Berry phase in Q.M.

Consider a quantum Hamiltonian which depends on a parameter λ. This could be a 'tuning knob' like magnetic or electric field, or an internal parameter like momentum in BZ, or more generally some set of parameters which combine the two.

Let us consider a gapped eigenstate of the Hamiltonian, call it $|n\rangle$. What happens to this state as we 'adiabatically' vary $\lambda \equiv \lambda(t)$?

Let us write

$$|n(t)\rangle = \overbrace{\underbrace{e^{-i\int_0^t dt'\, \mathcal{E}_n(\lambda(t'))}}_{\substack{\text{dynamical}\\ \text{phase from}\\ \text{instantaneous}\\ \text{energy}}} \cdot \underbrace{e^{-i\gamma_n(t)}}_{\substack{\text{"extra}\\ \text{possible}\\ \text{phase"}}}}^{\mathcal{F}(t)} \cdot \underbrace{|n(\lambda(t))\rangle}_{\substack{\text{stationary state}\\ \text{at instantaneous}\\ \text{parameter } \lambda(t)\\ \text{(normalized)}}}$$

$$\mathcal{H}\,|n(\lambda(t))\rangle = \mathcal{E}_n(\lambda(t))\,|n(\lambda(t))\rangle \Leftarrow$$

$$\left(i\frac{\partial}{\partial t} - \mathcal{H}\right)|n(t)\rangle = \cancel{\mathcal{E}_n(\lambda(t))\,\mathcal{F}(t)\,|n(\lambda(t))\rangle} + \frac{\partial\gamma_n}{\partial t}\mathcal{F}(t)\,|n(\lambda(t))\rangle$$

$$+\ \mathcal{F}(t)\, i\frac{\partial}{\partial t}|n(\lambda(t))\rangle - \cancel{\mathcal{H}\,\mathcal{F}(t)\,|n(\lambda(t))\rangle} = 0$$

$$\Rightarrow \quad \frac{\partial\gamma_n}{\partial t}|n(\lambda(t))\rangle = -i\frac{\partial}{\partial t}|n(\lambda(t))\rangle$$

Cyclic path $\Rightarrow$

$$\therefore \quad \gamma_n = -i \cdot \int_0^T dt\, \langle n(\lambda(t))|\frac{\partial}{\partial t}|n(\lambda(t))\rangle$$

$$\therefore \quad \gamma_n = \oint d\lambda \left[\underbrace{-i\langle n(\lambda)|\,\partial_\lambda\,|n(\lambda)\rangle}_{A\ \sim\ \text{'vector potential' (Berry connection)}}\right]$$

Phase ambiguity $\Leftrightarrow$ gauge transformation on A

* E.g. Consider a spin-½ particle in a magnetic field: $\mathcal{H} = -\vec{h}\cdot\vec{\sigma}$

Gnd state wfn $\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}$ $\left.\begin{array}{l} \langle\psi|\partial_\theta|\psi\rangle = 0 \\ \langle\psi|\partial_\phi|\psi\rangle = i\sin^2\frac{\theta}{2} = \frac{i}{2}(1-\cos\theta) \end{array}\right\}$  $\gamma = \frac{1}{2}\Omega$

* Berry-Zak phase of 1D SSH model :

$$\mathcal{H}_{Bloch}(k) \equiv \begin{pmatrix} 0 & -t_1 - t_2 e^{-ik} \\ -t_1 - t_2 e^{ik} & 0 \end{pmatrix} \qquad \varepsilon_-(k) = -\sqrt{(t_1 + t_2 \cos k)^2 + (t_2 \sin k)^2}$$

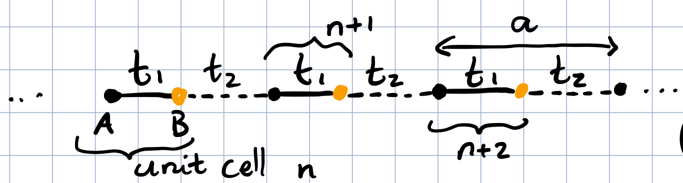
$$h_x = t_1 + t_2 \cos k \,; \; h_y = t_2 \sin k \qquad \psi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\phi_k} \end{pmatrix} \quad \because \theta = \frac{\pi}{2}$$

$$\phi_k = \tan^{-1}\left(\frac{t_2 \sin k}{t_1 + t_2 \cos k} \right)$$

$$\therefore \gamma = -i \int_0^{2\pi} dk \, \frac{1}{2} \left(1 \;\; e^{-i\phi_k}\right) \partial_k \begin{pmatrix} 1 \\ e^{i\phi_k} \end{pmatrix} = -\frac{i}{2} \int_0^{2\pi} dk \cdot i(\partial_k \phi_k)$$

$$\therefore \gamma = \frac{1}{2} \int_0^{2\pi} dk \, (\partial_k \phi_k) = \frac{1}{2} \left(\phi_{k \to 2\pi^-} - \phi_{k \to 0^+} \right) = \begin{cases} 0 : \text{trivial} \\ \pi : \text{topological} \end{cases}$$

