Symmetry Protected Topological Insulators and Semimetals

I. Introduction: Many examples of topological band phenomena

II. Recent developments:

- Line node semimetal

- 2D Dirac semimetal
  Young, Kane PRL 115, 126803 (2015).

- Double Dirac semimetal
  Wieder, Kim, Rappe, Kane, PRL 116, 186402 (2016).

Thanks to:
Gene Mele, Ben Wieder U. Penn. Physics Dept
Andrew Rappe, Youngkuk Kim U. Penn. Chemistry Dept.
Steve Young Naval Research Lab
“Single Particle” Topological Phases

Bulk Topological Invariant ↔ Boundary Topological Modes

2D  Integer quantum Hall effect

Bulk: Integer Chern invariant
Boundary: Chiral edge states

Topology + Time reversal symmetry

2D  topological insulator

Bulk: $\mathbb{Z}_2$ invariant
Boundary: Helical edge states

3D  topological insulator

Bulk: $\mathbb{Z}_2$ invariant
Boundary: Helical surface state

Topology + Particle-Hole symmetry

1D Topological Superconductor

Bulk: $\mathbb{Z}_2$ invariant
Boundary: Majorana zero mode

Quantum Hall state $\nu=1$

Quantum spin Hall insulator

3D TI

1D topo. SC
Periodic Table of Topological Insulators and Superconductors

Anti-Unitary Symmetries:
- Time Reversal: \( \Theta H(k)\Theta^{-1} = +H(-k) \); \( \Theta^2 = \pm 1 \)
- Particle - Hole: \( \Xi H(k)\Xi^{-1} = -H(-k) \); \( \Xi^2 = \pm 1 \)

Unitary (chiral) symmetry: \( \Pi H(k)\Pi^{-1} = -H(k) \); \( \Pi = \Theta \Xi \)

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>A</th>
<th>AIII</th>
<th>AI</th>
<th>BDI</th>
<th>D</th>
<th>DIII</th>
<th>AII</th>
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<td>1</td>
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Kitaev, 2008
Schnyder, Ryu, Furusaki, Ludwig 2008

T broken insulator  ➔  T broken superconductor  ➔  T invariant superconductor  ➔  T invariant insulator ➔
Topological Crystalline Phases

Crystal symmetry introduces new topological states

Weak Topological Insulator

Layered 2D topo. insulator
Protected by translation symmetry $T_z$
3 $Z_2$ “Miller Indices”

Topological Crystalline Insulator

Protected by Mirror symmetry $M_z$
Mirror Chern Number defined in mirror invariant plane:
$M_z = \pm i$ : $n = n_{+i} - n_{-i}$

Surface states protected by crystal symmetry can remain even when symmetry is violated.

eg weak TI :

helical mode on domain wall

Average symmetry: absence of localization
Topological (semi) metals

Topological band classification without symmetries, for \( k \in S_d = \partial B_{d+1} \)

<table>
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<th>d</th>
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<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
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<td>0</td>
<td>( \mathbb{Z} )</td>
<td>0</td>
<td>( \mathbb{Z} )</td>
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Fermi Liquid:

The Fermi surface of a metal is “topological”

\[
\begin{align*}
\partial B_1 &= S_0 \\
E_F &= \text{gap}
\end{align*}
\]

Weyl semimetal:

\[
\begin{align*}
\partial B_3 &= S_2 \\
H &\sim \mathbf{v} \cdot \mathbf{k}
\end{align*}
\]

\[
\begin{align*}
n_0 &\text{ characterizes } k \in \partial B_1 = S_0 \\
&= \# \text{ Fermi crossings in } B_1
\end{align*}
\]

\[
\begin{align*}
n_2 &\text{ (Chern no.) characterizes } k \in \partial B_3 = S_2 \\
&= \# \text{ Weyl points in } B_3
\end{align*}
\]

\[
\begin{align*}
H &\sim \mathbf{v} \vec{\sigma} \cdot \mathbf{k}
\end{align*}
\]
Symmetry Protected Topological Semimetal

