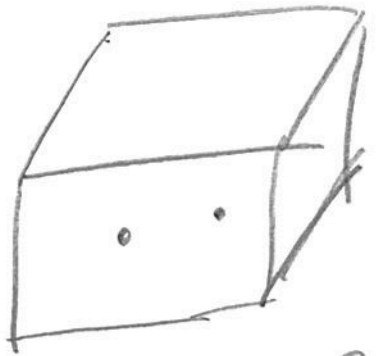
Topology of semi-metals

Following A. Turner and A. Vishwanath
arXiv: 1301.0330

Example Weyl semi-metal.
3D material

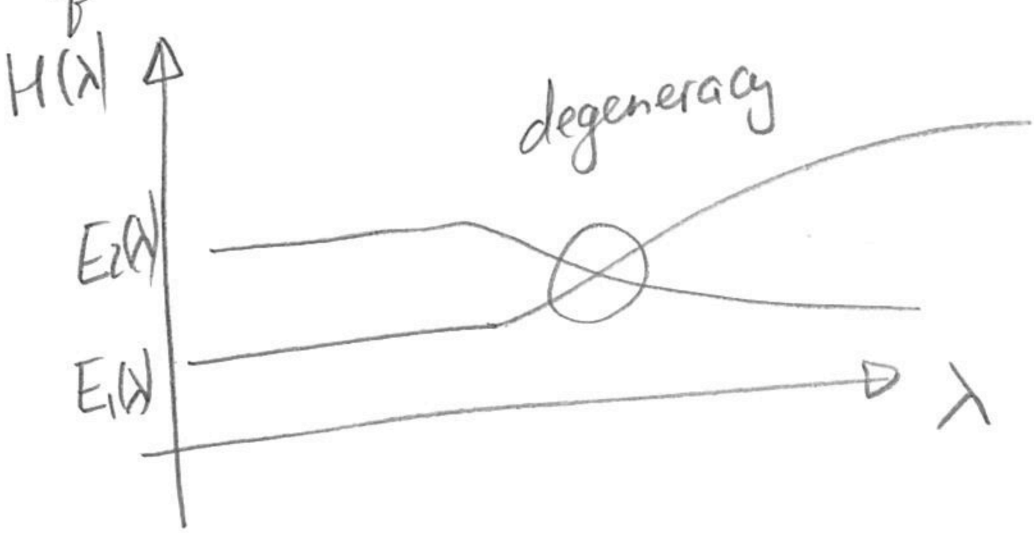


a number of degenerate points in the k-space.

k-space

Background

Accidental degeneracies
quantum mechanic Hamiltonian with a parameter



To have a degeneracy in q.M. you need 3 parameters to tune (unless there are symmetries).

For near degenerate situation any 2-level system has a Hamiltonian

$$H = f_0 \sigma_0 + f_x(\lambda)\sigma_x + f_y(\lambda)\sigma_y + f_z(\lambda)\sigma_z$$

The energy splitting

$$\Delta E = E_2 - E_1 = 2\sqrt{f_x^2(\lambda) + f_y^2(\lambda) + f_z^2(\lambda)}$$

Therefore

$f_x(\lambda) = f_y(\lambda) = f_z(\lambda)$ and if these functions are independent λ has to have 3 components.

Symmetry may change this argument, because they may force to be coeff. of some of the pauly matrix to vanish.

Dirac Equation (Relativistic physics)

$$i\partial_t \Psi = -\vec{\alpha}\cdot(-i\vec{\nabla}\Psi) + m\beta\Psi = 0$$

$\vec{\alpha}$, β are 4×4 matrix

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 0$$

$$\alpha^2 = \beta^2 = \mathbb{1} \qquad \alpha_i\beta + \beta\alpha_i = 0$$

$$E^2 = p^2 + m^2$$

For massless fermions $(m=0)$
and odd spatial dimension

4×4 matrix

$$\beta = \mathbb{1}\otimes\tau_x$$

$$\beta^2 = \mathbb{1}\otimes\mathbb{1}$$

$$\vec{\alpha} = \vec{\sigma}\otimes\tau_z$$

$$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$$

$\mathbb{1}\otimes\tau_z = i\alpha_1\cdot\alpha_2\cdot\alpha_3$ commutes with

$\alpha_1, \alpha_2, \alpha_3$

Check

$$[i\alpha_1\cdot\alpha_2\cdot\alpha_3, \alpha_3] =$$

$$= [\mathbb{1} \otimes \tau_{\cancel{z}}, \sigma_z \times \tau_z] = [1, \sigma_z] \otimes \tau_z = 0$$

$$= \cancel{\mathbb{1} \otimes [\tau_z, \tau_z] = 0}$$

$$[\mathbb{1} \otimes \tau_z, \alpha_2] = \cancel{1 \otimes \tau_z, 1}$$

$$= [1 \otimes \tau_z, \sigma_y, \tau_z] = [\mathbb{1}, \sigma_y] \otimes \tau_z = 0$$

