Topography and symmetry in topological semimetals: tutorial

Shuichi Murakami
Department of Physics, Tokyo Institute of Technology
TIES, Tokyo Institute of Technology
CREST, JST

(a) Weyl semimetal
(b) Dirac semimetal
(c) Nodal-line semimetal

Weyl node
Dirac node
Nodal line

No Kramers degeneracy
Kramers degeneracy
Various topological phases in electronic systems

(1) Bulk is an insulator: “topological insulator” in a broader sense

(1-1) Integer quantum Hall system (Chern insulator)
(1-2) topological insulator
(1-3) topological crystalline insulator

......

(2) Bulk is a metal: topological metal (topological semimetal)

(2-1) Dirac semimetal
(2-2) Weyl semimetal
(2-3) nodal-line semimetal

......
Band degeneracy occurs

- at high-symmetry points/lines
- At other general points, bands usually **anticross**.

→ Nevertheless, in some cases, anticrossing does not happen, and band degeneracy occurs at general k points

= **topological metal (topological semimetal)**

**(2) Bulk is a metal: topological metal (topological semimetal)**

- **Weyl semimetal**: No Kramers degeneracy
- **Dirac semimetal**: Kramers degeneracy
- **Nodal-line semimetal**: Nodal line
Degeneracies in electronic states in crystals

\[ H(\vec{k}) \rightarrow E_1(\vec{k}) , E_2(\vec{k}) , E_3(\vec{k}) , .... \]

- When do degeneracies appear?
- What conditions are required?
\[ E_n(\vec{k}) = E_m(\vec{k}) \]

**Case 1: symmetry**: High-dimensional irreducible representation of a little group

At high-symmetry points/lines, there might be degeneracies due to symmetry

https://www.tf.uni-kiel.de/matwis/amat/semi_en/kap_2/backbone/r2_1_5.html
Degeneracies in electronic states in crystals

Case 2: topology  “accidental degeneracy”

Wigner, Herring, Volovik, Murakami, ....

Simple example: general 2*2 Hamiltonian in k space

\[
H(\vec{k}) = \begin{pmatrix}
  a(\vec{k}) & b(\vec{k}) \\
  b^*(\vec{k}) & c(\vec{k})
\end{pmatrix}
\]

\[a(\vec{k}), c(\vec{k}) : \text{real}\]
\[b(\vec{k}) : \text{complex}\]

\[
\rightarrow E(\vec{k}) = \frac{a + c}{2} \pm \sqrt{\left(\frac{a - c}{2}\right)^2 + |b|^2}
\]

Degeneracy appears when

\[
\begin{cases}
a(\vec{k}) = c(\vec{k}) \\
\text{Re } b(\vec{k}) = 0 \\
\text{Im } b(\vec{k}) = 0
\end{cases}
\]

In 3D k space: they may have solutions
In 2D k space: they have no solutions (unless there are additional constraints)

Dimensionality matters!
Degeneracies in electronic states in crystals

Case 2: topology

\[ H(\vec{k}) = \begin{pmatrix} a(\vec{k}) & b(\vec{k}) \\ b^*(\vec{k}) & c(\vec{k}) \end{pmatrix} \rightarrow E(\vec{k}) = \frac{a + c}{2} \pm \sqrt{\left(\frac{a - c}{2}\right)^2 + |b|^2} \]

Degeneracy appears when

\[ \begin{cases} a(\vec{k}) = c(\vec{k}) \\ \text{Re} b(\vec{k}) = 0 \\ \text{Im} b(\vec{k}) = 0 \end{cases} \]

In 3D \( k \) space: they may have solutions:
isolated points in \( k \) space: \( k = k_0 \)

Apart from this degeneracy point at \( k_0 \),
energy separation between two bands is linear in wavevector
= forming a Dirac cone
\( k = k_0 \) : Weyl node (: not necessarily at high-symmetry point)

Note: this Weyl node cannot be removed perturbatively!
i.e. topologically stable
\[ H(\vec{k}) \rightarrow H(\vec{k}) + \delta H(\vec{k}) \]
Weyl nodes in 3D is topologically stable

3D Weyl node:

\[ H(\vec{k},m) = k_x \sigma_x + k_y \sigma_y + k_z \sigma_z + m \sigma_z \]

\[ = k_x \sigma_x + k_y \sigma_y + k_z + m \sigma_z \]

Weyl point moves but gap does not open

\[ (0,0,0) \rightarrow (0,0,-m) \]

3D Weyl node is topological.

