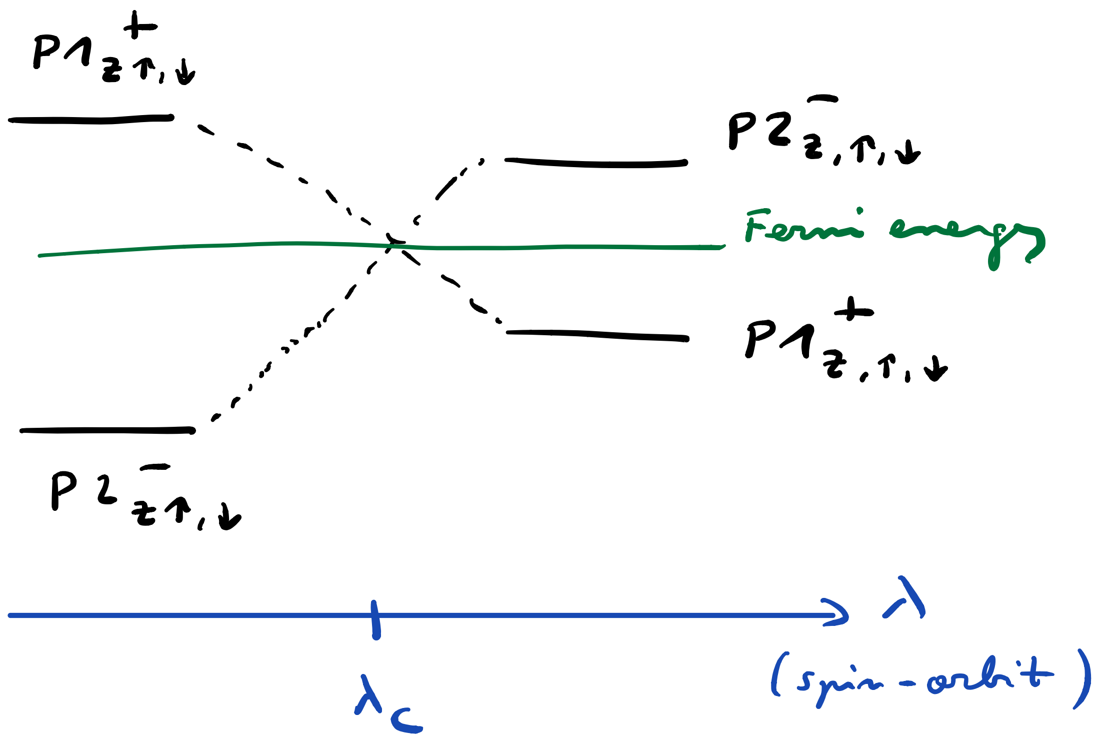
3.4 Bi_2Se_3

Low-energy states at $\vec{k} = 0$.



Low-energy basis:

$$\{ |P1^+_{z\uparrow}\rangle, |P1^+_{z\downarrow}\rangle, |P2^-_{z\uparrow}\rangle, |P2^-_{z\downarrow}\rangle \}$$

* Effective Hamiltonian:

$h_{eff}(\vec{k}) = 4\times 4$ matrix

Denote: $\sigma^z = \uparrow, \downarrow$ ("spin")

$\tau^z = P1, P2$ ("orbital")

TRS:

$$h_{eff}(\vec{k}) = \Theta\, h_{eff}(-\vec{k})\, \Theta^{-1}, \qquad (1)$$

where $\Theta = i\sigma^y \underline{K}$

SIS:

$$h_{eff}(\vec{k}) = \Pi\, h_{eff}(-\vec{k})\, \Pi^{-1}, \qquad (2)$$

where $\Pi = \tau^z$

$$\left(\begin{array}{l} \Pi\,|P1\rangle = |P1\rangle \\ \Pi\,|P2\rangle = -|P2\rangle \end{array} \right)$$

Using (1) and (2) as constraints, the form of $h_{eff}(\vec{k})$ is

$$\boxed{\begin{aligned} h_{eff}(\vec{k}) = \; & \epsilon_0(\vec{k}) \; + \\ & + \vec{d}(\vec{k}) \cdot \vec{\sigma} \, \tau^x \\ & + M(\vec{k}) \, \tau^z \end{aligned}}$$

where

$$M(\vec{k}) = M(-\vec{k})$$

$$\epsilon_0(\vec{k}) = \epsilon_0(-\vec{k})$$

$$\vec{d}(\vec{k}) = -\vec{d}(-\vec{k})$$

Small $\vec{k}$ expansion near Γ, assuming rotational symmetry:

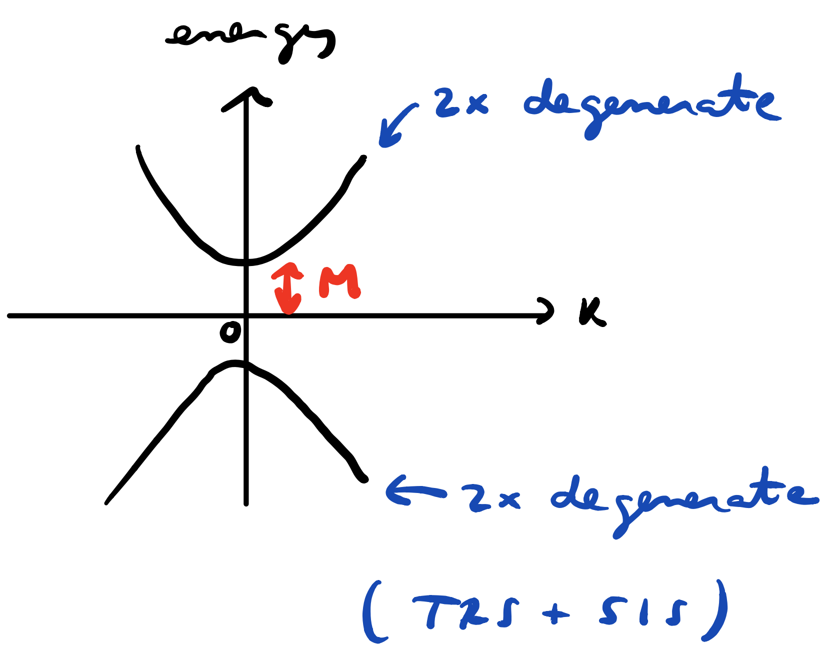
$$\boxed{\begin{aligned} \vec{d}(\vec{k}) &= A\,\vec{k} \\ M(\vec{k}) &= M + B\,\vec{k}^2 \\ \epsilon_0(\vec{k}) &= C + D\,\vec{k}^2 \end{aligned}}$$

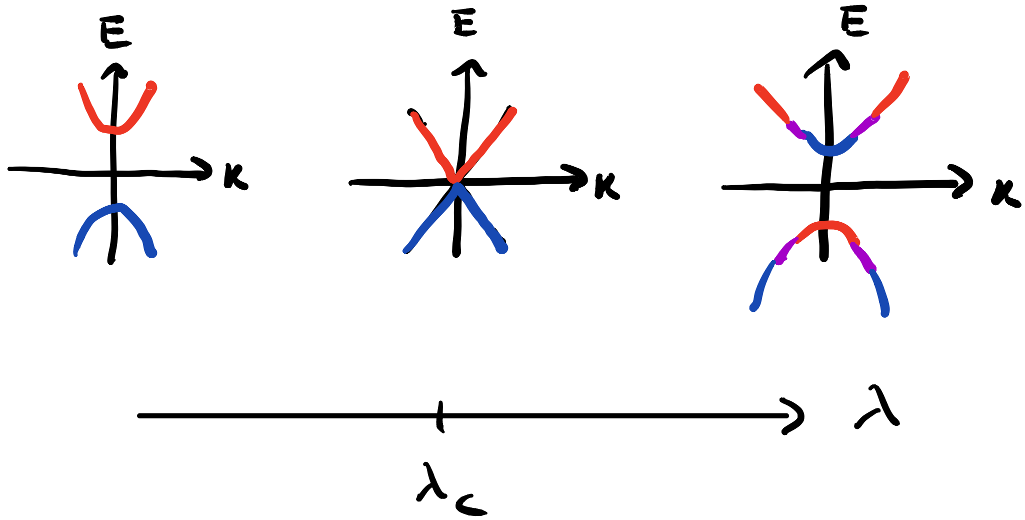
A, B, C, D : band parameters

(can be extracted from DFT)