Therefore we can classify all eigen states of Weyl equation in accordance with their eigen values of an operator

$$1 \otimes \tau_z = i \alpha_1 \alpha_2 \alpha_3 \equiv \gamma_5$$

$$1 \otimes \tau_z \Psi_\pm = \pm \Psi_\pm$$

Therefore the 4×4 matrices are reduced to 2×2 matrices

$$H_\pm = \pm \vec{\sigma} \cdot (-i \vec{\nabla}) \qquad 2 \times 2 \text{ matrices}$$

Weyl Hamiltonian

We needed odd spatial dimensions

$[\alpha_i, \alpha_1, \ldots \alpha_d] = 0$ because it is α_i and one commutes even number remaining anticommute, together commute.

Berry curvature and Chern number

conduction band

valence band

$$|u_k\rangle$$

$$\mathcal{A}_a(k) = -i\langle u(k)|\frac{\partial}{\partial k_a} u(k)\rangle$$ Berry connection

$$F_{ab}(k) = \frac{\partial \mathcal{A}_b}{\partial k_a} - \frac{\partial \mathcal{A}_a}{\partial k_b}$$ Berry curvature

Integral of $\vec{A}$ on a loop $\oint_C \vec{\mathcal{A}}_a(k)\, d\vec{k}$ is

γ

a Berry phase

In 2 dimension

$$\int_{\text{Brillouine zone}} F(k) \frac{d^2k}{(2\pi)} = C$$

Chern number

($C \in$ integerys)

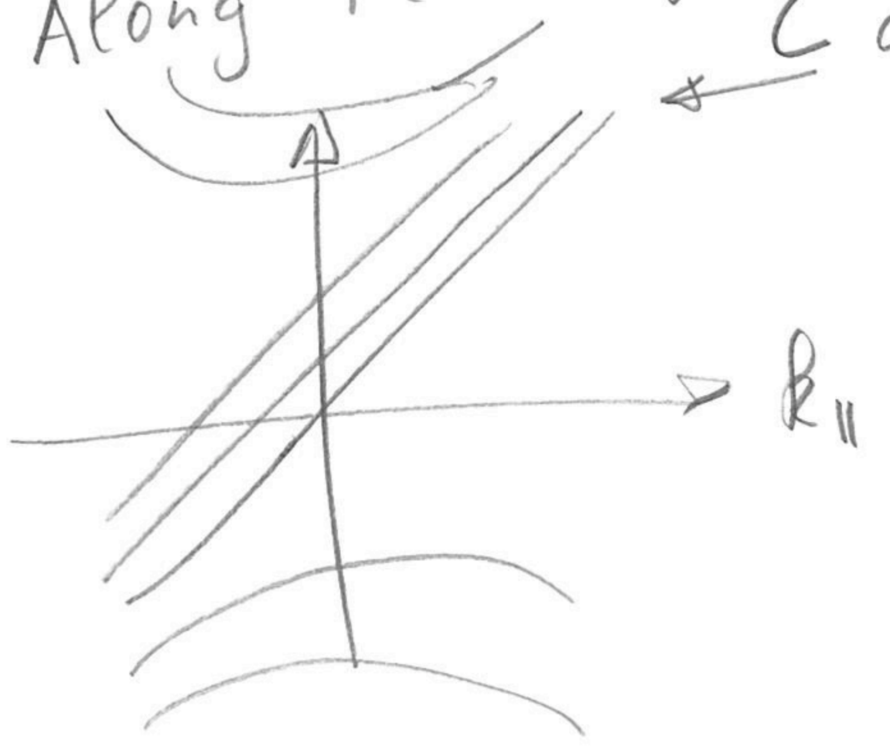
$C \in \mathbb{Z}$

$\oint (\nabla \times A) ds$

The physical interpretation of a system with a Chern number is quantization of the Hall conductunce

