Gamma Matrix Generalizations of the Kitaev Model

D. P. Arovas, UCSD

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

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

Jorge Cham © 2007

www.phdcomics.com
**Kitaev toric code (2003):**

\[ \mathcal{H} = -J_E \sum_{+} \sigma^z_a \sigma^z_b \sigma^z_c \sigma^z_d - J_M \sum_{-} \sigma^x_i \sigma^x_j \sigma^x_k \sigma^x_l \]

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):**

\[ \mathcal{H} = J_1 \sum_{\langle ij \rangle} \sigma^x_i \sigma^x_j + J_2 \sum_{\langle ij \rangle} \sigma^y_i \sigma^y_j + J_3 \sum_{\langle ij \rangle} \sigma^z_i \sigma^z_j \]

\( (0, 0, 1) \)
\( (J_1, J_2, J_3) \)
\( (1, 0, 0) \)
\( (0, 1, 0) \)

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

\( 2N \) Majoranas \( \Rightarrow 2^N \) states

\( \{ c, c^\dagger \} = 1 \)

\( S = \frac{1}{2} \) algebra represented with Majoranas

Four Majorana species: \( \theta^a \quad (a = 0, 1, 2, 3) \)

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

Constraint: \( \theta^0 \theta^1 \theta^2 \theta^3 = 1 \)

Projector onto constraint sector: \( P = \frac{1}{2} \left( 1 + \theta^0 \theta^1 \theta^2 \theta^3 \right) \)
2D Toric Code

Apply unitary transformation $U = e^{i \frac{\pi}{4} \sigma_y}$ to all NW/SE links: \[
\begin{cases}
\sigma^x \\
\sigma^z
\end{cases} \rightarrow \begin{cases}
-\sigma^z \\
\sigma^x
\end{cases}
\]

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

\[
\mathcal{H} = - J_E \sum_{\square,E} \sigma^x_i \sigma^z_j \sigma^x_k \sigma^z_l - J_M \sum_{\square,M} \sigma^x_i \sigma^z_j \sigma^x_k \sigma^z_l
\]

(Wen, 2003)

Define the $\mathbb{Z}_2$ gauge fields $u_{ij} = -i \theta^a_i \theta^a_j$ ($a = 0, 1, 2, 3$) \[u_{ij} = \pm 1\]

Magic: Sticks of same color never share a vertex means that the gauge fields $u_{ij}$ commute! \[[u_{ij}, u_{kl}] = 0 \Rightarrow \text{classical } \mathbb{Z}_2 \text{ gauge theory.} \]

\[
\sigma^x = i \theta^0 \theta^1 = -i \theta^2 \theta^3 \\
\sigma^y = i \theta^0 \theta^2 = +i \theta^1 \theta^3 \\
\sigma^z = i \theta^0 \theta^3 = -i \theta^1 \theta^2
\]

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

\[ \mathcal{H} = J_1 \sum' \sigma_i^x \sigma_j^x + J_2 \sum' \sigma_i^y \sigma_j^y + J_3 \sum' \sigma_i^z \sigma_j^z \]

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

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

\[
\begin{aligned}
2^N &= \left(\sqrt{2^4}\right)^N \\
\text{too many!}
\end{aligned}
\]

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

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

$\Rightarrow \frac{1}{2}N + 1$ 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:

$$|\Psi_0\rangle = \sum_g R_g |\psi_0(u)\rangle \otimes |\phi(u)\rangle$$

Starting from some $$|\Psi_0\rangle$$ we can build the Hilbert space multiplying by products of even numbers of Majoranas $$\theta_i^0$$. $$\mathcal{H}$$ 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 $\mathcal{T} = \mathcal{R} \mathcal{K}$

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

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

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

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

$N_p = \#$ 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:

\[ \sigma_i^z \sigma_j^y \sigma_k^x = i \theta_0^0 \theta_0^0 u_{ij} u_{jk} \]

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 $THT^{-1} = \mathcal{H}$

(Yao and Kivelson 2007)
Lieb’s theorem  (Lieb, 1994)

Consider a general single species Majorana Hamiltonian $\mathcal{H} = \frac{i}{4} A_{i,j} \theta_i \theta_j$ 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 $u_{i,j} = \text{sgn}(A_{i,j})$. 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:

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

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

The Hamiltonian may be reexpressed in terms of Dirac fermions:

\[ \mathcal{H} = i \sum_k A_{st}(k) \left( c_{ks}^\dagger c_{kt} - \frac{1}{2} \delta_{st} \right) + \frac{i}{4} \sum_Q A_{st}(Q) \xi_{s}(Q) \xi_t(Q) \]