* Hamiltonian & Polarization :-



Alternating hopping strengths arises from spontaneous dimerization

(Let us set lattice constant $a = 1$)

$$\mathcal{H} = -t_1 \sum_n (c_{nA}^{+} c_{nB} + c_{nB}^{+} c_{nA}) - t_2 \sum_n (c_{n+1A}^{+} c_{nB} + c_{nB}^{+} c_{n+1A})$$

Large t_1 Large t_2

Charge within unit cell moved by ½ unit cell distance $\Delta P = (e \cdot \frac{d}{2})/d$

Strictly speaking, ambiguous and really $\Delta P = e/2 + ne$ (n: integer)

Shift of electron cloud can be obtained by studying Wannier func^n

Recall Wannier function is Fourier transform of Bloch Wfn.

$$|w_{nR}\rangle = \int \frac{dk}{2\pi} \underbrace{|\psi_{nk}\rangle}_{\text{Band wfn}} \underbrace{e^{-ikR}}_{\text{Fourier}}$$

R: lattice site around which localized

$\langle r | W_{nR} \rangle = W_{nR}(r)$; $\langle r | \psi_{nk} \rangle = u_{nk} \, e^{ikr}$

{ use choice of phases of u_{nk} → get localized Wannier (not always possible)

1D: exponentially localized.

* Mean position in Wannier orbital ("Wannier Center")

$$\langle W_{nR}|\hat{r}-R|W_{nR}\rangle = \int dr\, |W_{nR}(r)|^2 (r-R) = \int dr \cdot (r-R) \int \frac{dk}{2\pi} \cdot \frac{dk'}{2\pi} \psi^*_{nk}(r)\psi_{nk'}(r)\, e^{ikR}\, e^{-ik'R}$$

$$= \int dr\,(r-R) \cdot \int \frac{dk}{2\pi}\frac{dk'}{2\pi}\, u^*_{nk}(r)\, u_{nk'}(r)\, e^{-ik(r-R)}\, e^{ik'(r-R)}$$

Let $\bar{r} = r-R$ $\quad u_{nk'}(r) = u_{nk'}(\bar{r}+R) = u_{nk'}(\bar{r})$ :: periodic

$$= \int d\bar{r} \int \frac{dk}{2\pi}\frac{dk'}{2\pi}\, u^*_{nk}(\bar{r})\, u_{nk'}(\bar{r})\, e^{-ik\bar{r}} \left(-i\partial_{k'} e^{ik'\bar{r}} \right)$$

$$= \int d\bar{r} \int \frac{dk}{2\pi}\frac{dk'}{2\pi} \left[u^*_{nk}(\bar{r})\;\; i\partial_{k'} u_{nk'}(\bar{r}) \right] \cdot e^{-ik\bar{r}}\, e^{ik'\bar{r}}$$

We can split $\bar{r}$ integral into $\sum_{cell} \int d\bar{r}_c$ where $\bar{r}_c$ is within unit cell.

Will lead to

$$\langle W_{nR}|\hat{r}-R|W_{nR}\rangle = \int d\bar{r}_c \int \frac{dk}{2\pi}\frac{dk'}{2\pi} \cdot u^*_{nk}(\bar{r}_c) \cdot i\partial_k \cdot u_{nk}(\bar{r}_c) \cdot 2\pi \cdot \delta(k-k')$$

$$= \int_0^{2\pi} \frac{dk}{2\pi} \langle u_{nk}| i\partial_k |u_{nk}\rangle$$

$\rightsquigarrow$ view k as a "parameter" & BZ being "cyclic"

$\Rightarrow$ Berry phase

$$\langle \bar{r} \rangle_n = \int_0^{2\pi} \frac{dk}{2\pi} \langle u_{nk}| i\partial_k |u_{nk}\rangle = \frac{\gamma_n}{2\pi} \rightarrow \begin{cases} 0 \mod (1) & : \text{trivial} \\ \frac{1}{2} \mod (1) & : \text{topological} \end{cases}$$

$$\Delta P = e \times \Delta \langle \bar{r} \rangle_n = \frac{e}{2}$$

* 2D Chern insulator model :-

Square lattice model $\quad H = \sum_{\langle ij \rangle} \left(t_{ij}^{\alpha\beta} C_{i\alpha}^{\dagger} C_{j\beta} + h.c. \right)$

$$H = -\sum_{k} \begin{pmatrix} C_{k\uparrow}^{\dagger} & C_{k\downarrow}^{\dagger} \end{pmatrix} \left[\sin k_x \sigma_1 + \sin k_y \sigma_2 + (2 - \cos k_x - \cos k_y - m)\, \sigma_3 \right] \begin{pmatrix} C_{k\uparrow} \\ C_{k\downarrow} \end{pmatrix}$$