2D Weyl node:

\[ H(\vec{k},m) = k_x \sigma_x + k_y \sigma_y + m \sigma_z \]

Parameter \( m \) opens a gap.

\[ m = 0 \]

\[ m \neq 0 \]
Apart from 2-band model:

How one can topologically characterize Weyl nodes?

**Berry curvature**

\[
\vec{B}_n(\vec{k}) = i \left\langle \frac{\partial u_n}{\partial \vec{k}} \right| \times \left| \frac{\partial u_n}{\partial \vec{k}} \right
\]
Berry curvature in k space

**Berry curvature**
\[
\mathbf{B}_n(\mathbf{k}) = i \left\langle \frac{\partial u_n}{\partial \mathbf{k}} \right| \times \right| \frac{\partial u_n}{\partial \mathbf{k}} \right\rangle
\]

\(u_{nk}\): periodic part of the Bloch wave function.

\[
\psi_{nk}(\mathbf{x}) = u_{nk}(\mathbf{x}) e^{i \mathbf{k} \cdot \mathbf{x}} \quad (n: \text{band index})
\]

**Monopole density**
\[
\rho_n(\mathbf{k}) = \frac{1}{2\pi} \nabla_{\mathbf{k}} \cdot \mathbf{B}_n(\mathbf{k})
\]

Quantization of monopole charge
\[
\rho_n(\mathbf{k}) = \sum_i q_l \delta(\mathbf{k} - \mathbf{k}_l) \quad q_l: \text{integer}
\]

Position of Weyl node

"magnetic field in k-space"
3D Weyl nodes = monopole or antimonopole for Berry curvature

\[
B_n(\vec{k}) = i\left\langle \frac{\partial u_{nk}}{\partial k} \times \frac{\partial u_{nk}}{\partial k} \right\rangle \quad \text{: Berry curvature}
\]
\[
\rho_n(\vec{k}) = \frac{1}{2\pi} \nabla_k \cdot \vec{B}_n(\vec{k}) \quad \text{: monopole density}
\]

- Weyl nodes are either monopole or antimonopole
- Quantization of monopole charge
  \[ Q = \pm 1 \]

- Weyl nodes can be created only as a monopole-antimonopole pair

Weyl semimetal and Fermi arc
**Weyl semimetal**


= Bulk 3D Dirac cones **without** degeneracy at or around the Fermi energy

- Weyl nodes are either monopole or antimonopole for Berry curvature

\[
B_n(\vec{k}) = i \left< \frac{\partial u_{nk}}{\partial k} \times \frac{\partial u_{nk}}{\partial k} \right>
\]

\[
\rho_n(\vec{k}) = \frac{1}{2\pi} \nabla_{\vec{k}} \cdot \vec{B}_n(\vec{k})
\]

- Surface Fermi arc
  - connecting between Weyl nodes

TaAs surface Fermi arc
(Xu et al., Lv et al., Yang et al. ’15)
3D system with Weyl node

Even in 3D, one can consider the plane, $k_z=$const., to be a 2D system and consider its Chern number.

$$Ch_{(n)}(k_z) = \frac{1}{2\pi} \int_{k_z=\text{const.}} B\left(\vec{k}\right) \cdot \vec{n} dS$$

This Chern number depends on $k_z$

When a monopole (Weyl node with $Q=1$) is at $k_z^W$ the Chern number jumps by $+1$

E.g. 

$$\begin{align*}
Ch_{(n)}(k_z^W - \delta) &= 0 \\
Ch_{(n)}(k_z^W + \delta) &= 1
\end{align*}$$

but at $k_z > k_z^W$

$\rightarrow$ Surface states starting from the Weyl node projection = Fermi arc

Wan et al. (2011)
Symmetry and monopole density

- Time-reversal symmetry
  \[ \rightarrow \text{Monopoles distribute symmetrically w.r.t. } k=0 \]

- Inversion symmetry
  \[ \rightarrow \text{Monopoles distribute antisymmetrically with respect to } k=0 \]

- Total monopole charge in the whole BZ vanishes.

