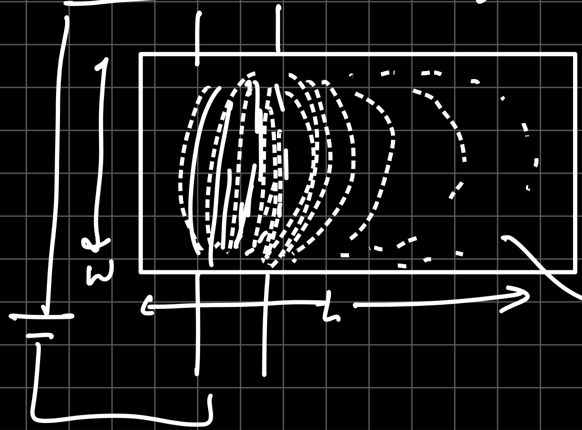
(Lec 23 in MDi)

some recap of the CdTe- HgTe heterostructure



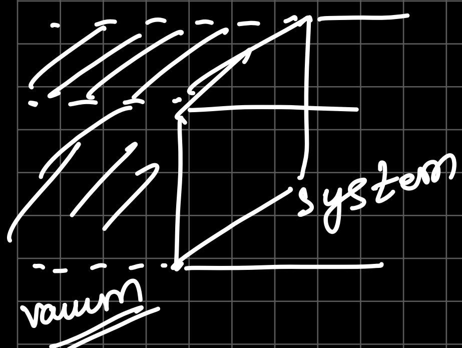
diffusive transport

$\to i \sim \exp(-W/L)$

however

3 dim Dirac eqn

$$\Delta H_{3D} = v p_y \sigma_y + v p_z \alpha_z - B(p_y^2+p_z^2)\beta$$



$$H_{eff} = \left[\left(\langle\psi_1|,\langle\psi_2|\right)\Delta H_{3D}\left(|\psi_1\rangle,|\psi_2\rangle\right)^T\right]$$

$$\psi_1 = \begin{pmatrix} \mathrm{sgn} \\ 0 \\ 0 \\ i \end{pmatrix}\left(e^{-x/\xi_+} - e^{-x/\xi_-}\right) e^{i(k_y y + k_z z)}$$

$$\psi_2 = \begin{pmatrix} 0 \\ \mathrm{sgn}\,B \\ i \\ 0 \end{pmatrix}\left(e^{-x/\xi_+} - e^{-x/\xi_-}\right) e^{i(k_y y + k_z z)}$$

$$\langle\psi_1|\Delta H_{eff}|\psi_1\rangle = v p_y\,\mathrm{sgn}(B)\,\sigma_z \xrightarrow{\text{from}} \sigma_y$$

$$\langle\psi_1|\alpha_z|\psi_1\rangle = \langle\psi_1|\begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}\begin{pmatrix} \mathrm{sgn}B \\ 0 \\ 0 \\ i \end{pmatrix} = \langle\psi_1|\begin{pmatrix} 0 \\ -i \\ \mathrm{sgn}B \\ 0 \end{pmatrix} = 0$$

But $\langle\psi_2|\alpha_z|\psi_1\rangle = (0 \;\; \mathrm{sgn}B \;\; -i \;\; 0)\begin{pmatrix} 0 \\ -i \\ \mathrm{sgn}B \\ 0 \end{pmatrix} = -2i\,\mathrm{sgn}\,B$

$$\therefore \langle \psi_2 | v p_z \alpha_z | \psi_1 \rangle = -2v\, p_z \,\mathrm{sgn}B\; i$$

$$\therefore (v p_z \alpha_z)_{2\times 2} = \begin{pmatrix} 0 & +i \\ -i & 0 \end{pmatrix} v\, p_z \,\mathrm{sgn}B = \underline{\underline{-v\, p_z \,\mathrm{sgn}B\, \sigma_y}}$$

(ignoring 2)

$$\therefore \Delta H = v p_y \,\mathrm{sgn}B\, \sigma_z - v p_z \,\mathrm{sgn}B\, \sigma_y = v\,\mathrm{sgn}B\,(p_y \sigma_z - p_z \sigma_y)$$

$$= v\,\mathrm{sgn}B\,(\vec{p}\times\vec{\sigma})_x$$

But now redefine

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle - i|\psi_2\rangle\right)$$

