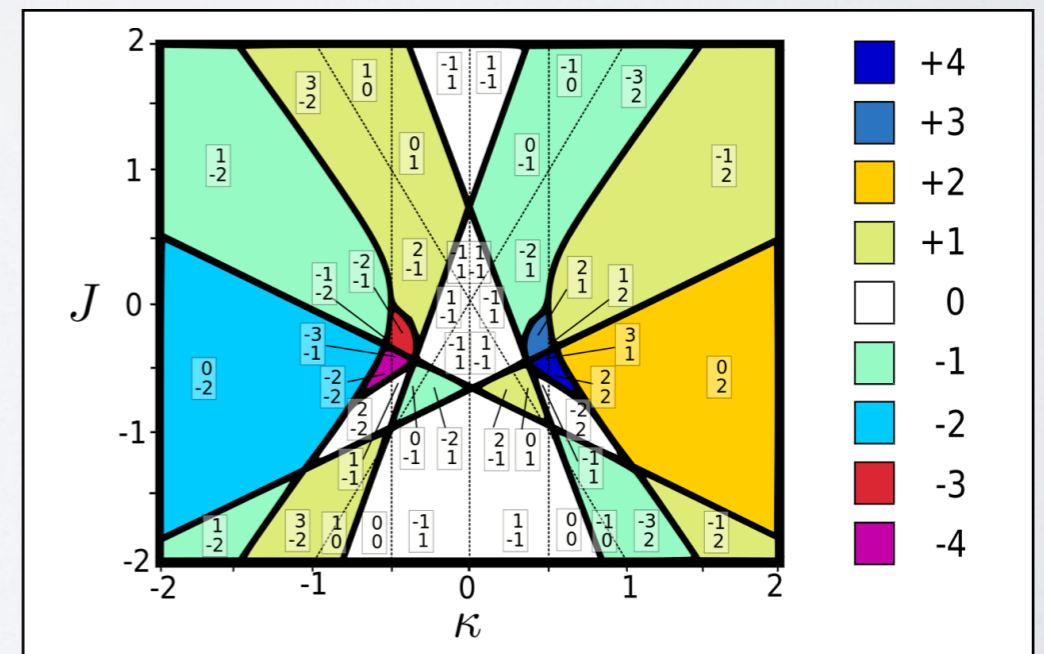
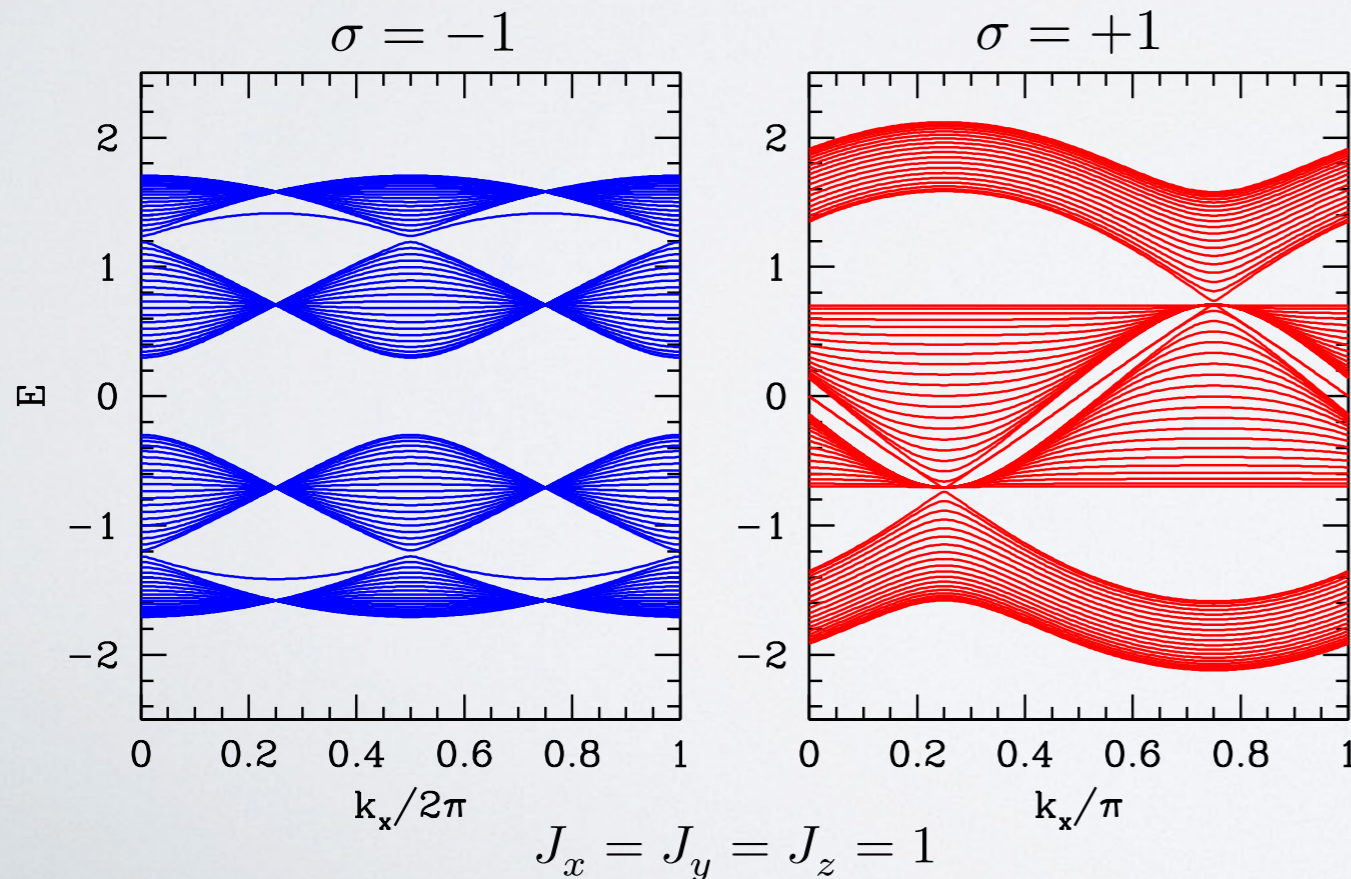
Spin-metal in the square-octagon model

Yang *et al.* 2007
 Baskaran *et al.* 2009
 Kells *et al.* 2010



Lowest energy flux configuration consistent with Lieb's theorem has $\sigma = -1$, but adding ring terms such as $\sigma_1^z \sigma_2^z \sigma_3^z \sigma_4^z = -\phi_4$ to the Hamiltonian can stabilize the phase with $\phi_4 = \phi_8 = +1$, which has a Fermi surface (Baskaran *et al.* 2009).

Adding next-nearest-neighbor $\sigma_i^x \sigma_j^y \sigma_k^z$ terms explicitly breaks T and generates new phases, some with exotic Chern numbers (Kells *et al.* 2010).



with explicit T -breaking terms $\sigma_i^x \sigma_j^y \sigma_k^z$
 (Kells *et al.* 2010)

Gamma matrices and Clifford algebras

Clifford algebra : $\{\Gamma^a, \Gamma^b\} = 2\delta^{ab}$ $a, b \in \{1, \dots, \mathcal{N}\}$

When $\mathcal{N} = 2k$, a representation of the CA can be constructed by tensor products of k Pauli matrices, viz.

$$\begin{aligned}\Gamma^1 &= \sigma^x \otimes 1 \otimes \dots \otimes 1 \otimes 1 & \Gamma^{2k-1} &= \sigma^z \otimes \sigma^z \otimes \dots \otimes \sigma^z \otimes \sigma^x \\ \Gamma^2 &= \sigma^y \otimes 1 \otimes \dots \otimes 1 \otimes 1 & \Gamma^{2k} &= \sigma^z \otimes \sigma^z \otimes \dots \otimes \sigma^z \otimes \sigma^y \\ \Gamma^3 &= \sigma^z \otimes \sigma^x \otimes \dots \otimes 1 \otimes 1 & \Gamma^{2k+1} &= \sigma^z \otimes \sigma^z \otimes \dots \otimes \sigma^z \otimes \sigma^z\end{aligned}$$

In even dimensions, define $\Gamma^{2k+1} = (-i)^k \Gamma^1 \Gamma^2 \dots \Gamma^{2k}$.

Majorana fermion representation

With $2k + 2$ Majorana fermions θ^a ($0 \leq a \leq 2k + 1$) satisfying $\{\theta^a, \theta^b\} = 2\delta^{ab}$.

Then take $\Gamma^a = i\theta^0\theta^a$ ($a = 1, \dots, 2k + 1$). The following product is fixed :

$$\theta^0 \theta^1 \dots \theta^{2k+1} = i^{k-1}$$

$k = 1$: Pauli matrices

$k = 2$: Dirac matrices

Interactions $\Gamma_i^a \Gamma_j^a = i \theta_i^0 \theta_j^0 u_{ij}$ where $u_{ij} = -i \theta_i^a \theta_j^a = \pm 1$.

$k = 1$: Pauli matrices $\Gamma^1 = \sigma^x$, $\Gamma^2 = \sigma^y$, $\Gamma^3 = -i \Gamma^1 \Gamma^2 = \sigma^z$

$k = 2$: Dirac matrices $\Gamma^5 = -\Gamma^1 \Gamma^2 \Gamma^3 \Gamma^4$

In addition to 1 and five Γ^a , ten others : $\Gamma^{ab} = \frac{i}{2} [\Gamma^a, \Gamma^b] = i \theta^a \theta^b$

These form a basis for 4x4 Hermitian matrices.

$k > 2$: The construction can be continued for $2^k \times 2^k$ Hermitian matrices :

class	number	$k = 1$	$k = 2$	$k = 3$	$k = 4$
1	1	1	1	1	1
$i \theta^0 \theta^a$	$2k + 1$	3	5	7	9
$i \theta^a \theta^b$	$\binom{2k+1}{2}$	—	10	21	36
$\theta^0 \theta^a \theta^b \theta^c$	$\binom{2k+1}{3}$	—	—	35	84
$\theta^a \theta^b \theta^c \theta^d$	$\binom{2k+1}{4}$	—	—	—	126
total	4^k	4	16	64	256
rank	2^k	2	4	8	16

The symmetry of these various classes under time-reversal must be worked out in detail and depends on conventions for the charge conjugation operator.

Complex conjugation : one can always take $\mathcal{K} \theta^a \mathcal{K} = (-1)^a \theta^a$

this is consistent with the constraint $\theta^0 \theta^1 \dots \theta^{2k+1} = i^{k-1}$

Charge conjugation : for $k = 1$ take $\mathcal{R} = i\Gamma^2$; for $k = 2$ take $\mathcal{R} = (i\Gamma^2)(i\Gamma^4)$

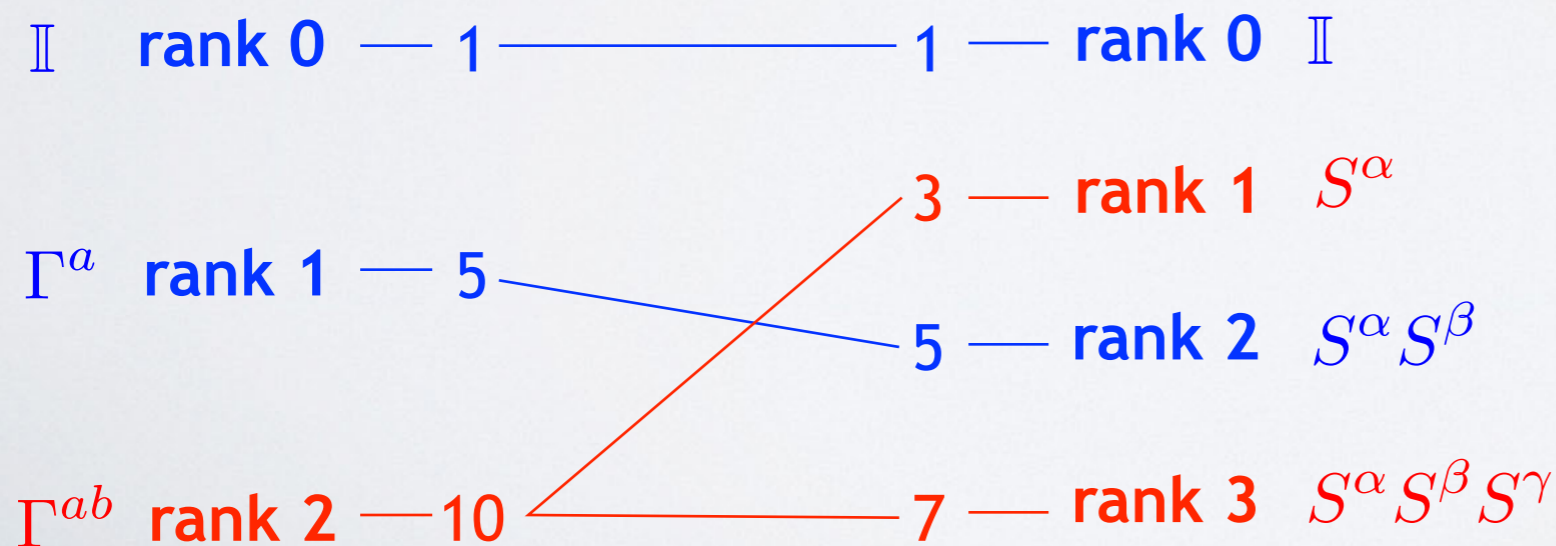
ε	Γ^1	Γ^2	Γ^3	Γ^4	Γ^5
$\varepsilon_{\mathcal{K}}$	E	O	E	O	E
$\varepsilon_{\mathcal{R}}$	O	E	O	E	O
$\varepsilon_{\mathcal{T}}$	O	O	O	O	O

$k = 2$	1	$i\theta^0\theta^a$	$i\theta^a\theta^b$
matrices	\mathbb{I}	Γ^a	Γ^{ab}
multiplicity	1	5	10
$\varepsilon_{\mathcal{T}}$	E	E	O

Correspondence to $S = \frac{3}{2}$ spin tensor algebra for $k = 2$:

Murakami et al. 2004
Yao et al. 2009
Chua et al. 2011

$$16 = 1 + 3 + 5 + 7$$



$$\Gamma^1 = \frac{1}{\sqrt{3}} \{S^y, S^z\}$$

$$\Gamma^2 = \frac{1}{\sqrt{3}} \{S^z, S^x\}$$

$$\Gamma^3 = \frac{1}{\sqrt{3}} \{S^x, S^y\}$$

$$\Gamma^4 = \frac{1}{\sqrt{3}} (S^x S^x - S^y S^y)$$

$$\Gamma^5 = S^z S^z - \frac{5}{4}$$

Models with $k=2$

Wu et al. 2009

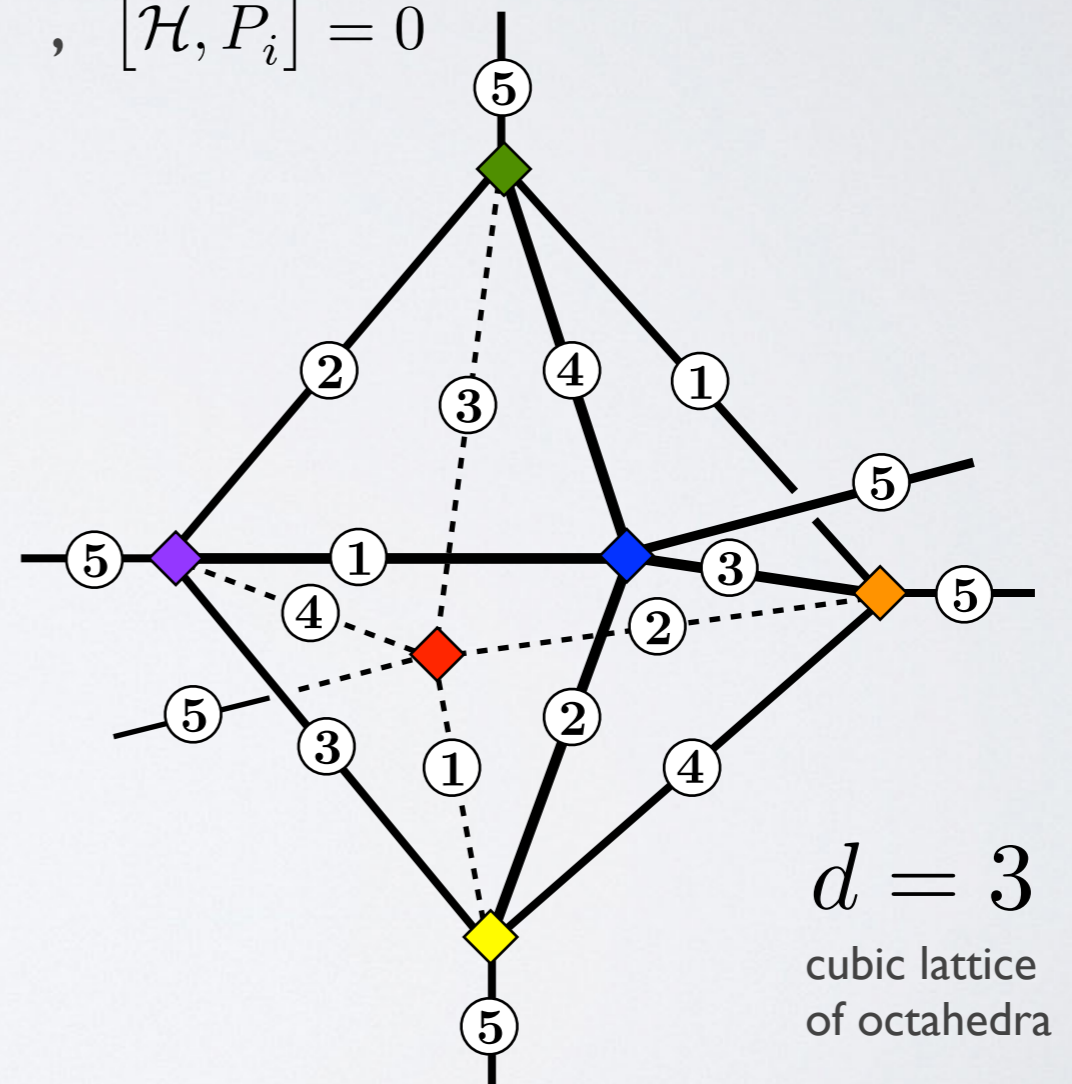
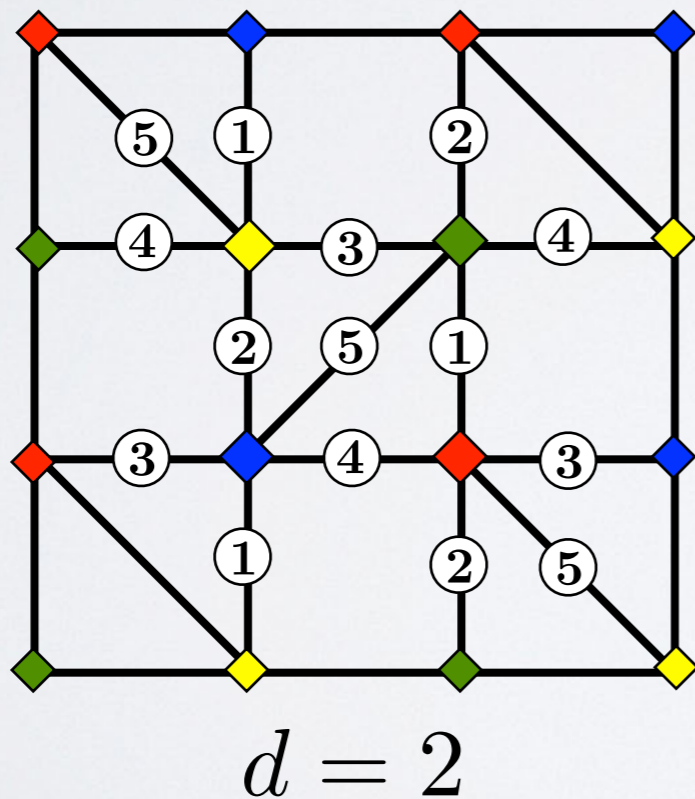
Yao et al. 2009

Consistent with “magic stick rule” we look for a 5-fold coordinated lattice and impose the Hamiltonian

$$\mathcal{H} = \sum_{a=1}^5 J_a \sum_{\langle ij \rangle_{a\text{-type}}} \Gamma_i^a \Gamma_j^a = \sum_{\langle ij \rangle} J_{ij} i\theta_i^0 \theta_j^0 u_{ij}$$

Local projector : $P_i = \frac{1}{2} (1 - i\theta_i^0 \theta_i^1 \theta_i^2 \theta_i^3 \theta_i^4 \theta_i^5)$, $[\mathcal{H}, P_i] = 0$

Examples of viable lattices :



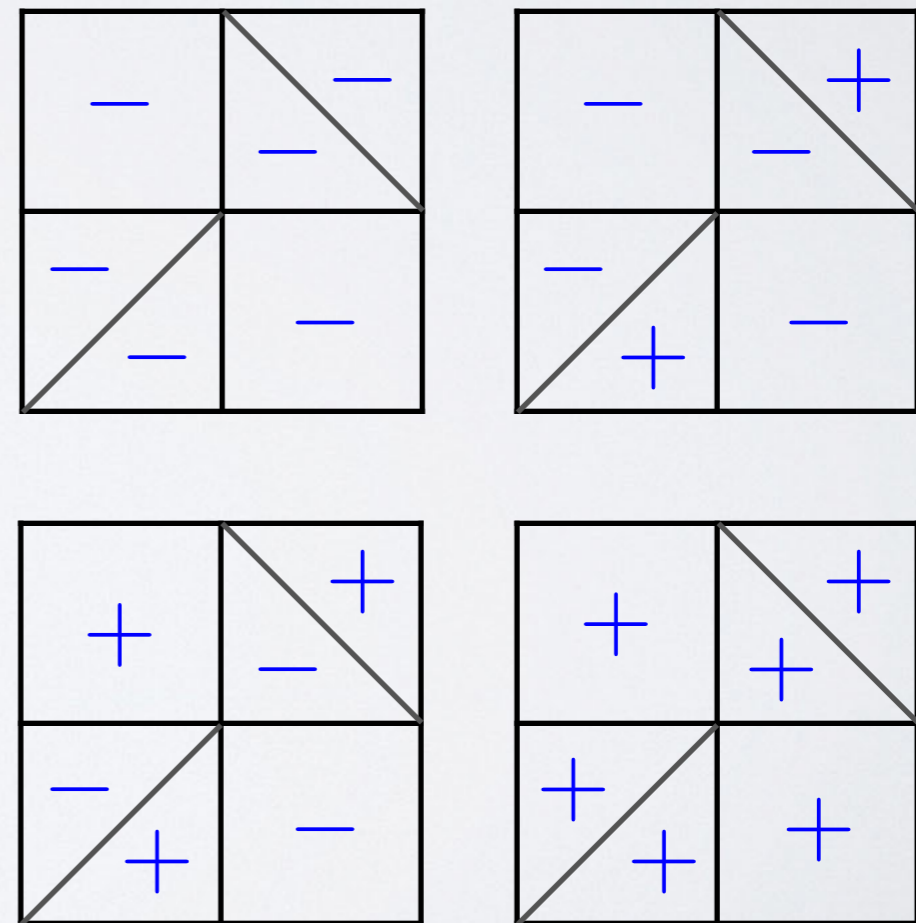
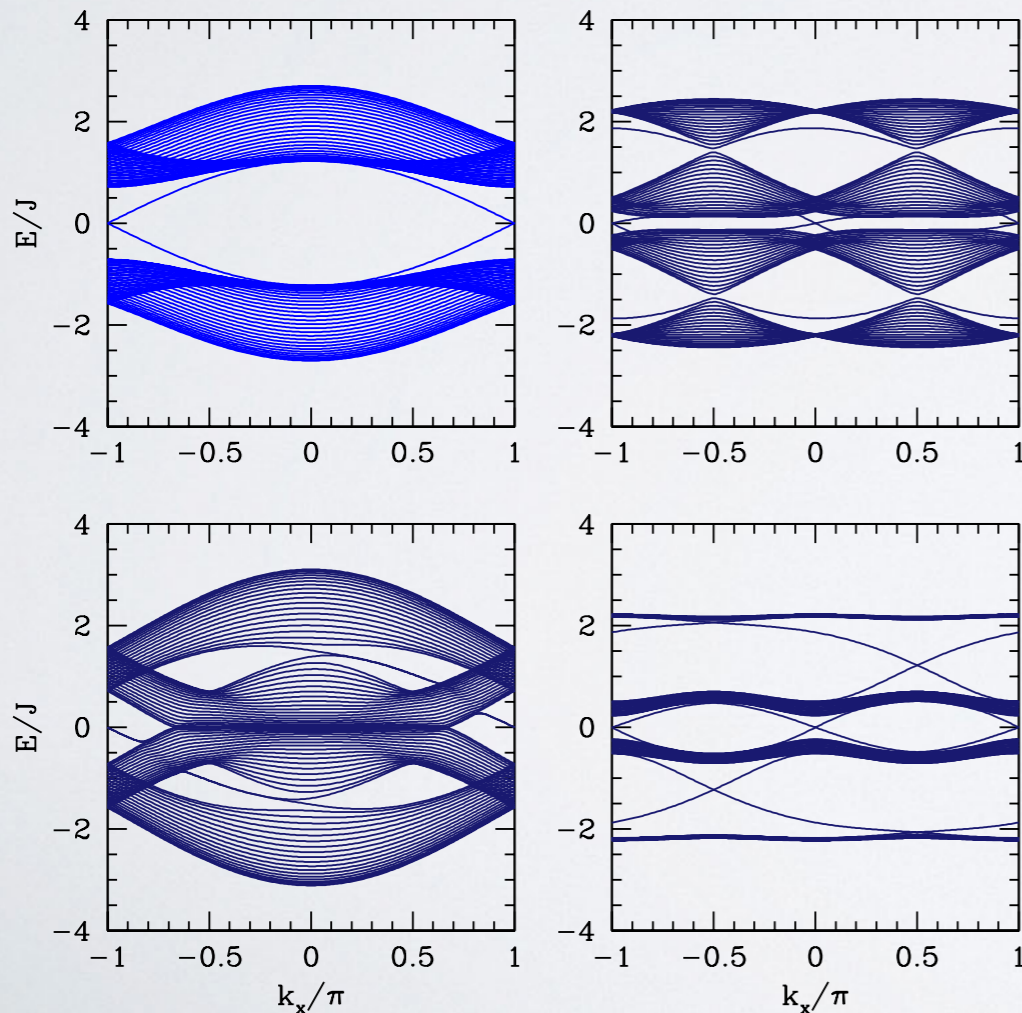
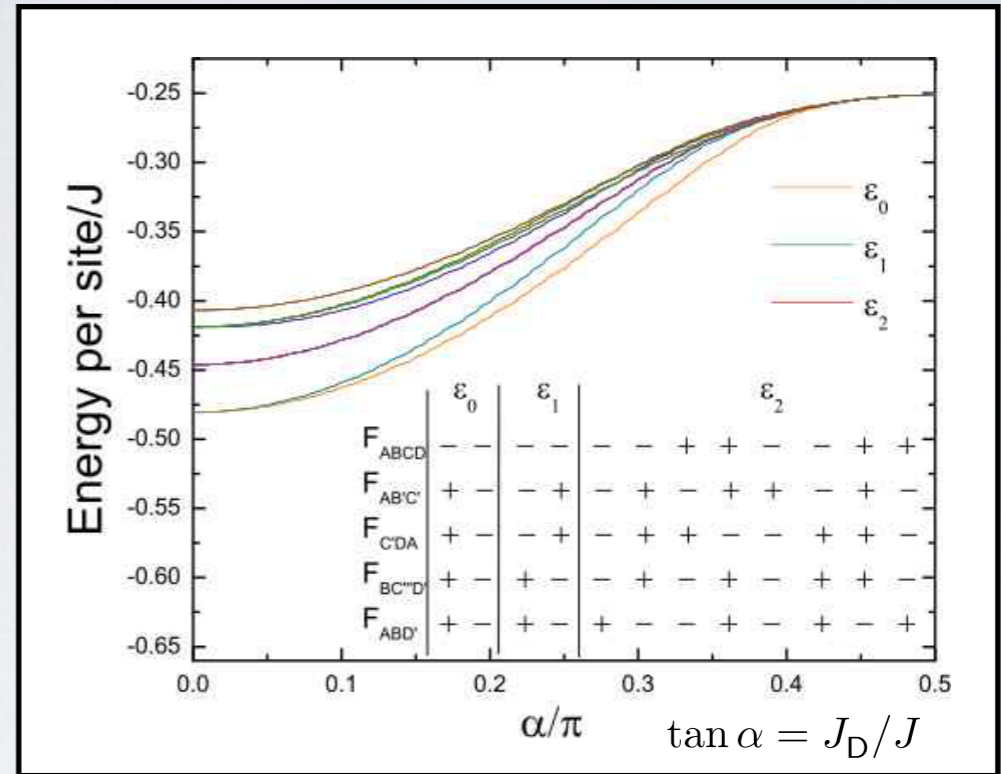
Both contain triangular plaquettes and will have T -breaking ground states.

For the decorated square lattice model, the lowest energy flux configuration is that in which all square plaquettes have $\phi_{\square} = -1$ and all triangle fluxes are the same, with $\phi_{\Delta} = \pm 1$.