(time reversal invariant momenta \( Q = \frac{1}{2} G \))

The spectrum of \( iA(k) \) satisfies \( \text{spec} \left\{ iA(k) \right\} = -\text{spec} \left\{ iA(-k) \right\} \)

The spectrum consists of the positive eigenvalues of \( iA_{st}(k) \) (plus half the zeros).
Spin-metal in the square-octagon model

Lowest energy flux configuration consistent with Lieb’s theorem has $\sigma = -1$, but adding ring terms such as $\sigma_1^{\cdot} \sigma_2^{\cdot} \sigma_3^{\cdot} \sigma_4^{\cdot} = -\phi_4$ 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).
Gamma matrices and Clifford algebras

Clifford algebra : \[ \{ \Gamma^a, \Gamma^b \} = 2\delta^{ab} \quad a, b \in \{1, \ldots, \mathcal{N}\} \]

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

\[
\begin{align*}
\Gamma^1 &= \sigma^x \otimes 1 \otimes \cdots \otimes 1 \otimes 1 \\
\Gamma^2 &= \sigma^y \otimes 1 \otimes \cdots \otimes 1 \otimes 1 \\
\Gamma^3 &= \sigma^z \otimes \sigma^x \otimes \cdots \otimes 1 \otimes 1 \\
\Gamma^{2k-1} &= \sigma^z \otimes \sigma^z \otimes \cdots \otimes \sigma^z \otimes \sigma^x \\
\Gamma^{2k} &= \sigma^z \otimes \sigma^z \otimes \cdots \otimes \sigma^z \otimes \sigma^y \\
\Gamma^{2k+1} &= \sigma^z \otimes \sigma^z \otimes \cdots \otimes \sigma^z \otimes \sigma^z
\end{align*}
\]

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

Majorana fermion representation

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

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

\[
\theta^0 \theta^1 \ldots \theta^{2k+1} = i^{k-1}
\]

\( k = 1 \) : Pauli matrices \hspace{1cm} 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 \( \Gamma^a \), 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 :

<table>
<thead>
<tr>
<th>class</th>
<th>number</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 1 )</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( i \theta^0 \theta^a )</td>
<td>( 2k + 1 )</td>
</tr>
<tr>
<td>( i \theta^a \theta^b )</td>
<td>( \binom{2k+1}{k} )</td>
</tr>
<tr>
<td>( \theta^0 \theta^a \theta^b \theta^c )</td>
<td>( \binom{2k+1}{k+1} )</td>
</tr>
<tr>
<td>( \theta^a \theta^b \theta^c \theta^d )</td>
<td>( \binom{2k+1}{k+1} )</td>
</tr>
<tr>
<td>total</td>
<td>( 4^k )</td>
</tr>
<tr>
<td>rank</td>
<td>( 2^k )</td>
</tr>
</tbody>
</table>

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

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

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$\Gamma^1$</th>
<th>$\Gamma^2$</th>
<th>$\Gamma^3$</th>
<th>$\Gamma^4$</th>
<th>$\Gamma^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_{\mathcal{K}}$</td>
<td>E</td>
<td>O</td>
<td>E</td>
<td>O</td>
<td>E</td>
</tr>
<tr>
<td>$\varepsilon_{\mathcal{R}}$</td>
<td>O</td>
<td>E</td>
<td>O</td>
<td>E</td>
<td>O</td>
</tr>
<tr>
<td>$\varepsilon_{\mathcal{T}}$</td>
<td>O</td>
<td>O</td>
<td>O</td>
<td>O</td>
<td>O</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$k = 2$</th>
<th>1</th>
<th>$i\theta^0 \theta^a$</th>
<th>$i\theta^a \theta^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>matrices</td>
<td>$\mathbb{I}$</td>
<td>$\Gamma^a$</td>
<td>$\Gamma^{ab}$</td>
</tr>
<tr>
<td>multiplicity</td>
<td>1</td>
<td>5</td>
<td>10</td>
</tr>
</tbody>
</table>

$\varepsilon_{\mathcal{T}}$

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

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

$\mathbb{I}$ rank 0 — 1 — rank 0 $\mathbb{I}$

$\Gamma^a$ rank 1 — 5

$\Gamma^{ab}$ rank 2 — 10

3 — rank 1 $S^\alpha$

5 — rank 2 $S^\alpha S^\beta$

7 — rank 3 $S^\alpha S^\beta S^\gamma$

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

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

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

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

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

Murakami et al. 2004
Yao et al. 2009
Chua et al. 2011
Models with $k=2$

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

$$\mathcal{H} = \sum_{a=1}^{5} J_a \sum_{\langle ij \rangle} \Gamma^a_i \Gamma^a_j = \sum_{\langle ij \rangle} J_{ij} i\theta_i^0 \theta_j^0 u_{ij}$$

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

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 \( \phi_\triangle = \pm 1 \).

