Weyl semimetal

A. Classification of Weyl node

B. Linear Weyl node

    1. Multiplet of nodes due to symmetry

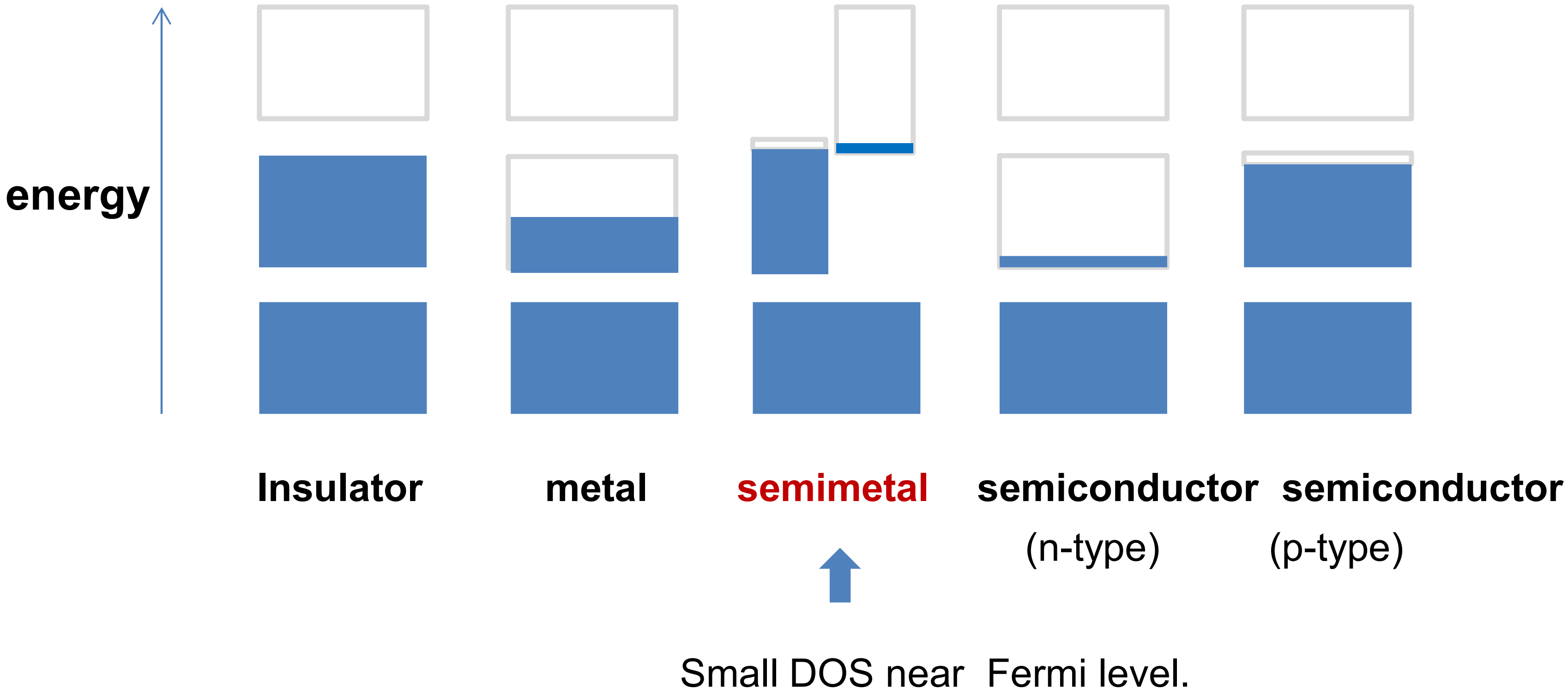
C. From Dirac to Weyl

D. The Burkov-Balent multilayer model

    1. Fermi arc of surface states

    2. Property of Fermi arc

Band theory of solids



Accidental degeneracy: 2 levels (2D, 3D)

The degeneracy that occurs coincidentally, without the protection by symmetry

- Wigner-von Neumann "theorem" (1929):

It is necessary to adjust 3 parameters in to obtain a 2-fold degeneracy.

Consider a system with 2 levels,

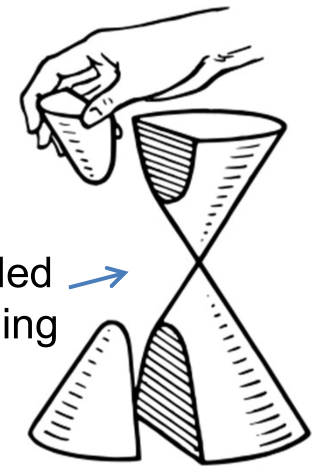
$$H = d_0(\vec{k}) + d_x(\vec{k})\sigma_x + d_y(\vec{k})\sigma_y + d_z(\vec{k})\sigma_z$$

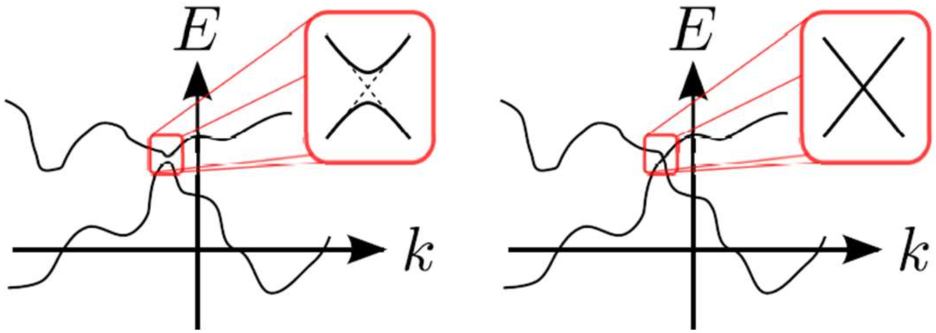
$$\rightarrow E_\pm = d_0 \pm \sqrt{d_x^2 + d_y^2 + d_z^2}$$

$$\rightarrow \text{degeneracy only when } d_x = d_y = d_z = 0$$ (i.e., Co-dimension is 3)

- 3D: one (or several) point degeneracy in 3D ***k***-space
- 2D: unlikely to have a point degeneracy in 2D ***k***-space

Avoided crossing





Avoided crossing

Crossing

Fig. from Meng's thesis

Level crossing leads to Dirac cone

- 2 level crossing in 2D (SS of TI, graphene)

e.g., $\mathrm{H}_{SS} = \alpha(\boldsymbol{\sigma} \times \mathbf{k})_z + O(k^2)$