Recall under $\mathcal{T}$: $\quad \mathcal{H}(k) \mapsto \mathcal{U}_{\tau}^{\dagger} \mathcal{H}^{*}(-k)\, \mathcal{U}_{\tau}$

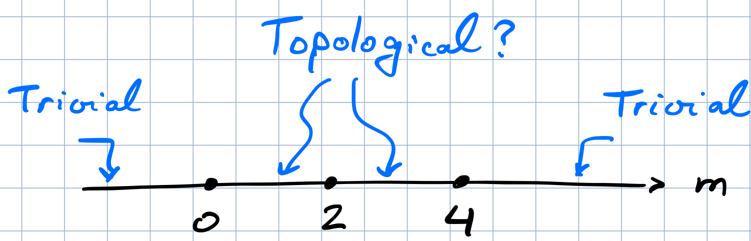
$$\mathcal{U}_{\tau} = i\sigma_2 \quad \therefore \mathcal{H}(k) \longmapsto \sigma_2 \mathcal{H}^{*}(-k)\, \sigma_2$$

$\sin k_x \sigma_1$: even , $\quad \sin k_y \sigma_2$: even , $\quad (2 - \cos k_x - \cos k_y)\, \sigma_3$: odd

Band energies $\quad \pm E(k) \equiv \pm \sqrt{\sin^2 k_x + \sin^2 k_y + (2 - \cos k_x - \cos k_y - m)^2}$

Zero gap $\Rightarrow$

k_x	k_y		m
0	0	$\rightarrow$	0
0	π	$\rightarrow$	2
π	0	$\rightarrow$	2
π	π	$\rightarrow$	4



$h_x = \sin k_x \quad ; \quad h_y = \sin k_y \quad ; \quad h_z = (2 - \cos k_x - \cos k_y - m)$

$$\vec{\mathcal{A}}^{(n)} = -i \langle u_n(\vec{k}) | \vec{\partial} u_n(\vec{k}) \rangle \qquad \alpha = x, y \; ; \; \partial_\alpha \equiv \partial_{k_\alpha}$$

"winding #" not robust $\because$ all $h_i \neq 0$ but "winding #" differences may be topological?

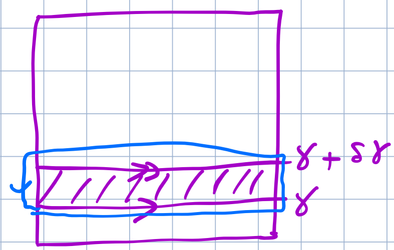
$$\mathcal{H} = -\begin{pmatrix} h_z & h_x - ih_y \\ h_x + ih_y & -h_z \end{pmatrix} ; \quad u_- = \frac{1}{\sqrt{2h(h+h_z)}} \begin{pmatrix} h_z + h \\ h_x + ih_y \end{pmatrix}$$

Consider k_y as "some parameter" for a series of 1D models with k_x as 1D momentum:

$$\gamma_-(k_y) = \int_0^{2\pi} dk_x \; \mathrm{Im} \langle u_-(\vec{k}) | \partial_x u_-(\vec{k}) \rangle$$

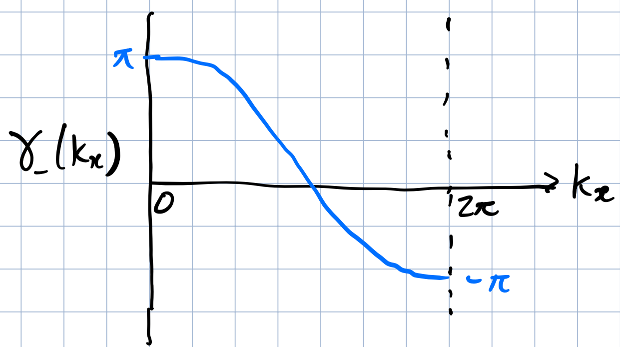
$$u_- \equiv \mathcal{N}\begin{pmatrix} h_z + h \\ h_x + i h_y \end{pmatrix} \Rightarrow \mathrm{Im}\langle u_- | \partial_x u_- \rangle = \mathcal{N}^2 \left[h_x \partial_x h_y - h_y \partial_x h_x \right]$$

