Time-Reversal Breaking Weyl Metals and Non-symmorphically Protected Fermions

Maia G. Vergniory

in collaboration with

Barry Bradlyn, Jennifer Cano, Zhijun Wang, Arthur Ernst, Evgueni Chulkov, Robert Cava, Claudia Felser and B. Andrei Bernevig
Outline

1. **Time-Reversal Breaking Weyl Metals**
   - Introduction-Motivation
   - Electronic and Magnetic Structure
   - Weyl Physics
   - Alloying and Fermi Arcs
   - Conclusions

2. **Non-symmorphically Protected Fermions**
   - Introduction
   - Non-symmorphic Space Groups
   - Topological Classification
   - Materials Search
   - Conclusions
Time-Reversal Breaking Weyls

- Weyls fermions are described by massless Weyl equation with fixed chirality

\[
H_D = E_0 \mathcal{I} + \mathbf{v}_0 \cdot \mathbf{q} \mathcal{I} + \sum_{i=1}^{3} \mathbf{v}_i \cdot \mathbf{q} \sigma_i
\]

\[
\mathbf{q} = \mathbf{k} - \mathbf{k}_0
\]

\[
\Delta E = \mathbf{v}_0 \cdot \mathbf{q} \pm \sqrt{\sum_{i=1}^{3} (\mathbf{v}_i \cdot \mathbf{q})^2}
\]

- We can also assign a chirality: \( c = \text{sgn}(\mathbf{v}_1 \cdot \mathbf{v}_2 \times \mathbf{v}_3) \)

- Stable in 3D: Perturbation can shift the position of the crossing point but it cannot remove it.
• They act like magnetic monopoles in momentum space whose charge is given by the chirality

The Berry connection, is defined as

\[ \vec{A}(\vec{k}) = \sum_n \langle n\,\vec{k}|\vec{\nabla}_k|n\,\vec{k}\rangle \]

Can be consider as the magnetic field of momentum space

\[ \vec{B}(\vec{k}) = \vec{\nabla}_k \times \vec{A}(\vec{k}) \]

Then these Weyls points are just like magnetic monopoles in momentum space

\[ \vec{\nabla}_k \vec{B}(\vec{k}) = \pm \delta(\vec{k} - \vec{k}_0) \]
• Weyl nodes appear in multiples of 2, with time reversal symmetry this number raises to 4

The TaAs family presents 24 Weyl nodes, due to several others mirror symmetries

Rise complicated transport and spectroscopic properties

Motivation : Look for Time-Reversal breaking Weyls
• We propose candidates for Weyl metals that are XCo2Z (X=V,Zr,Ti,Nb,Hf; Z=Si,Ge,Sn), VCo2Al and VCo2Ga
  
  ![Diagram of crystal structure]

  sg 225, C₄ and I

  • They follow the Slater-Pauling rule: \( m = N_v - 24 \)

  • Half metallic magnetism with 2 \( u_B \) per formula unit

  • In the following we are gonna focus in ZrCo2Sn that has been synthesized experimentally

Electronic structure:

(1) On site Coulomb interaction

ANISOTROPY
easy axis [110]

(2) SOC vs NSOC

GGA+U PBE
Symmetry analysis and Weyls physics

(a) Energy-momentum dispersion near Fermi surface with SOC.

(b) Surface Fermi arc and inversion point in the inset. (d) Weyl points emerge with SOC.

The [110] magnetism, opening a small gap in the 3D system: the product of the inversion eigenvalues of the occupied bands at the inversion symmetric points is signaling the presence of an odd number of pairs of Weyls. The coordinates of these WPs (W1, W2), related by inversion symmetry configuration), as they can be moved by all the three generators of the magnetism group. As a result, the position of the WPs is of a trivial nature. The color code represents the Wilson-loop method applied on a sphere (illustrated as dashed circles) enclosing a Weyl point. The filled (unfilled) circles indicate Chern number +1 (−1).