➡ Berry curvature

$$F_z^{\pm} = \mp\pi\delta^2(\mathbf{k})$$

- 2 level crossing in 3D (Weyl semi-metal)

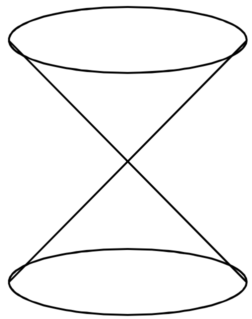
e.g., $H_{2\times2}(\vec{k}) = \vec{k}\cdot\vec{\sigma}$

➡ $\vec{F}_{\pm} = \mp\frac{1}{2}\frac{\hat{k}}{k^2}$ (Recall the Berry curvature of Zeeman coupling)

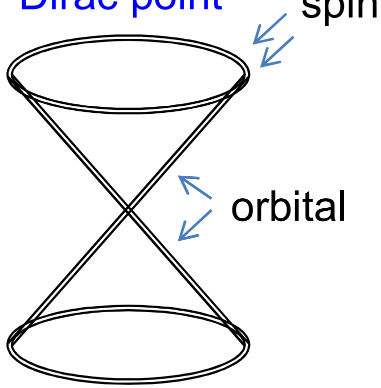
- A degenerate point is a “monopole” in momentum space (source or sink of Berry flux)

- From now one, we will call the degenerate point between 2 levels (in 3D) as a Weyl point, instead of a Dirac point.

2-level crossing
Weyl point

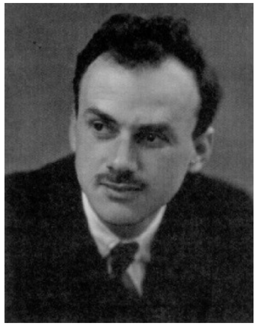


4-level crossing
Dirac point



Types of fermion in
Particle physics

Realizations in
Solid-state phys



- Dirac fermion (1928)
  - Relativistic spin ½ fermion
  - 4 components
  - Electron, proton …

$$\begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \end{pmatrix}$$

Graphene with spin
(2004)

- Weyl fermion (1929)
  - Massless ½ fermion
  - 2 components
  - Not found in nature

$$\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$$

TaAs… 砷化鉭
(2015)

- Majorana fermion (1937)
  - Being its own anti-particle
  - 2 *independent* components
  - Neutrino?

$$\begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_1^* \\ \varphi_2^* \end{pmatrix}$$

Semi-SC hybrid
structure …
(2012, 14, 16 …)

Chirality of Weyl point

- Near a Weyl point

$$H_{2\times 2}(\vec{q}) = h_0(\vec{q}) + \vec{h}(\vec{q})\cdot\vec{\sigma}, \qquad \vec{q} \equiv \vec{k}_0 + \vec{k}$$

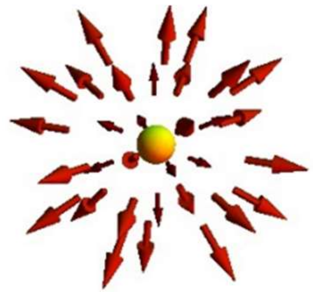
$$\simeq h_0(\vec{q}) + \vec{h}\left(\vec{k}_0\right)\cdot\vec{\sigma} + \underline{\frac{\partial h_i}{\partial k_j} k_j\, \sigma_i}$$

$$= \vec{v}_i \cdot \vec{k}\, \sigma_i$$

手徵 Chirality (or helicity)

$$\chi \equiv \mathrm{sgn}\left[\det\left(\frac{\partial h_i}{\partial k_j}\right)\right] \text{ or } \mathrm{sgn}(\vec{v}_1\cdot\vec{v}_2\times\vec{v}_3)$$

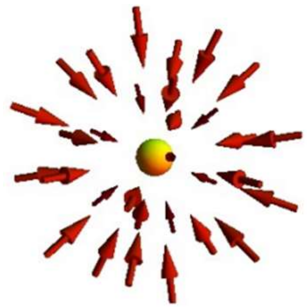
e.g., $H = \pm v_F \vec{k}\cdot\vec{\sigma}, \qquad \chi = \pm$



$\chi = +$

Berry curvature

$$\vec{F}_-^{\chi} = \frac{\chi}{2}\frac{\hat{k}}{k^2}$$



$\chi = -$

- Berry flux (~monopole charge) is quantized

$\Phi_F = 2\pi C_1$.

Stability of Weyl point

Weyl point is stable against perturbation

$$H = \pm v_F \vec{\sigma} \cdot \vec{k} + H'$$

a general perturbation:

$$H' = a(\vec{k}) + \vec{b}(\vec{k}) \cdot \vec{\sigma}$$

$$\rightarrow H' \cong a(\vec{k}) + \vec{b}(0) \cdot \vec{\sigma} + \frac{\partial b_i\,(0)}{\partial k_j} k_j \sigma_i$$

Shift position of node   Renormalize v_F

e.g., $$H = v_F \vec{\sigma} \cdot \vec{k} + m\sigma_z$$

- Weyl node can only appear/disappear by pair creation/annihilation

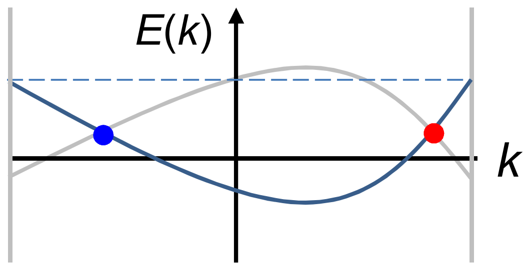
二宮正夫

Nielsen-Ninomiya theorem (1981):

Aka Fermion-doubling theorem, no-go theorem

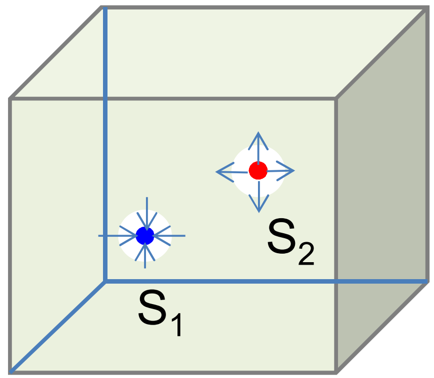
In a lattice, massless Weyl fermions must appear in pairs with opposite chiralities.

- Energy band in 1D BZ



Crossings need to appear in pairs

- Energy band in 3D BZ



Total Berry flux from Weyl points needs to be zero.

