Majorana metals
in spin-orbit entangled quantum matter

APS March Meeting
San Antonio, March 2015

Simon Trebst
University of Cologne

PRB 89, 235102 (2014)
arXiv:1411.7379
Collaborators

Maria Hermanns
University of Cologne
Emmy-Noether junior research group

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

![Phase diagram for electronic materials](image)
**j=1/2 Mott insulators**

Most common **Iridium valence** \( \text{Ir}^{4+} (5d^5) \)

Octahedral crystal field

- \( e_g \) ~ 3eV
- \( t_{2g} \)

IrO\(_6\) cage

Spin-orbit coupling

\( \vec{L} \cdot \vec{\sigma} \)

Electronic correlations

\( j = 1/2 \)

\( j = 3/2 \)

\( U \)

**Why** are these spin-orbit entangled \( j=1/2 \) Mott insulators **interesting**?

**Sr\(_2\)IrO\(_4\)** exhibits cuprate-like magnetism

Superconductivity?  

**\((\text{Na, Li})_2\)IrO\(_3\)** exhibits Kitaev-like magnetism

Spin liquids?  
G. Jackeli, G. Khaliullin, J. Chaloupka  
PRL 102, 017205 (2009); PRL 105, 027204 (2010)
Family of Li$_2$IrO$_3$ compounds

hexagonal layers

Na$_2$IrO$_3$

α-Li$_2$IrO$_3$

see also RuCl$_3$

hyper-honeycomb

β-Li$_2$IrO$_3$

γ-Li$_2$IrO$_3$

and higher harmonics

hyper-octagon
Spin liquids in 3D Kitaev models

Spin-orbit entangled j=1/2 Mott insulators in \( \text{Li}_2\text{IrO}_3 \) realize two- and three-dimensional **Kitaev models**.

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

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

\[
\text{spin-1/2} \quad \sigma_j^{\gamma} = i b_j^{\gamma} c_j + Z_2 \text{ gauge field}
\]

Emergent Majorana fermions form **Majorana metals** reflecting the underlying lattice structure.
The hyper-honeycomb lattice

$\beta$-$\text{Li}_2\text{IrO}_3$

novel crystalline form of $\text{Li}_2\text{IrO}_3$

Hide Takagi’s group  
PRL (2015)

James Analytis’s group  
Nature Comm. (2014)

3D tricoordinated Ir lattice

space group $\text{Fdd}d$ (no. 70)

3D prints @ www.shapeways.com/designer/trebst
The hyper-octagon lattice

δ-Li$_2$IrO$_3$?

3D tricoordinated Ir lattice
space group I4$_1$32 (no. 214)
possibly crystalline form of Li$_2$IrO$_3$?
How do you find these lattices?

medial and premedial lattices

kagome lattice  \(\rightarrow\)  medial lattice  \(\leftarrow\)  premedial lattice  \(\rightarrow\)  honeycomb lattice
Medial and premedial lattices

The hyperkagome is **chiral**.

The hyperhoneycomb is **not chiral**!
Medial and premedial lattices

Medial lattice of triangles

hyperkagome \rightarrow \text{medial lattice of triangles} \rightarrow \text{hyperoctagon}

\text{square-octagon projection}

\text{square-octagon projection}
Hyperoctagon – space group symmetries

**four-fold skew** symmetry  
**three-fold** symmetry  
**two-fold** symmetry

space group \( \text{i4}_1\text{32} \) (no. 214)
A three-dimensional Kitaev model

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

\[ J_x + J_z + J_y = \text{const.} \]

**gapped** spin liquid

**gapless** spin liquid with Majorana Fermi surface

- \( xx \) – bond
- \( yy \) – bond
- \( zz \) – bond
Let’s solve this model

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

Step 2: Bond operators $\hat{u}_{jk} = i\alpha_j^\alpha \alpha_k^\alpha$ realize an emergent $\mathbb{Z}_2$ gauge field
Physics of the $\mathbb{Z}_2$ gauge field

$\mathbb{Z}_2$ gauge field is **static** due to presence of additional conserved quantities

Six fundamental **loop operators** (per unit cell) $W_l = \prod_{\langle \alpha, \beta \rangle \in l} \sigma_\alpha^{\gamma_{\alpha,\beta}} \sigma_\beta^{\gamma_{\alpha,\beta}}$

only two loop operators per unit cell are linearly independent

$W_{l_a} W_{l_b} W_{l_c} = 1$
Majorana Fermi surface

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

gapped spin liquid

gapless spin liquid with Majorana Fermi surface

$E(K)$

momentum $K$
The hyperoctagon Kitaev model exhibits a full two-dimensional Majorana Fermi surface.
Majorana Fermi surface