Circuit composition rule for \mathbb{Z}_2 flux :

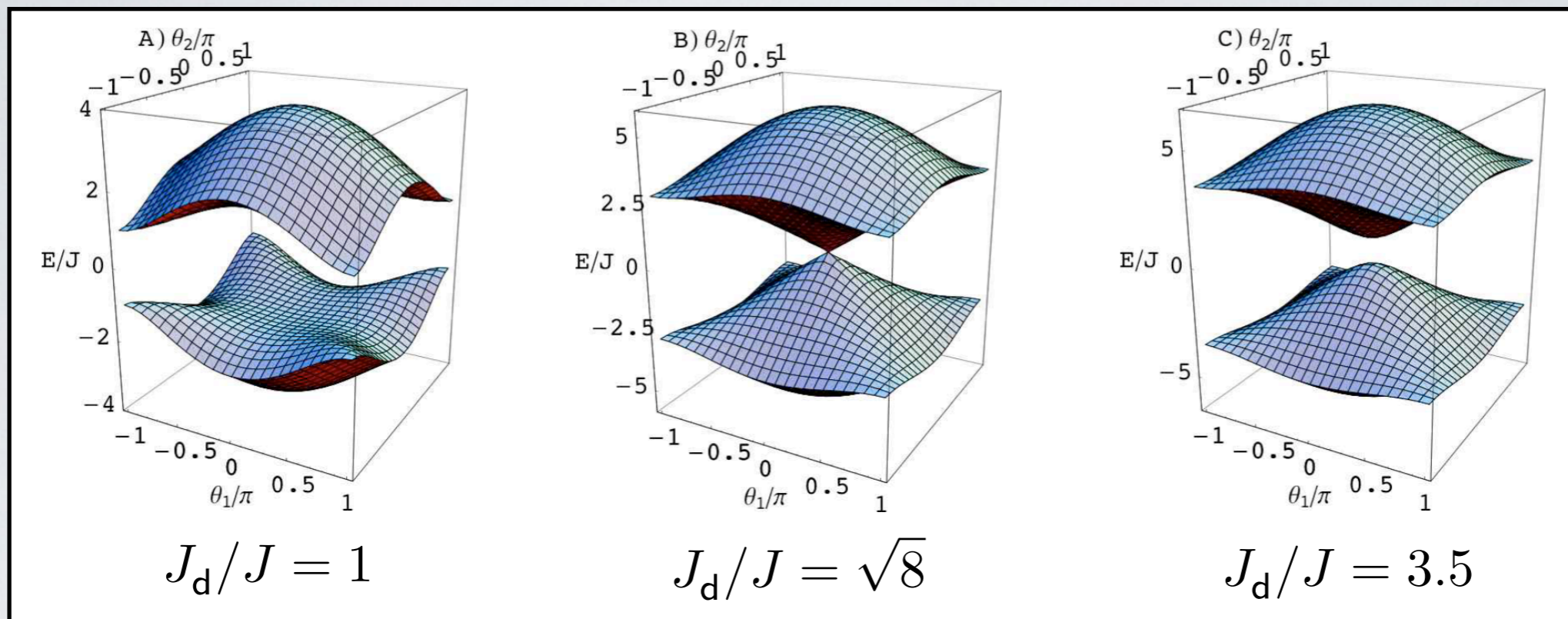
$$\phi_{cc'} = (-1)^{N(c,c')} \phi_c \phi_{c'}$$

↑
of common links



$$J_x = J_y = J_d = 1$$

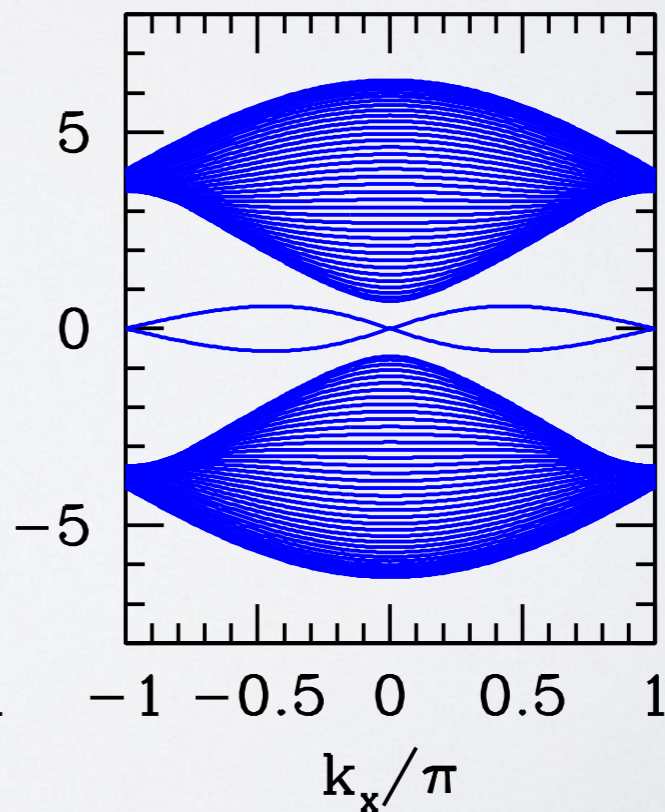
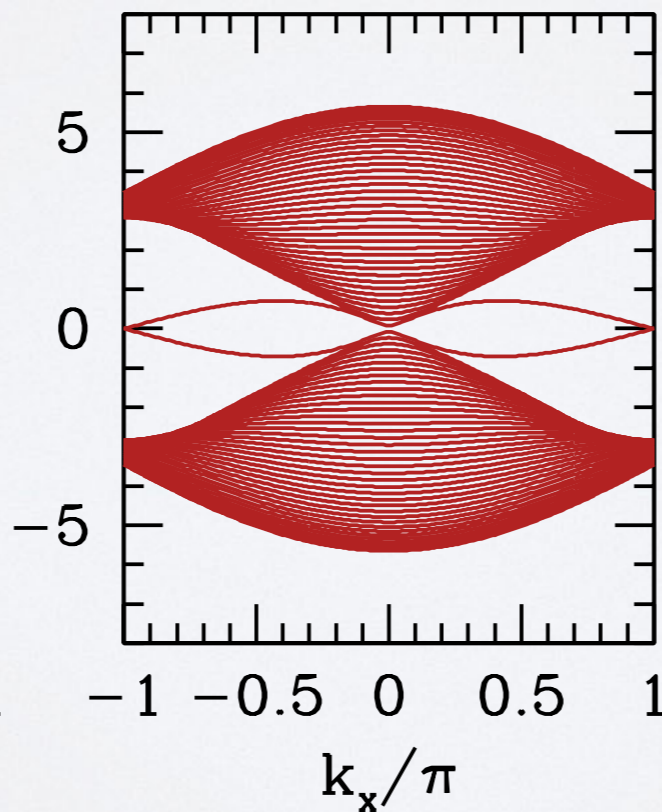
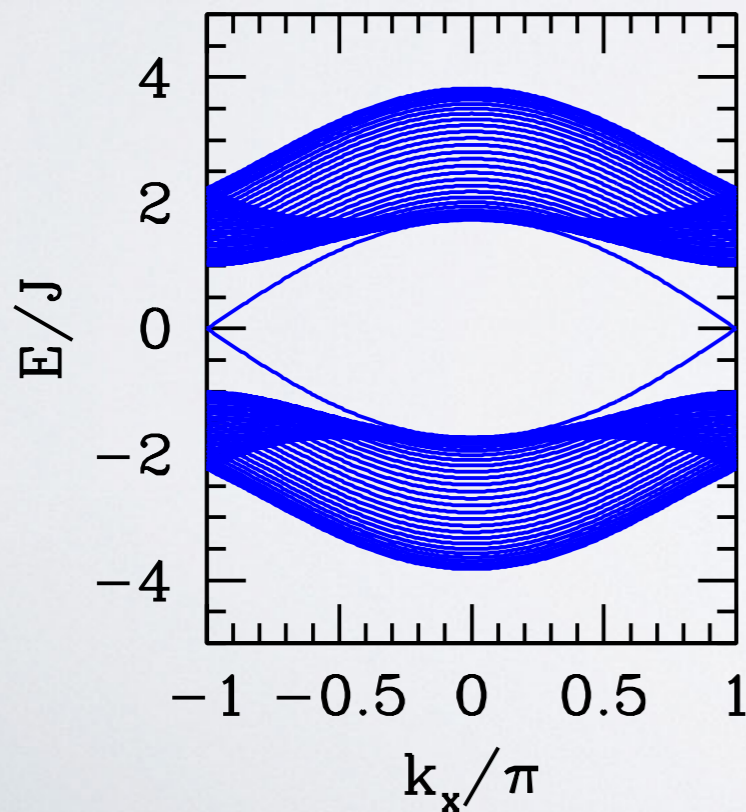
ground state : bulk energy bands



Chern number = ± 1
topologically nontrivial

edge state structure

Chern number = 0
topologically trivial



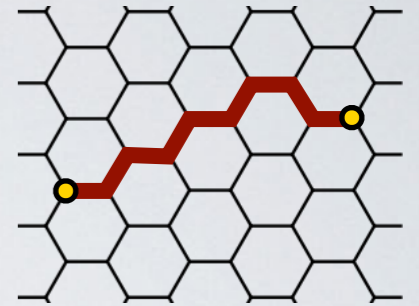
Spin correlations

The ground state, when properly projected onto the constraint subspace, is a sum over all gauge configurations consistent with a given flux pattern: $|\Psi_G[\phi]\rangle = P |\Psi[\mathbf{u}]\rangle$

Only gauge-invariant objects can have an expectation value. Thus,

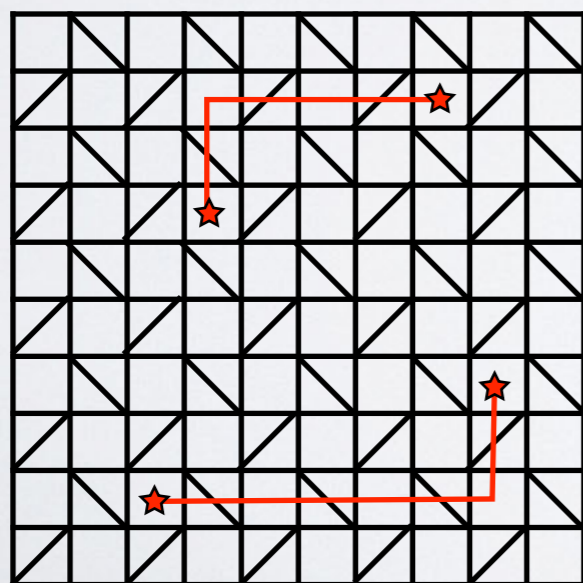
$$\langle \Psi_G | \Gamma_i^a \Gamma_m^a | \Psi_G \rangle = 0 \quad \text{if} \quad J_{im} = 0$$

$$\langle \Psi_G | \Gamma_i^a \Gamma_j^{ab} \Gamma_k^{bc} \cdots \Gamma_l^{da} \Gamma_m^a | \Psi_G \rangle \neq 0 \quad \text{if} \quad J_{ij} J_{jk} \cdots J_{lm} \neq 0$$

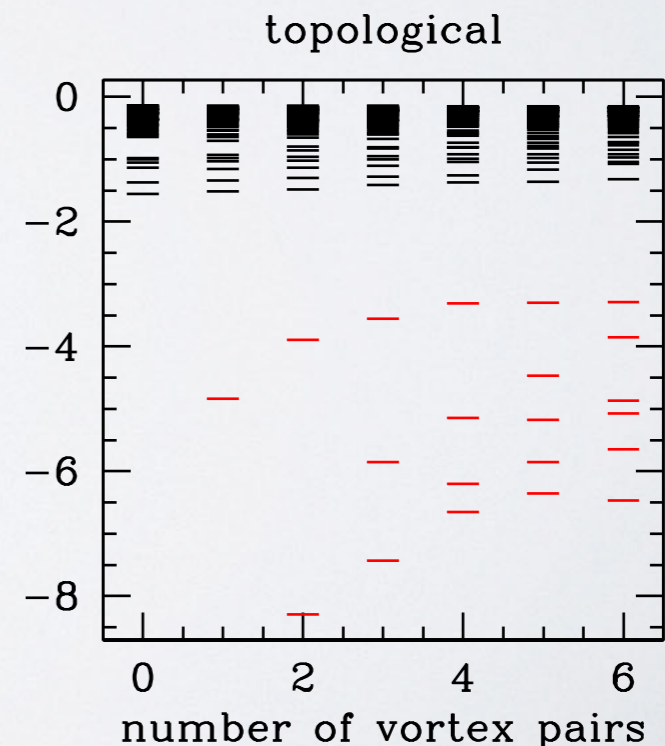
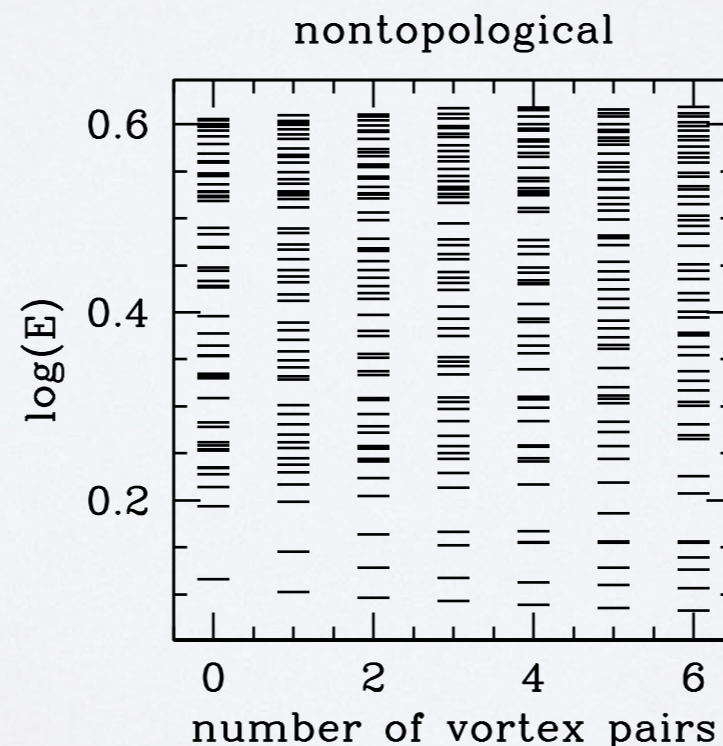


Nonabelions for $J_d < \sqrt{8} J$

Kitaev showed how each \mathbb{Z}_2 vortex binds an odd number of Majorana zero modes in a phase where the Chern number is odd. Yao and Kivelson (2007) observed a degeneracy 2^{n+1} for n well-separated vortices. We find (at fixed $W_{H/V}$) n Dirac zero modes for $2n$ vortices.



\mathbb{Z}_2 vortices and gauge strings



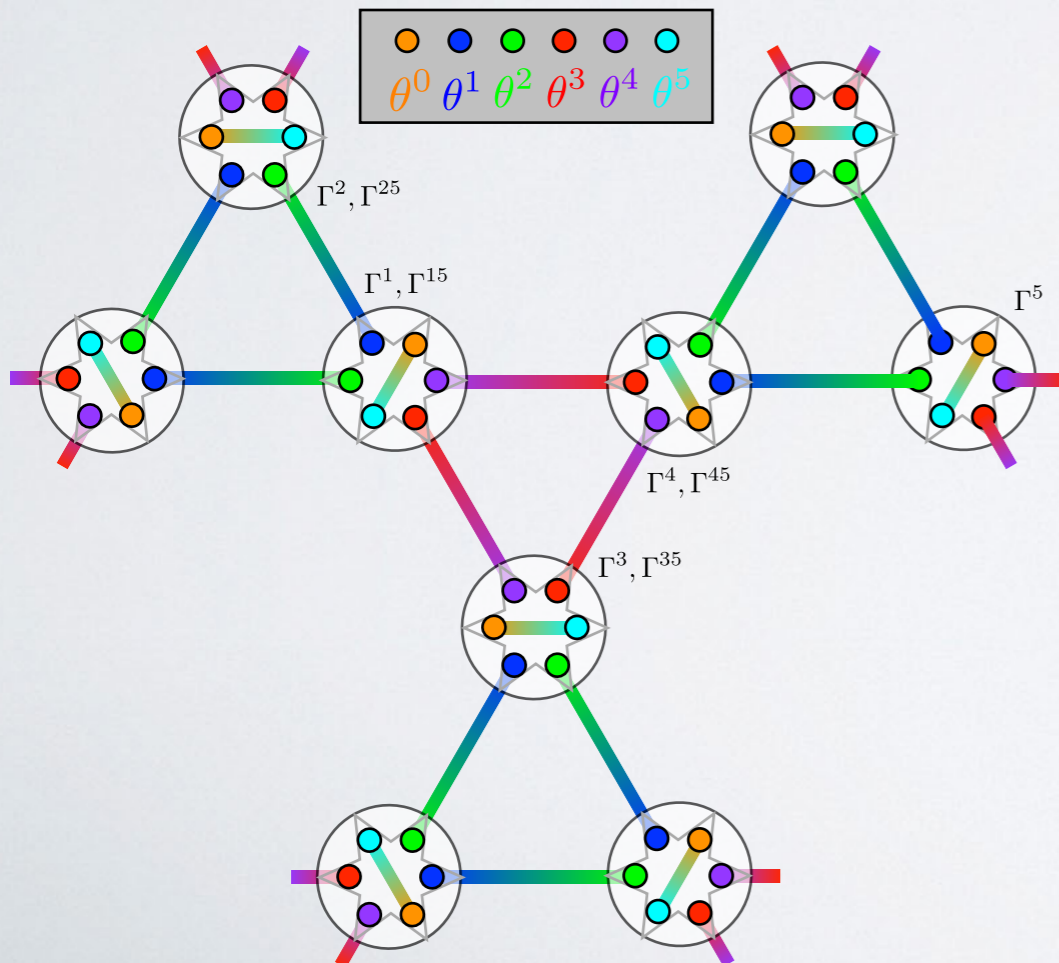
Kagome chiral spin liquid

(Chua, Yao, and Fiete, 2009)