Prototype example: Graphene

Dirac points protected by
- Inversion symmetry (P)
- Time reversal symmetry (T)
- Absence of spin-orbit ($T^2 = +1$)

Berry Phase: $\gamma_C = 0$ or $\pi$
Loop C: 1 parameter family $H(\mathbf{k})$ in class AI:

$$[H(\mathbf{k}), PT] = 0$$

$$d = 0 \text{ - } 1 \mod 8$$

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<thead>
<tr>
<th>$d$</th>
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<th>-1</th>
<th>0</th>
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<td>$Z_2$</td>
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</table>

3D Generalizations:

Weyl semimetal: topologically protected but “symmetry prevented”. Must break T or P.

3D Dirac line node semimetal

3D Dirac semimetal: 4 fold degenerate Dirac point protected by crystal symmetry
- “topological” Dirac semimetal
- “non-symmorphic Dirac semimetal”
3D Dirac Line Node Semimetal

Kim, Wieder, Kane, Rappe, PRL 115, 036806 (2015)

In absence of spin-orbit, P and T \((T^2 = +1)\) allows symmetry protected line nodes.

\[ C : \text{Berry phase } 0, \pi \]

Z\(_2\) Topological Invariants:

\[ N_{abcd} = \# \text{DLN passing through } PT \text{ invariant plane spanned by } \Gamma_{a,b,c,d} \]

\[ (-1)^{N_{abcd}} = \xi_a \xi_b \xi_c \xi_d \]

\[ \xi_a = \prod_n \xi_n(\Gamma_a) \]

Similar to invariants for TI and WTI with spin orbit

Band Inversion:

Inversion of opposite parity bands leads to a \textbf{Dirac Circle}
Realizations


Ca$_3$P$_2$  Xie, Schoop, Seibel, Gibson, Xi, Cava, APL Mat. 3, 083602 (2015).


Cu$_3$N: Uninverted insulator  
Band inversion can be controlled by doping with transition metal atoms X
Nearly Flat Surface Bands

- Curvature of surface band depends on effective masses: \( \frac{1}{m_{\text{surf}}} = \frac{1}{m_c} - \frac{1}{m_v} \)
- Surface is electrically neutral when surface band is half filled.
- Interesting platform for strong correlation physics.

\[ \text{Cu}_3\text{N Zn} \]

slab calculation:
More classes of Line Node semimetals:

Nodal rings protected by P,T that can not be shrunk to zero (weak spin orbit)

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<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Fang, Chen, Kee and Fu, PRB 92, 081201 (2015).

Nodal rings protected by mirror symmetries (weak spin orbit)

Line degeneracies connecting multiple bands are linked

Weng, Fang, Fang, Bernevig, Dai, PRX 5, 011029 (2015)

Doubly degenerate line nodes (strong spin orbit) Impossible to ‘uninvert’: non-symmorphic symmetry

Fang, Chen, Kee and Fu, PRB 92, 081201 (2015).
“Topological” Dirac Semimetal

Dirac Points on a line via band inversion

- Consequence of band inversion in presence of spin orbit and C\textsubscript{3} rotational symmetry
- Located on C\textsubscript{3} rotation invariant line in Brillouin zone due to band inversion of opposite parity states in presence of spin orbit and C\textsubscript{3} rotational symmetry

Almost a topological insulator

- Opening a gap by lowering symmetry leads to TI
- Surface states similar to topological insulator

Realizations

- Predicted and observed in Na\textsubscript{3}Bi and Cd\textsubscript{2}As\textsubscript{3}

Wang, Sun, Chen, Franchini, Xu, Weng, PRB ‘12
Wang, Weng, Wu, Dai, and Fang, PRB ‘13

Borisenko, Gibson, Evtushinsky, Zabolotnyy, Buchner, Cava, PRL 14
“Non-Symmorphic” Dirac Semimetal