Upon introducing SOC, with a magnetization along the [110] direction, the mirror symmetries related by inversion must be broken. Hence, the (110) mirror plane breaks up into other mirror planes. As these Weyls are generic points without any symmetry protection, their Chern numbers can be calculated.

In conclusion we have predicted theoretically that a Hf-CoSn solid solution has two (110) Weyl nodes under SOC. Other four Weyls are found, which are related to each other by inversion. The coordinates of the other Weyl points are related to the ones of SOC would form nodal lines.

In (b) we plot the surface spectral function for the (001)-surface of (1,-1,0) plane =3. By inversion we find two Weyl points related by (110) mirror plane. As these Weyls are generic points without any symmetry protection, their Chern numbers can be calculated.

We have plotted the surface spectral function for the (001)-surface at 0.5 eV. Only the bulk projections of the unalloyed compound. The WPs Sn, to ZrCo and Nb and showed that these two Weyls can be shifted to the same energy level, thus reducing the gap. To determine the spontaneous magnetization, Departamento de Educaci´on, Universidades e Investigaciones, Steinmetz Center for research on quantum phenomena, Universidad Nacional de Colombia, and Schmidt Fellowship.

The coordinates of the Weyl points are given in Table I. After carefully checking other possible initial points as depicted in Fig. 2(b). As the energy level of Weyl points is interrupted by the resid-

<table>
<thead>
<tr>
<th>Weyl points</th>
<th>coordinates</th>
<th>Chern number $E - E_F$ (eV)</th>
</tr>
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<tbody>
<tr>
<td>W</td>
<td>$(0.334, 0.334, 0)$</td>
<td>$-1$</td>
</tr>
<tr>
<td>W1</td>
<td>$(0.58, -0.0005, 0)$</td>
<td>$+1$</td>
</tr>
<tr>
<td>W2</td>
<td>$(0.40, 0.001, ±0.28)$</td>
<td>$-1$</td>
</tr>
</tbody>
</table>

Chern number of (1,-1,0) plane =3

$W$: C2_{110}

$W_1$: I and C2_{110}

$W_2$: generic (no stable)

NSOC: $M_X, M_Y, M_Z$

SOC
Coherent Potential Approximation

Based on scattering theory

\[ T_C(E) = \sum_i c_i T_i(E). \]

CPA equation for a binary alloy:

\[ c_A G_A + c_B G_B = G_C \]

\[
\begin{bmatrix}
  C & C & C \\
  C & A & C \\
  C & C & C
\end{bmatrix}
+ c_A
\begin{bmatrix}
  C & C & C \\
  C & B & C \\
  C & C & C
\end{bmatrix}
\]

\[
\begin{bmatrix}
  C & C & C \\
  C & C & C \\
  C & C & C
\end{bmatrix}
\]
(001 surface)  Fermi Arcs

![Fermi Arcs](image-url)
The diagram shows the electronic band structure for various compounds, including HfCo$_2$Sn, TiCo$_2$Ge, TiCo$_2$Si, TiCo$_2$Sn, VCo$_2$Al, and VCo$_2$Ga. The x-axis represents the momentum points (Γ, L, W, K, X), and the y-axis represents the energy relative to the Fermi level (E-EF). The color bar on the right indicates the orbital localization.
**Ti_{0.9}V_{0.1}Co_{2}Sn**

![Band Structures](image)

- **HfCo_{2}Sn**
- **TiCo_{2}Ge**
- **TiCo_{2}Si**
- **TiCo_{2}Sn**
- **VC_{2}Al**
- **VC_{2}Ga**

** Orbital Localization**

![Color Scale](image)
Conclusions

• We have predicted theoretically that a new family of Co-base Heuslers realize Weyls systems

• By means of ab initio calculations we have determined the easy axis of ZrCo2Sn to be [110]

• Symmetry analysis shows there are 2 Weyls separated in momentum space of the order of $2\pi$