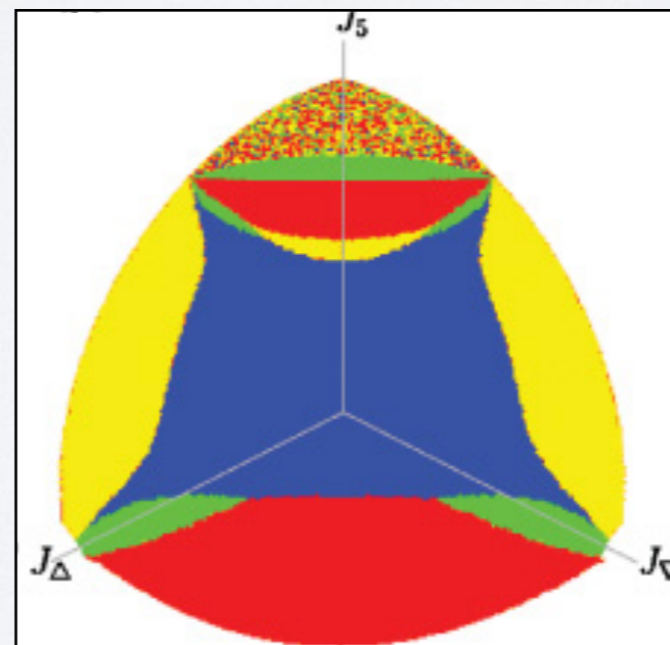
Building on the work of Yao, Zhang, and Kivelson, considered the following model :

$$\begin{aligned} \mathcal{H} &= J_{\Delta} \sum_{\langle ij \rangle \in \Delta} \Gamma_i^1 \Gamma_j^2 + J_{\nabla} \sum_{\langle ij \rangle \in \nabla} \Gamma_i^3 \Gamma_j^4 + J'_{\Delta} \sum_{\langle ij \rangle \in \Delta} \Gamma_i^{15} \Gamma_j^{25} + J'_{\nabla} \sum_{\langle ij \rangle \in \nabla} \Gamma_i^{35} \Gamma_j^{45} + J_5 \sum_i \Gamma_i^5 \\ &= i \sum_{\langle ij \rangle \in \Delta} (J_{\Delta} \theta_i^0 \theta_j^0 + J'_{\Delta} \theta_i^5 \theta_j^5) u_{ij} + i \sum_{\langle ij \rangle \in \nabla} (J_{\nabla} \theta_i^0 \theta_j^0 + J'_{\nabla} \theta_i^5 \theta_j^5) u_{ij} + i J_5 \sum_i \theta_i^0 \theta_i^5 \end{aligned}$$

where $u_{ij} = -i \theta_i^1 \theta_j^2$ (Δ) or $u_{ij} = -i \theta_i^3 \theta_j^4$ (∇). This model has at least two interesting phases : (i) a gapped chiral spin liquid ($C = \pm 2$) with abelian vortices, and (ii) a gapless spin liquid with a stable spin Fermi surface (possibly stabilized by additional flux energy terms cf. Baskaran et al. 2007).

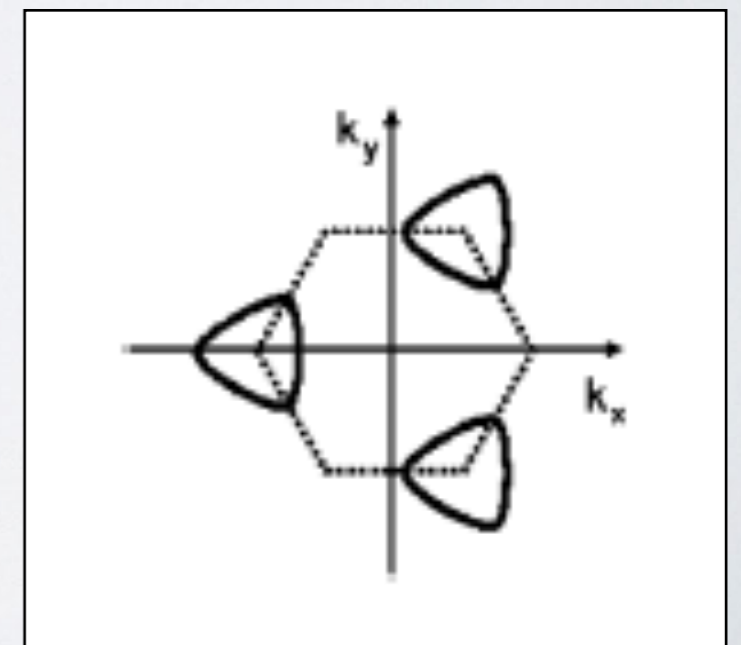


phase diagram



$$J_{\Delta} = J'_{\Delta} , J_{\nabla} = J'_{\nabla}$$

Fermi surface



$$(J_{\Delta}, J_{\nabla}, J'_{\Delta}, J'_{\nabla}, J_5) = (1.0, 0.3, 0.8, 0.5, 1.4)$$

Diamond lattice model

diamond = two interpenetrating FCC lattices , $z = 4$

Our model : $k=2$ (4x4 Γ matrices). Start with

$$\mathcal{H}_0 = \sum_{\mathbf{R}} \sum_{a=1}^4 J_a \Gamma_{\mathbf{R}}^a \tilde{\Gamma}_{\mathbf{R}+\hat{e}_a}^a$$

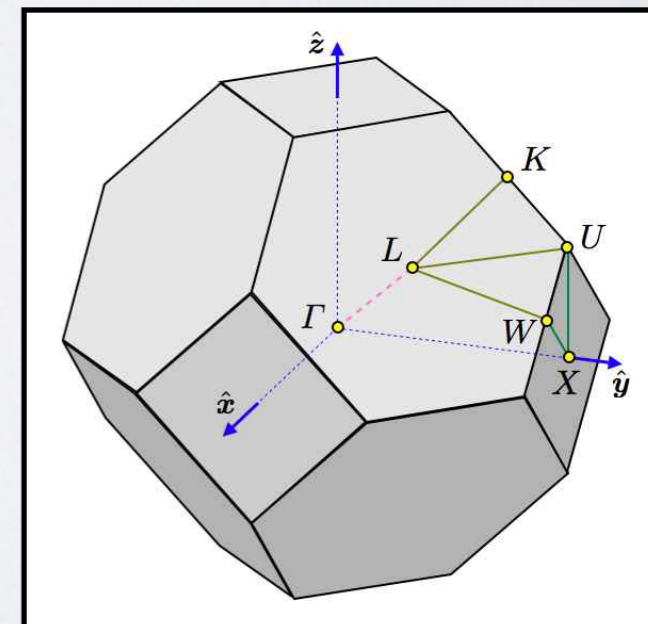
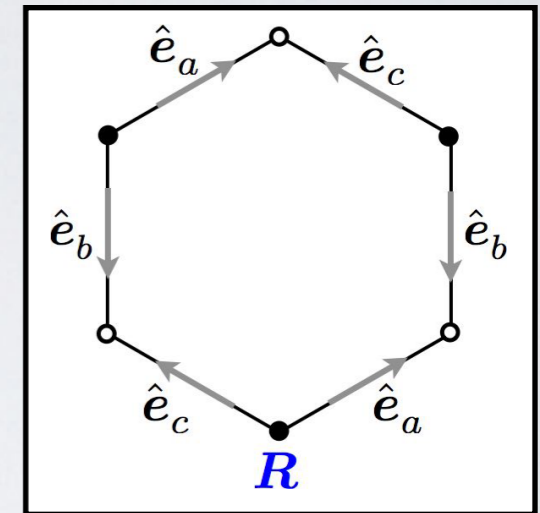
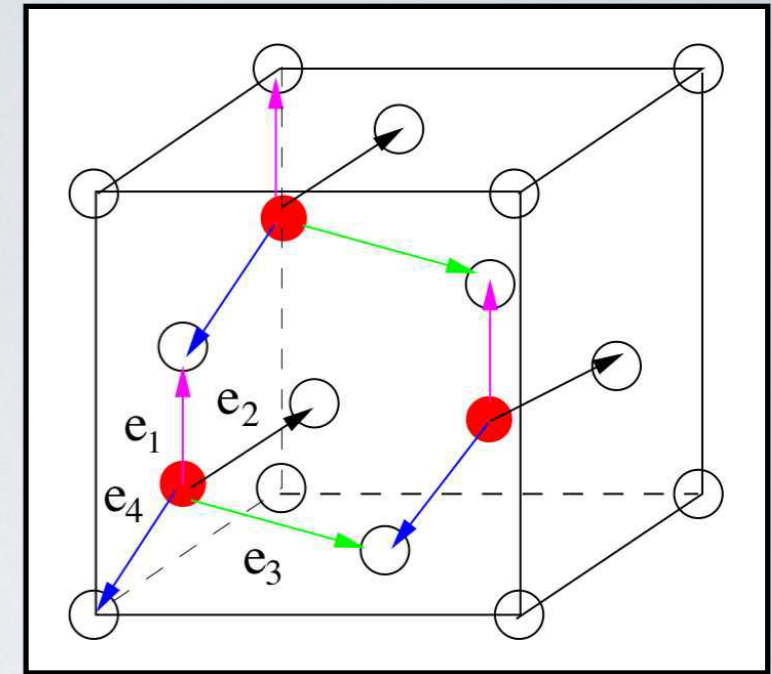
and add

$$\mathcal{H}_1 = \sum_{\mathbf{R}} \sum_{a<b}^4 (h_{ab} V_{\mathbf{R}}^{ab} + \tilde{h}_{ab} \tilde{V}_{\mathbf{R}}^{ab})$$

where

$$V_{\mathbf{R}}^{ab} = \Gamma_{\mathbf{R}}^a \tilde{\Gamma}_{\mathbf{R}+\hat{e}_a}^{ab} \Gamma_{\mathbf{R}+\hat{e}_a-\hat{e}_b}^b, \quad \tilde{V}_{\mathbf{R}}^{ab} = \tilde{\Gamma}_{\mathbf{R}+\hat{e}_a}^a \Gamma_{\mathbf{R}}^{ab} \tilde{\Gamma}_{\mathbf{R}+\hat{e}_b}^b$$

This Hamiltonian exhibits deformed Dirac cones at the three inequivalent X points on the Brillouin zone square faces. The spectrum is linear in two directions and quadratic in the third.



So far we've only used $\theta^{0,1,2,3,4}$. We now add in corresponding terms where

$\Gamma^a = i\theta^0\theta^a$ ($a = 1, 2, 3, 4$) is replaced by $\Gamma^{5a} = i\theta^5\theta^a$ ($a = 1, 2, 3, 4$). Then

$$H(\mathbf{k}) = \begin{pmatrix} \omega(\mathbf{k}) & 0 & \Delta(\mathbf{k}) & 0 \\ 0 & -\omega(\mathbf{k}) & 0 & -\Delta(\mathbf{k}) \\ \Delta^*(\mathbf{k}) & 0 & -\omega(\mathbf{k}) & 0 \\ 0 & -\Delta^*(\mathbf{k}) & 0 & \omega(\mathbf{k}) \end{pmatrix} \begin{array}{l} \leftarrow \theta_A^0 \\ \leftarrow \theta_A^5 \\ \leftarrow \theta_B^0 \\ \leftarrow \theta_B^5 \end{array}$$

$$= \omega(\mathbf{k})\gamma^4 - \text{Re } \Delta(\mathbf{k})\gamma^{14} + \text{Im } \Delta(\mathbf{k})\gamma^{45}$$

where $\omega(\mathbf{k}) = \sum_{a<b}^4 h_{ab} \sin(\psi_a - \psi_b)$ and $\Delta(\mathbf{k}) = i \sum_a^4 J_a e^{i\psi_a}$ with $\psi_a \equiv \mathbf{k} \cdot \mathbf{b}_a$ ($\psi_4 \equiv 0$). primitive RLVs
↓

Here γ^{ab} are a gamma-matrix basis for 4x4 Hermitian - not spin operators!

Defining a pseudo-time reversal operator $\mathcal{T} = i\gamma^{24}\mathcal{K}$ and parity $\mathcal{P} = \gamma^{45}\mathcal{K}$, we consider the most general model which is symmetric under both. This allows for the addition of a hybridization term,

$$\mathcal{H}_{\text{hyb}} = m \sum_{\mathbf{R}} (\Gamma_{\mathbf{R}}^5 + \tilde{\Gamma}_{\mathbf{R}+\hat{e}_4}^5) + \sum_{\mathbf{R}} \left(g_{ab} \Gamma_{\mathbf{R}}^a \tilde{\Gamma}_{\mathbf{R}+\hat{e}_a}^{ab} \Gamma_{\mathbf{R}+\hat{e}_1-\hat{e}_b}^{5b} + \tilde{g}_{ab} \tilde{\Gamma}_{\mathbf{R}+\hat{e}_a}^a \Gamma_{\mathbf{R}}^{ab} \tilde{\Gamma}_{\mathbf{R}+\hat{e}_b}^{5b} \right)$$

This preserves the essential 'solvability' of the model in terms of its representation as two Majorana species (0 and 5) hopping in a static \mathbb{Z}_2 gauge background.

The Hamiltonian then becomes

$$\begin{aligned}
 H(\mathbf{k}) &= \begin{pmatrix} \omega(\mathbf{k}) & \beta(\mathbf{k}) & \Delta(\mathbf{k}) & 0 \\ \beta^*(\mathbf{k}) & -\omega(\mathbf{k}) & 0 & -\Delta(\mathbf{k}) \\ \Delta^*(\mathbf{k}) & 0 & -\omega(\mathbf{k}) & \beta(\mathbf{k}) \\ 0 & -\Delta^*(\mathbf{k}) & \beta^*(\mathbf{k}) & \omega(\mathbf{k}) \end{pmatrix} \\
 &= \omega(\mathbf{k}) \gamma^4 - \text{Re } \Delta(\mathbf{k}) \gamma^{14} + \text{Im } \Delta(\mathbf{k}) \gamma^{45} \\
 &\quad + \text{Re } \beta(\mathbf{k}) \gamma^{34} + \text{Im } \beta(\mathbf{k}) \gamma^{24}
 \end{aligned}$$

where $\beta(\mathbf{k}) = im + i \sum_{a<b}^4 g_{ab} e^{i(\psi_a - \psi_b)}$. Pseudo-time reversal symmetry $\Rightarrow \text{Im } \beta(\mathbf{k}) = 0$: $m = 0$
 $g = -g^T$

We can set $\text{Im } \omega(\mathbf{k}) = 0$. Now let $J_4 \neq J_{123} \equiv J$, following Fu, Kane, and Mele (2007). Then the Dirac nodes at the X points acquire a mass gap proportional to $|J_4 - J|$. The system is then topologically nontrivial when $J_4 > J$, and there are an odd number of surface Dirac cones.