$$\sigma_{xy} = C \frac{e^2}{h}$$

Along the edge C chiral modes



Weyl semimetals

TR $\quad T^2 = -1$

$$H_{\vec{S}}(k_x, k_y, k_z) \xrightarrow{T} H_{-\vec{S}}(-\vec{k})$$

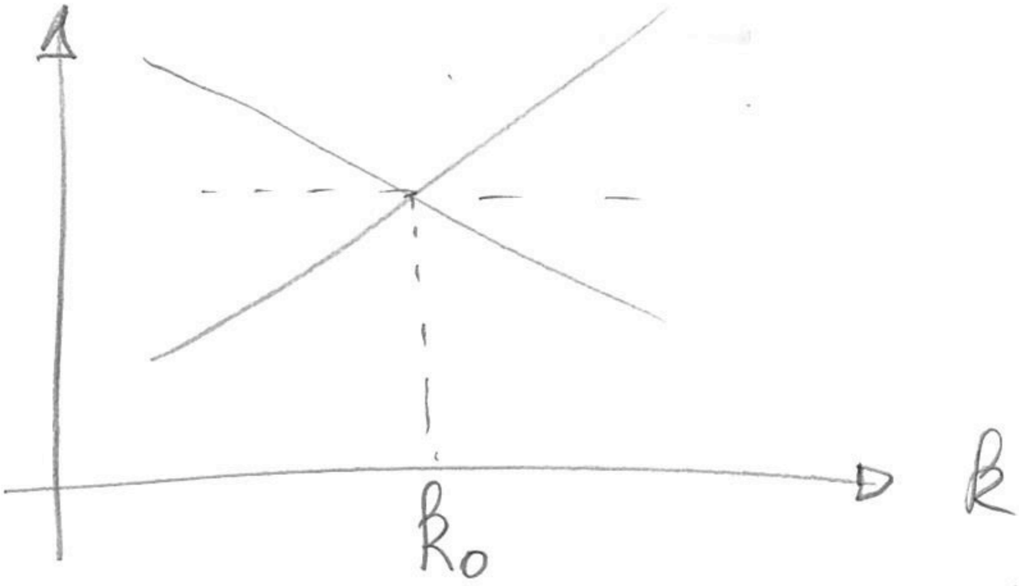
Inversion symmetry (I)

$$H_{-S}(-\vec{k}) \xrightarrow{I} H_{-\vec{S}}(\vec{k})$$

Both inversion and TR mean that states at each $\vec{k}$ are double degenerate. If we break either TR or inversion the band is <u>not</u> double degenerate. Otherwise it is

To have Weyl semimetal we need to break at least one.

Crossing of bands



Close to the crossing point

$$H(k_0+\delta k) = f_0(k_0+\delta k)\, I + \vec{f}\,(k_0+\delta k)\cdot\vec{\sigma}$$

$$f_1(k_0) = f_2(k_0) = f_3(k_0) = 0$$

$$f_\mu(k_0+\delta k) = \vec{\delta k}\cdot\frac{\partial}{\partial\vec{k}} f_\mu(k)\Big|_{k=k_0} = \vec{v}_\mu\,\vec{\delta k}$$

$$H_0(k+\delta k) = \vec{v}_0\,\vec{\delta k}\cdot\vec{1} + \sum_a \vec{v}_a\cdot\vec{\delta k}\,\sigma^a$$

For simple limit

$$\vec{v}_0 = 0 \qquad v_a = \delta_{a,i}\cdot v_F$$

$$H_0(k+\delta k) = v_F\,\vec{\delta k}\cdot\vec{\sigma}$$

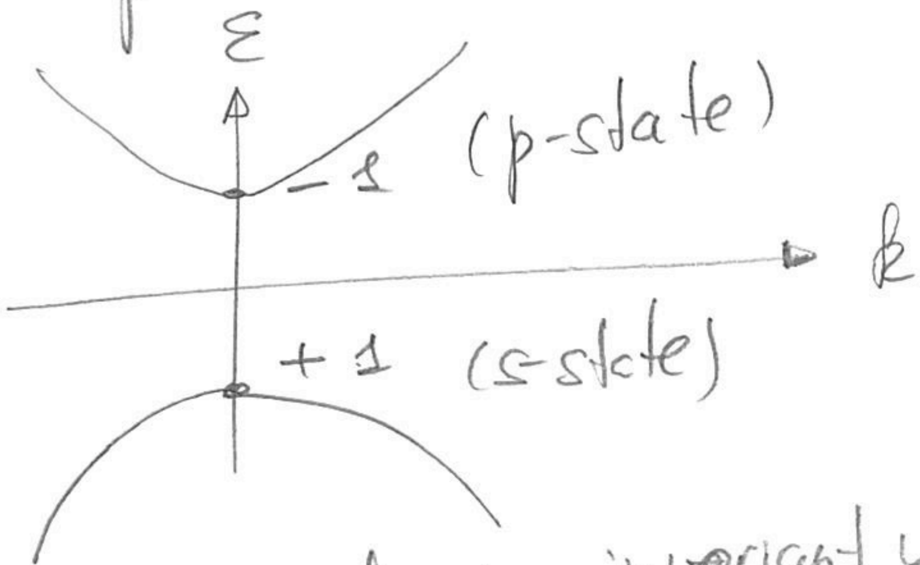
The existance of Weyl node has to do with 3 parameters in the band structure of 3d materials.

