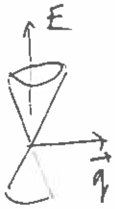
LECTURE 23

(II) Weyl semimetals in 3D

Suppose we have low-energy hamiltonian in a 3D system of the form:



$$H_{eff} = v\,\vec{\sigma}\cdot\vec{q} \qquad \vec{q} = (q_x, q_y, q_z)$$

$$E(\vec{q}) = \pm v|\vec{q}|$$ – gapless linear dispersion in all 3 directions.

"Weyl spectrum" Herman Weyl 1927

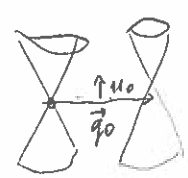
• **Note:** (i) to have such a non-degenerate spectrum either $\mathcal{T}$ or $\mathcal{P}$ must be broken (otherwise all bands at least doubly degenerate).

(ii) Such Weyl point is absolutely stable: there is no possible mass term one can add to open a gap:

most general perturbation

$$H_{Weyl} \to H_{Weyl} + \delta H \qquad \delta H = \mu_0 + \vec{q}_0\cdot\vec{\sigma}$$

$$E(\vec{q}) \to \mu_0 \pm v|\vec{q}-\vec{q}_0|$$



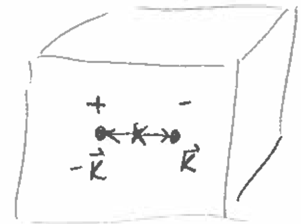
(iii) Anisotropic version:

$$H_{eff} = v_i \sigma_i q_i$$

Chirality: $\chi = \mathrm{sgn}(v_x v_y v_z) = \pm 1$

(iv) In a system defined on the lattice such Weyl points must come with pairs of opposite chirality

$$H^{(\pm)}_{Weyl} = \pm v \vec{\sigma} \cdot (\vec{q} \pm \vec{K})$$



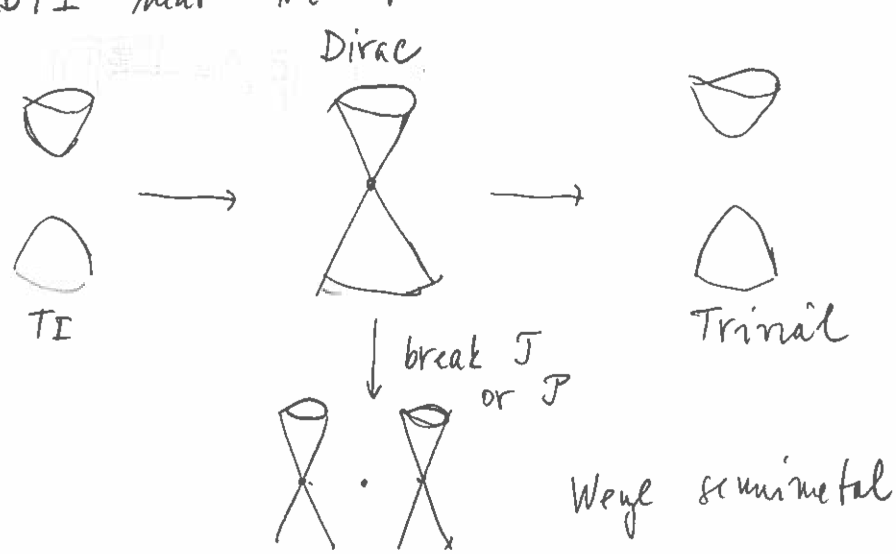
3D BZ

(v) The only way to remove Weyl points is by moving them to the same (high-symmetry) point in the BZ. Then one gets a doubly degenerate Dirac point which can be gapped out

$$H_{Dirac} = \begin{pmatrix} v\vec{\sigma}\cdot\vec{q} & M \\ M & -v\vec{\sigma}\cdot\vec{q} \end{pmatrix}$$

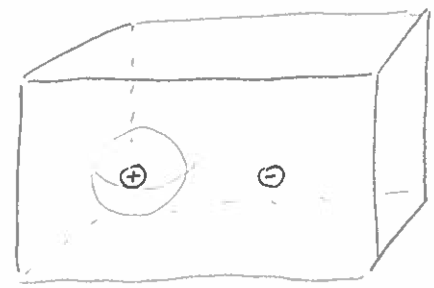
$$E(\vec{q}) = \pm\sqrt{v^2 q^2 + M^2} \qquad \text{gapped spectrum}$$

(vi) One way to think about Weyl semimetal is to take a 3D TI near the transition to the trivial insulator



Topological invariant and fermi arcs on the surface

Consider a sphere centered around a Weyl point, evaluate the Berry flux through the sphere:



3D BZ

$$H = \vec{d} \cdot \vec{\sigma}, \qquad \vec{d} = v(q_x, q_y, q_z) = vq(\cos\varphi \sin\theta, \sin\varphi \sin\theta, \cos\theta)$$

$$\Omega^{(+)} = \int d\vec{S} \cdot \mathcal{F}$$

Problem set #2: $\mathcal{F}_{\theta\varphi} = \frac{1}{2}\sin\theta$

$$= \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \left(\frac{1}{2}\sin\theta\right)$$

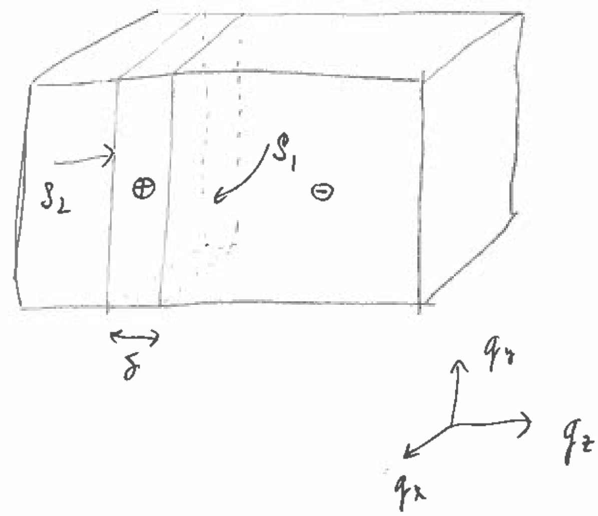
$$= \frac{2\pi}{2} \int_0^{\pi} \sin\theta \, d\theta = 2\pi$$

$$\Omega^{(-)} = -2\pi$$

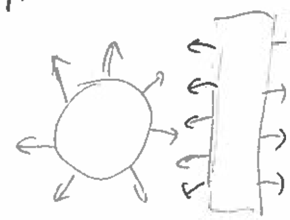
$\Omega^{(+)} + \Omega^{(-)} = 0$ - the total Berry flux in the BZ vanishes.

$$\int^{\pi} \sin\theta = \left[-\cos\theta\right]_0^{\pi} = 2$$

- Now deform the sphere into a rectangular box



$\rightarrow$ $\Omega^{(+)}$ is contributed by the large flat surfaces only when $\delta \to 0$.



$$\Omega^{(+)} = \underbrace{\int_{S_1} \mathcal{F}\, dq_x dq_y}_{\Omega_1} + \underbrace{\int_{S_2} \mathcal{F}\, dq_x dq_y}_{\Omega_2} = 2\pi$$

- Regard each $q_z = \text{const.}$ slice of the 3D BZ as a fictitious 2D system

Then $C_1 = \frac{\Omega_1}{2\pi}$ and $C_2 = -\frac{\Omega_2}{2\pi}$ are Chern numbers characterising that 2D system

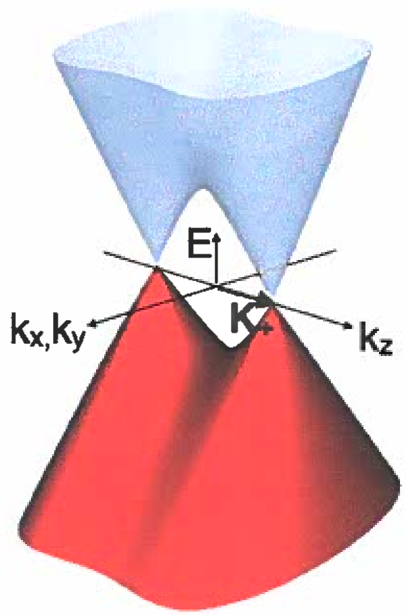
$$\Rightarrow \quad \boxed{C_1 - C_2 = 1}$$

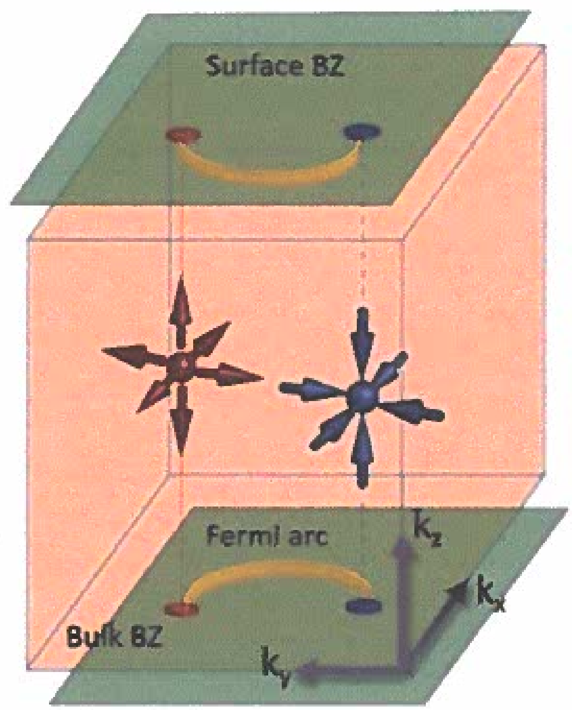
> One of the 2D systems is a Chern insulator with protected surface states