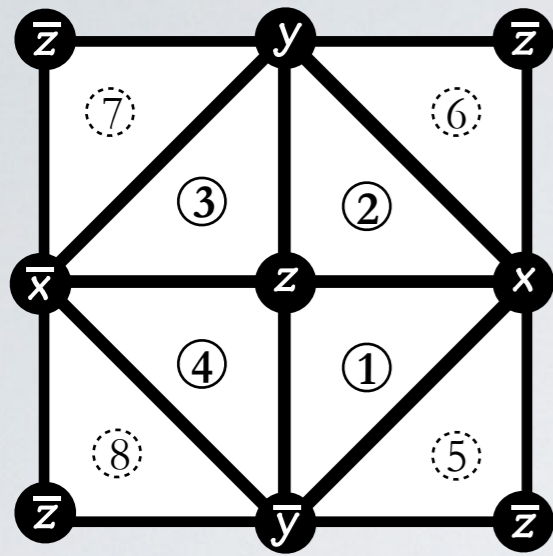
γ	class	\mathcal{T}	\mathcal{P}	\mathcal{PT}	γ	class	\mathcal{T}	\mathcal{P}	\mathcal{PT}
\mathbb{I}	-	+	+	+	γ^{14}	-	-	-	+
γ^1	+	-	+	-	γ^{15}	-	+	-	-
γ^2	-	-	+	-	γ^{23}	-	-	+	-
γ^3	+	-	+	-	γ^{24}	+	-	-	+
γ^4	-	-	-	+	γ^{25}	+	+	-	-
γ^5	-	+	-	-	γ^{34}	-	-	-	+
γ^{12}	-	-	+	-	γ^{35}	-	+	-	-
γ^{13}	+	-	+	-	γ^{45}	+	+	+	+

Table 1: Symmetry properties of the γ -matrices.

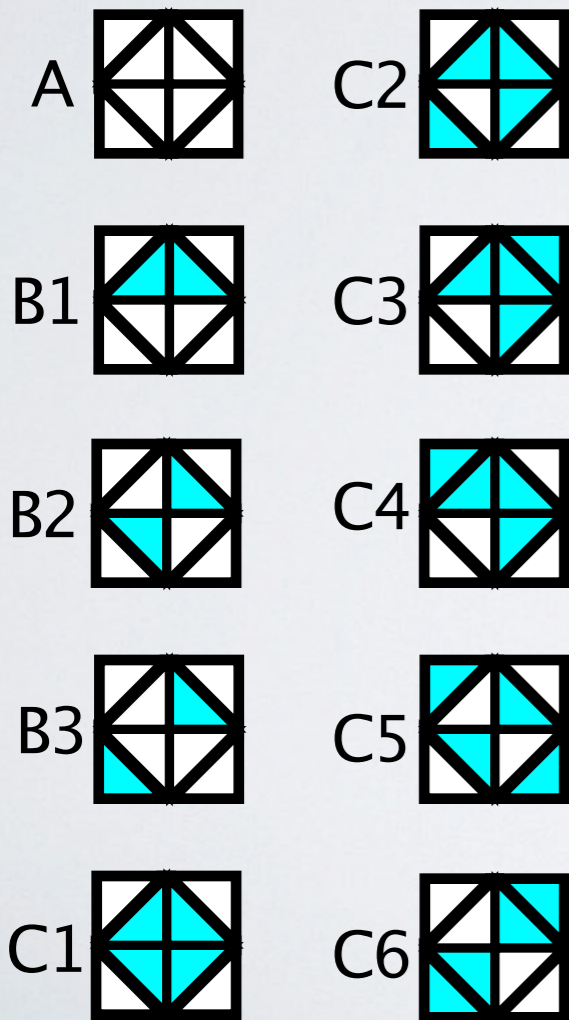
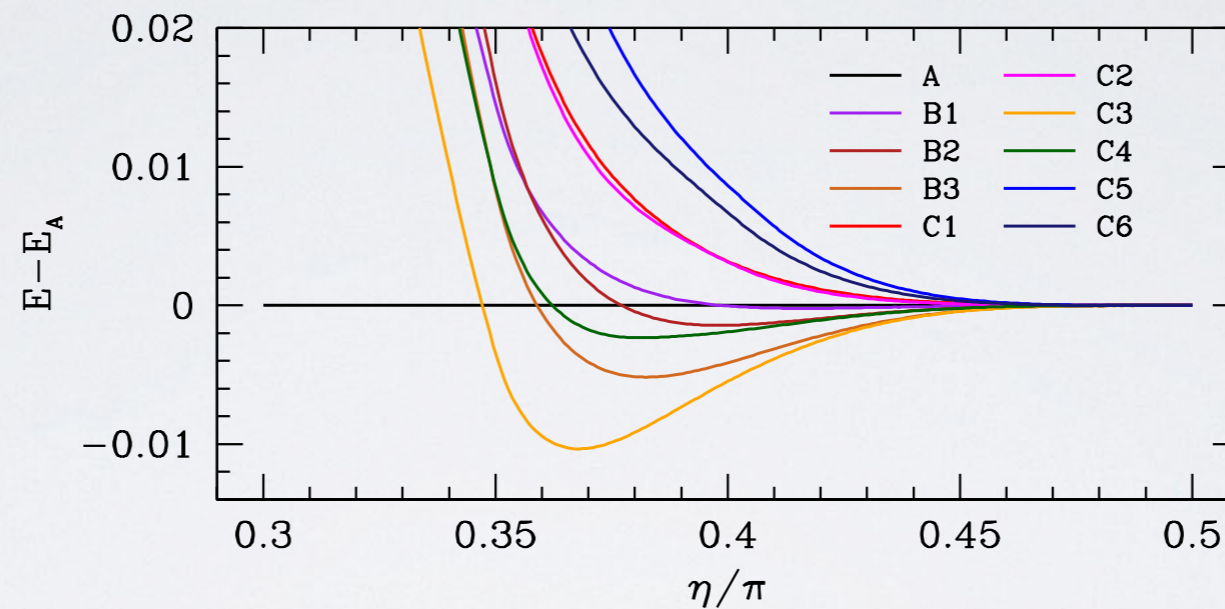
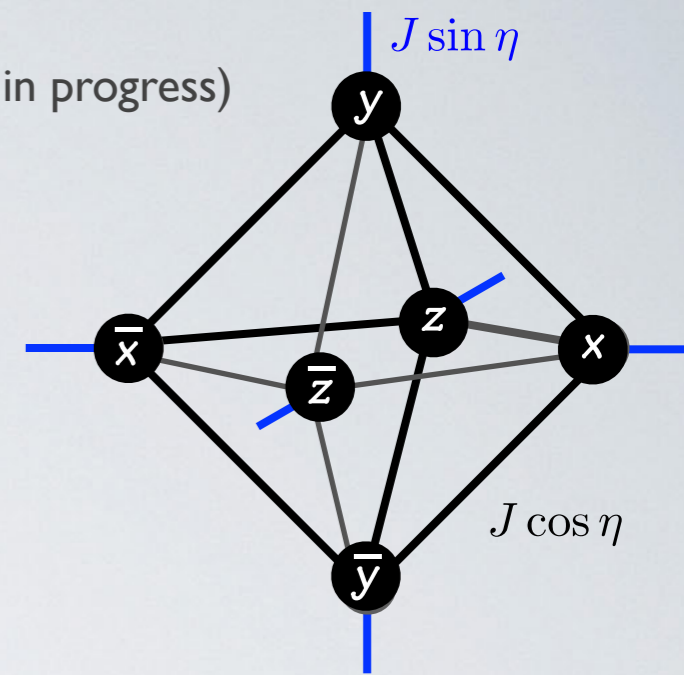
Finally, if we relax the requirement of separate \mathcal{T} and \mathcal{P} symmetries and require only \mathcal{PT} then the band structure is richer, with $\gamma^4, \gamma^{14}, \gamma^{45}, \gamma^{24}$, and γ^{34} terms in the Hamiltonian, potentially allowing for a more diverse set of possibilities.

Octahedron cubic lattice model

(Z. Huang and DPA, in progress)

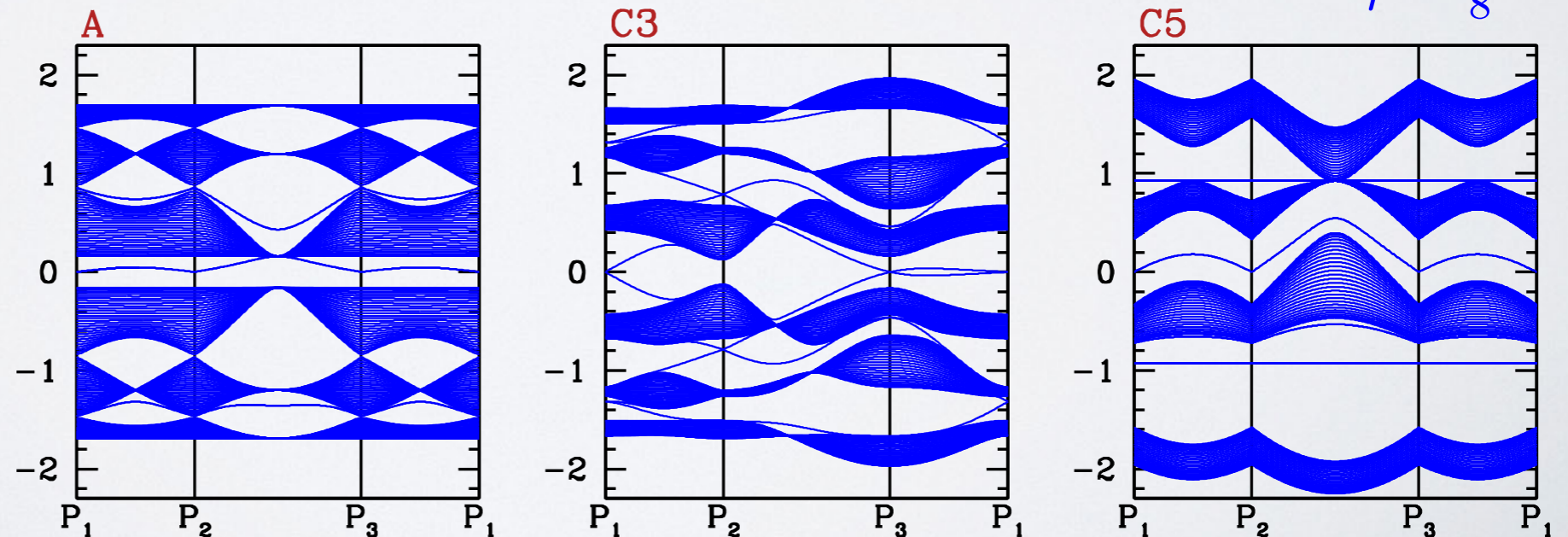


If we assume a single cube unit cell, there are ten distinct flux assignments for each octahedron (modulo time reversal).



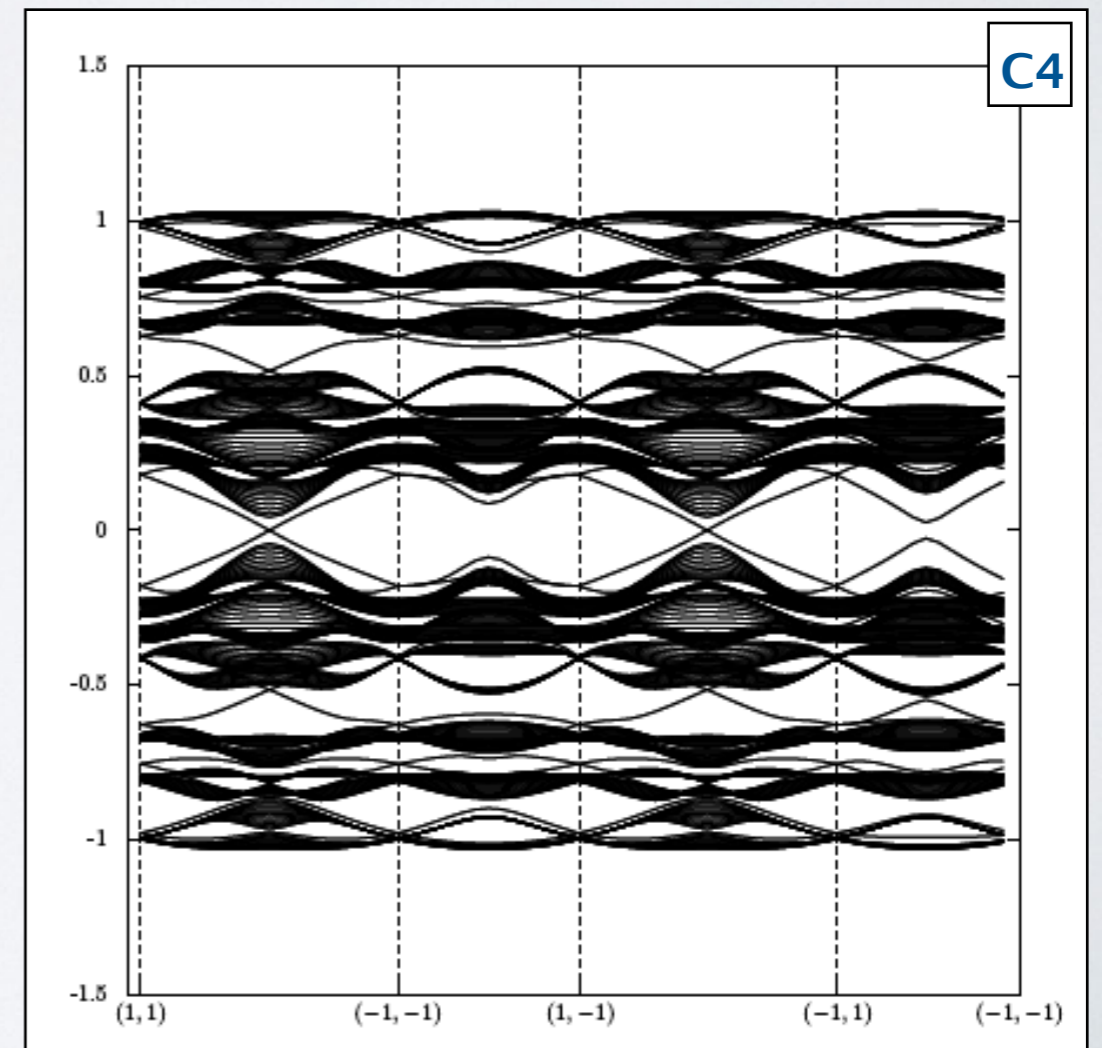
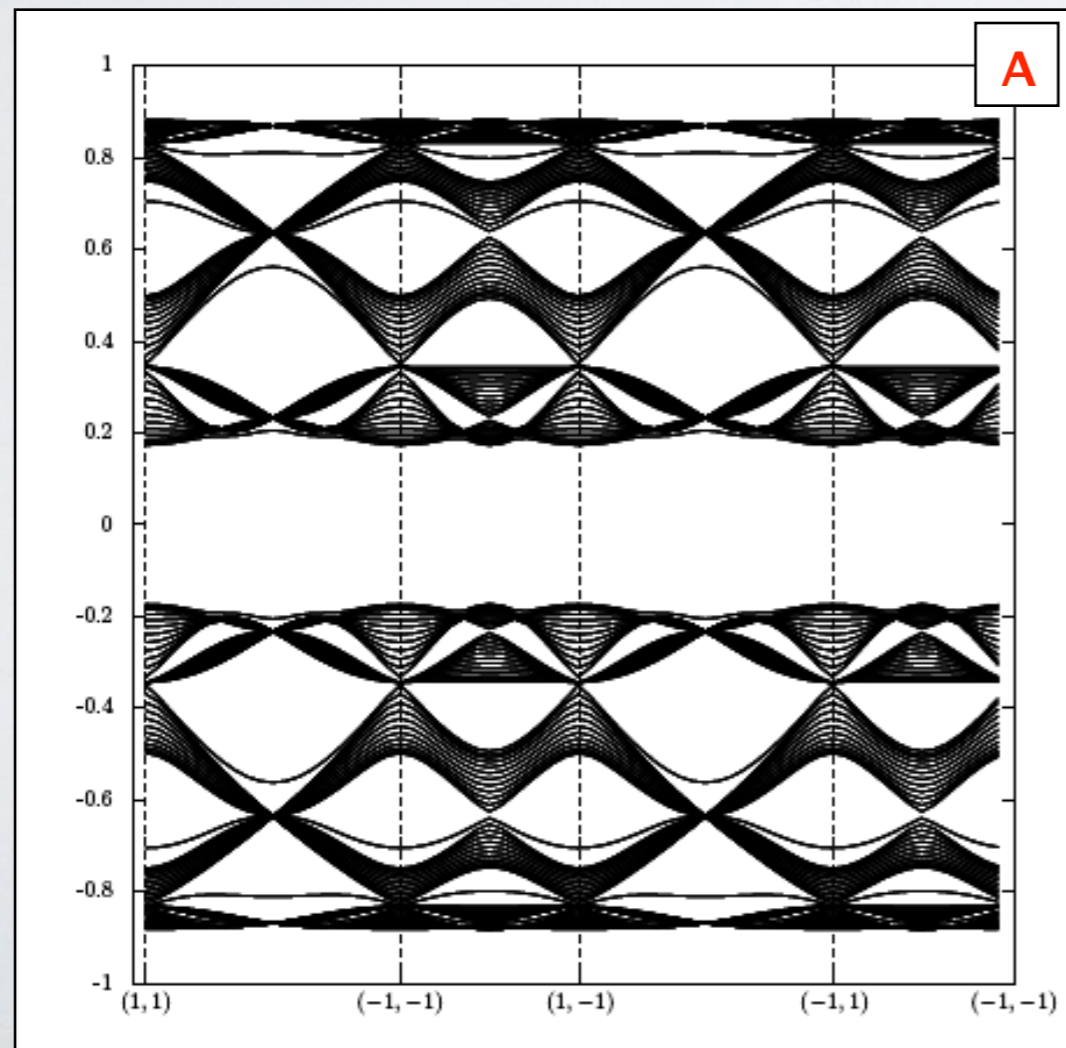
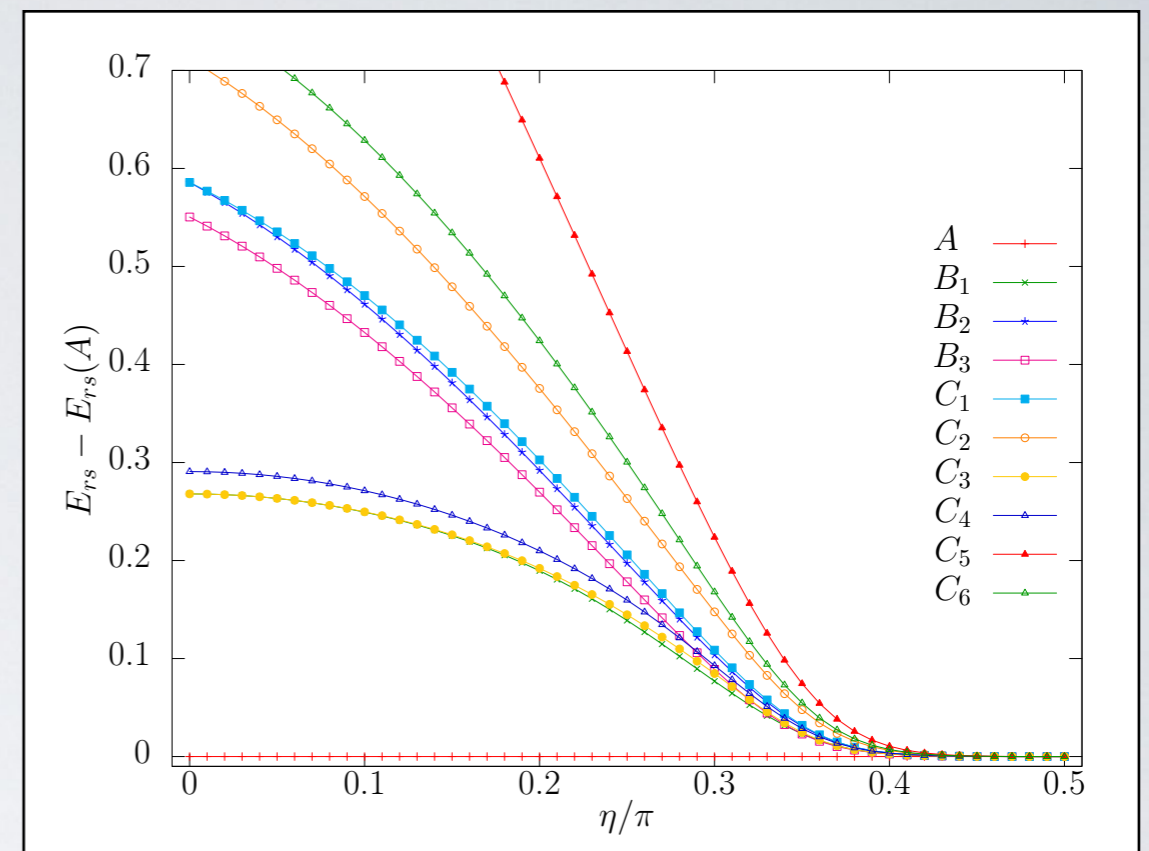
Several potentially interesting phases appear :

