Topological Semimetals: Weyl Semimetals, Dirac Semimetals

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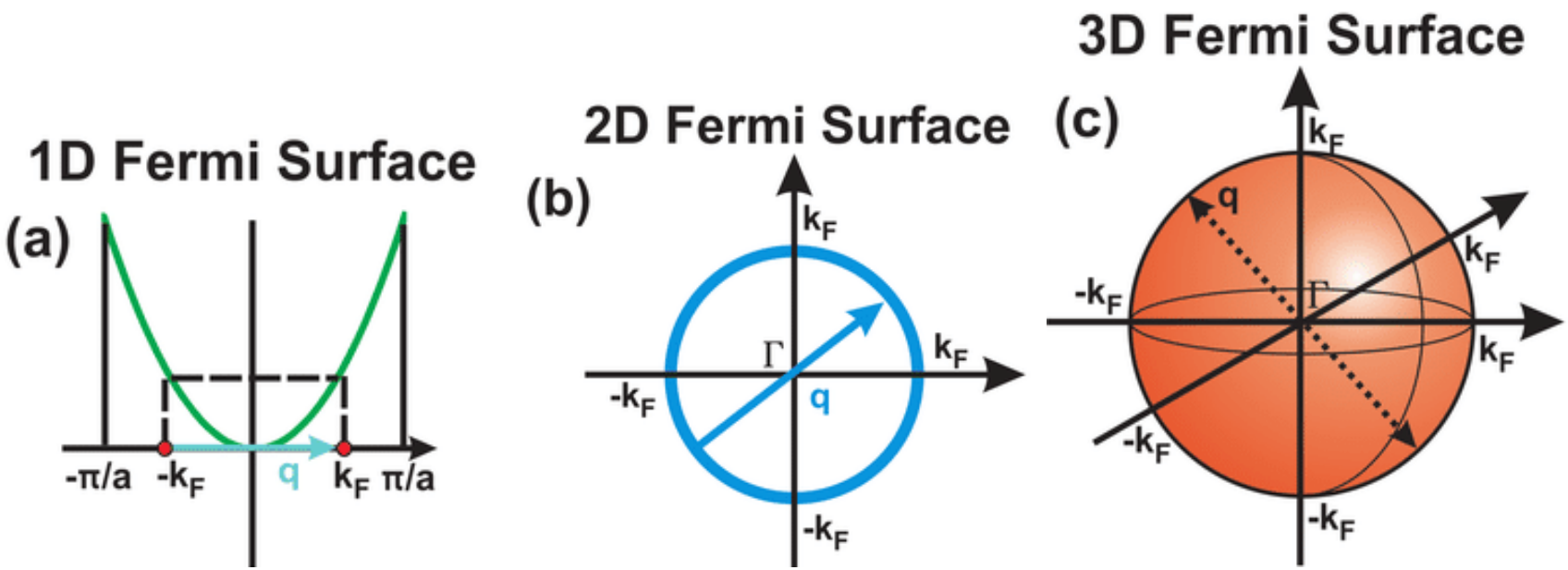
Some basic definitions

Fermi Surface (FS)

- The surface created by the highest occupied electronic states in the momentum space (k_x, k_y, k_z) is known as FS.
- Schematics of FS of non interacting electrons:



(a) (b) (c)

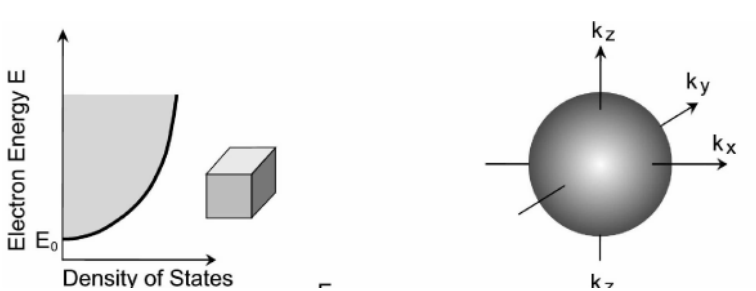
Some basic definitions

Density of states (DOS)

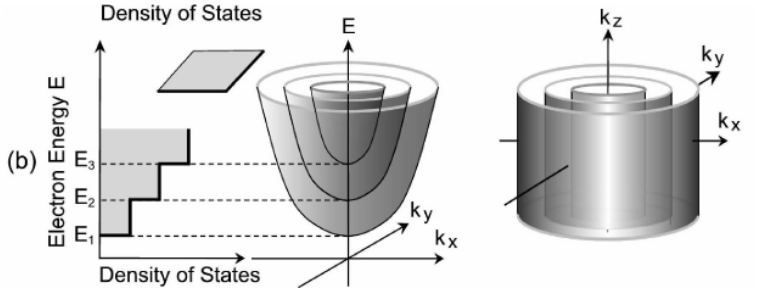
- Number of states lying in the energy range dE around energy $E(k)$.
- It is defined as:

$$D(E) = \int dk_x dk_y dk_z \, \frac{1}{|\nabla_k \; E(k_x, k_y, k_z)|} \tag{1}$$