- To be precise, for a lattice in odd space dimensions, without breaking translation symmetry and chiral symmetry, massless Weyl fermions must appear in pairs. (defined in high energy. For massless fermion, chirality = helicity)

- 1. This doubling property used to be a problem in lattice QCD

  2. In 2 dim, chirality is not well-defined. For example, it's possible to open only one Dirac point in graphene.

Symmetry and Weyl point

$$H = \pm v_F \vec{\sigma} \cdot (\vec{k} - \vec{k}_0)$$ A monopole at $\boldsymbol{k}_0$

- TR Symm $\vec{k} \to -\vec{k}, \quad \vec{\sigma} \to -\vec{\sigma}$

$$H \to H' = \pm v_F \vec{\sigma} \cdot \left(\vec{k} + \vec{k}_0\right)$$

→ A monopole at $-\boldsymbol{k}_0$ with the *same* chirality

- SI Symm $\vec{k} \to -\vec{k}, \quad \vec{\sigma} \to \vec{\sigma}$

$$H \to H' = \mp v_F \vec{\sigma} \cdot \left(\vec{k} + \vec{k}_0\right)$$

→ A monopole at $-\boldsymbol{k}_0$ with the *opposite* chiralities

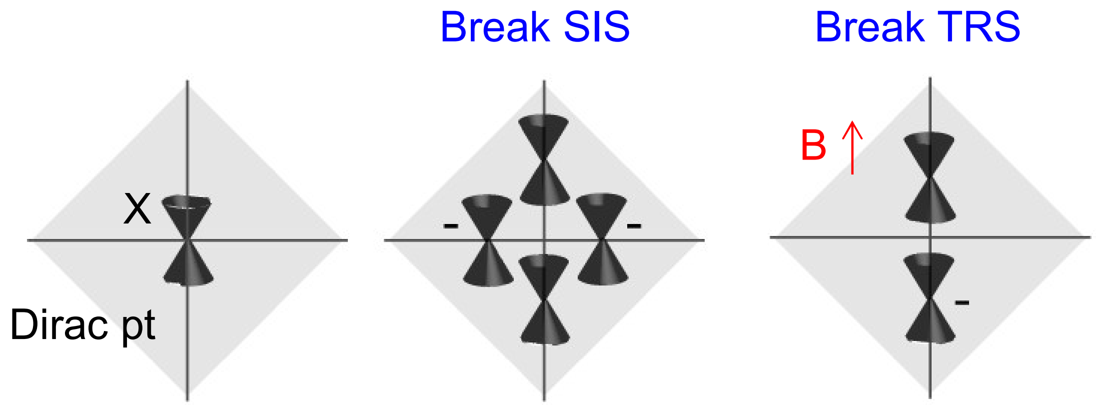
- Nielsen-Ninomiya theorem: always a pair with *opposite* chirality

TRS	IS	Implications	Min. number
×	×	Weyl nodes can be at any $\vec{k}$ and may have different energies.[113]	2
✓	×	Weyl node at $\vec{k}_0 \Leftrightarrow$ Weyl node of *same* chirality at $-\vec{k}_0$.	4
×	✓	Weyl node at $\vec{k}_0 \Leftrightarrow$ Weyl node of *opposite* chirality at $-\vec{k}_0$.	2
✓	✓	Not topologically stable	none

Dirac point (but can be protected by crystal symmetry)

Meng T thesis 2012

From Dirac SM to Weyl SM



Not topo stable

Young et al, PRL 2012

Candidates of Weyl semi-metals

(Fermi energy needs to be near a Weyl point)

Theory

- Iridium pyrochlores

  ($R_2Ir_2O_7$, R is Rare Earth, Wan et al, PRB 2011)

- Ferromagnetic spinel

  ($HgCr_2Se_4$, Xu et al, PRL 2011, double Weyl)

- Transition metal monopnictide (break SIS)

  (TaAs, Huang, Nat Comm 2015, PRX 2015; Weng, PRX 2015

  NbAs, theory and exp't, Xu, Nat Phys 2015; TaP…)

- strontium silicide

  ($SrSi_2$, Huang, PNAS 2016, double Weyl)

- WTe_2 (… Li et al, Nature Comm 2017)

Experiment

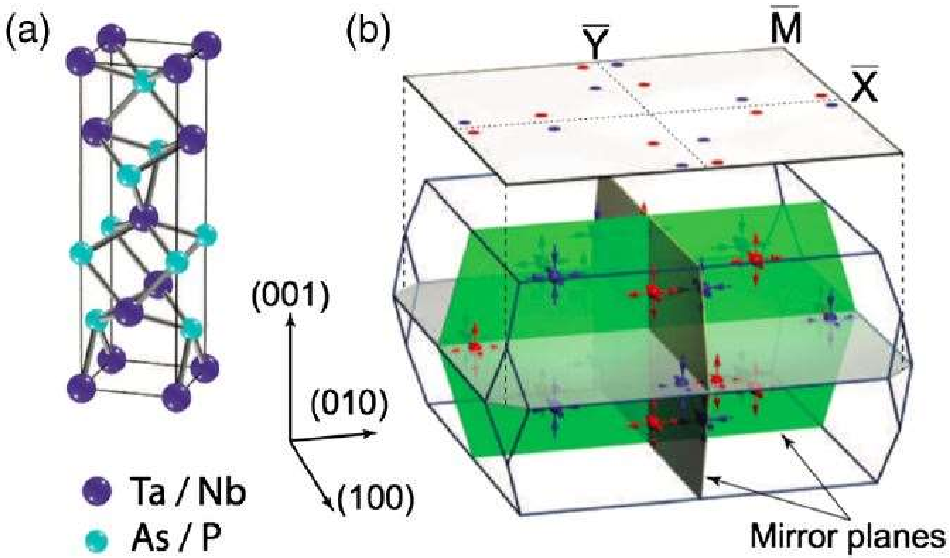
- Xu et al, Science 2015
- Lv et al, PRX 2015
- Lv et al, Nat Phys 2015
- Yang et al, Nat Phys 2015

Also, line node, Cu_3PdN, Yu, PRL 2015, $PbTaSe_2$, Bian 1505.03069
And more.

See Armitage, Mele, and Vishwanath, Rev Mod Phys (2018).