• We doped the compound to shift the Weyls to Fermi level

• We have also obtained the Fermi arc structure of this materials

arXiv:1603.00479v1
see also Chandra Shekhar et al. arXiv:1604.01641
Non-symmorphically protected fermions

1. The existence of 3-fold and higher degeneracies has been known from band theory

\textit{The Mathematical Theory of Symmetry in Solids}
\textit{Irreducible representations in space groups}

2. The topological classification of these degeneracies is still missing

3. We will look for irreducible representations at high symmetry points, being the dimension of these irreps the number of bands that meet at high symmetry point.
Degeneracy may occur at the Fermi point if they lack inversion symmetry. Energy bands away from the Fermi level correspond to the number of bands that meet at a Fermi point. Since we are interested in fermions with spin-orbit coupling, we consider only the doubly-degenerate representations of the fermion type. The overall energy scale is sufficiently small to not require approximations from the others in the above table.

### Table I

<table>
<thead>
<tr>
<th>SG</th>
<th>La</th>
<th>k</th>
<th>d</th>
<th>Generators</th>
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<tbody>
<tr>
<td>198</td>
<td>cP</td>
<td>R</td>
<td>6</td>
<td>{C_{3,111}</td>
</tr>
<tr>
<td>199</td>
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<td>P</td>
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<td>{C_{3,111}</td>
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<tr>
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<td>H</td>
<td>8</td>
<td>{C_{4z}</td>
</tr>
</tbody>
</table>

**cP:** cubic primitive  
**cB:** cubic body-centered  
**tP:** tetragonal primitive

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All space groups include non-symmorphic generators.
- 3-fold degeneracies at P point in BZ

- P is non TR invariant

- 3fold at -P

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cP: cubic primitive
CB: cubic body-centered
tP: tetragonal primitive