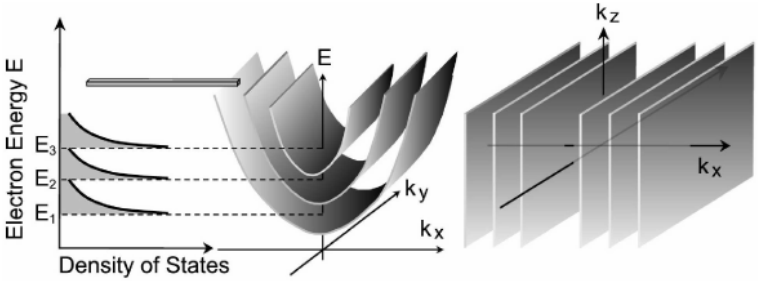
DOS and FS in 0D, 1D, 2D, 3D



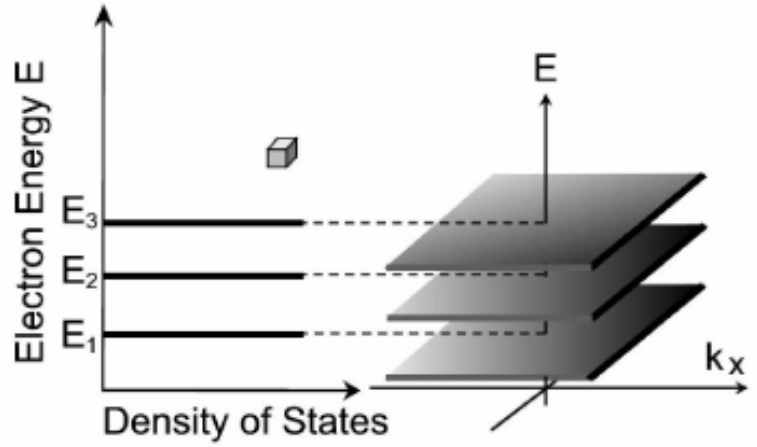
(a) 3D, Volume



(b) 2D, Plane



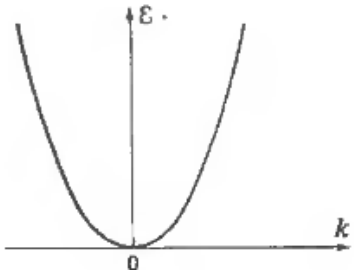
(c) 1D, Line



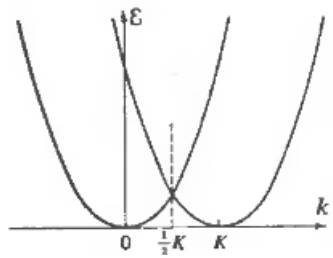
(d) 0D, Dot

Band gap appears due to crystal potential

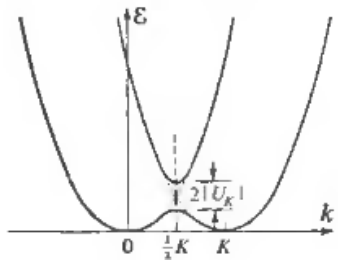
Appearance of band gap when free electron is put in the weak periodic potential.



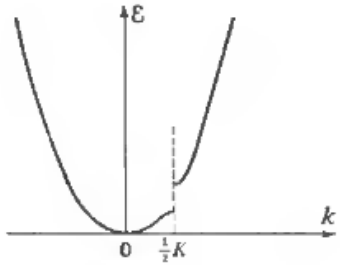
(a) Free Electron



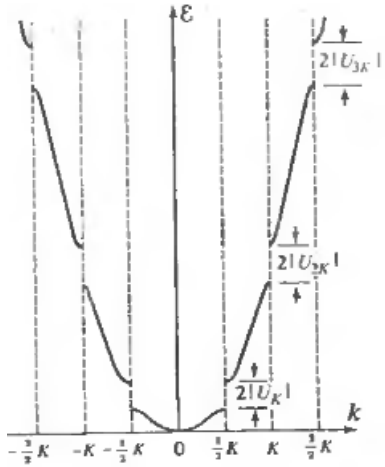
(b) In weak pot.



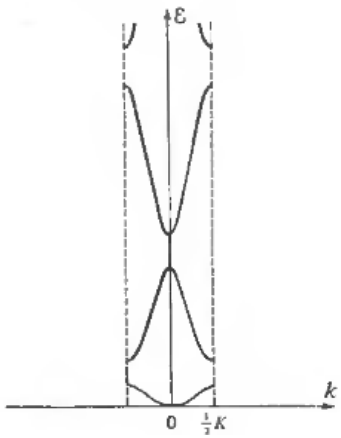
(c) Split of Band



(d) Alter. Rep.