$$\eta = \frac{3}{8}\pi$$



However, all these phases violate Lieb's theorem, which applies here because of the presence of reflection planes. For each octahedral flux configuration, the energy is minimized with a reflection-symmetric extension to the full lattice, requiring a $2 \times 2 \times 2$ cubic unit cell. The A phase always has the lowest energy.

Surface energy plots at $\eta = \frac{7\pi}{20}$:



$k=3$ and beyond...

Constraint is $\theta^0\theta^1\theta^2\theta^3\theta^4\theta^5\theta^6\theta^7 = -1$. Try $\mathcal{R} = i\Gamma^2 \xrightarrow{k=1} (i\Gamma^2)(i\Gamma^4) \xrightarrow{k=2} (i\Gamma^2)(i\Gamma^4)(i\Gamma^6) \xrightarrow{k=3} ?$

If $\mathcal{K}\theta^a\mathcal{K} = (-1)^a\theta^a$, then $\mathcal{T}^2 = +1$ -- not conventional time-reversal!

$k=3$	1	$i\theta^0\theta^a$	$i\theta^a\theta^b$	$\theta^0\theta^a\theta^b\theta^c$
matrices	\mathbb{I}	Γ^a	Γ^{ab}	Γ^{abc}
multiplicity	1	7	21	35
$\varepsilon_{\mathcal{T}}$	E	O	O	E

How to represent using $S = \frac{7}{2}$ algebra?

$$1 + 3 + 5 + 7 + 9 + 11 + 13 + 15 = 8^2 = 64$$

The 21 and 35 multiplets are of mixed symmetry under the familiar time reversal operation.

(i.e. $21 = 3+5+13$, $35 = 9+11+15$).

Solution : Take $\mathcal{R} = \Gamma^1\Gamma^3\Gamma^5$, which results in $\mathcal{T}^2 = -1$. Then Γ^7 is odd under time reversal, while $\Gamma^{1,2,3,4,5,6}$ are all even :

$k=3$	1	$i\theta^0\theta^a$	$i\theta^0\theta^7$	$i\Gamma^7\Gamma^a$	$i\theta^a\theta^b$	$\theta^0\theta^7\theta^a\theta^b$	$\theta^0\theta^a\theta^b\theta^c$
matrices	\mathbb{I}	Γ^a	Γ^7	Γ^{7a}	Γ^{ab}	Γ^{7ab}	Γ^{abc}
multiplicity	1	6	1	6	15	15	20
\mathcal{T} symmetry	E	E	O	E	O	E	O

$$a, b, c \in \{1, 2, 3, 4, 5, 6\}$$

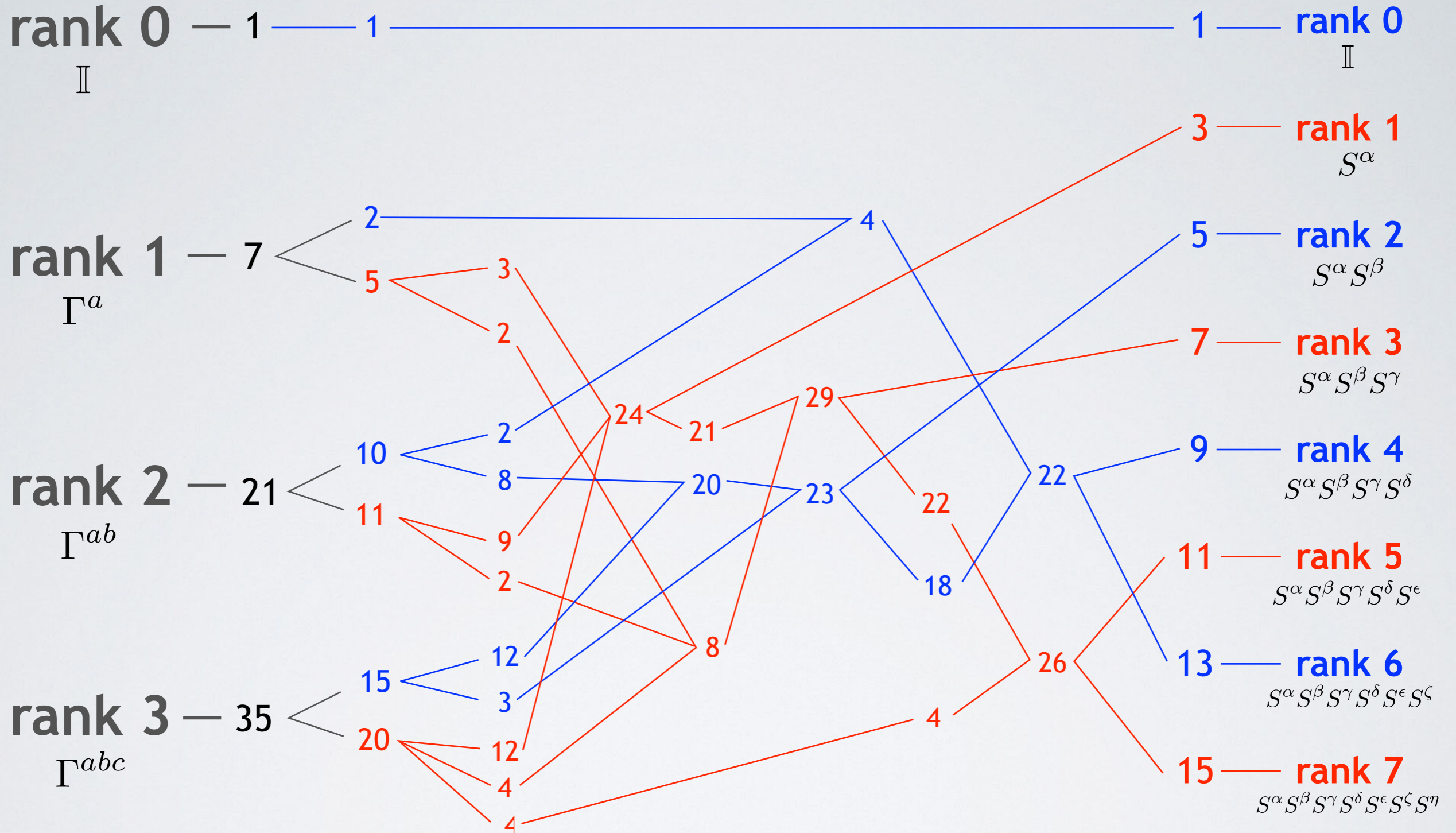
$$1 + 6 + 1 + 6 + 15 + 15 + 20 = 1 + 3 + 5 + 7 + 9 + 11 + 13 + 15$$

28 EVEN , 36 ODD

gamma matrices

k=3 Gamma matrix decomposition table
(courtesy of Y. Li)

spin tensors



$$S^x = \frac{\sqrt{7}-\sqrt{15}}{4} i \Gamma^1 \Gamma^4 - \frac{\sqrt{7}+\sqrt{15}}{4} i \Gamma^5 \Gamma^6 - \frac{\sqrt{3}}{2} i \Gamma^3 \Gamma^4 + \frac{\sqrt{3}}{2} i \Gamma^2 \Gamma^5 + \frac{1}{2} i \Gamma^1 \Gamma^3 \Gamma^4 + \frac{1}{2} i \Gamma^1 \Gamma^2 \Gamma^5 + \frac{1}{2} i \Gamma^2 \Gamma^4 \Gamma^6 - \frac{1}{2} i \Gamma^3 \Gamma^5 \Gamma^6$$

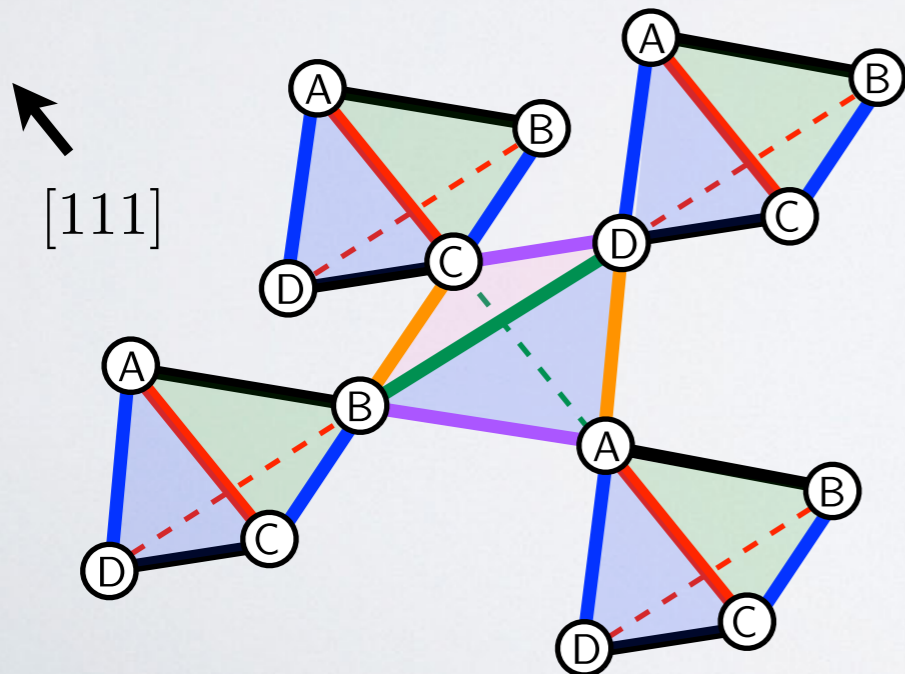
$$S^y = \frac{\sqrt{7}-\sqrt{15}}{4} i \Gamma^1 \Gamma^5 + \frac{\sqrt{7}+\sqrt{15}}{4} i \Gamma^4 \Gamma^6 + \frac{\sqrt{3}}{2} i \Gamma^3 \Gamma^5 + \frac{\sqrt{3}}{2} i \Gamma^2 \Gamma^4 - \frac{1}{2} i \Gamma^3 \Gamma^4 \Gamma^6 - \frac{1}{2} i \Gamma^2 \Gamma^5 \Gamma^6 + \frac{1}{2} i \Gamma^1 \Gamma^2 \Gamma^4 - \frac{1}{2} i \Gamma^1 \Gamma^3 \Gamma^5$$