Transition metal monopnictide 磷族

- With nonsymmorphic space group
- DP → WP by breaking SIS



24 Weyl nodes

Huang et al, Nature Comm 2015

Physics related to Weyl fermions

1. Anomalous Hall effect
2. Fermi arc of surface state

Use
Burkov-Balent model
as an example

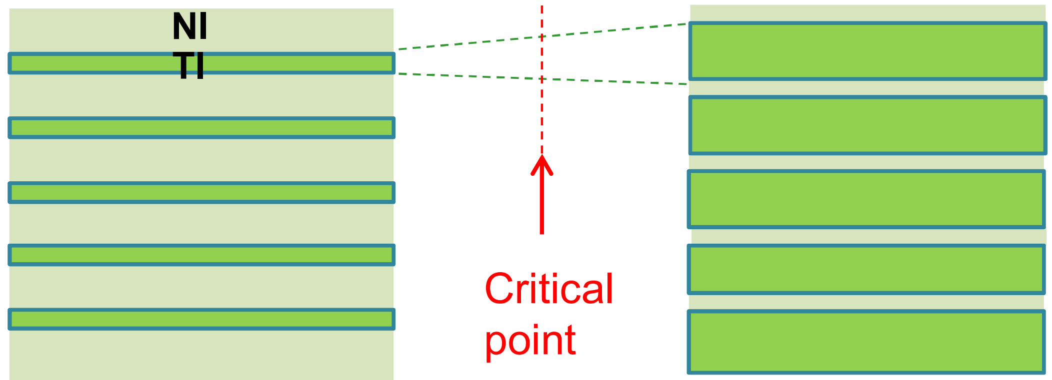
3. Chiral anomaly
4. Chiral magnetic effect
5. Bulk photovoltaic effect (Weng, Nat material, 18, 428, 2019)
6. …

WP as a critical point of QPT:

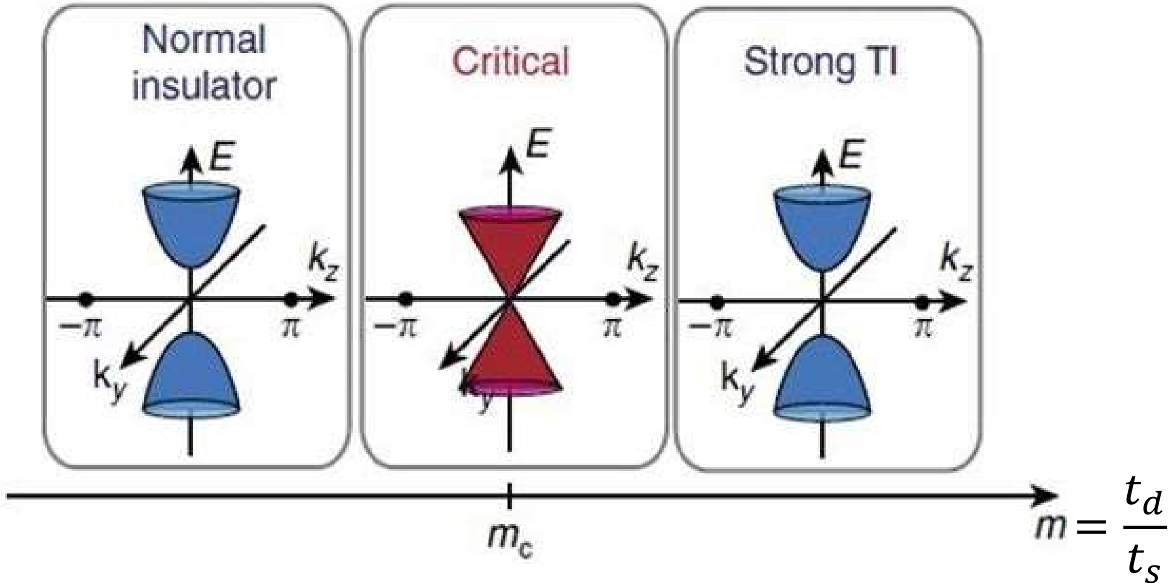
Burkov-Balent model - multi-layer heterostructure

(Burkov and Balent PRL 2011)

Normal insulator
Topological insulator



Coupling between surface states: $t_s > t_d$: **normal insulator** $t_s < t_d$: **topological insulator**



Two SS's from one TI slab $\quad \mathsf{H} = v\tau_z \otimes (\boldsymbol{\sigma} \times \mathbf{k}_\perp) \cdot \hat{z} + m1 \otimes \sigma_z + t_s\tau_x \otimes 1$

Multiple layers

$$\hat{\mathsf{H}} = \sum_l [v\tau_z(\boldsymbol{\sigma} \times \mathbf{k}_\perp) \cdot \hat{z} + m\sigma_z + t_s\tau_x] c_l^\dagger c_l + \sum_l t_d(\tau_+ c_l^\dagger c_{l+1} + \tau_- c_l^\dagger c_{l-1}),$$

$$\tau_\pm = (\tau_x \pm i\tau_y)/2, \; c_l = (c_{lu}, c_{ld})^T$$

Fourier transform

$$c_l^\dagger = \frac{1}{\sqrt{N}} \sum_{k_z} e^{ildk_z} c_{k_z}^\dagger$$

$$\begin{aligned} \Rightarrow \hat{\mathsf{H}} &= \sum_{k_z} \Big[v\tau_z(\boldsymbol{\sigma} \times \mathbf{k}_\perp) \cdot \hat{z} c_{k_z}^\dagger c_{k_z} \\ &+ m\sigma_z c_{k_z}^\dagger c_{k_z} \\ &+ t_s\tau_x c_{k_z}^\dagger c_{k_z} \\ &+ t_d(e^{-ik_zd}\tau_+ c_{k_z}^\dagger c_{k_z} + e^{ik_zd}\tau_- c_{k_z}^\dagger c_{k_z}) \Big] \\ &= \sum_{k_z} \begin{pmatrix} \mathsf{h}_0 + m\sigma_z & t_s + t_d e^{-ik_zd} \\ t_s + t_d e^{ik_zd} & -\mathsf{h}_0 + m\sigma_z \end{pmatrix} c_{k_z}^\dagger c_{k_z} \\ &\equiv \sum_{k_z} \mathsf{H}_{k_z} c_{k_z}^\dagger c_{k_z}, \end{aligned}$$

Each k_z is an independent subsystem

$$
\begin{aligned}
\mathsf{H}_{k_z} &= \tau_z \mathsf{h}_0 + m\sigma_z \\
&+ t_s\tau_x + t_d(e^{-ik_z d}\tau_+ + e^{ik_z d}\tau_-)
\end{aligned}
$$

$$
\mathsf{h}_0 = v(\boldsymbol{\sigma} \times \mathbf{k}_\perp) \cdot \hat{z}
$$

We'd like to block-diagonalize the 4x4 matrix:

Unitary rotation

$$
\mathsf{U} = \begin{pmatrix} 1 & 0 \\ 0 & \sigma_z \end{pmatrix} \qquad UU^\dagger = U^\dagger U = 1
$$

$$
\begin{aligned}
\tau_{x,y} &\to \mathsf{U}^\dagger \tau_{x,y} \mathsf{U} = \tau_{x,y}\sigma_z, \\
\sigma_{x,y} &\to \mathsf{U}^\dagger \sigma_{x,y} \mathsf{U} = \tau_z \sigma_{x,y}.
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow \quad \mathsf{H}_{k_z} &= \mathsf{h}_0 + m\sigma_z \\
&+ [t_s\tau_x + t_d(e^{-ik_z d}\tau_+ + e^{ik_z d}\tau_-)]\sigma_z
\end{aligned}
$$

$$
\begin{aligned}
\mathsf{H}_{k_z} &= \mathsf{h}_0 + \underbrace{\left[m + \tau_z\sqrt{t_s^2 + t_d^2 + 2t_s t_d \cos(k_z d)}\right]}_{M_{\tau_z}(k_z)} \sigma_z \\
&= v(\boldsymbol{\sigma} \times \mathbf{k}_\perp) \cdot \hat{z} + M_{\tau_z}(k_z)\sigma_z,
\end{aligned}
$$

Effective mass for layer-k_z

Band structure

$$\varepsilon_{\pm}^{\tau_z} = \pm\sqrt{v^2(k_x^2 + k_y^2) + M_{\tau_z}^2(k_z)}$$

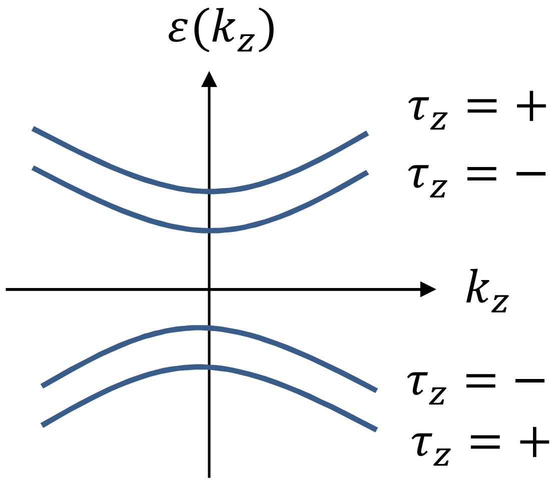
$$M_{\tau_z}(\mathrm{k_z}) = m + \tau_z\sqrt{t_s^2 + t_d^2 + 2t_s t_d \cos(k_z d)}$$

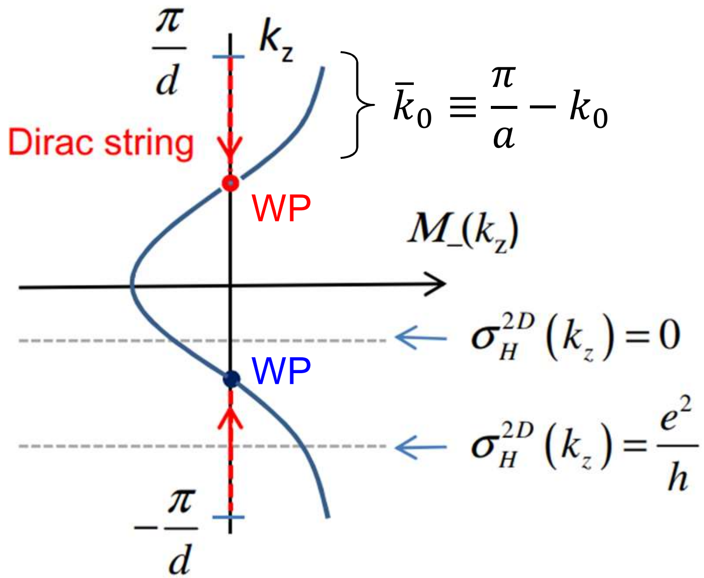
- Gap closes when

$$\cos(k_0 d) = \frac{m^2 - (t_s^2 + t_d^2)}{2t_s t_d}$$

- k_0 exists when

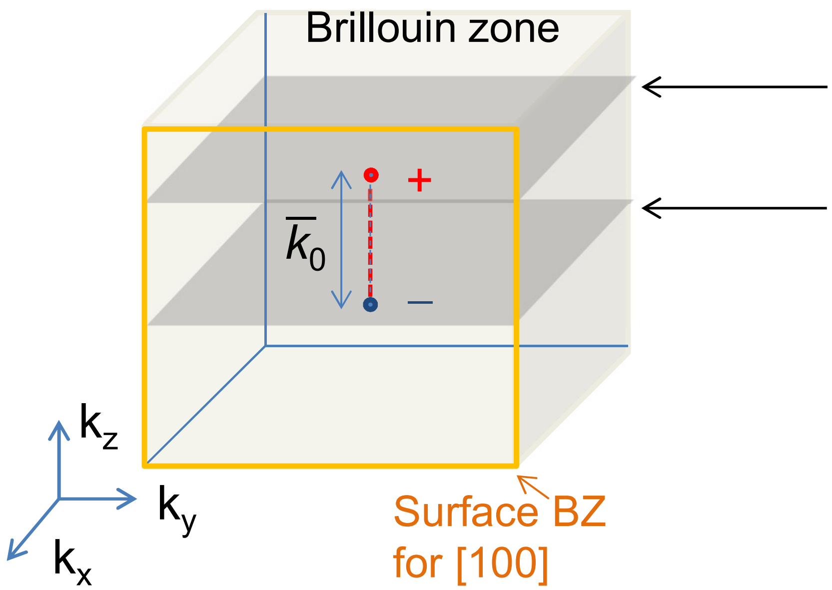
$$\underbrace{|t_s - t_d|}_{m_{c1}} \le m \le \underbrace{|t_s + t_d|}_{m_{c2}}$$





1. Anomalous QHE in Weyl SM

(Shift the BZ along z-axis by half)



One 2D layer for each k_Z

Hall conductivity

$$\sigma_H^{2D}(k_z) = 0$$

$$\sigma_H^{2D}(k_z) = \frac{e^2}{h}$$

Cut through Dirac string (the center of vortex)