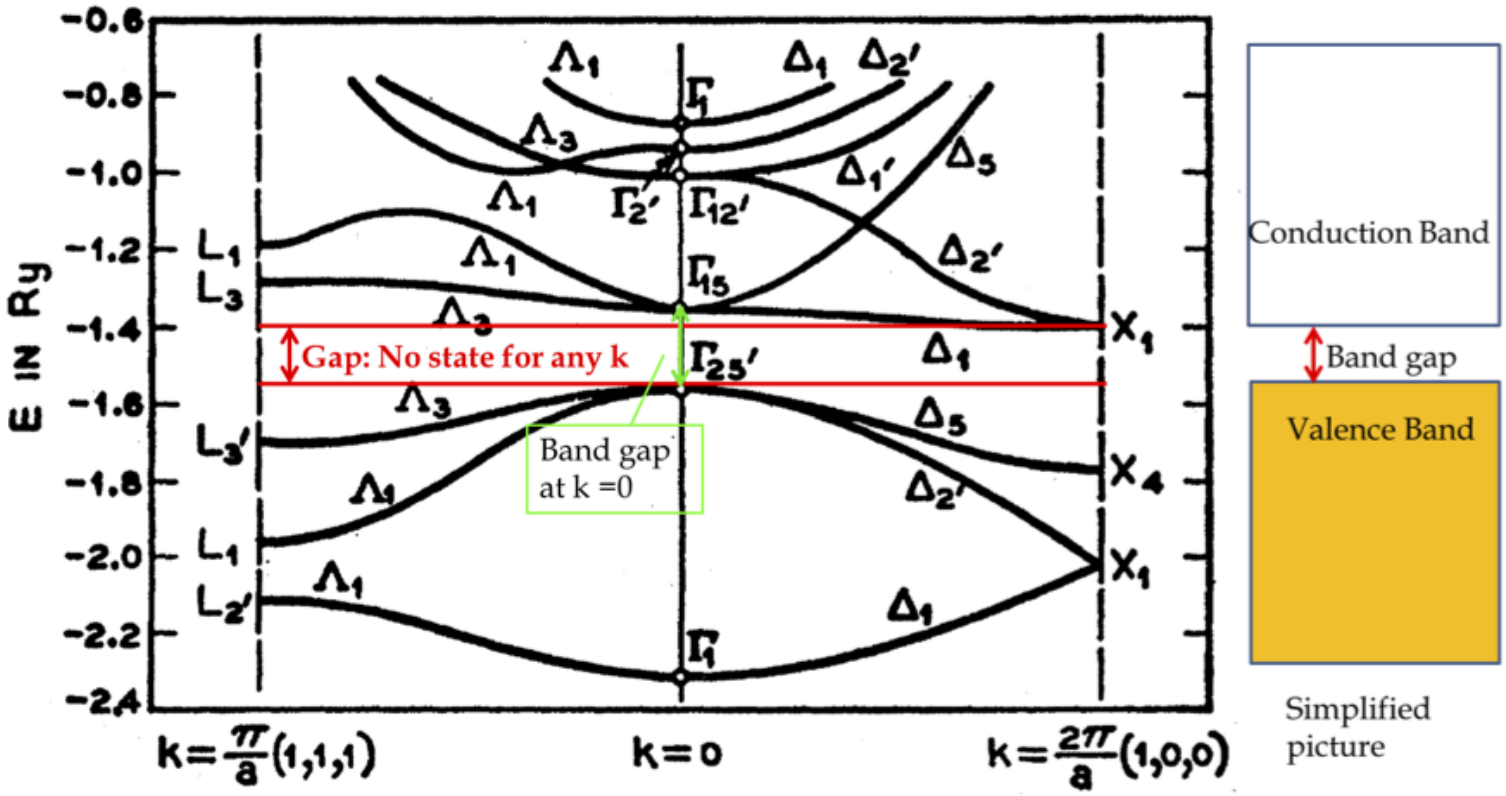


(e) Higher Ener.



(f) Reduced BZ.

Band structure of real materials is more complicated



Metals, Semimetal, Semiconductor, Insulator

- Metal: Conduction and Valence band overlaps at Fermi Energy (E_F). DOS has large values at E_F.
- Semimetal: Conduction and Valence band touch each other at E_F, but vanishing DOS at E_F
- Semiconductor: Conduction and Valence band don't touch each other at E_F, and DOS at E_F is zero. The band gap is $E_g \gtrsim k_B T$.
- Insulator: Conduction and Valence band don't touch each other at E_F, and DOS at E_F is zero. The band gap is $E_g \gg k_B T$.