Consider Weyl semimetal

Break TR, preserve Inversion

s orbital
p orbital
on each cite

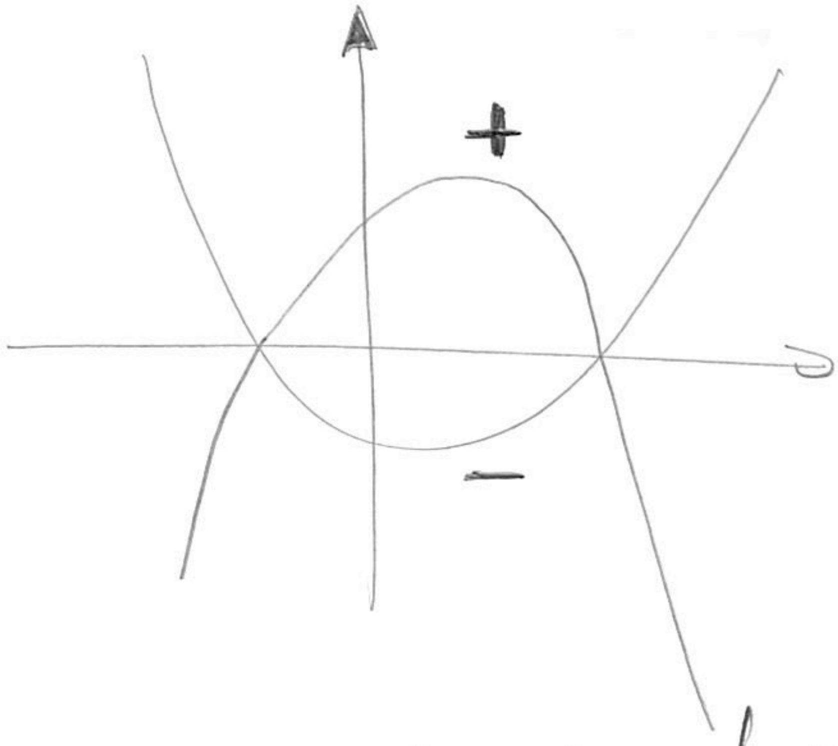
s orbital $I = +1$
p orbital $I = -1$
inversion eigen-value



insulator.

$k=0$ state in invariant under I therefore $\psi_{k=0}$ can be labeled by inversion eigen-values

Band inversion



The example of such spectrum

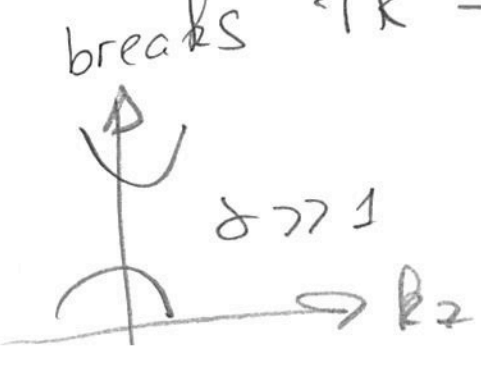
$$H(k) = t(2+\gamma - \cos k_x - \cos k_y - \cos k_z)\,\tau_z + t'\sin k_x\,\tau_x + t''\sin k_y\,\tau_y$$

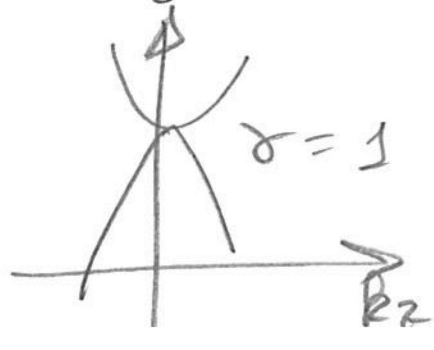
$-1 < \gamma < 1$

invariant under inversion

$k \to -k \qquad \tau_y \to -\tau_y$

breaks TR symmetry





Examples of Weyl semimetals

$Pr\,Al\,Ge_{1-x}\,Si_x$

$TaAs$

AaP

$NbAs$

For a review

Binghai Yan and Claudia Felser,
Annual Review of cond. matter phys. 8
p. 337 (2017).

Experimental signatures:

Fermi arcs