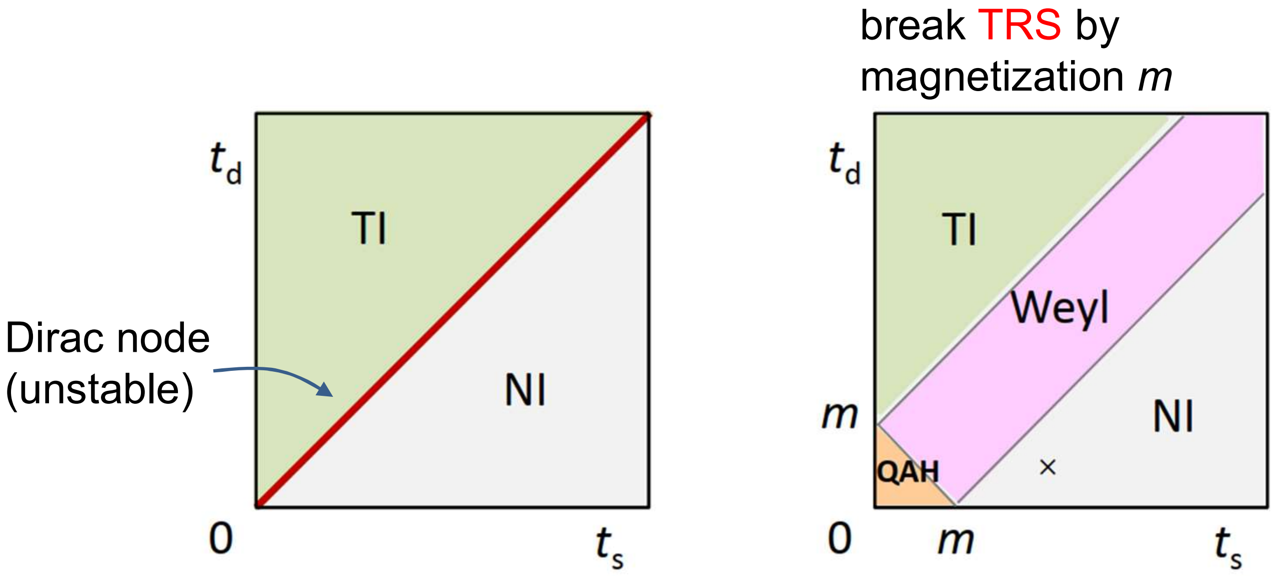
Total Hall conductivity

$$\sigma_H^{3D} = \frac{1}{L_z}\sum_{k_Z}\sigma_H^{2D}(k_Z) = \frac{e^2}{h}\frac{\overline{k}_0}{2\pi}$$

Semi-quantized
Hall conductivity

- 2 Weyl nodes are created at origin
- They are linked by a string of gauge singularity (Dirac string)

Phase diagram of Burkov-Balent model



(a) m=0

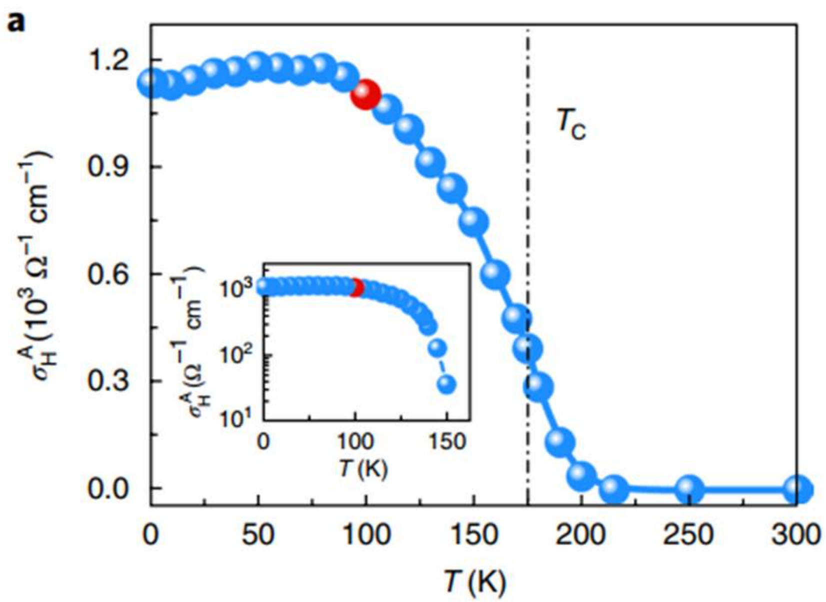
(b) m≠0

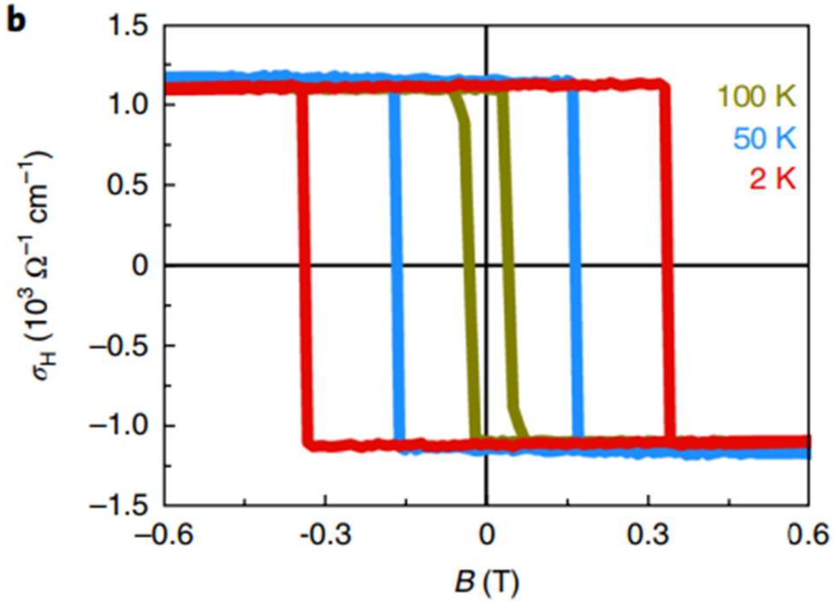
Weyl:

$$\underbrace{|t_S - t_D|}_{m_{c1}} < m < \underbrace{t_S + t_D}_{m_{c2}}$$

Anomalous Hall effect in *ferromagnetic* Weyl SM

- Temperature dependence of the anomalous Hall conductivity at B=0
- Field dependence of the Hall conductivity