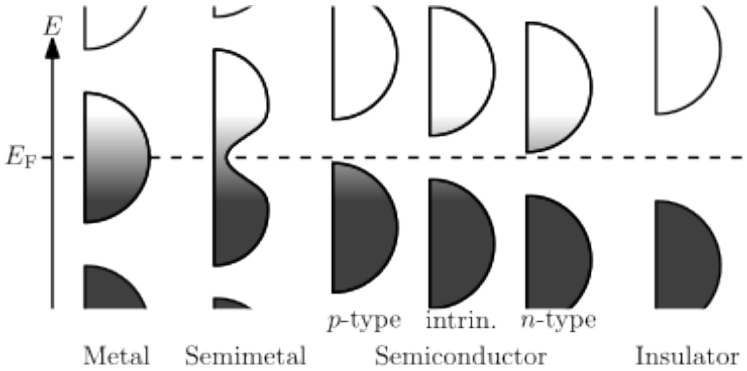


Figure: Distribution of DOS in valence (lower, black) and conduction (upper, white) bands at Fermi energy.

Representation of Hamiltonian at band touching points

- The simplest case is the two bands touching each other at as single points in momentum space.
- The (hermitian) Hamiltonian at the band touching point can be written in terms of the Pauli matrices.

$$H = \begin{bmatrix} a(k) + b(k) & c(k) + \imath d(k) \\ c(k) - \imath d(k) & a(k) - b(k) \end{bmatrix} = a(k)\sigma_0 + c(k)\sigma_1 + d(k)\sigma_2 + b(k)\sigma_3 \quad (2)$$

  where $k \equiv [k_x, k_y, k_z]$.
- The solution (energy) of the Hamiltonian is:

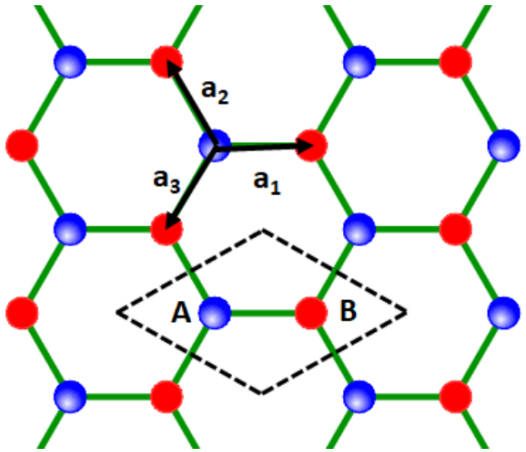
$$E = a(k) \pm \sqrt{c(k)^2 + d(k)^2 + b(k)^2} \quad (3)$$

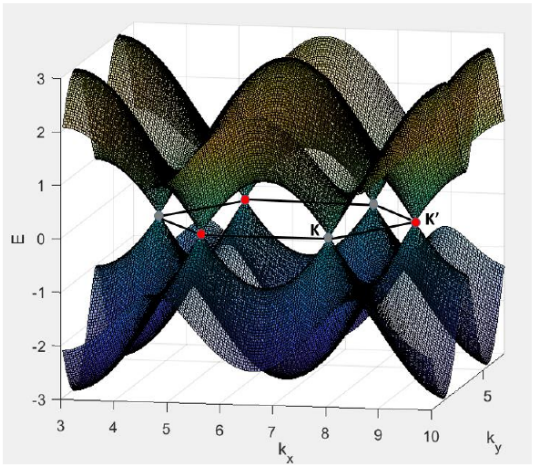
- The band touching points (gapless) occurs when $b(k) = c(k) = d(k) = 0$; gap appears when either of $b(k)$, $c(k)$, $d(k)$ is non-zero.

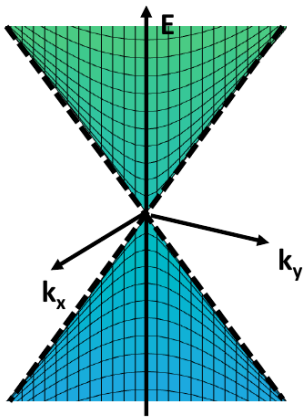
Hamiltonian of the Graphene

- The Hamiltonian of Graphene with nearest neighbour hopping:

$$H = \begin{bmatrix} 0 & \sum_{i=1}^{3} e^{\imath k a_i} \\ \sum_{i=1}^{3} e^{-\imath k a_i} & 0 \end{bmatrix} = t_1 \left(\sum_i \cos k a_i \right) \sigma_x + t_1 \left(\sum_i \sin k a_i \right) \sigma_y . \quad (4)$$