$h_{eff}(\vec{k})$ = 3D Dirac Hamiltonian,

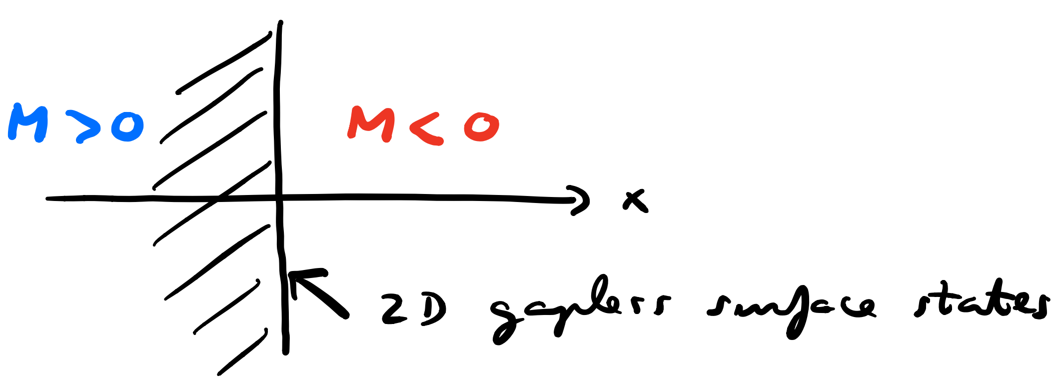
with mass $M(\vec{k})$.





Sign of the Dirac mass changes sign across a band inversion.

* Connection to Jackiw-Rebbi theory:



* Calculation of $\mathbb{Z}_2$ invariant:

lattice regularisation:

$$k_i \longrightarrow \frac{1}{a} \sin(k_i a)$$

$$k_i^2 \longrightarrow \frac{2}{a^2} \left(1 - \cos(k_i a)\right)$$

$$(-1)^{\nu_0} = \prod_{i=1}^{8} \delta_i$$

3.5 Axion electrodynamics

Review: A. Sekine and K. Nomura, J. Appl. Phys. 129, 141101 (2021)

* Lagrangian density for electromagnetic fields in an insulator:

$$\mathcal{L}_{EM} = \frac{1}{2} \left(\epsilon \vec{E}^2 - \frac{\vec{B}^2}{\mu} \right)$$

$$- \rho \phi - \vec{j} \cdot \vec{A}$$

$\vec{E}$ = electric field $= -\vec{\nabla}\phi - \dfrac{\partial \vec{A}}{\partial t}$

$\vec{B}$ = magnetic " $= \vec{\nabla} \times \vec{A}$

$$S_{EM} = \int dt\, d^3x\, \mathcal{L}_{EM}$$

$$\frac{\delta S_{EM}}{\delta \phi} = \frac{\delta S_{EM}}{\delta \vec{A}} = 0$$

$$\Rightarrow \quad \vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon_0}$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{B} = \mu_0 \vec{j} + \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}$$

* Axion term:

$$\mathcal{L}_{EM} \rightarrow \mathcal{L}_{EM} + \mathcal{L}_{ax} = \mathcal{L}$$

where

$$\mathcal{L}_{ax} = \underbrace{\theta}_{\text{dimensionless \#}} \frac{e^2}{2\pi h} \vec{E} \cdot \vec{B} .$$

$\mathcal{L}_{ax}$ is present in 3D insulators with time-reversal symmetry.

$\mathcal{L}_{ax} \rightarrow$ magnetoelectric coupling

$$\underbrace{\vec{P}}_{\text{electric polarisation}} = \frac{\partial \mathcal{L}}{\partial \vec{E}} = \epsilon \vec{E} + \theta \frac{e^2}{2\pi h} \vec{B}$$

$$\underbrace{\vec{M}}_{\text{magnetization}} = \frac{\partial \mathcal{L}}{\partial \vec{B}} = \frac{\vec{B}}{\mu} + \theta \frac{e^2}{2\pi h} \vec{E}$$

magnetization

* θ is defined modulo 2π.

$$S_{ax} = \int d^3x \, dt \, \mathcal{L}_{ax}$$

$$= \theta \, \frac{e^2}{2\pi h} \int d^3x \, dt \, \vec{E}\cdot\vec{B}$$

suppose θ = const in space and time

integer for closed space-time!

$$= n\,\theta$$

Partition function for EM fields:

$$Z = \int D\phi \, D\vec{A} \; e^{iS}$$

$e^{i S_{ax}} = e^{i n \theta}$ invariant under $\theta \to \theta + 2\pi$. $\Rightarrow$ θ is defined mod 2π.

* What are the possible values of θ in a 3D insulator with time reversal symmetry?