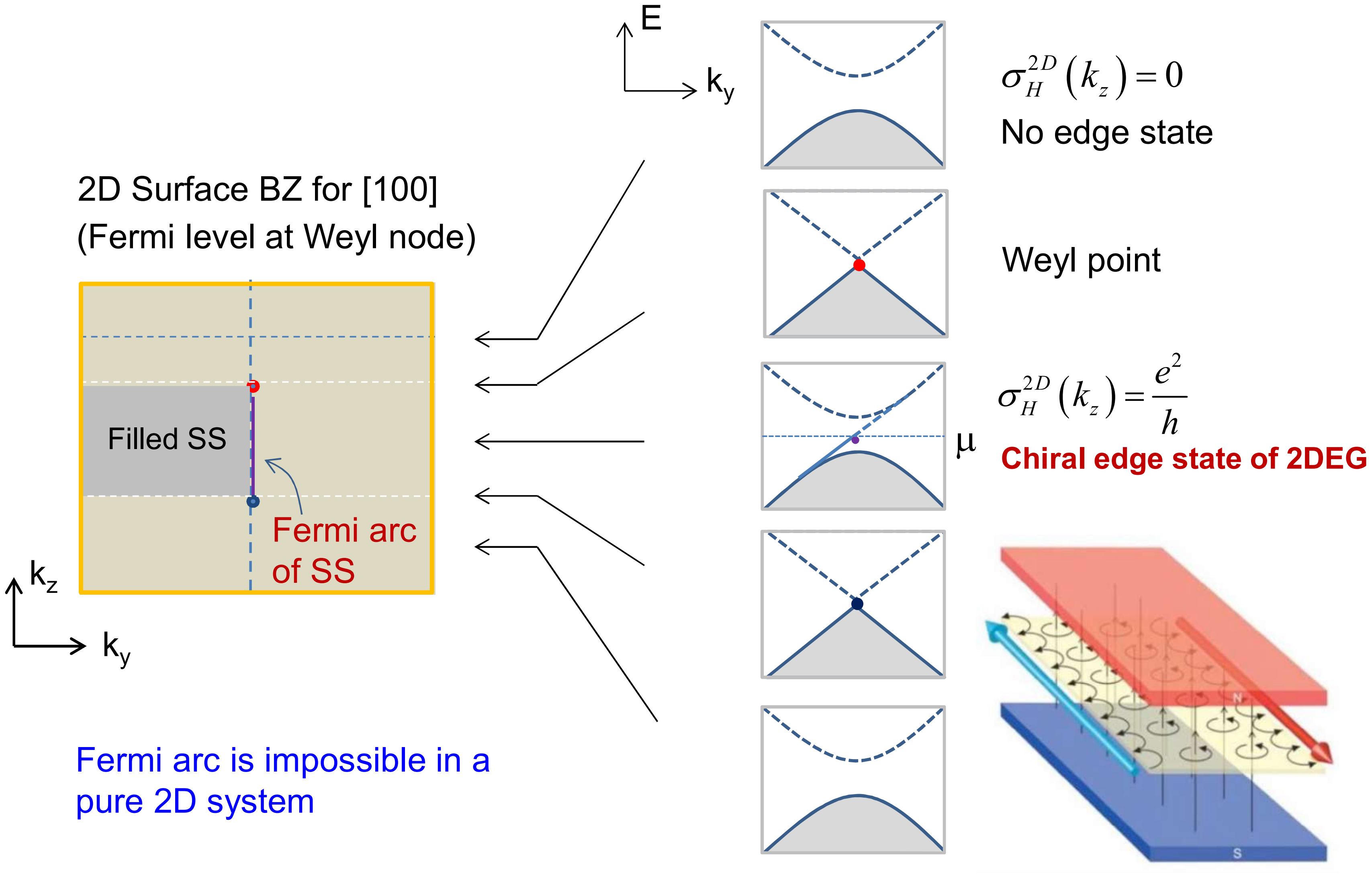




Below 100 K, σ_H is roughly constant, indicating that the AHE is not governed by scatterings.

$Co_3Sn_2S_2$, Liu et al, Nat Phys 2018

2. Surface state and Fermi arc (Wan et al, PRB 2011)



Fermi arc is impossible in a pure 2D system

Consider a semi-infinite WSM

$$m(x) \; < \; |t_s - t_d| \text{ for } x<0, \text{ or } M_-(k_z)<0 \text{ (NI)}$$
$$m(x) \; > \; |t_s - t_d| \text{ for } x>0, \text{ or } M_-(k_z)>0 \text{ (WSM)}$$

$$\mathsf{H}_{k_z} = \mathsf{h}_0 + \underbrace{\left[m(x) - \sqrt{t_s^2 + t_d^2 + 2t_s t_d \cos(k_z d)}\right]}_{M_-^{k_z}(x)} \sigma_z$$

Re-quantized Hamiltonian for the middle 2 bands,

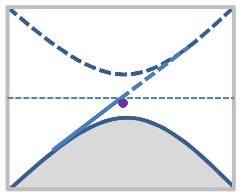
$$\begin{pmatrix} M_-^{k_z}(x) & v\left(\frac{\partial}{\partial x} + k_y\right) \\ v\left(-\frac{\partial}{\partial x} + k_y\right) & -M_-^{k_z}(x) \end{pmatrix} \phi_s^{k_z} = \varepsilon_s^{k_z}(k_y)\phi_s^{k_z}$$

Surface state

$$\phi_s^{k_z}(x) = e^{-\frac{1}{v}\int_0^x dx' M_-^{k_z}(x)} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Energy level of surface state

$$\varepsilon_s^{k_z}(k_y) = v k_y$$



Chiral edge state

Weyl point and Fermi arc (3D view)