Symmetry Protected Dirac Point

• Located at T invariant point X on Brillouin zone boundary

• Filling enforced semimetal
  All states at X are fourfold degenerate.
  Groups of 4 bands “stick together”

• Protected (and guaranteed) by non-symmorphic symmetry

• Symmetry tuned to transition between topological and trivial insulator: Lowering symmetry (e.g. by compressive or tensile strain) can lead to either TI or I

Realizations:

• Toy model: diamond lattice

  Fu, Kane, Mele, PRL ’07

• Predicted (not yet observed) in BiO₂, BiZnSiO₄

  Young, Zaheer, Teo, Kane, Mele, Rappe PRL ’12
  Steinberg, Young, Zaheer, Kane, Mele, Rappe PRL ’14
Non-Symmorphic Symmetry

Simplest examples: Glide Plane, Screw Axis

- \( \{g|t\} \): point group operation \( g \) + fractional translation \( t \)
- e.g. \( d=1 \) with screw symmetry \( \{ C_2 | a/2 \} \)
- Guarantees bands “stick together”
- For \( k \) on \( g \) invariant line (plane), \( \{ g | t \} u_k^\pm = \pm \lambda e^{ik \cdot t} \) with \( e^{iG \cdot t} = -1 \)

No additional symmetries:
- Two bands cross between \( k \) and \( k+G \) \( (G=2\pi/a) \)
Non-Symmorphic Symmetry

Simplest examples: Glide Plane, Screw Axis

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- Two bands cross between \( k \) and \( k+G \) \( (G=2\pi/a) \)

Time reversal \( (T^2=+1) \):
- Crossing at zone boundary \( G/2 \)
Non-Symmorphic Symmetry

Simplest examples: Glide Plane, Screw Axis

- \( \{g|t\} : \) point group operation \( g + \) fractional translation \( t \)
- e.g. \( d=1 \) with screw symmetry  \( \{ C_2 \mid a/2 \} \)
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No additional symmetries:

- Two bands cross between \( k \) and \( k+G \) (\( G=2\pi/a \))

Time reversal (\( T^2=+1 \)):
- Crossing at zone boundary \( G/2 \)

Time reversal (\( T^2=-1 \)):
- Kramers degeneracies split by spin-orbit
- Four bands cross between \( k \) and \( k+G \)
Non-Symmorphic Symmetry

Simplest examples: Glide Plane, Screw Axis

- \{g|t\} : point group operation g + fractional translation t
- e.g. d=1 with screw symmetry \{ C_2 | a/2 \}
- Guarantees bands “stick together”
- For k on g invariant line (plane), \( \{ g | t \} u_k^{\pm} = \pm \lambda e^{i k \cdot t} \), with \( e^{i G \cdot t} = -1 \)

No additional symmetries:

- Two bands cross between k and k+G (G=2\pi/a)

Time reversal (T^2=+1):

- Crossing at zone boundary G/2

Time reversal (T^2=-1):

- Kramers degeneracies split by spin-orbit
- Four bands cross between k and k+G

Inversion P and T (T^2=-1):

- Degenerate crossing at zone boundary G/2
Filling Enforced Semimetals with Strong Interactions

Watanabe, Po, Vishwanath, Zaletel, PNAS ‘15

Treat crystal with twisted periodic boundary conditions.

e.g. $d=1$:

- $\# \text{unit cells} = N + \frac{1}{2}$
- band filling $\nu = \#e/\text{cell}$
- $\#e = 2M$ necessary for energy gap (Kramers’ thm)
- $2M = \nu (N + \frac{1}{2})$ \textbf{band filling = multiple of 4 required for insulator}

Generalization to 3D:

- Put crystal on one of 10 flat 3D “Bieberbach manifolds”
- Determines WPVZ bound on band filling for all 230 space groups
2D Dirac Semimetal


- 2D Dirac points with strong spin orbit interaction
- Symmetry tuned to transition between 2D Topological and Trivial Insulator
- Toy model: Deformed Square lattice