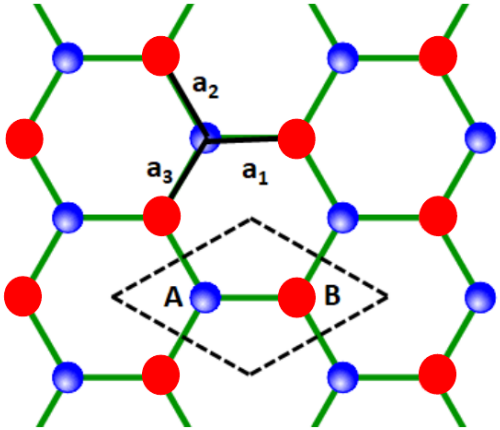




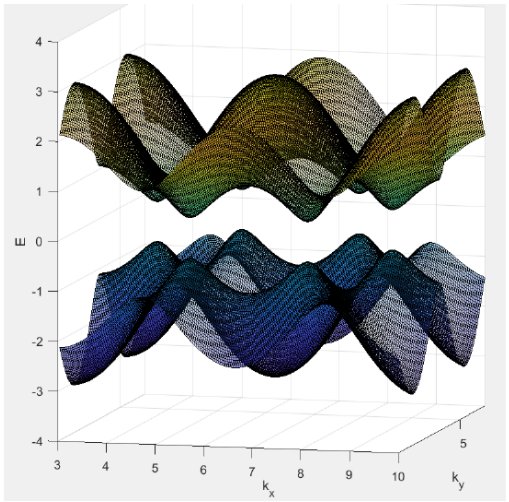
A way to open a gap: break inversion symmetry

- Adding a single mass term the Hamiltonian reads:

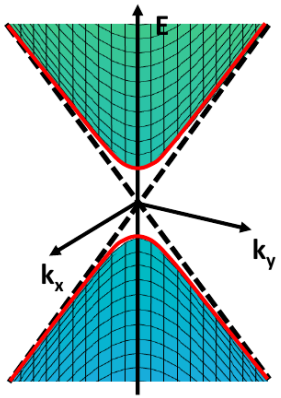
$$H = \begin{bmatrix} M & \sum_{i=1}^{3} e^{\imath k a_i} \\ \sum_{i=1}^{3} e^{-\imath k a_i} & -M \end{bmatrix} . = t_1 \left(\sum_i \cos k a_i \right) \sigma_x + t_1 \left(\sum_i \sin k a_i \right) \sigma_y + M \sigma_z . \tag{5}$$



hBN lattice



Band structure with $V = 0.1t_1$

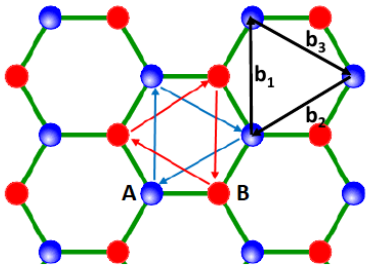


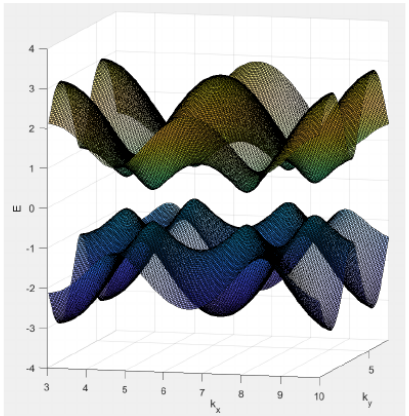
Another way to open gap: Haldane model

- A periodic local magnetic field such that the total flux through a unit cell is zero.
- Second-neighbor hopping: each hop along the arrows has a complex hopping $-t_2 e^{\imath\phi}$ (The consequence of Aharonov-Bohm effect)

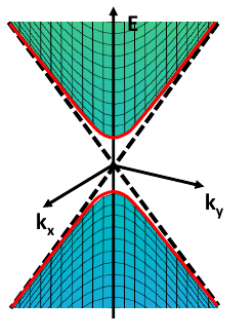
$$H = \begin{bmatrix} t_2 \sum \left(e^{\imath\phi} e^{-\imath k b_i} + e^{-\imath\phi} e^{\imath k b_i} \right) & t_{b1} \sum e^{\imath k a_i} \\ t_1 \sum e^{-\imath k a_i} & t_2 \sum \left(e^{-\imath\phi} e^{-\imath k b_i} + e^{\imath\phi} e^{\imath k b_i} \right) \end{bmatrix}. \tag{6}$$

$$\begin{aligned} H =& t_1 \left(\sum_i \cos k a_i \right) \sigma_x + t_1 \left(\sum_i \sin k a_i \right) \sigma_y \\ &+ 2 t_2 \cos\phi \left(\sum \cos k b_i \right) \sigma_0 - 2 t_2 \sin\phi \left(\sum \sin k b_i \right) \sigma_z. \end{aligned} \tag{7}$$