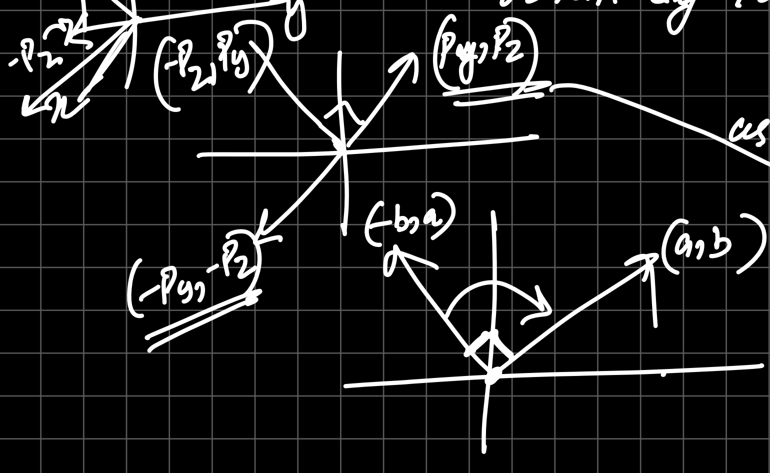
$$|\phi_2\rangle = \frac{-i}{\sqrt{2}}\left(|\psi_1\rangle + i|\psi_2\rangle\right)$$

or
$$\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} = \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & +1\end{pmatrix}}_{\frac{M}{\sqrt{2}}}\begin{pmatrix}|\psi_1\rangle \\ |\psi_2\rangle\end{pmatrix} \Rightarrow \Phi = M\Psi$$

$$\Delta H\,(\phi_1,\phi_2 \text{ basis}) = \Psi^{+}\Delta H\,\Psi = 2\;\Psi^{+} M^{+}(M\Delta H M^{+})M\Psi$$

$$\therefore \Delta H \to \underbrace{M\,\Delta H\, M^{+}}$$ but $$M = \frac{1 - i\sigma_x}{\sqrt{2}} = e^{-\frac{i\sigma_x}{2}\frac{\pi}{2}}$$

rotate by 90° →



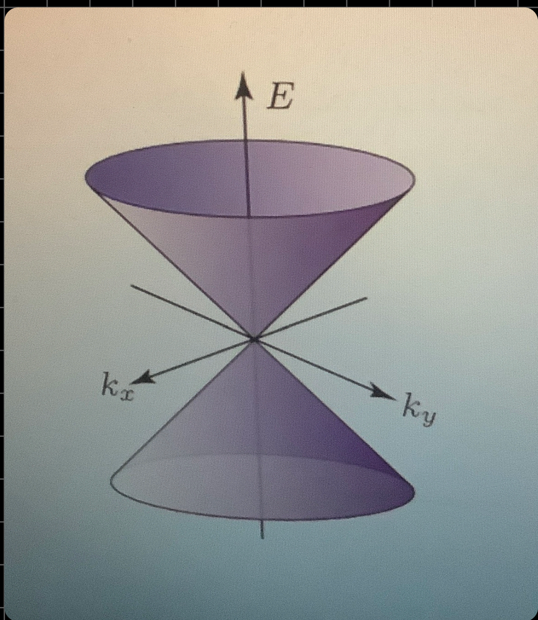
$$\Delta H = -v\,\mathrm{sgn}B\,(p_y\sigma_y + p_z\sigma_z)$$

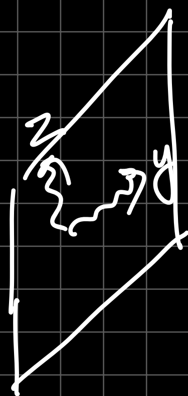
as -90° rotation occurs

$$\Delta H = \underbrace{v\,\mathrm{sgn}B\,(p_y\sigma_y + p_z\sigma_z)}_{\text{again a dirac Hamiltonian}}$$

$\epsilon_{\pm} = \pm v p$, $p = \sqrt{p_y^2 + p_z^2}$ $\Rightarrow$ "Dirac like disp., but for a propagating boundary mode"

We get a "Dirac Cone" but for surface states

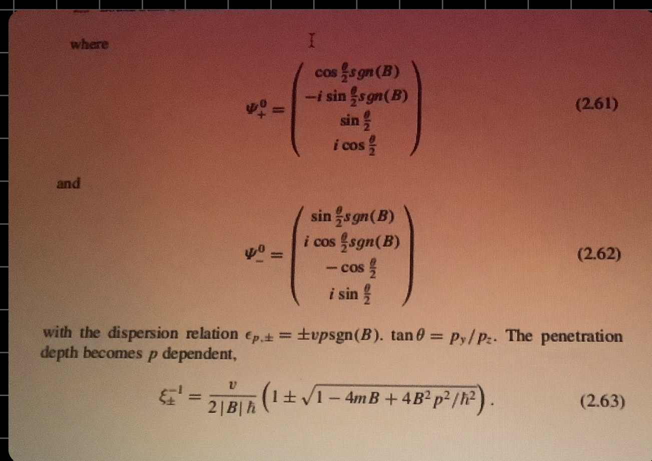




note:-

① σ_i are not "real" spin dof

② exact soln



where

$$\Psi_+^0 = \begin{pmatrix} \cos\frac{\theta}{2} sgn(B) \\ -i\sin\frac{\theta}{2} sgn(B) \\ \sin\frac{\theta}{2} \\ i\cos\frac{\theta}{2} \end{pmatrix} \tag{2.61}$$