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

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

Symmetry relations

<table>
<thead>
<tr>
<th>Symmetry Type</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Particle-hole</strong></td>
<td>$\epsilon(k) = -\epsilon(-k)$</td>
</tr>
<tr>
<td><strong>Sublattice</strong></td>
<td>$\epsilon(k) = -\epsilon(k - k_0)$</td>
</tr>
<tr>
<td><strong>Time-reversal</strong></td>
<td>$\epsilon(k) = \epsilon(-k + k_0)$</td>
</tr>
<tr>
<td><strong>Inversion</strong></td>
<td>$\epsilon(k) = \epsilon(-k + k_0)$</td>
</tr>
</tbody>
</table>

$k_0$ is the reciprocal lattice vector of the translation vector of the sublattice.
Why is the Fermi surface stable?

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

\[
H = \begin{pmatrix}
0 & if(k) \\
-if^*(k) & 0
\end{pmatrix} \quad \text{complex-valued function} \quad E(k) = \pm |f(k)|
\]

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

\[
H = \begin{pmatrix}
0 & A \\
A^\dagger & 0
\end{pmatrix} \quad \text{complex matrix} \quad E(k) = \pm |\lambda_j(k)|
\]

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

\[
H = \begin{pmatrix}
0 & A \\
A^\dagger & \ddots & A \\
& \ddots & \ddots & \ddots \\
& & \ddots & A^\dagger & 0
\end{pmatrix} \quad \text{generic band Hamiltonian with TR symmetry}
\]

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

(conplex) fermion

conventional BCS instability

Generic form of the induced interactions between Majorana fermions

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

order parameter distribution

M. Hermanns, S. Trebst & A. Rosch, in preparation
Experimental signatures?

**correlation functions**

spin-spin correlations $\langle S_i^z S_j^z \rangle$ decay exponentially.

bond-bond energy correlations $\langle (S_i^z)^2 (S_j^z)^2 \rangle$ exhibit algebraic divergence on Majorana Fermi surface.

**specific heat**

<table>
<thead>
<tr>
<th>System</th>
<th>$C(T)$ Expression</th>
<th>$\gamma = C/T$ State</th>
</tr>
</thead>
<tbody>
<tr>
<td>U(1) spin liquid</td>
<td>$C(T) \propto T \ln(1/T)$</td>
<td>diverges</td>
</tr>
<tr>
<td>$Z_2$ spin liquid with spinon Fermi surface</td>
<td>$C(T) \propto T$</td>
<td>constant</td>
</tr>
<tr>
<td>$Z_2$ spin liquid with spinon Fermi line</td>
<td>$C(T) \propto T^2$</td>
<td>vanishes</td>
</tr>
</tbody>
</table>
Breaking time-reversal symmetry

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

hyper-octagon

Fermi surface

Fermi surface deforms

\( \kappa = 0.1 \)

\( \kappa = 0.5 \)

\( \kappa = 0.75 \)

hyper-honeycomb

Fermi line

Fermi line gaps out, but two Weyl nodes remain
Weyl physics – energy spectrum

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

\[ \kappa > 0 \]
Weyl nodes are sources or sinks of Berry flux

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

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

\( \kappa = 0.05 \)
Weyl physics – surface states

Evolution of **Weyl nodes** in the **bulk**

Evolution of **Fermi arcs** on the **surface**

\[ \kappa = \frac{1}{2} \]

\[ \kappa = \frac{1}{2} \sqrt{\frac{3}{5}} \approx 0.39 \]
Experimental signatures?

**specific heat**

Specific heat has bulk and surface contributions

\[
C(T) \sim a_{\text{bulk}} \cdot L^3 \cdot T^3 + a_{\text{surf}} \cdot L^2 \cdot T
\]

Could be distinguished via sample size variation.

**thermal Hall effect**

Applying a thermal gradient to the system, a net heat current perpendicular to the gradient arises due to the chiral nature of the surface modes.

Thermal Hall conductance given by

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

Spin-orbit entangled j=1/2 Mott insulators in Li$_2$IrO$_3$ realize two- and three-dimensional Kitaev models.

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

Kitaev models are paradigmatic examples for spin fractionalization.

$$\sigma_j^\gamma = i b_j^\gamma c_j$$  Majorana fermion + $\mathbb{Z}_2$ gauge field

Emergent Majorana fermions form a remarkably rich variety of Majorana metals reflecting the underlying lattice structure.