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<td>198</td>
<td>cP</td>
<td>R</td>
<td>6</td>
<td>{C_{3,111}^{-}{010}, {C_{2x}\quad 1\over 2 \over 2 \over 0}, {C_{2y}\quad 0\over 3 \over 1 \over 2 \over 2}}</td>
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<td>P</td>
<td>3</td>
<td>{C_{3,111}^{-}{101}, {C_{2x}\quad 1\over 2 \over 2 \over 0}, {C_{2y}\quad 0\over 1 \over 1 \over 2 \over 2}}</td>
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<td>6</td>
<td>{C_{3,111}^{-}{010}, {C_{2x}\quad 1\over 2 \over 2 \over 0}, {C_{2y}\quad 0\over 3 \over 1 \over 2 \over 2}, {I}{000}}</td>
</tr>
<tr>
<td>206</td>
<td>cB</td>
<td>P</td>
<td>6</td>
<td>{C_{3,111}^{-}{101}, {C_{2x}\quad 1\over 2 \over 2 \over 0}, {C_{2y}\quad 0\over 1 \over 1 \over 2 \over 2}}</td>
</tr>
<tr>
<td>212</td>
<td>cP</td>
<td>R</td>
<td>6</td>
<td>{C_{2x}\quad 1\over 2 \over 2 \over 0}, {C_{2y}\quad 0\over 1 \over 1 \over 2 \over 2}, {C_{3,111}^{-}{000}, {C_{2,110}\quad 1\over 1 \over 1 \over 1 \over 4 \over 4 }}</td>
</tr>
<tr>
<td>213</td>
<td>cP</td>
<td>R</td>
<td>6</td>
<td>{C_{2x}\quad 1\over 2 \over 2 \over 0}, {C_{2y}\quad 0\over 1 \over 1 \over 2 \over 2}, {C_{3,111}^{-}{000}, {C_{2,110}\quad 3\over 3 \over 3 \over 3 \over 4 \over 4 }}</td>
</tr>
<tr>
<td>214</td>
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<td>P</td>
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<td>{C_{3,111}^{-}{101}, {C_{2x}\quad 1\over 2 \over 2 \over 0}, {C_{2y}\quad 0\over 1 \over 1 \over 2 \over 2}}</td>
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<tr>
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<td>P</td>
<td>3</td>
<td>{C_{3,111}^{-}{01\over 2 \over 2 \over 2}, {C_{2y}\quad 0\over 1 \over 1 \over 2 \over 2}, {C_{2x}\quad 3\over 3 \over 2 \over 0}, {IC_{4x}\quad 1\over 1 \over 11}}</td>
</tr>
<tr>
<td>230</td>
<td>cB</td>
<td>P</td>
<td>6</td>
<td>{C_{3,111}^{-}{01\over 2 \over 2 \over 2}, {C_{2y}\quad 0\over 1 \over 1 \over 2 \over 2}, {C_{2x}\quad 3\over 3 \over 2 \over 0}, {IC_{4x}\quad 1\over 1 \over 11}}</td>
</tr>
<tr>
<td>130</td>
<td>tP</td>
<td>A</td>
<td>8</td>
<td>{C_{4x}\quad 0\over 0 \over 0 \over 0}, {\sigma_{xy}\quad 0\over 1 \over 0 \over 2 \over 2}{I}{1\over 1 \over 1 \over 2 \over 2}}</td>
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<td>{C_{2x}\quad 0\over 0 \over 0 \over 0}, {C_{2y}\quad 0\over 0 \over 0 \over 0}, {C_{3,111}^{-}{001}, {\sigma_{xy}\quad 1\over 1 \over 1 \over 2 \over 2}}</td>
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<tr>
<td>222</td>
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<td>R</td>
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<td>{C_{4x}\quad 0\over 0 \over 0 \over 0}, {C_{2x}\quad 0\over 0 \over 0 \over 0}, {C_{3,111}^{-}{010}, {I}{1\over 1 \over 1 \over 2 \over 2}}</td>
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<th>Bravais lattice</th>
<th>Lattice vectors</th>
<th>Reciprocal lattice vectors</th>
</tr>
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<tbody>
<tr>
<td>Primitive cubic</td>
<td>(a, 0, 0), (0, a, 0), (0, 0, a)</td>
<td>2\pi { 0, 1, 0 }, 2\pi { 0, 1, 0 }, 2\pi { 0, 0, 1 }</td>
</tr>
<tr>
<td>Body-centered cubic</td>
<td>2\pi { -1, 1, 1 }, 2\pi { -1, 1, 1 }, 2\pi { -1, 1, 1 }</td>
<td>2\pi { 0, 0, 1 }, 2\pi { 0, 1, 0 }, 2\pi { 1, 0, 0 }</td>
</tr>
<tr>
<td>Primitive tetragonal</td>
<td>(a, 0, 0), (0, a, 0), (0, 0, c)</td>
<td>2\pi { 1, 0, 0 }, 2\pi { 0, 1, 0 }, 2\pi { 0, 0, 1 }</td>
</tr>
</tbody>
</table>

TABLE I. Lattice and reciprocal lattice vectors
In addition, SGs 222 are in fact necessary ingredients for the 3-, 6- and 8-band crossings (irreps) of the (little) group of lattice symmetries which do not change the size of the 3d irrep, are also present. Consider the case when the little group at a particular high-symmetry point has three generators, which display either a 3- or 6-fold rotation about the z-axis. Similarly, there exists a 3d irrep. Before proving this, we comment that Eq. (S4) places tight constraints on the operators: in particular, we will first find the little group without time reversal symmetry, where it will display either a 3- or 6-fold rotation in the full symmetry group. 