$\mathcal{L}$ must be invariant under time-reversal

$$\mathcal{L}_{ax} = \theta \frac{e^2}{2\pi h} \vec{E} \cdot \vec{B}$$

$$\xrightarrow[TR]{} -\theta \frac{e^2}{2\pi h} \vec{E} \cdot \vec{B}$$

$(\vec{E} \to \vec{E})$
$(\vec{B} \to -\vec{B})$

$$\mathcal{L}_{ax} = -\mathcal{L}_{ax} \Leftrightarrow \theta = -\theta$$

$$\Leftrightarrow \theta = 0 \text{ or } \pi$$

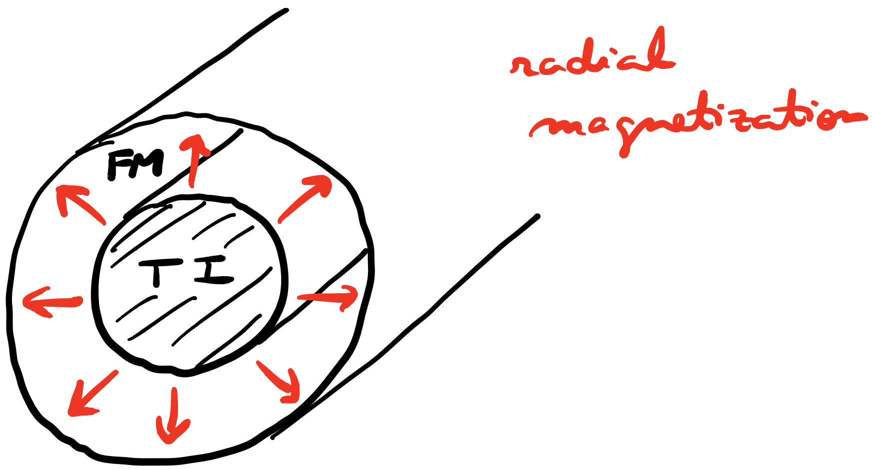
* If $\theta = 0$, the insulator is topologically trivial.

  If $\theta = \pi$, the insulator is topological.

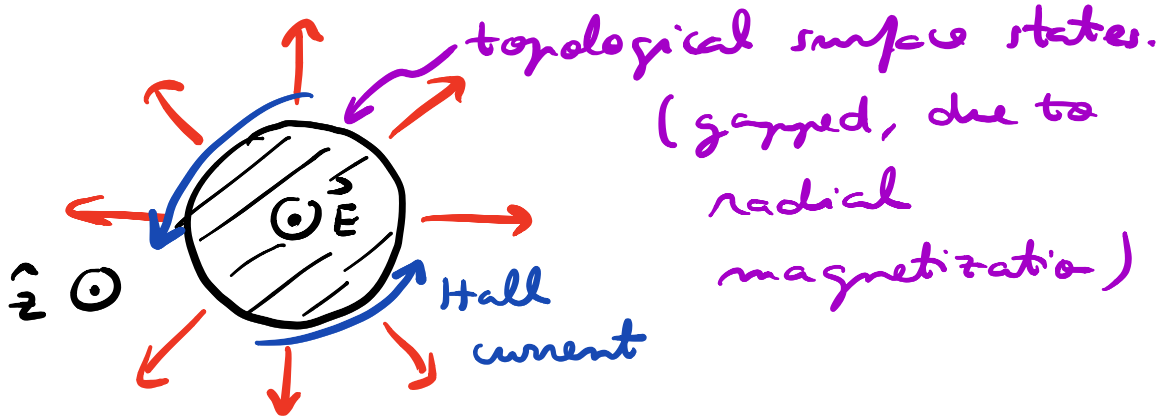
$$\theta = \pi \underbrace{\nu_0}_{\substack{\uparrow \\ \text{strong topological index.}}}$$

* Phenomenological justification of $\theta = \pi \nu_0$:

Consider a TI cylinder surrounded by a ferromagnetic layer:



Apply an electric field $\vec{E}$ parallel to cylinder.



Hall current density:

$$\vec{j}_H = \sigma_H \underbrace{\hat{n}}_{} \times \vec{E}$$

unit vector normal to surface

$$= \frac{e^2}{2h} \hat{n} \times \vec{E} = \frac{e^2}{2h} E \underbrace{\hat{\phi}}_{}$$

2D massive Dirac fermions

azimuthal unit vector (cylindrical coords.)

Magnetic moment associated with $\vec{j}_H$:

$$\vec{m} = \underbrace{I}_{} \underbrace{A}_{} \hat{z}$$

total current (Ampères)

cross section area of the TI cylinder

$$I = \underbrace{L}_{\text{length of cylinder}} \; j_H$$

$$\Rightarrow \vec{m} = j_H \underbrace{V}_{\text{volume of TI cylinder}} \hat{z}$$

Then,

$$\boxed{\vec{M}} = \text{induced magnetization}$$

$$= \frac{\vec{m}}{V} = j_H \, \hat{z}$$

$$= \frac{e^2}{2h} E \, \hat{z} = \boxed{\frac{e^2}{2h} \vec{E}}$$

This is compatible w/

$$\vec{M}_{ax} = \theta \frac{e^2}{2\pi h} \vec{E} \quad \text{with } \theta = \pi .$$

If the insulator was trivial, we'd have no Chern insulator and $\sigma_H = 0 \Rightarrow \vec{M} = 0$.