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

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

\# of common links

\[
E/J = \frac{\epsilon_0}{J} \left( \cos^2 \left( \frac{k_x}{\pi} \right) + \cos^2 \left( \frac{k_y}{\pi} \right) \right)
\]

\[
J_x = J_y = J_d = 1
\]
ground state: bulk energy bands

\[ J_d/J = 1 \]

\[ J_d/J = \sqrt{8} \]

\[ J_d/J = 3.5 \]

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: $| \Psi_G[\Phi] \rangle = P | \Psi[u] \rangle$

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

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

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

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 $\mathcal{W}_{\text{H/V}}$) $n$ Dirac zero modes for $2n$ vortices.
Building on the work of Yao, Zhang, and Kivelson, considered the following model:

\[ \mathcal{H} = J_\Delta \sum_{\langle ij \rangle \in \Delta} \Gamma^1_i \Gamma^2_j + J_\nabla \sum_{\langle ij \rangle \in \nabla} \Gamma^3_i \Gamma^4_j + J'_\Delta \sum_{\langle ij \rangle \in \Delta} \Gamma^{15}_i \Gamma^{25}_j + J'_\nabla \sum_{\langle ij \rangle \in \nabla} \Gamma^{35}_i \Gamma^{45}_j + J_5 \sum_i \Gamma^5_i \]

\[ = i \sum_{\langle ij \rangle \in \Delta} (J_\Delta \theta^0_i \theta^0_j + J'_\Delta \theta^5_i \theta^5_j) u_{ij} + i \sum_{\langle ij \rangle \in \nabla} (J_\nabla \theta^0_i \theta^0_j + J'_\nabla \theta^5_i \theta^5_j) u_{ij} + i J_5 \sum_i \theta^0_i \theta^5_i \]

where \( u_{ij} = -i \theta^1_i \theta^2_j (\Delta) \) or \( u_{ij} = -i \theta^3_i \theta^4_j (\nabla) \). 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).

\( \text{Kagome chiral spin liquid} \) (Chua, Yao, and Fiete, 2009)
Diamond lattice model

diamond = two interpenetrating FCC lattices, \( z = 4 \)

Our model: \( k = 2 \) (4x4 \( \Gamma \) matrices). Start with

\[
\mathcal{H}_0 = \sum_{R} \sum_{a=1}^{4} J_a \Gamma^a_R \tilde{\Gamma}^a_{R+\hat{e}_a}
\]

and add

\[
\mathcal{H}_1 = \sum_{R} \sum_{a<b}^{4} (h_{ab} V^{ab}_R + \tilde{h}_{ab} \tilde{V}^{ab}_R)
\]

where

\[
V^{ab}_R = \Gamma^a_R \tilde{\Gamma}^{ab}_{R+\hat{e}_a} \Gamma^b_{R+\hat{e}_a-\hat{e}_b}, \quad \tilde{V}^{ab}_R = \tilde{\Gamma}^a_{R+\hat{e}_a} \Gamma^{ab}_R \tilde{\Gamma}^b_{R+\hat{e}_b}
\]

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

$$H(k) = \begin{pmatrix}
\omega(k) & 0 & \Delta(k) & 0 \\
0 & -\omega(k) & 0 & -\Delta(k) \\
\Delta^*(k) & 0 & -\omega(k) & 0 \\
0 & -\Delta^*(k) & 0 & \omega(k)
\end{pmatrix} \leftarrow \begin{pmatrix}
\theta^0_A \\
\theta^5_A \\
\theta^0_B \\
\theta^5_B
\end{pmatrix}$$

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

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

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

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

$$\mathcal{H}_{hyb} = m \sum_R (\Gamma^{5_R} + \bar{\Gamma}^{5_R+E_4}) + \sum_R \left( g_{ab} \Gamma^a_R \bar{\Gamma}^{ab}_{R+E_1-E_2} \Gamma^{5b}_{R+E_1-E_2} + \bar{g}_{ab} \bar{\Gamma}^a_{R+E_1-E_2} \Gamma^{5b}_{R+E_1-E_2} \right)$$