and

$$\Psi_-^0 = \begin{pmatrix} \sin\frac{\theta}{2} sgn(B) \\ i\cos\frac{\theta}{2} sgn(B) \\ -\cos\frac{\theta}{2} \\ i\sin\frac{\theta}{2} \end{pmatrix} \tag{2.62}$$

with the dispersion relation $\epsilon_{p,\pm} = \pm vp\text{sgn}(B)$. $\tan\theta = p_y/p_z$. The penetration depth becomes p dependent,

$$\xi_\pm^{-1} = \frac{v}{2|B|\hbar}\left(1 \pm \sqrt{1 - 4mB + 4B^2p^2/\hbar^2}\right). \tag{2.63}$$

Gapless propagating edge modes

$\Downarrow$

"Dirac like Hamiltonian"

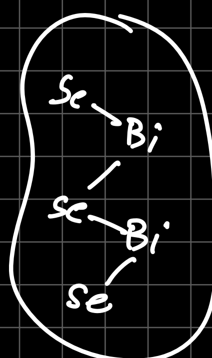
for surface

Topological Insulators & Expt relevance

Real material: Bi_2Se_3 — Quintiple layer

$6s^2 6p^3$ $4s^2 4p^4$

only P_z orbitals matter



→ people looked in 3d where a similar "Band inversion" happens. For e.g. Alloys $Pb_x Sn_{1-x}$ → x can be tuned to go into int. band situation

$x=0$, one type of symmetry of bonds

$x=1$, other type of bonds

→ 3d materials (alloys can be used to tune the band)

↳ as function of x, it has band inversion

bulk ≡ insulator

surface ≡ gapless modes

⇒ $Bi_2 Se_3$ → among the 1st materials to be scanned

→ by ARPES → shine light on the crystal at a fixed relative angle & look at the outgoing electron

↓

can detect its $\vec{k}$ & Energy of it.

Allows you to map bandstructure

↓

measure "filled states"

→ $Bi_2 Se_3$ → known to be SC for alot of time

↳ but inside the gap, ∃ a few states (edge states)

↓

"they saw cones touching each other"

↳ 0~50 meV where it's valid.

↓

dispersion of surface state looks like $H \sim (\sigma_x p_x + \sigma_y p_y)$ [as our calc]

Diff from graphene ⇒ no info about Spin

→ but here the $H^{eff}_{surface}$ has info spin is coupled to momenta → spin resolved photoemission spectroscopy ⇐ about spin of the electrons.

can give info about spin resolved bandstructure.

∃ (in real materials) even/odd # of dirac cones.

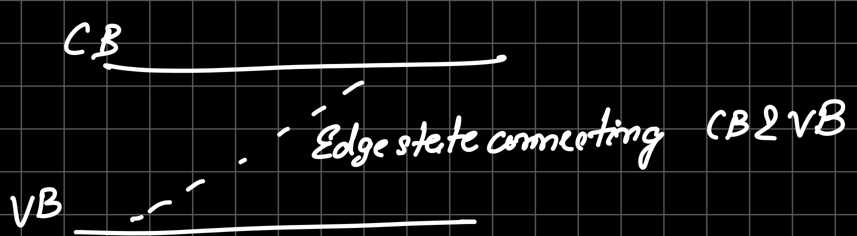
for even, it's not a strong topological insulator as even # can be roughly equated to having no cones in Bandstructure.

odd

→ strong topo. insulator

→ cannot make the dirac cones disappear

Check:- Vanderbilt's book for a discussion of the invariance of topological systems.