Band structure with $t_2 = 0.1 t_1$ and $\varphi = \pi/2$

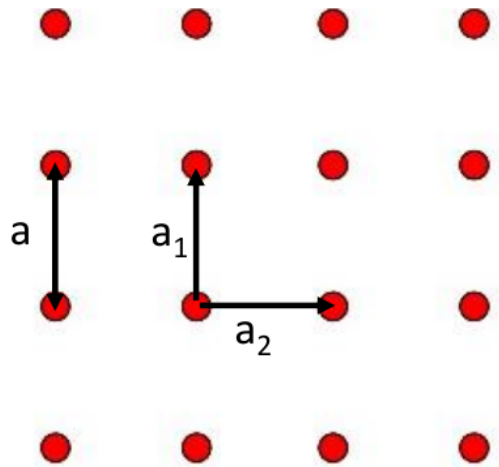


Band-inversion Top. Insulator

- Each lattice site has two orbital s and p.
- M indicates the potential difference of two orbitals.
- Hopping t_1 indicates the coupling between s and p orbitals.
- Hopping t_2 indicates the intra-orbital hopping.

$$H = t_1 \sin(k_x a_x)\sigma_x + t_1 \sin(k_y a_y)\sigma_y t_2 \left[\frac{M}{t_2} - \cos(k_x a) - \cos(k_y a)\right]\sigma_z. \quad (8)$$

- $-2 < M/t_2 < 2$ - non-trivial (band-inversion insulator); otherwise (trivial insulator)

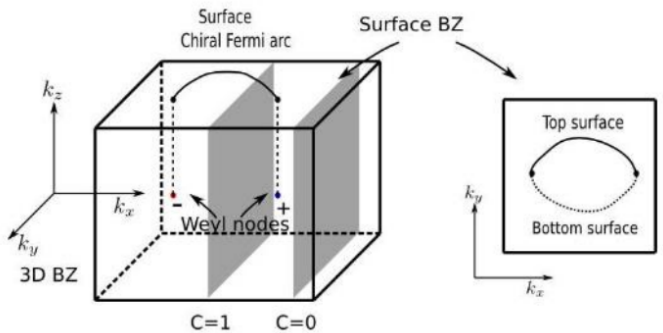


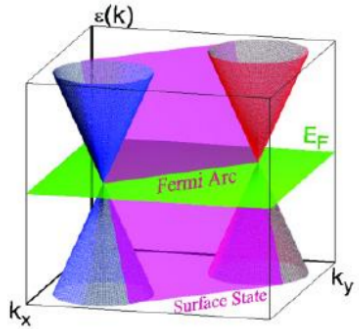
3D topological system: Weyl semimetal

- Hamiltonian of half-filled 3D two band model:

$$H = [2t_x(\cos k_x - \cos k_0) + m(2 - \cos k_x - \cos k_z)]\,\sigma_x + 2t_y \sin k_y \sigma_y + 2t_z \sin k_z \sigma_z. \tag{9}$$

- This model breaks time reversal symmetry and hosts two weyl nodes at $\pm(k_0, 0, 0)$.





Weyl semimetals from the band theory

- Consider the bands are filled upto fermi levels and we have band touching points $\pm(\pm k_x \mp k_0, k_y, k_z)$.
- Expanding hamiltonian at these high symmetry points:

$$\begin{aligned} H_{pm} &= v_x \left[p_\pm\right]_x \sigma_x + v_y \left[p_\pm\right]_y \sigma_y + v_z \left[p_\pm\right]_z \sigma_z \\ E &= \left[v.p_{pm}\right]^2 . \end{aligned} \tag{10}$$

  Here, $v_x = 2t_x \sin k_0$, $v_{y,z} = -2t_{y,z}$.
- Above Hamiltonian is closely related to the Weyl hamiltonian:

$$H^{\pm}_{\text{Weyl}} = \pm c\mathbf{p}.\sigma$$

.

General description of Weyl semimetals

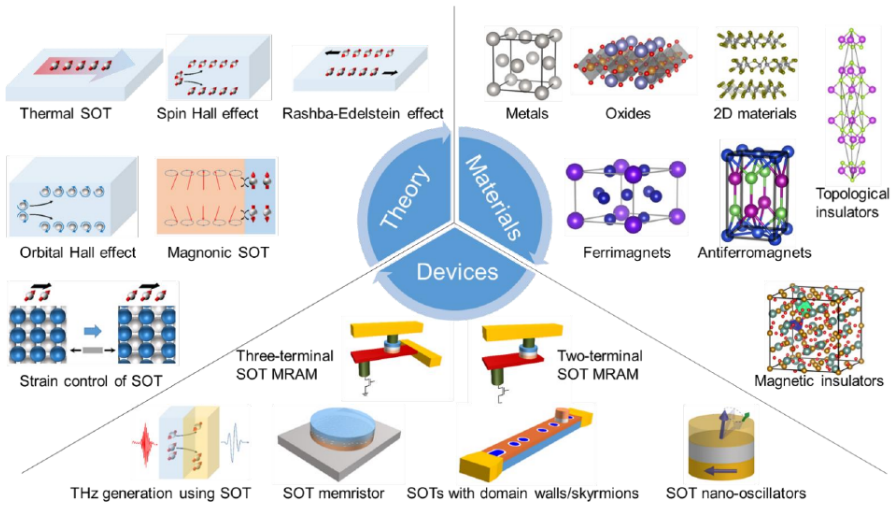
- More generally the low-energy theory of a Weyl point is in general an anisotropic version of the above Weyl equation:

$$H = \sum_i v_i \left(\hat{n}_i \cdot \mathbf{p}\right) \sigma_i + v_0 \left(\hat{n}_0 \cdot p\right) I. \tag{11}$$