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

\[ H(\mathbf{k}) = \begin{pmatrix} \omega(\mathbf{k}) & \beta(\mathbf{k}) & \Delta(\mathbf{k}) & 0 \\ \beta^*(\mathbf{k}) & -\omega(\mathbf{k}) & 0 & -\Delta(\mathbf{k}) \\ \Delta^*(\mathbf{k}) & 0 & -\omega(\mathbf{k}) & \beta(\mathbf{k}) \\ 0 & -\Delta^*(\mathbf{k}) & \beta^*(\mathbf{k}) & \omega(\mathbf{k}) \end{pmatrix} \]

\[ = \omega(\mathbf{k}) \gamma^4 - \text{Re} \Delta(\mathbf{k}) \gamma^{14} + \text{Im} \Delta(\mathbf{k}) \gamma^{45} + \text{Re} \beta(\mathbf{k}) \gamma^{34} + \text{Im} \beta(\mathbf{k}) \gamma^{24} \]

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

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.

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>class</th>
<th>( T )</th>
<th>( P )</th>
<th>( PT )</th>
<th>( \gamma )</th>
<th>class</th>
<th>( T )</th>
<th>( P )</th>
<th>( PT )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( J )</td>
<td>-</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>( \gamma^4 )</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>( \gamma^1 )</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>( \gamma^5 )</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( \gamma^2 )</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>( \gamma^6 )</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>( \gamma^3 )</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>( \gamma^7 )</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( \gamma^4 )</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>+</td>
<td>( \gamma^8 )</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>( \gamma^5 )</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>( \gamma^9 )</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
</tbody>
</table>

Table 1: Symmetry properties of the \( \gamma \)-matrices.

Finally, if we relax the requirement of separate \( T \) and \( P \) symmetries and require only \( PT \) then the band structure is richer, with \( \gamma^4, \gamma^{14}, \gamma^{45}, \gamma^{24}, \) and \( \gamma^{34} \) terms in the Hamiltonian, potentially allowing for a more diverse set of possibilities.
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 2x2x2 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 $\mathcal{R} = i\Gamma^2 \rightarrow (i\Gamma^2)(i\Gamma^4) \rightarrow (i\Gamma^2)(i\Gamma^4)(i\Gamma^6)$.

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

<table>
<thead>
<tr>
<th>$k=3$</th>
<th>1</th>
<th>$i\theta^0\theta^a$</th>
<th>$i\theta^a\theta^b$</th>
<th>$\theta^0\theta^a\theta^b\theta^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>matrices</td>
<td>$\mathbb{I}$</td>
<td>$\Gamma^a$</td>
<td>$\Gamma^{ab}$</td>
<td>$\Gamma^{abc}$</td>
</tr>
<tr>
<td>multiplicity</td>
<td>1</td>
<td>7</td>
<td>21</td>
<td>35</td>
</tr>
<tr>
<td>$\varepsilon_{\mathcal{T}}$</td>
<td>E</td>
<td>O</td>
<td>O</td>
<td>E</td>
</tr>
</tbody>
</table>

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 $\Gamma^7$ is odd under time reversal, while $\Gamma^{1,2,3,4,5,6}$ are all even:

<table>
<thead>
<tr>
<th>$k=3$</th>
<th>1</th>
<th>$i\theta^0\theta^a$</th>
<th>$i\theta^0\theta^7$</th>
<th>$i\Gamma^7\Gamma^a$</th>
<th>$i\theta^a\theta^b$</th>
<th>$\theta^0\theta^7\theta^a\theta^b$</th>
<th>$\theta^0\theta^a\theta^b\theta^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>matrices</td>
<td>$\mathbb{I}$</td>
<td>$\Gamma^a$</td>
<td>$\Gamma^7$</td>
<td>$\Gamma^{7a}$</td>
<td>$\Gamma^{ab}$</td>
<td>$\Gamma^{7ab}$</td>
<td>$\Gamma^{abc}$</td>
</tr>
<tr>
<td>multiplicity</td>
<td>1</td>
<td>6</td>
<td>1</td>
<td>6</td>
<td>15</td>
<td>15</td>
<td>20</td>
</tr>
<tr>
<td>$\mathcal{T}$ symmetry</td>
<td>E</td>
<td>E</td>
<td>O</td>
<td>E</td>
<td>O</td>
<td>E</td>
<td>O</td>
</tr>
</tbody>
</table>