$$S^z = -2 \Gamma^7 - i \Gamma^2 \Gamma^3 - \frac{1}{2} i \Gamma^4 \Gamma^5 .$$

$k=3$ on the pyrochlore lattice

Z. Huang (PhD thesis, 2014)

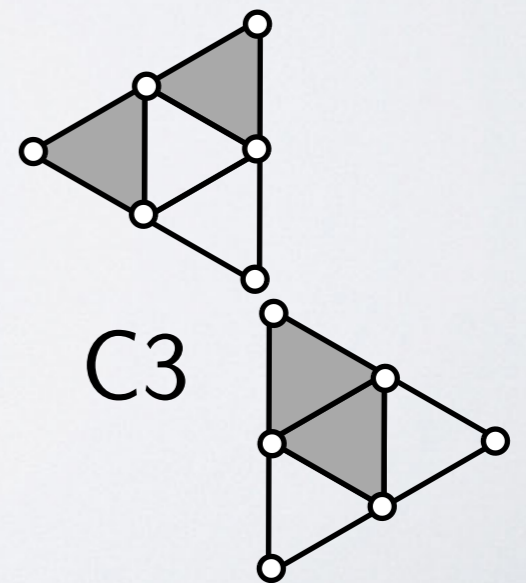
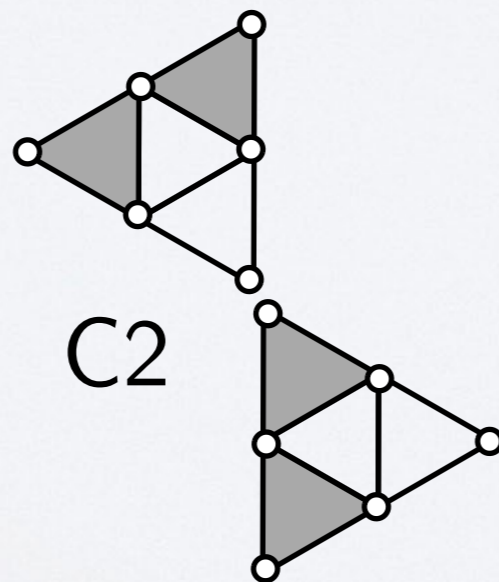
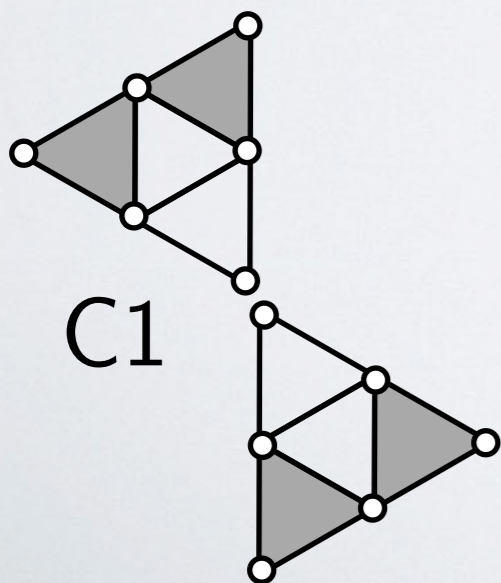
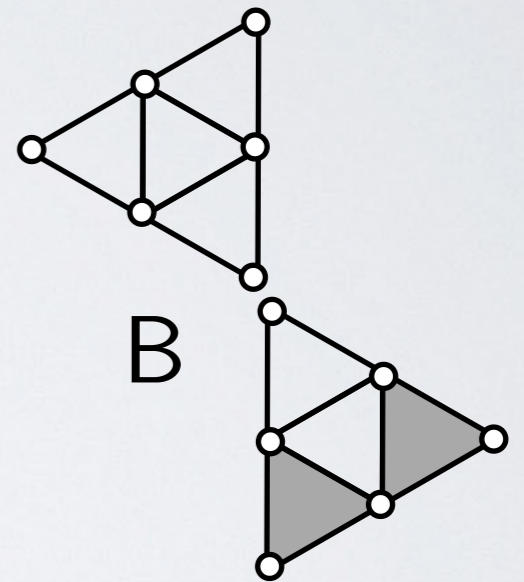
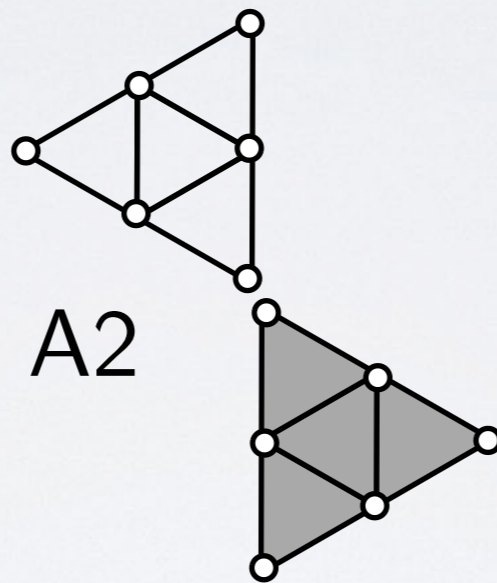
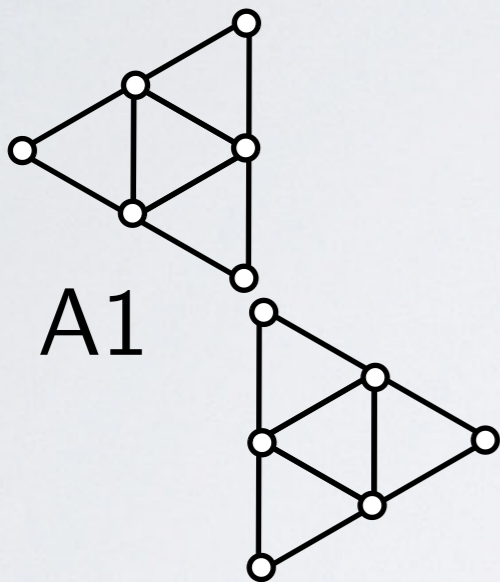
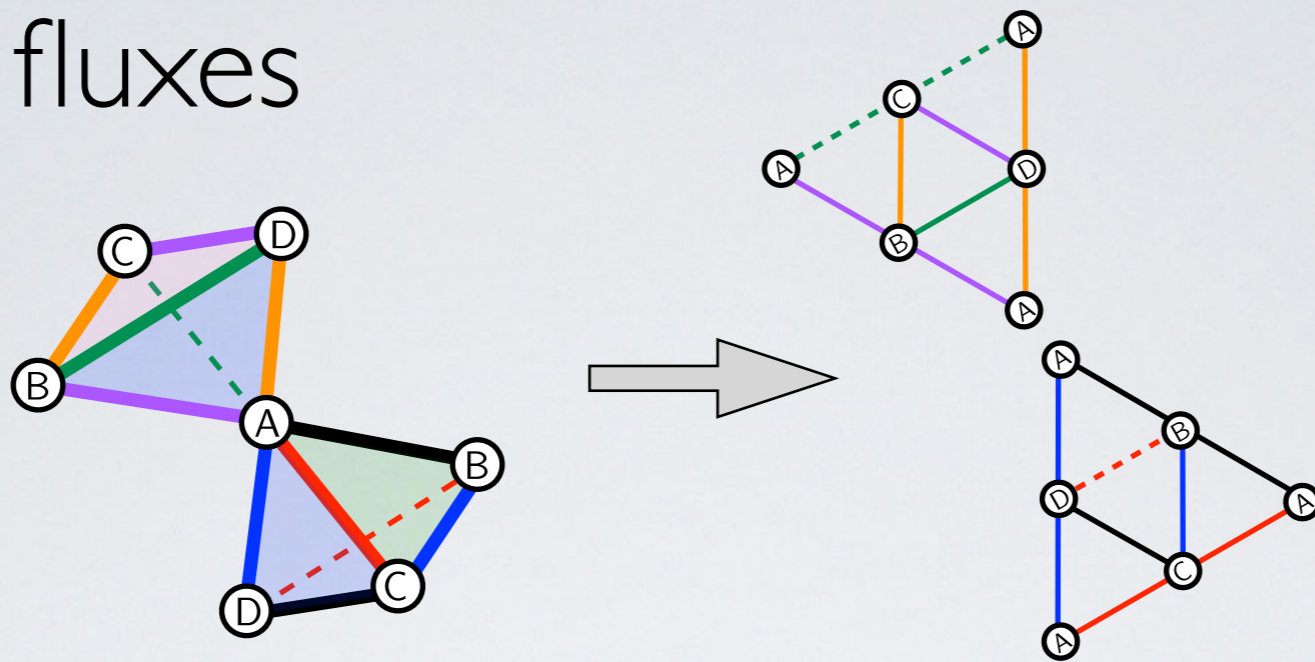
$$\begin{aligned}
 \mathcal{H} &= J_{\Delta} \sum_{t \in [111]} \left[\Gamma_{tA}^1 \Gamma_{tB}^1 + \Gamma_{tC}^1 \Gamma_{tD}^1 + \Gamma_{tA}^2 \Gamma_{tC}^2 + \Gamma_{tB}^2 \Gamma_{tD}^2 + \Gamma_{tA}^3 \Gamma_{tD}^3 + \Gamma_{tB}^3 \Gamma_{tC}^3 \right] \\
 &+ J'_{\Delta} \sum_{t \in [111]} \left[\Gamma_{tA}^{17} \Gamma_{tB}^{17} + \Gamma_{tC}^{17} \Gamma_{tD}^{17} + \Gamma_{tA}^{27} \Gamma_{tC}^{27} + \Gamma_{tB}^{27} \Gamma_{tD}^{27} + \Gamma_{tA}^{37} \Gamma_{tD}^{37} + \Gamma_{tB}^{37} \Gamma_{tC}^{37} \right] \\
 &+ J_{\nabla} \sum_{\bar{t} \in [\bar{1}\bar{1}\bar{1}]} \left[\Gamma_{\bar{t}A}^4 \Gamma_{\bar{t}B}^4 + \Gamma_{\bar{t}C}^4 \Gamma_{\bar{t}D}^4 + \Gamma_{\bar{t}A}^5 \Gamma_{\bar{t}C}^5 + \Gamma_{\bar{t}B}^5 \Gamma_{\bar{t}D}^5 + \Gamma_{\bar{t}A}^6 \Gamma_{\bar{t}D}^6 + \Gamma_{\bar{t}B}^6 \Gamma_{\bar{t}C}^6 \right] \\
 &+ J'_{\nabla} \sum_{\bar{t} \in [\bar{1}\bar{1}\bar{1}]} \left[\Gamma_{\bar{t}A}^{47} \Gamma_{\bar{t}B}^{47} + \Gamma_{\bar{t}C}^{47} \Gamma_{\bar{t}D}^{47} + \Gamma_{\bar{t}A}^{57} \Gamma_{\bar{t}C}^{57} + \Gamma_{\bar{t}B}^{57} \Gamma_{\bar{t}D}^{57} + \Gamma_{\bar{t}A}^{67} \Gamma_{\bar{t}D}^{67} + \Gamma_{\bar{t}B}^{67} \Gamma_{\bar{t}C}^{67} \right] + K \sum_i \Gamma_i^7 \\
 &= i \sum_{\langle ij \rangle}^{[111]} \left(J_{\Delta} \theta_i^0 \theta_j^0 + J'_{\Delta} \theta_i^7 \theta_j^7 \right) u_{ij} + i \sum_{\langle ij \rangle}^{[\bar{1}\bar{1}\bar{1}]} \left(J_{\nabla} \theta_i^0 \theta_j^0 + J'_{\nabla} \theta_i^7 \theta_j^7 \right) u_{ij} + i \sum_i K \theta_i^0 \theta_i^7
 \end{aligned}$$



This generalizes the model of Chua, Yao, and Fiete to a $k=3$ system. The hybridization term $K\Gamma^7$ may or may not break time reversal.

Once again, there are two Majorana species hopping in the presence of a single \mathbb{Z}_2 gauge field, and with on-site hybridization.

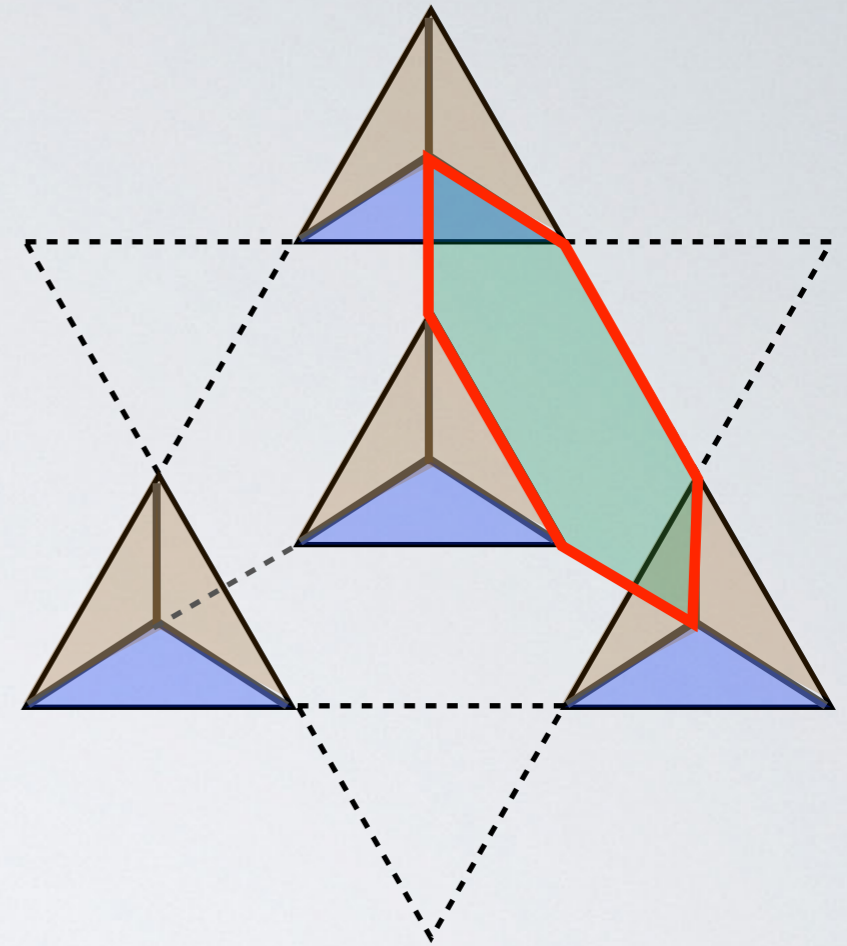
tetrahedra fluxes



hexagon fluxes

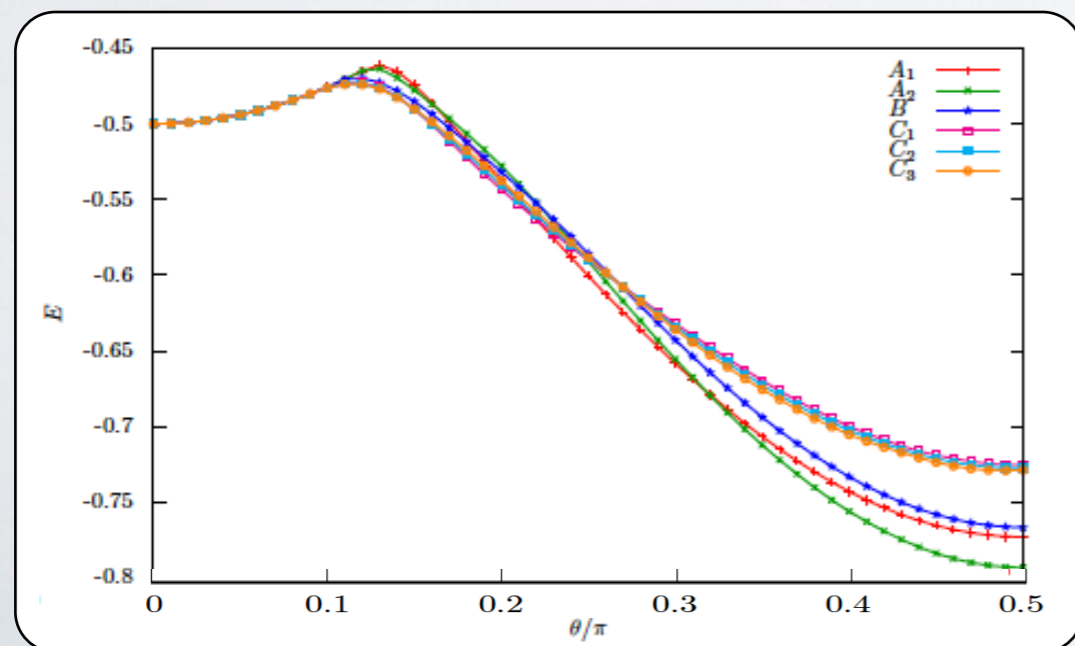
Fixing the fluxes through all the triangular faces of the tetrahedra still leaves the hexagonal faces in all the Kagome planes unconstrained. On a supertetrahedron containing four elementary tetrahedra, there are four hexagonal faces, and we can flip an even number of them :