This is consistent w/ $\theta = 0$.

* Modified Maxwell's eqs:

$$S = \int d^3x \, dt$$

$$\left[\frac{1}{2} \left(\epsilon \vec{E}^2 - \frac{\vec{B}^2}{\mu} \right) + \theta \frac{e^2}{2\pi h} \vec{E} \cdot \vec{B} \right]$$

$$\frac{\delta S}{\delta \phi} = \frac{\delta S}{\delta \vec{A}} = 0 \Rightarrow$$

$$\vec{\nabla} \cdot \vec{E} = \frac{1}{\epsilon_0} \left[\rho - \underbrace{\frac{e^2}{2\pi h} \vec{\nabla}\theta \cdot \vec{B}}_{\text{new}} \right]$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} = - \frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{B} = \mu_0 \left(\vec{J} + \overbrace{\frac{e^2}{2\pi h} \frac{\partial \theta}{\partial t} \vec{B}}^{\text{new}} \right)$$

$$+ \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t}$$

4 Topological crystalline insulator

Can a symmetry, other than chiral, particle-hole or time-reversal lead to protected topological phases?

yes. Crystal symmetries can.

Consider a mirror plane $\perp \hat{z}$: M_z.

$$M_z = \underbrace{C_2^z}_{\substack{\uparrow \\ \text{180° rotation} \\ \text{around } z}} \underbrace{\Pi}_{\uparrow \text{ space inversion}}$$

$$= i\sigma^z \, \Pi$$

$$M_z^{-1} = -i\sigma^z \, \Pi$$

$$(k_x, k_y, k_z) \xrightarrow{M_z} (k_x, k_y, -k_z)$$

$$(\sigma^x, \sigma^y, \sigma^z) \xrightarrow[M_z]{} (-\sigma^x, -\sigma^y, \sigma^z)$$

$$M_z^2 = -\mathbb{1} \quad (\text{like } \Theta^2 = -\mathbb{1})$$

For a 2D insulator invariant under M_z,

$$[\,h(\vec{k}),\ M_z\,] = 0 \text{ for all } \vec{k}.$$

$\Rightarrow$ Bloch states $|u_{\vec{k}}\rangle$ are also eigenstates of M_z.

Two types of Bloch states:

$|u_{\vec{k},\alpha}\rangle$, where $\alpha = \pm i$.

For each class, one can define a Chern # C_α.

Total Chern # : $C_{+i} + C_{-i}$

Mirror Chern # : $C_{+i} - C_{-i}$

If the crystal has TRS,

$C_i + C_{-i} = 0$. But,

$C_i - C_{-i}$ can be nonzero.

(analogous to spin Chern # of 2D insulator)

If so, there are gapless states at the boundary. These states are robust only if mirror symmetry is present.

Review: Y. Ando and L. Fu, Ann. Rev. Cond. Matt. Phys. 6, 361 (2015).

5 Weyl and Dirac semimetals in 3D

N. P. Armitage, E. J. Mele and A. Vishwanath, RMP 90, 015001 (2018).

CH. 5: ADDITIONAL TOPICS

1 Topological superconductors in 3D

Review: M. Sato and Y. Ando, Rep. Prog. Phys. 80, 076501 (2017)

② Classification of topological phases

What kind of topological phases (invariants) can we have?

"Periodic table":

C.-K. Chiu, J.C.Y. Teo and A.P. Schnyder, RMP 88, 035005 (2015)

"Topological quantum chemistry":

J. Cano and B. Bradlyn, Ann. Rev. Cond. Matt. Phys. 12, 225 (2020).

(3) Interacting topological phases

S. Rachel, Rep. Prog. Phys. 81, 116501 (2018).

Topological order:

X.-G. Wen, RMP 89, 041004 (2017)

(4) Floquet topological phases

Can we induce topological phases out of equilibrium? Yes.

T. Oka and S. Kitamura, Ann. Rev. Cond. Matt. Phys. 10, 387 (2019)

(5) Topological wave insulators

Topological phases for nonelectronic systems (photons, phonons, magnons, excitons, polaritons ...)

F. Zangeneh-Nejad, A. Alù and R. Fleury,

Comptes Rendus Physique 21, 467 (2020).