Undeformed square lattice (doubled unit cell)
2D Dirac Semimetal


- 2D Dirac points with strong spin orbit interaction
- Symmetry tuned to transition between 2D Topological and Trivial Insulator
- Toy model: Deformed Square lattice

Out of plane deformation: allows 2nd neighbor spin-orbit \( i\lambda_{so} \vec{\sigma} \cdot (\vec{d}_1 \times \vec{d}_2) \)

Non-symmorphic screw and glide symmetries

3 Dirac Points
Symmetry Inequivalent
2D Dirac Semimetal


• 2D Dirac points with strong spin orbit interaction

• Symmetry tuned to transition between 2D Topological and Trivial Insulator

• Toy model: Deformed Square lattice

Lower symmetry further:

Two equivalent Dirac points protected by \(\{C_{2x} \mid \hat{x}\}\)

2 Dirac Points
Symmetry Equivalent
Iridium oxide superlattice grown along [001] with certain rotations of IrO$_6$ octahedra.
Double Dirac Semimetal

3D Semimetal with 8-fold degenerate double Dirac point

Wieder, Kim, Rappe, Kane, PRL 116, 186402 (2016).

7 of the 230 space groups host double Dirac points

Space groups 130, 135* : filling enforced semimetal.

Tight binding models:

<table>
<thead>
<tr>
<th>Space Group</th>
<th>K</th>
<th>Reps at K</th>
</tr>
</thead>
<tbody>
<tr>
<td>130 $P4/ncc$</td>
<td>$\Gamma D^8_{4h}$</td>
<td>$A$</td>
</tr>
<tr>
<td>135 $P4_2/mbc$</td>
<td>$\Gamma D^{13}_{4h}$</td>
<td>$A$</td>
</tr>
<tr>
<td>218 $P43m$</td>
<td>$\Gamma c T^4_{d}$</td>
<td>$R$</td>
</tr>
<tr>
<td>220 $P43d$</td>
<td>$\Gamma u T^6_{d}$</td>
<td>$H$</td>
</tr>
<tr>
<td>222 $Pn3n$</td>
<td>$\Gamma c O^2_{h}$</td>
<td>$R$</td>
</tr>
<tr>
<td>223 $Pm3n$</td>
<td>$\Gamma c O^2_{h}$</td>
<td>$R$</td>
</tr>
<tr>
<td>230 $Ia3d$</td>
<td>$\Gamma c O^{10}_{h}$</td>
<td>$H$</td>
</tr>
</tbody>
</table>
Features of the Double Dirac Point

Multiple T–invariant mass terms introduced by lowering symmetry

\[ H = \gamma_x k_x + \gamma_y k_y + \gamma_z k_z + m_{B_{1g}} \Gamma_1 + m_{B_{2g}} \Gamma_2 + m_{A_{2g}} \Gamma_3 \]

Both topological and trivial Insulators can be created with uniaxial compression

Topological line defects host 1D helical modes
Towards Materials Realization:

Known materials hosting double Dirac points:

130: Bi$_2$AuO$_5$
135: Pb$_3$O$_4$
223: GaMo$_3$
Strong Interactions

Space group 130:

- WPVZ bound = 8
- Filling enforced semimetal even for strong interactions
- Single DPs along RZ in addition to double DP at A.

Space group 135:

- WPVZ bound = 4
- Band Theory and WPVZ bound disagree
- Could there be an insulator for strong interactions?
Conclusion

Topological Band Phenomena are both Rich and Feasible

Dirac Semimetals come in two varieties

• “topological” vs non-symmorphic Dirac semimetals

2D Dirac Semimetal

• Protected by non-symmorphic symmetry
• At intersection between topological and trivial insulator

3D Dirac line node semimetal

• Driven by band inversion in absence of spin-orbit
• Dirac Circle
• Many variants

Double Dirac semimetal

• Hosted by certain space groups
• Multiple mass terms give new handle for topological states
• Target for band structure engineering
• Interesting question for strong interactions