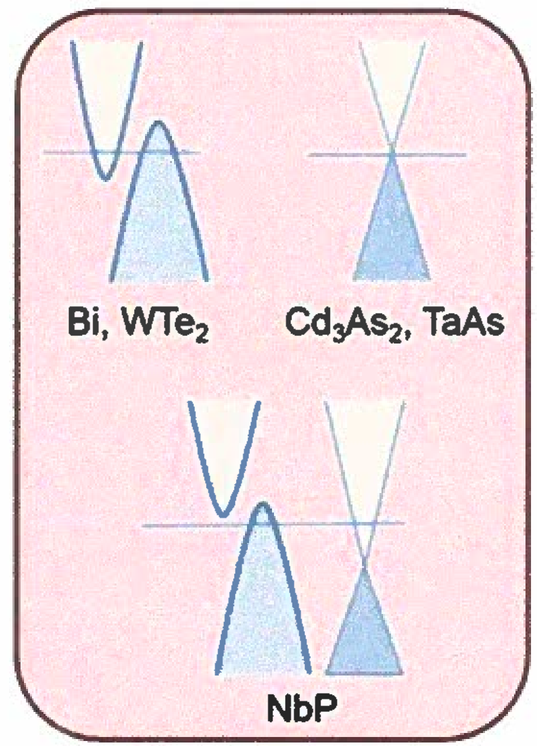
"Fermi arcs" connecting the $\oplus$ and $\ominus$ Weyl points.

Dirac and Weyl semimetals

- 3D materials with bulk gapless Dirac or Weyl points
- surface Fermi arcs

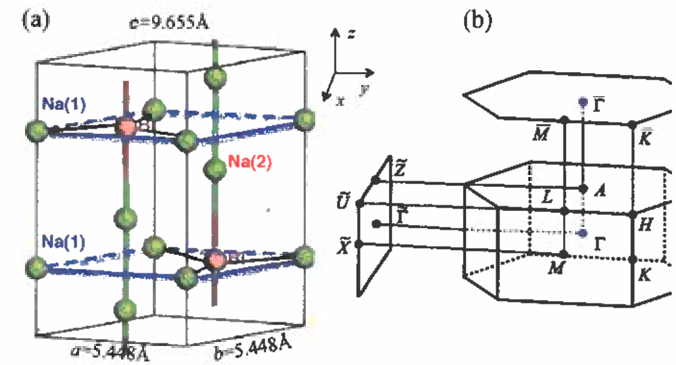






[Figure by Chandra Shekhar MPI Munchen]

Back to 3D: Model for Cd_3As_2 and Na_3Bi Dirac semimetals



In the basis of spin-orbit coupled states

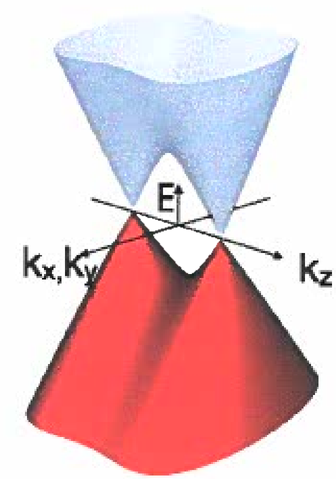
$$|P_{\frac{3}{2}},\tfrac{3}{2}\rangle, |S_{\frac{1}{2}},\tfrac{1}{2}\rangle, |S_{\frac{1}{2}},-\tfrac{1}{2}\rangle, |P_{\frac{3}{2}},-\tfrac{3}{2}\rangle$$

the tight-binding model reads:

$$H^{\mathrm{latt}} = \epsilon_{\boldsymbol{k}} + \begin{pmatrix} h^{\mathrm{latt}} & 0 \\ 0 & -h^{\mathrm{latt}} \end{pmatrix}$$

$$h^{\mathrm{latt}}(\boldsymbol{k}) = m_{\boldsymbol{k}}\tau^z + \Lambda(\tau^x \sin a_x k_x + \tau^y \sin a_y k_y),$$

$$m_{\boldsymbol{k}} = t_0 + t_1 \cos a k_z + t_2(\cos a k_x + \cos a k_y)$$



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