  - v_i: Anisotropy of Weyl points
  - $\hat{n}_i$: Principal direction
  - Helicity of the weyl points $\kappa = \text{sign}\left[\hat{n}_1 \left(\hat{n}_2 \times \hat{n}_3\right)\right]$.

Motivation of the paper

- Large SOC is needed to generate spin current through electric current.
- This spin current will apply the spin orbit torque (SOT) to create effective magnetic field.
- Large SOT is generated through large current, which give rise to the Joule effect.
- To avoid the Joule loss we need the large SOT at low current.



Use of non-dissipative transport

- To generate SOT one can use the transverse Hall current which uses the topological band properties (topological SOT).
- Using linear response theory and mixed berry curvature (MBC) it is found that topological SOT is large compared to the bulk SOT in Ti_2MnAl.

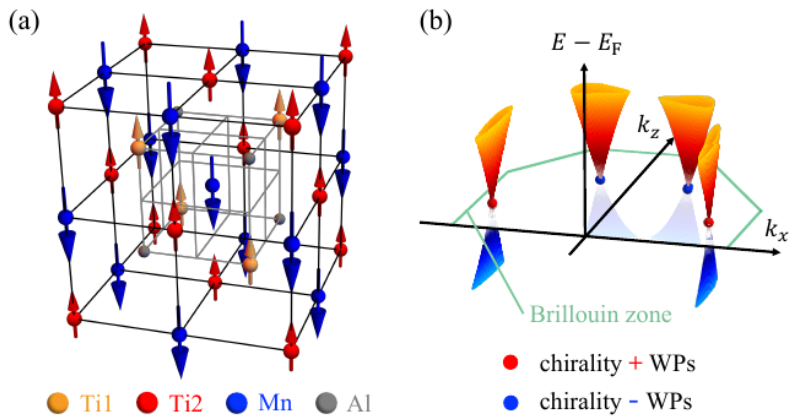


FIG. 1. (a) Crystal structure of Ti_2MnAl. Ti and Mn are responsible for the compensated ferrimagnetic ordering. (b) The energy dispersion around the WPs on $k_y = 0$ plane.

Comparison of topological and bulk SOT driven parameters

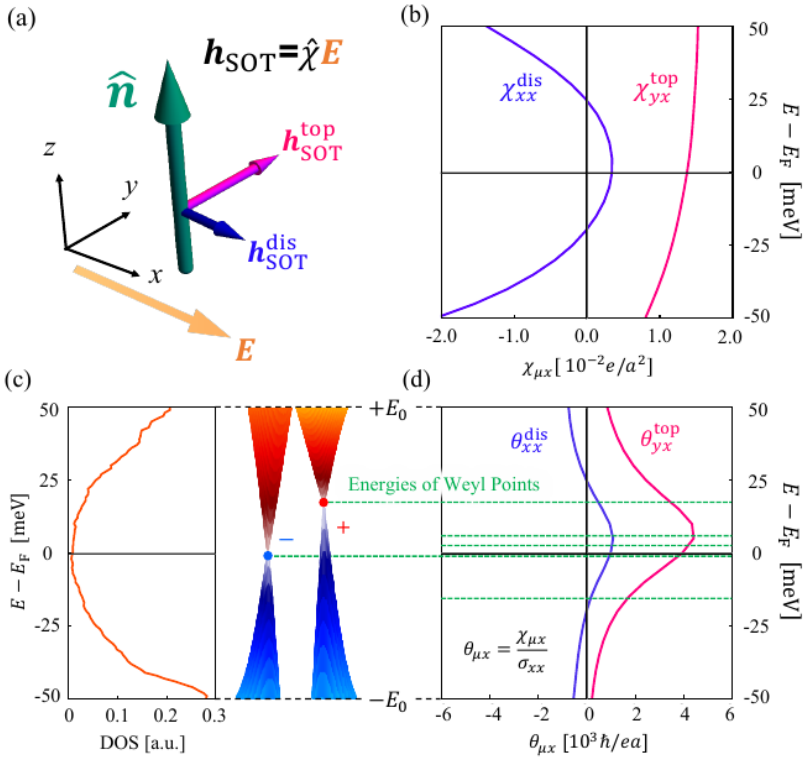


FIG. 3. (a) The effective magnetic fields form dissipative and topological response, acting on the compensated ferrimagnetic ordering $\hat{\boldsymbol{n}}$. (b) The energy dependences of the response coefficients $\chi^{\rm dis}_{xx}$ and $\chi^{\rm top}_{yx}$. (c) The density of states and one of the energy dispersion around WPs. The inversion symmetry breaking in Ti_2MnAl causes energy differences between WPs. (d) The energy dependences of efficiencies of SOT $\theta^{\rm dis}_{xx}$ and $\theta^{\rm top}_{yx}$.