In the presence of TR symmetry, six space groups can be closed (i.e., they cannot be made to open by a two-fold screw rotation in the full symmetry group). These are space groups 198, 205, 206, 212, 213 and 214. Full details of the construction of the most general Hamiltonian consistent with the cubic and icosahedral symmetries, SGs 218 and SG 220. These, as shown below, the resulting fermions fall into distinct sectors. Here we are exploring fermions beyond the Weyl and Dirac points that the little group at the prescribed point has an irrep of the correct degeneracy to support the band crossings (since we are interested in 3-, 6-, and 8-band crossings, we do not include in our search 4d irreps that remain the same as in the absence of TR symmetry). There exists a possibility for unique fermions with an arbitrary number of bands, which we now illustrate 

In this appendix, we prove a sufficient condition for a Fermi arc to exist, where the arc must be an isolated line segment. Similarly, we prove that the Fermi arc is necessarily closed. As a simple, illustrative example, we consider the case where the Fermi arc connects two adjacent high-symmetry points in the Brillouin zone.

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<tr>
<td>Body-centered cubic</td>
<td>(\frac{2\pi}{a}(-1, 1, 1), \frac{2\pi}{a}(1, -1, 1), \frac{2\pi}{a}(1, 1, -1))</td>
<td>(\frac{2\pi}{a}(0, 1, 1), \frac{2\pi}{a}(1, 0, 1), \frac{2\pi}{a}(1, 1, 0))</td>
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**SG cP**: cubic primitive  
**SG cB**: cubic body-centered  
**SG tP**: tetragonal primitive
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<tr>
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<td>(\frac{\pi}{2}(-1,1,1), \frac{\pi}{2}(1,-1,1), \frac{\pi}{2}(1,1,-1))</td>
<td>(\frac{\pi}{a}(0,1,1), \frac{\pi}{a}(1,0,1), \frac{\pi}{a}(1,1,0))</td>
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<td>Primitive tetragonal</td>
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<td>(\frac{\pi}{a}(1,0,0), \frac{\pi}{a}(0,1,0), \frac{\pi}{a}(0,0,1))</td>
</tr>
</tbody>
</table>

**TABLE I.** Lattice and reciprocal lattice vectors.
Low-energy effective Hamiltonians consistent with the symmetries of the little group

A special case: 3-fold Degeneracy (in several symmetry groups)

\[ \mathbf{k} \cdot \mathbf{S} \]

Spin 1 matrices

In SPG-214 not needed to stabilize the fermion: New Chiral Anomaly and anomalous transport

(a) SGs 199 and 214
3-fold, 6-fold, 8-fold Crossings: All Different Fermions

For 8-fold see also Benjamin J. Wieder, Youngkuk Kim, A. M. Rappe, C. L. Kane, arXiv:1512.00074

k dot p models

3-fold degeneracy,
Line-nodes on $|\delta k_x| = |\delta k_y| = |\delta k_z|$ (b) SG 220

6-fold degeneracy,
Surface-nodes on $\delta k_i = 0$ of the BZ (c) SGs 198, 212 and 213

4-fold degenerate at corner of BZ: Dirac Line Nodes (a) SGs 130 and 135
The Different Classes of New Fermions: 3, 6, 8 Fold

AsPdS, K3BiTe3
M3(XS)2 where M = Ni, Pd, X = Pb, Bi
A2 B2 O3 (A = K, Rb, B = Ge, Sn, Pb)
PdSb2

CsSn

A4Pn3 where A = Ca, Sr, Ba, Eu and R = La, Ce and Pn = pnictogen (As, Sb, Bi)
MPd3S4 where M = rare earth (see La very close to the Fermi level)
X3Y where X = Nb, Ta and Y = A−IV; A−V (Sb for ex)
Th3P4, PdBi2O4, AuBi2O5, WO3, CsSn, CsSi

FeS2
PtP2
KBiF6
Li2(Pd/Pt)3B
Re2(W/Mo)3C
La3PbI3
Conclusions

• We have given all possible non-symmorphic space groups where 3fold, 6fold and 8 fold degeneracies can occur

• We have also given some possible experimental signatures

• A list of potential candidates displaying these properties has been reported.

arXiv:1603.03093v2