- Inversion + Time-reversal
  \[ \rightarrow \text{monopoles do not exist} \]
  \[ \rightarrow \text{Weyl semimetal cannot be realized} \]
  \[ \text{(Dirac semimetal is possible)} \]
Topological metals with bulk Dirac cones

**Dirac semimetals** =
bulk 3D Dirac cone with Kramers degeneracy
Both inversion- or time-reversal symmetry are required

- $\beta$-BiO$_2$ (Young et al., (2011))
- A$_3$Bi (A = Na, K, Rb) (Wang et al., (2011))
- Cd$_3$As$_2$ (Wang et al., (2012))
- NI/TI multilayer (Burkov, Balents)

**Weyl semimetals** =
bulk 3D Dirac cone without Kramers degeneracy
Either inversion- or time-reversal symmetry should be broken

- pyrochlore iridates
  (Wan et al., PRB (2011), Yang et al., PRB(2011))
- NI/TI multilayer (Burkov, Balents)
- TaAs
- YbMnBi$_2$ …
Effective model: insulator – Weyl semiemtal

\[ H = \gamma (k_x^2 - m)\sigma_x + v (k_y\sigma_y + k_z\sigma_z) \]

Bulk dispersion

\[ E = \pm \sqrt{\gamma^2 (k_x^2 - m)^2 + v^2 k_y^2 + v^2 k_z^2} \]

\( m<0 \): bulk gap = \( 2\gamma|m| \)

= topological or normal insulator

\( m>0 \): bulk is gapless

gap closed at \( W_{\pm} \): \( k = (\pm \sqrt{m}, 0, 0) \)

= Weyl semimetal

Surface Fermi arc : effective model calc.

Bulk band structure

Bulk + surface

Fermi arcs
top surface
bottom surface

Weyl semimetal TaAs

Weng et al., PRX (2015): theory

Lv et al., Xu et al. (2015):

Fermi arc

(a) Weyl node

(b) Fermi arc
Multilayers of a Weyl semimetal and a normal insulator

K. Yokomizo and S. Murakami

Multilayer (Pattern A)

\[ H = \gamma \left( k_x^2 - m(z) \right) \sigma_x + \nu \left( k_y \sigma_y - i \partial_z \sigma_z \right) \]

Spatial modulation

The multilayer becomes the WSM phase by increasing the thickness of the WSM layer.
Multilayer (Pattern B)

Hamiltonian

\[ H = \gamma \left( -\partial_x^2 - m(x) \right) \sigma_x + \nu (k_y\sigma_y + k_z\sigma_z) \]

Spatial modulation

(1) WSM phases periodically emerge
(2) Quantum anomalous Hall (QAH) phases which have different Chern number periodically emerge
Trajectory of the Weyl nodes in multilayer (Pattern B)

thickness of the WSM layer: increase
thickness of the NI layer: const

K. Yokomizo and S. Murakami
Nodal-line semimetal
Nodal-line semimetal: bulk gap closes along a loop in k space

2 typical mechanisms

(i) **Mirror symmetric system:**

Mirror eigenvalues are different between the valence and the conduction bands

\[
\begin{align*}
& \text{spinless (SOC=0)} & M = \pm 1 \\
& \text{spinful (nonzero SOC)} & M = \pm i
\end{align*}
\]

→ No anticrossing between the two bands
  (\(\leftarrow\) prohibited hybridization)
→ Nodal line on a mirror plane

**Dirac line node**
- Carbon allotropes
- Cu3PdN
- Ca3P2
- LaN
- CaAgX (X=P,As)

**Weyl line node**
- HgCr2Se4
- TiTaSe2
2 typical mechanisms

(ii) Spinless (SOC=0) & time-reversal sym. & inversion symm.

topological nodal line at generic position in k space

(Example)

\[
H(\vec{k}) = \begin{pmatrix}
    a(\vec{k}) & b(\vec{k}) \\
    b^*(\vec{k}) & c(\vec{k})
\end{pmatrix}
\]

\[a(\vec{k}), c(\vec{k}) : \text{real}\]
\[b(\vec{k}) : \text{complex}\]

With the above 3 conditions \(\rightarrow\) Hamiltonian is a real matrix.

\[b(\vec{k}) : \text{real}\]

Degeneracy appears when

\[
\begin{cases}
a(\vec{k}) = c(\vec{k}) \\
\text{Re } b(\vec{k}) = 0
\end{cases}
\]

2 conditions \(\rightarrow\) nodal line

Topological characterization:

\(\pi\) Berry phase around the nodal line
Rewrite the matrix in terms of Pauli matrices. Omit the trace part.

\[
H(\vec{k}) = \begin{pmatrix}
a_z(\vec{k}) & a_x(\vec{k}) \\
a_x(\vec{k}) & -a_z(\vec{k})
\end{pmatrix}
\]

\[a_x(\vec{k}), a_z(\vec{k}) : \text{real}\]

Phase of \( z(\vec{k}) = a_x(\vec{k}) + ia_z(\vec{k}) \) winds by \( 2\pi \) around the nodal line.