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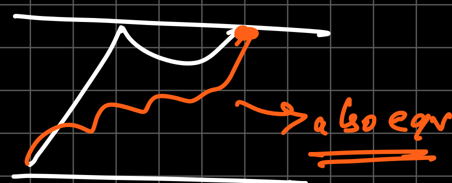
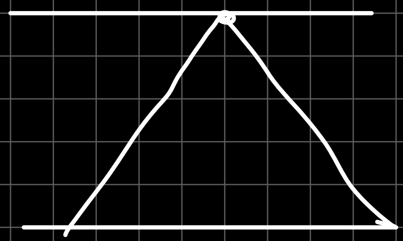
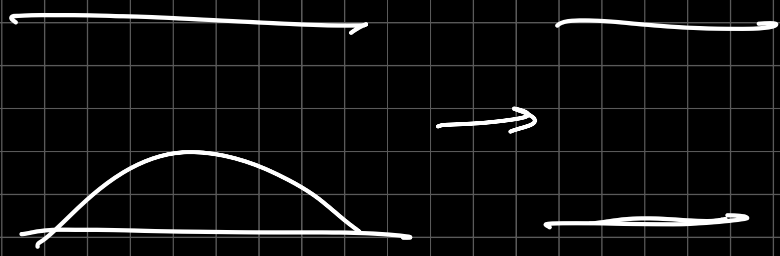


topologically same but can be transformed by suitably perturbing the H.



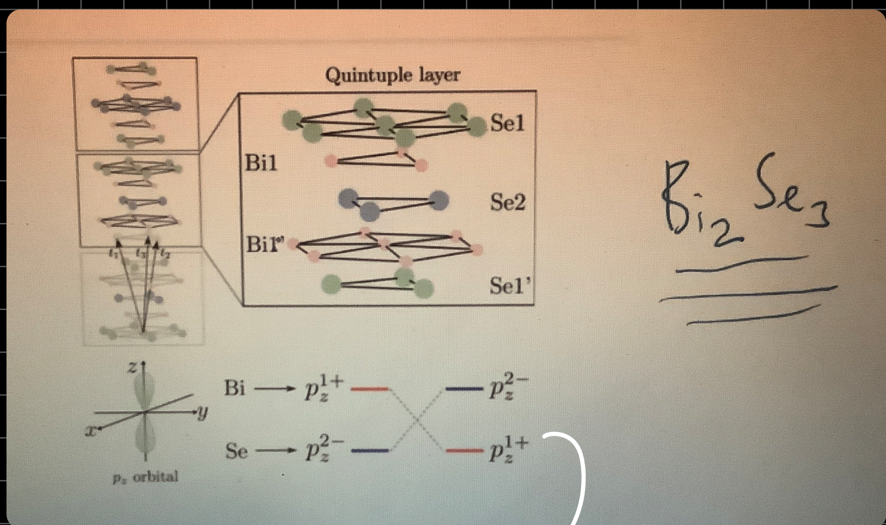
even # of
dirac cones

deformation
$\longrightarrow$
possible



Q. How is the deformation done exactly?
$\Rightarrow$ "$\mathbb{Z}_2$ index" related to it
$\hookrightarrow$

Bi_2Se_3 :-



coupling b/w Quintiple layers is vdw (weak) but intra layer is strong

have "partially filled" P_z orbitals $\rightarrow$ imp for what happens close to fermi energy.

"inversion symmetry present"

- Basis:- Close to fermi energy

$$|P_z^{1+}, \uparrow\rangle, \ |P_z^{1+}, \downarrow\rangle, \ |P_z^{2-}, \uparrow\rangle, \ |P_z^{2-}, \downarrow\rangle$$

(probably spin polarized)

$Bi_2Se \rightarrow$ large Z, so large SOC & hence spin attributed basis is chosen.

The effective hamiltonian

$$\boxed{\mathcal{H} = \mathcal{E}(p) + \sum_{i=1,2,3} v_i p_i \alpha_i + (M - \Sigma B p_i^2)\beta}$$

$$\mathcal{E}(p) = -D_{\parallel}(p_x^2 + p_y^2) - D_{\perp} p_z^2$$

→ Heuristics → • A gen decomp into α_i, β is ofc possible, $\mathcal{H}$ being 4×4

• now wkt TRS is present, we apply $\vec{k} \cdot \vec{p}$

⇓

$\alpha_i \xrightarrow{TRS} -\alpha_i$ ↳ pair with odd terms in momentum.

$\beta \xrightarrow{TRS} \beta$ ↳ pair with even terms of $\vec{p}$

in $\vec{k} \cdot \vec{p}$, you'll get terms like $\mathcal{E}(k) + f(\vec{k}) \cdot \vec{p} + \frac{p^2}{2m}$

demand $f(\vec{k})$ be odd under TRS

↓

gives rise to $v p_i \alpha_i$ type terms

give rise to βp^2 terms of $\mathcal{H}$.

[sidenote:- Kane & mele → Gaps out Graphene & introduces SOC

↳ ribbon geo was done in lecture]

→ @ Shoucheng Zhang ⇒ used HgTe-CdTe → bands invert & "at the edges, the mode is topological"

→ Graphene (weak SOC) when put on an insulator (strong SOC)

can be proximetized to have a strong SOC.

→ probably

Kane & mele can be realized on it

but Bi_2Se_3 also generates

an eqv model.