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

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

28 EVEN, 36 ODD
\[
S^x = \frac{\sqrt{7} - \sqrt{15}}{4} \mathrm{i} \Gamma^1 \Gamma^4 - \frac{\sqrt{7} + \sqrt{15}}{4} \mathrm{i} \Gamma^5 \Gamma^6 - \frac{\sqrt{3}}{2} \mathrm{i} \Gamma^3 \Gamma^4 + \frac{\sqrt{3}}{2} \mathrm{i} \Gamma^2 \Gamma^5 + \frac{1}{2} \mathrm{i} \Gamma^1 \Gamma^3 \Gamma^4 + \frac{1}{2} \mathrm{i} \Gamma^1 \Gamma^2 \Gamma^5 + \frac{1}{2} \mathrm{i} \Gamma^2 \Gamma^4 \Gamma^6 - \frac{1}{2} \mathrm{i} \Gamma^3 \Gamma^5 \Gamma^6
\]

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

\[
S^z = -2 \Gamma^7 - \mathrm{i} \Gamma^2 \Gamma^3 - \frac{1}{2} \mathrm{i} \Gamma^4 \Gamma^5
\]
$k=3$ on the pyrochlore lattice

$$
\mathcal{H} = J_\Delta \sum_{t \in [111]} \left[ \Gamma^1_{tA} \Gamma^1_{tB} + \Gamma^1_{tA} \Gamma^1_{tC} + \Gamma^1_{tB} \Gamma^1_{tD} + \Gamma^2_{tA} \Gamma^2_{tB} + \Gamma^2_{tA} \Gamma^2_{tD} + \Gamma^2_{tB} \Gamma^2_{tD} + \Gamma^3_{tA} \Gamma^3_{tD} + \Gamma^3_{tB} \Gamma^3_{tC} \right] 
+ J'_\Delta \sum_{t \in [111]} \left[ \Gamma^{17}_{tA} \Gamma^{17}_{tB} + \Gamma^{17}_{tA} \Gamma^{17}_{tC} + \Gamma^{27}_{tA} \Gamma^{27}_{tB} + \Gamma^{27}_{tB} \Gamma^{27}_{tD} + \Gamma^{37}_{tA} \Gamma^{37}_{tD} + \Gamma^{37}_{tB} \Gamma^{37}_{tC} \right] 
+ J_\nabla \sum_{\bar{t} \in [\bar{111}]} \left[ \Gamma^4_{\bar{t}A} \Gamma^4_{\bar{t}B} + \Gamma^4_{\bar{t}A} \Gamma^4_{\bar{t}C} + \Gamma^5_{\bar{t}A} \Gamma^5_{\bar{t}C} + \Gamma^5_{\bar{t}B} \Gamma^5_{\bar{t}D} + \Gamma^6_{\bar{t}B} \Gamma^6_{\bar{t}D} + \Gamma^6_{\bar{t}B} \Gamma^6_{\bar{t}C} \right] 
+ J'_\nabla \sum_{\bar{t} \in [\bar{111}]} \left[ \Gamma^{47}_{\bar{t}A} \Gamma^{47}_{\bar{t}B} + \Gamma^{47}_{\bar{t}A} \Gamma^{47}_{\bar{t}C} + \Gamma^{57}_{\bar{t}A} \Gamma^{57}_{\bar{t}C} + \Gamma^{57}_{\bar{t}B} \Gamma^{57}_{\bar{t}D} + \Gamma^{67}_{\bar{t}A} \Gamma^{67}_{\bar{t}D} + \Gamma^{67}_{\bar{t}B} \Gamma^{67}_{\bar{t}C} \right] + K \sum_i \Gamma^7_i 
$$

$$
= i \sum_{\langle ij \rangle} \left( J_\Delta \theta^0_i \theta^0_j + J'_\Delta \theta^7_i \theta^7_j \right) u_{ij} + i \sum_{\langle ij \rangle} \left( J_\nabla \theta^0_i \theta^0_j + J'_\nabla \theta^7_i \theta^7_j \right) u_{ij} + i \sum_i K \theta^0_i \theta^7_i 
$$

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 \( (J_\triangle = J'_\triangle, J_\triangledown = J'_{\triangledown}, K) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \):

minimal unit cell: A2 ground state

free hexagon fluxes: A1 ground state
fermi surfaces

\[
\theta = 0.1080 \pi, \ \phi = 0.25 \pi
\]

\[
\theta = 0.1082 \pi, \ \phi = 0.25 \pi
\]

\[
\theta = 0.1084 \pi, \ \phi = 0.25 \pi
\]

\[
\theta = 0.095 \pi, \ \phi = 0.25 \pi
\]

\[
\theta = 0.100 \pi, \ \phi = 0.25 \pi
\]

\[
\theta = 0.110 \pi, \ \phi = 0.25 \pi
\]
Selected references


G. Kells et al., arXiv 1012.5376