\( \rightarrow \) Nodal line is topological

In general systems, the nodal line is characterized by \( \pi \) Berry phase.

\[
\phi = -i \oint_C \text{d} \vec{k} \cdot \left< u_n(\vec{k}) \right| \frac{\partial}{\partial \vec{k}} \left| u_n(\vec{k}) \right> = \pi
\]
Ca have nodal lines near $E_F$

Hirayama, Okugawa, Miyake, Murakami
Nat. Commun. 8, 14022 (2017)

Not semimetal at 0 GPa

Nodal line semimetal at 7.5 GPa

(cf.) previous works
nodal-line semimetal: drumhead surface states

Surface state often appears within the region surrounded by the nodal line:
- Similar to the flat-band edge states in graphene zigzag ribbon.
Nodal-line and Zak phase

Zak phase (Berry phase) for a given $\vec{k}_\parallel$ (= surface wavevector)

$$\theta(\vec{k}_\parallel) = -i \sum_{occ.} \int_0^{2\pi/a_\perp} dk_\perp \left\langle u_n(\vec{k}) \right| \frac{\partial}{\partial k_\perp} \left| u_n(\vec{k}) \right\rangle$$

$\theta(\vec{k}_\parallel) = 0$ or $\pi$

$\leftrightarrow$ Inversion+ time-reversal symmetries

Zak phase $\theta(\vec{k}_\parallel)$ jumps by $\pi$ at the nodal line

(111) Surface Brillouin zone in Ca

Zak phase $\theta(\vec{k}_\parallel) = \pi$

Zak phase $\theta(\vec{k}_\parallel) = 0$

Berry phase $= \pi$

$\theta(a) = \pi$

$\theta(b) = 0$
Zak phase and charge polarization

In 1D system:

\[ \text{Polarization } \sigma = \text{Zak phase } \times \frac{e}{2\pi} \left( \text{mod } e \right) \]

"modern theory of polarization"

Total polarization for 3D system (=surface polarization charge density)

\[ \sigma = \int \frac{d^2 \vec{k}_\parallel}{(2\pi)^2} \sigma(\vec{k}_\parallel) \]

(Note: only for insulators)

Charge profile in a slab along thickness direction

\[ \theta(\vec{k}_\parallel) = 0 \]

\[ \theta(\vec{k}_\parallel) = \pi \]

Charge is depleted by \( e/2 \)
Surface charge

Remarks:

- It is not ferroelectric $\leftrightarrow$ centrosymmetric fcc
- Where is the missing charge at $\pi$ Zak phase region?

The number of bulk occupied bands change at the nodal lines. Chemical potential will slightly change to accommodate missing charge.
Nodal-line and Berry phase

Area = 0.485*BZ

→ surface charge density = $0.485 \cdot \frac{e}{2}$ per surface unit cell

Huge surface polarization charge

→ In metals this charge is screened by carriers and lattice

→ Charge imbalance & lattice relaxation at the surface
Topological metals often appears between various topological insulator phases
Topological insulator multilayer without time-reversal symmetry

Burkov, Balents, PRL 107, 127205 (2011)

Magnetization

Quantum anomalous Hall:
Ch=1 for all $k_z$
=Chiral surface state for all $k_z$

Weyl semimetal:
Ch=1 for $k_z$ between the two Weyl nodes. = Fermi arc
Ch=0 otherwise

• By changing parameters, the Weyl nodes move in k-space.
• When they meet, they are annihilated in pair and the system becomes an insulator in the bulk (i.e. either QAH phase or an insulator phase).
NI-TI universal phase diagram in 3D

SM. Kuga, PRB ('08)
SM, Physica E43, 748 ('11)

Degree of inversion symmetry breaking

Weyl semimetal

Dirac semimetal

Normal insulator

Strong topological insulator

Weyl semimetal

external parameter (e.g.: pressure, atomic composition, SOC etc.)
Systems with inversion symmetry

- Gap closes at TRIM inversion of bands with opposite parities.
- Insulator-to-insulator transition

\[ \text{e.g. TlBi(S}_{1-x}\text{Se}_x)\text{2} \]

Xu et al., Science.332, 560 (’11)

Sato et al., Nature Phys.7, 840 (’11)
Systems without inversion symmetry

Weyl semimetal

Dirac semimetal

WTI (or NI)

STI

inversion symmetric ($\delta = 0$)

Surface state evolution

Okugawa, SM, PRB('14)