Comparison of topological and bulk SOT driven parameters

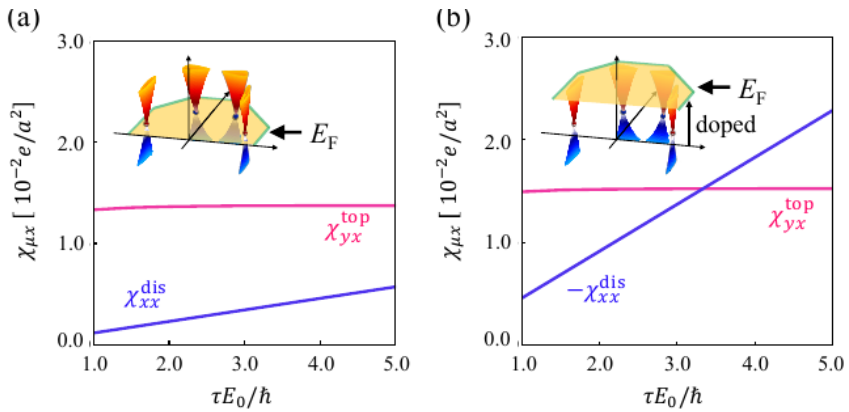


FIG. 4. Relaxation time dependences for response coefficients $\chi_{xx}^{\rm dis}$ and $\chi_{yx}^{\rm top}$ when (a) $E_{\rm F}$ is located at the energy of the WPs and (b) $E_{\rm F}$ is away from the energy of the WPs.

MBC

MBC is a BC extended in the composite parameter space $k, \hat{n}$ spanned by the momentum k and the ferrimagnetic ordering $\hat{n}$.

$$\Omega^{\boldsymbol{kk}}_{yx}(\boldsymbol{k}) = 2\,\mathrm{Im}\sum_{n\neq m} f_{n\boldsymbol{k}} \frac{\langle n\boldsymbol{k}|\partial_{k_y} H|m\boldsymbol{k}\rangle\langle m\boldsymbol{k}|\partial_{k_x} H|n\boldsymbol{k}\rangle}{(E_{n\boldsymbol{k}} - E_{m\boldsymbol{k}})^2},$$

$$\Omega^{\hat{\boldsymbol{n}}\boldsymbol{k}}_{yx}(\boldsymbol{k}) = 2\,\mathrm{Im}\sum_{n\neq m} f_{n\boldsymbol{k}} \frac{\langle n\boldsymbol{k}|\partial_{\hat{n}_y} H|m\boldsymbol{k}\rangle\langle m\boldsymbol{k}|\partial_{k_x} H|n\boldsymbol{k}\rangle}{(E_{n\boldsymbol{k}} - E_{m\boldsymbol{k}})^2}.$$

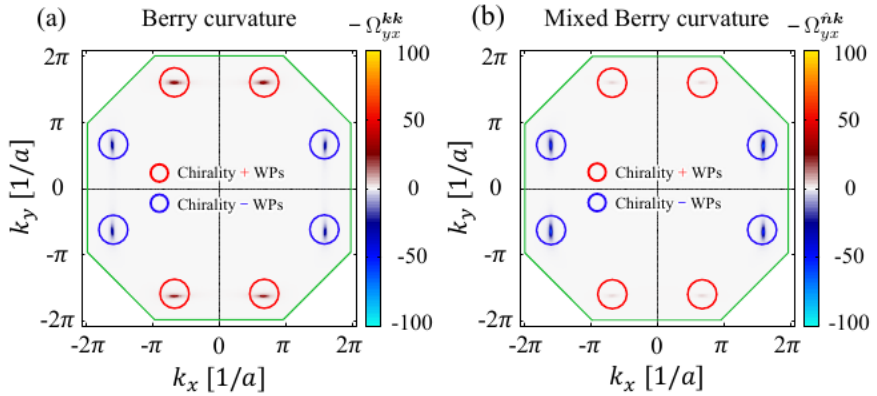


FIG. 5. The mapping of the yx component of (a) the BC $-\Omega^{\boldsymbol{kk}}_{yx}$ and (b) the MBC $-\Omega^{\hat{\boldsymbol{n}}\boldsymbol{k}}_{yx}$ on $k_z = 0.1[1/a]$ at E_F. In momentum space, the positions of the peaks/valleys of $-\Omega^{\boldsymbol{kk}/\hat{\boldsymbol{n}}\boldsymbol{k}}_{yx}$ correspond to the positions of the WPs.