$$1 + 6 + 1 = 8 \text{ hexagon configurations}$$

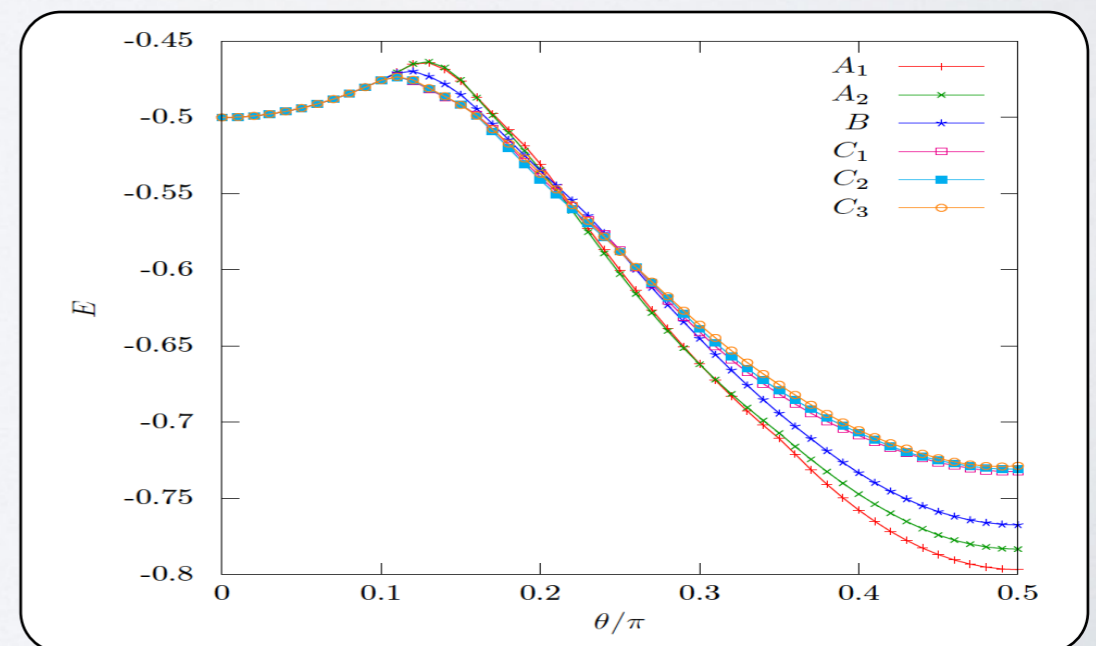


Total energies for $(J_{\Delta} = J'_{\Delta}, J_{\nabla} = J'_{\nabla}, K) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$:

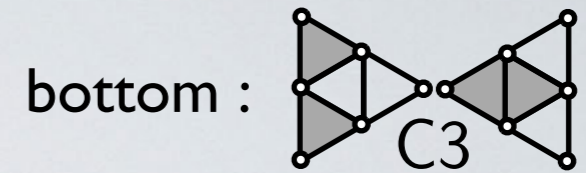
minimal unit cell : A2 ground state



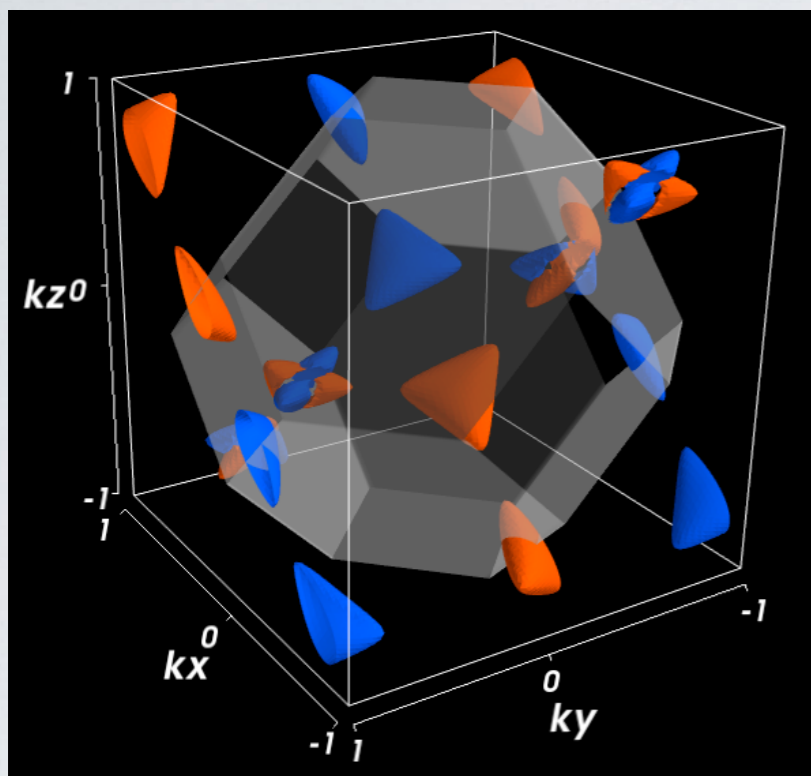
free hexagon fluxes : A1 ground state



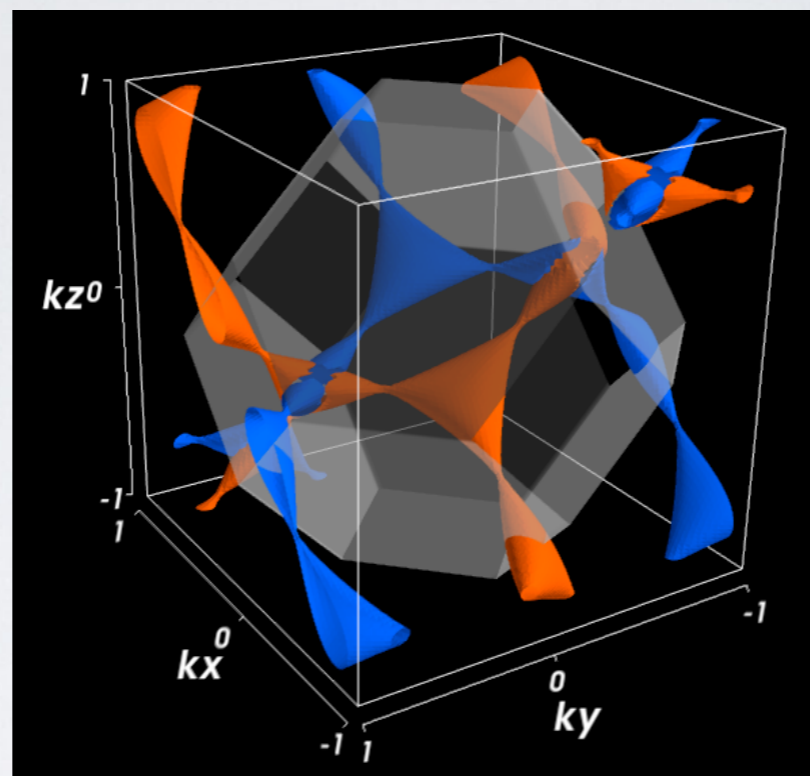
fermi surfaces



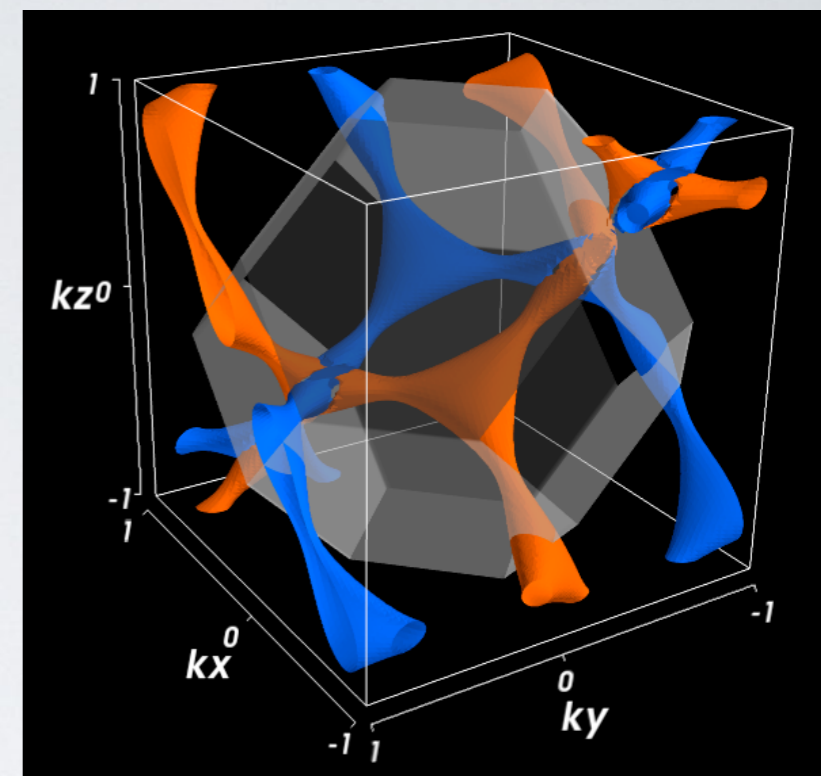
$$\theta = 0.1080 \pi, \phi = 0.25 \pi$$



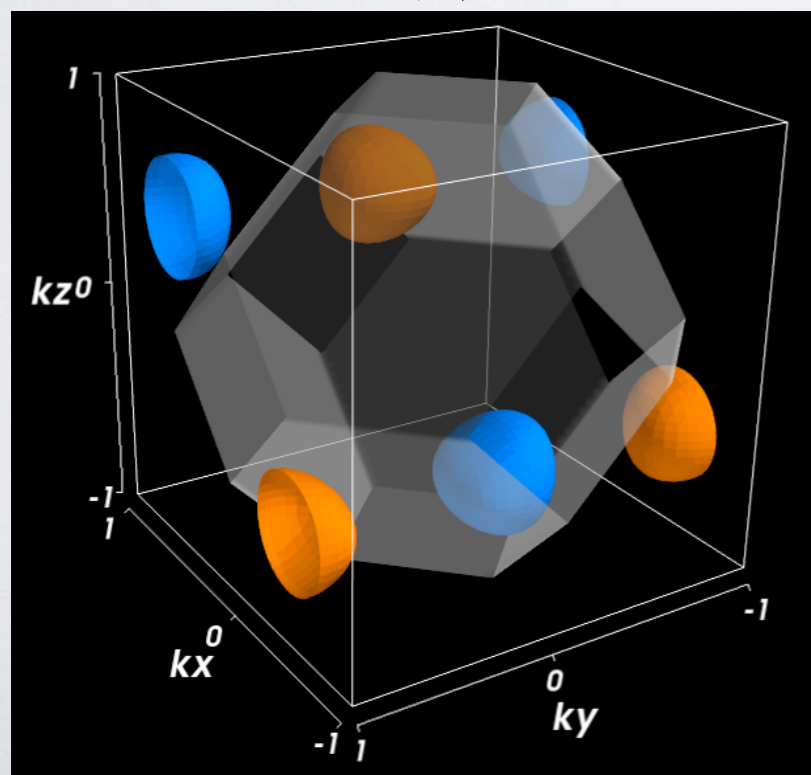
$$\theta = 0.1082 \pi, \phi = 0.25 \pi$$



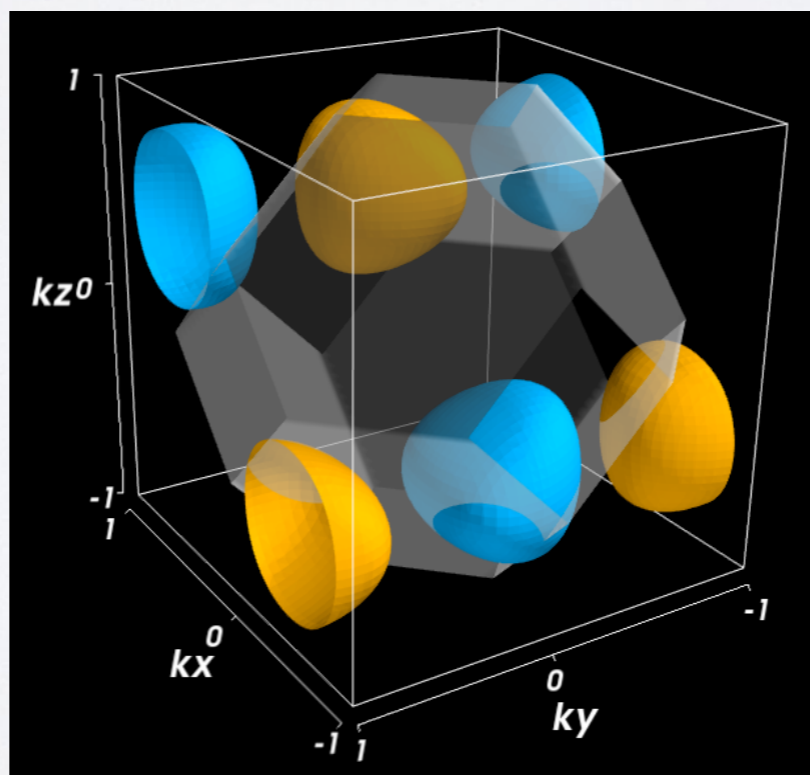
$$\theta = 0.1084 \pi, \phi = 0.25 \pi$$



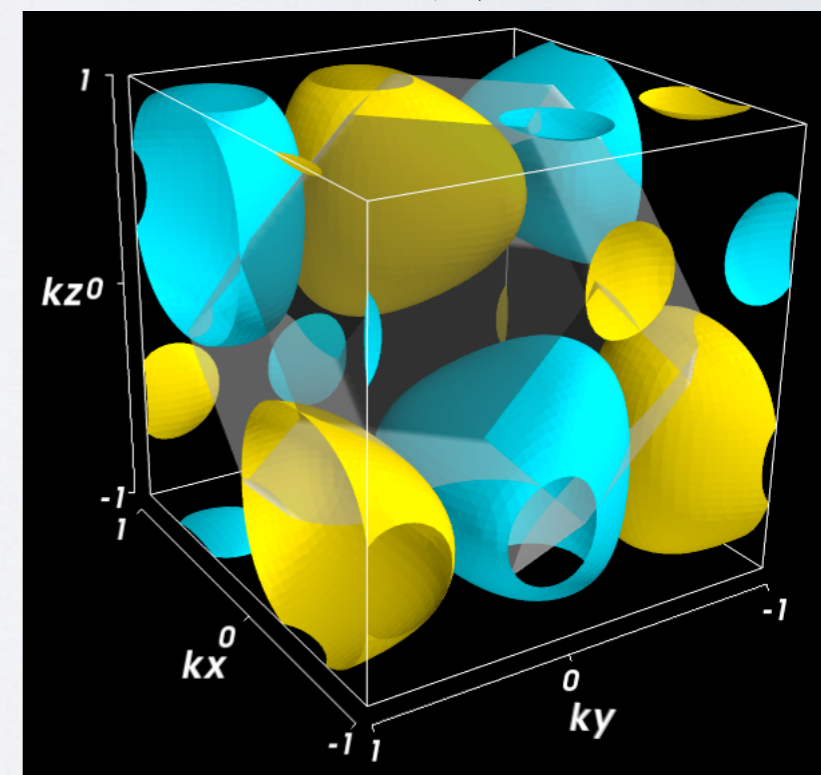
$$\theta = 0.095 \pi, \phi = 0.25 \pi$$



$$\theta = 0.100 \pi, \phi = 0.25 \pi$$



$$\theta = 0.110 \pi, \phi = 0.25 \pi$$



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