Fermi arc

WS

Dirac cone

STI

Okugawa, SM, PRB('14)

SM. Kuga, PRB ('08)
SM, Physica E('11)
Okugawa, SM, PRB('14)

Pair creation of Weyl nodes (monopole+antimonopole)

Pair annihilation

SM. Kuga, PRB ('08)
SM, Physica E('11)
Okugawa, SM, PRB('14)
$Z_2$ topological number $\nu$

$\nu = 0$: normal insulator (NI)
$\nu = 1$: topological insulator (TI)

(A) systems with inversion symmetry

\[ (-1)^\nu = \prod_i \prod_{m=1}^N \xi_{2m}(\Gamma_i) \]
Parity eigenvalue
+1 or -1

$\Gamma_i : \text{TRIM}$

Fu, Kane, PRB(2007)

(B) systems without inversion symmetry

\[ (-1)^\nu = \prod_i \sqrt{\frac{\text{det}[w(\Gamma_i)]}{\text{Pf}[w(\Gamma_i)]}} \]

\[ w_{mn}(\tilde{k}) = \langle u_{-k,m} | \Theta | u_{k,n} \rangle \]

Fu, Kane, PRB(2006)

Gap closes at TRIM
$\rightarrow$ parity eigenvalues are exchanged

Gap closes at generic points
$\rightarrow$ This gap closing should be a pair creation of Weyl nodes.
BiTeI under pressure

Liu, Vanderbilt, PRB (2015)
Rusinov et al., NJP (2016)
See also: Bahramy et al., Nat. Commun. (2012)

Trajectory of Weyl nodes

TI//NI superlattice without inversion sym.

Halasz, Balents, PRB (2012)

e.g., Fourfold rotational symmetry

Trajectory of Weyl nodes
HgTe$_x$S$_{1-x}$ under [001] strain


LaBi$_{1-x}$Sb$_x$Te$_3$, LuBi$_{1-x}$Sb$_x$Te$_3$


Trajectories of Weyl nodes in kz=0 plane

Trajectories of Weyl nodes (within kx-ky plane)
Problem:

Start from any band insulator \textit{without} inversion symmetry (spinful + time-reversal symm.)

→ suppose a gap closes by changing a parameter $m$

\textit{What phase appears next?}

Classification by space groups & $k$-points.

138 space groups without inversion symm.

(Example #1): $C_2$ symmetry  (i.e. $k$: invariant under $C_2$)

$C_2$ eigenvalue = $+i$ or $-i$

(i) **Same signs of $C_2$**

Weyl semimetal

Weyl nodes along $C_2$ line

(ii) **Different signs of $C_2$**

Gap cannot close at $k$ - level repulsion

$\text{C}_2$

$\text{C}_2$

$E$

$\text{monopole}$

$\text{anti-monopole}$
(Example #2): mirror symmetry  (i.e. \( k \) : invariant under \( M \))

\[ M \text{ eigenvalue} = +i \text{ or } -i \]

(i) **Same signs of** \( M \)

   gap closes at \( k \) on the mirror plane \( \rightarrow \) Weyl semimetal

(ii) **Different signs of** \( M \)

   nodal-line semimetal

   (gap closing along a loop on a mirror plane)
Semiconductors without inversion symmetry → Gap-closing always leads to topological semimetals

(a) Nodal-line semimetal (← mirror plane)

(b) Weyl semimetal

Only two possibilities. No insulator-to-insulator transition happens.
(in contrast to inversion symmetric systems)
- Chiral lattice with helical chains
- No inversion symmetry
- No mirror symmetry
→ Allow Weyl nodes

Insulator: gap=0.3eV

Weyl semimetal
Conclusions

- Weyl semimetals (in inversion asymmetric systems)
  - Appear in TI-NI phase transition
    e.g. Tellurium: Weyl semimetal at high pressure

  Murakami, NJP 9, 356 (2007)
  Murakami, Kuga, PRB78, 165313 (2008)
  Okugawa, Murakami, PRB 89, 235315 (2014)
  Hirayama et al., PRL 114, 206401 (2015)
  Murakami, Hirayama, Okugawa, Miyake,

- Nodal lines in alkaline earth metals Ca, Sr, Yb
  - nodal lines if spin-orbit coupling is neglected
  - large “polarization” for $k_\parallel$ inside the nodal line
  - surface Rashba SOC is enhanced e.g. Bi/Sr(111), Bi/Ag(111)

  Hirayama et al., Nat. Commun.8, 14022 (2017)