Surface Brillouin zone

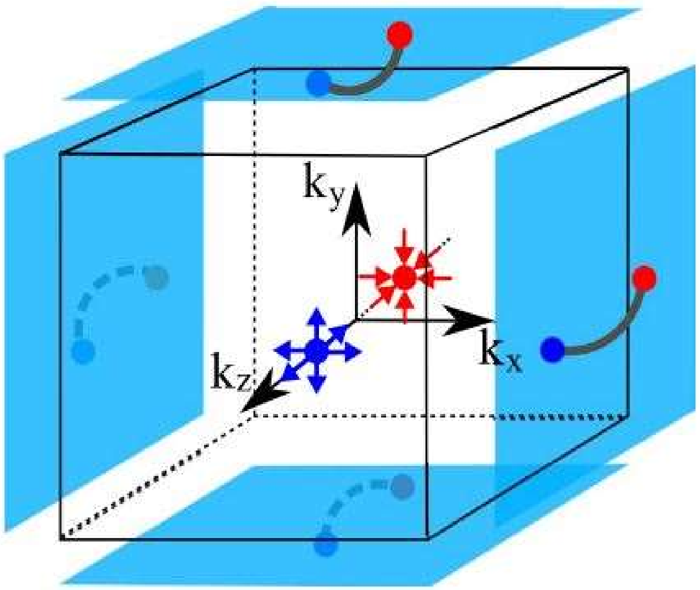
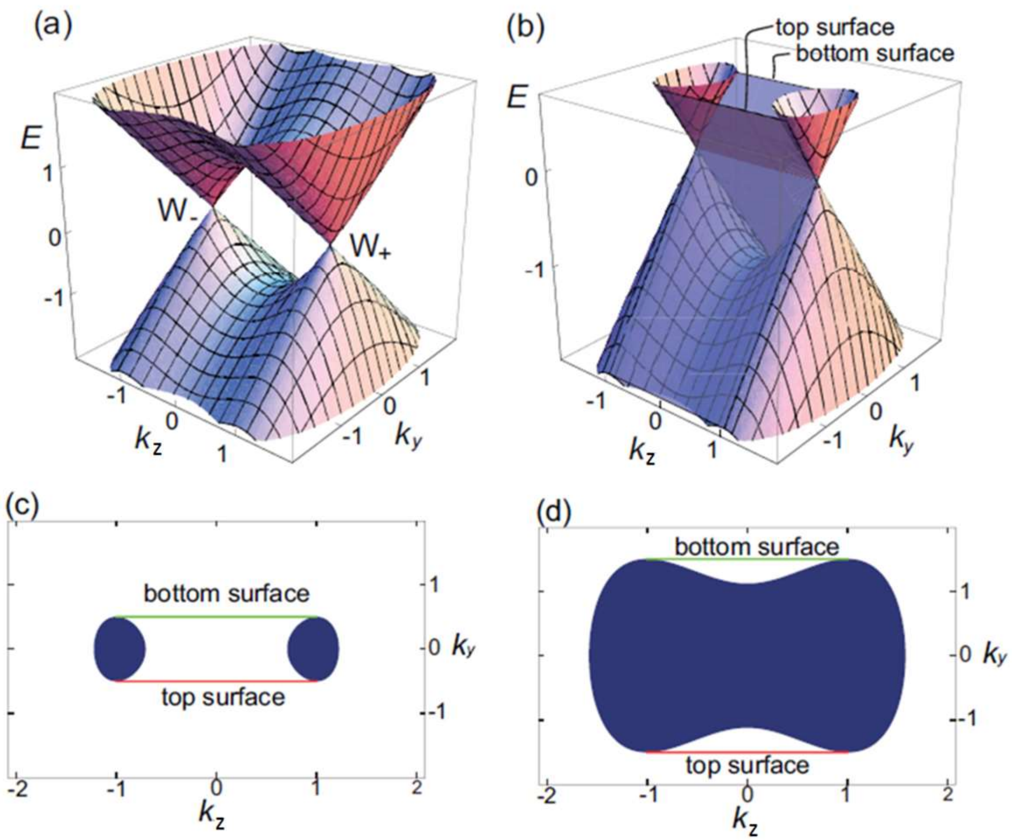


Fig from Kargarian et al, Sci Rep 2015

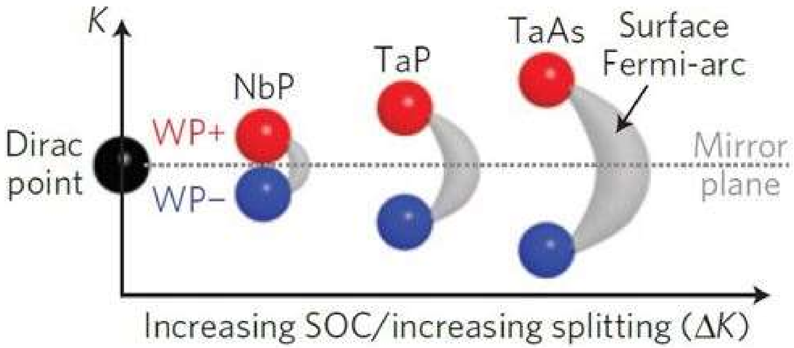


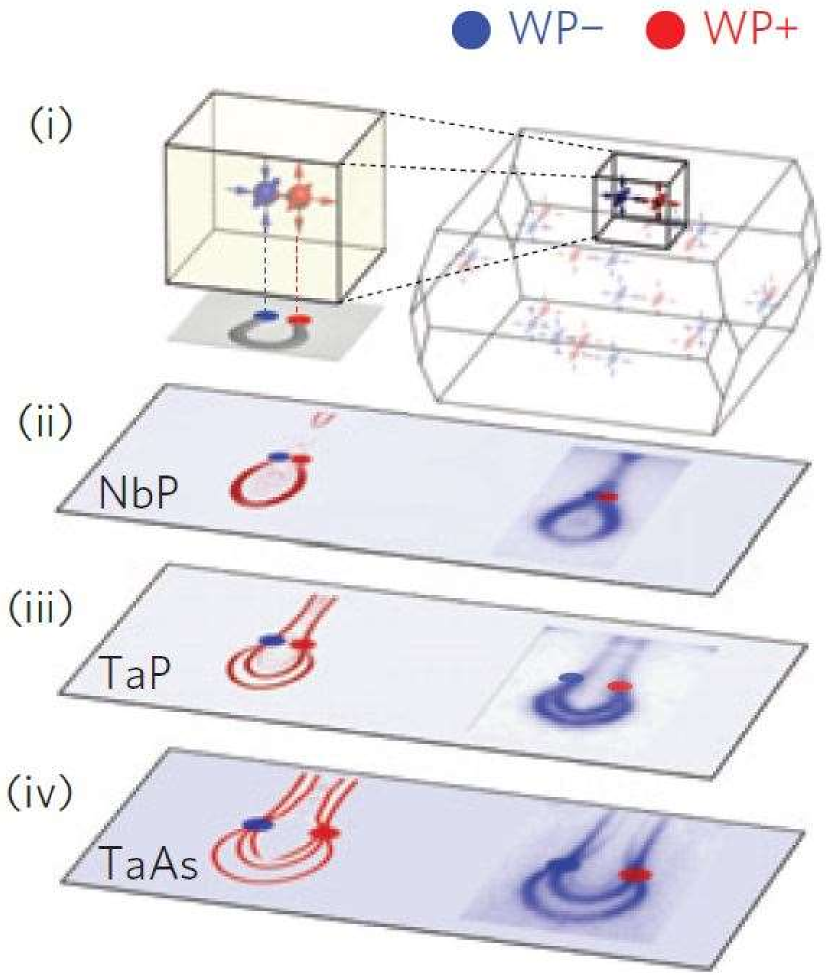
- SS connects to bulk states at Weyl nodes

Haldane 1401.0529

Fermi arc in Transition metal monopnictide

0.5 mm





theory

experiment (ARPES)

Z.K. Liu et al, Nature Material 2015