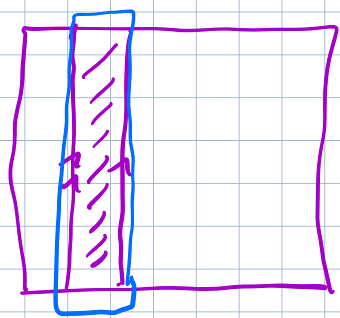
$\boxed{m=1}$



Total "flux" $= (-2\pi)$

Alternatively, view k_x as "parameter" & k_y as momentum





Total "flux" $= (-2\pi)$

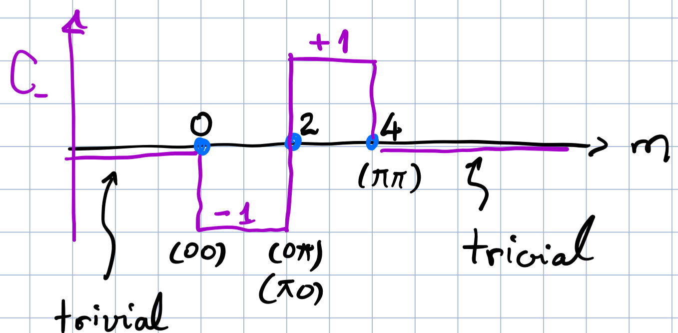
$$(\vec{\nabla} \times \vec{A})_\alpha = -i\, \varepsilon_{\alpha\beta\gamma}\, \partial_\beta \langle u_n(\vec{k}) | \partial_\gamma | u_n(\vec{k}) \rangle$$

$$= \underbrace{-i\, \varepsilon_{\alpha\beta\gamma} \langle \partial_\beta u_n(\vec{k}) | \partial_\gamma u_n(\vec{k}) \rangle}_{\text{taking complex conjugate} \Rightarrow \text{ check purely imaginary}}$$

$$\varepsilon_{\alpha\beta\gamma} \langle \partial_\beta u_n | \partial_\gamma u_n \rangle^* = \varepsilon_{\alpha\beta\gamma} \langle \partial_\gamma u_n | \partial_\beta u_n \rangle = -\varepsilon_{\alpha\beta\gamma} \langle \partial_\beta u_n | \partial_\gamma u_n \rangle$$

$\therefore \quad (\vec{\nabla} \times \vec{A})_z \equiv$ real #. $\longrightarrow$ "Berry curvature": $\Omega_z(k_x, k_y)$

$$C_n = \frac{1}{2\pi} \int \Omega_z^{(n)}(k_x, k_y) \cdot dk_x\, dk_y \quad = \text{ Chern number}$$



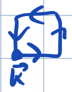
$\sim$ Every Dirac band inversion $\longrightarrow$ $\Delta C = \pm 1$

* Discretized BZ :-

$$\mathcal{L}^{(n)}(\vec{k},\vec{\Delta k}) \equiv \frac{\langle u^{(n)}_{\vec{k}} | u^{(n)}_{\vec{k}+\vec{\Delta k}}\rangle}{|\langle u^{(n)}_{\vec{k}} | u^{(n)}_{\vec{k}+\Delta \vec{k}}\rangle|} = e^{i\theta^{(n)}(\vec{k},\,\vec{k}+\Delta\vec{k})}$$

$\rightsquigarrow$ U(1) link variable for any band-n

$$W_{\vec{k}} = \prod e^{i\theta} = \underbrace{e^{i\Omega_z(\vec{k})}}_{\text{"Berry flux"} = \text{gauge invariant}} \Rightarrow -i\ln W_{\vec{k}} = \Omega_z(\vec{k})$$



finely discretize so that plaquette fluxes ~ small $\therefore$ no "ln" ambiguities

$$\int \frac{d^2\vec{k}}{2\pi}\, \Omega^{(n)}_z(\vec{k}) = C_n$$

For multiple "N" bands with degeneracies or band touchings (so they can't be isolated) total Chern # obtained by replacing $\mathcal{L}$ by $\mathcal{L} = \det\underbrace{[\langle u_n(\vec{k}) | u_m(\vec{k}+\vec{\delta k})\rangle]}_{N\times N \text{ matrix}}$

& $\mathcal{A} = \mathrm{Im}(\ln \mathcal{L})$ & $\Omega_z = \mathrm{Im}(\ln \prod_{\square} \mathcal{L})$.

* Removing wavefunction derivatives :-

$$\Omega^{(n)}_\alpha(\vec{k}) = \mathrm{Im}\; \epsilon_{\alpha\beta\gamma} \langle \partial_\beta u_n(\vec{k}) | \partial_\gamma u_n(\vec{k})\rangle$$

$$= \mathrm{Im}\; \epsilon_{\alpha\beta\gamma} \sum_{m\neq n} \langle \partial_\beta u_n(k) | u_m(k)\rangle\langle u_m(\vec{k}) | \partial_\gamma u_n(\vec{k})\rangle$$

{ $m=n$ term kept but vanishes $\because \mathrm{Im}\to 0$ }
{ $\langle u_n|\partial_\beta u_n\rangle$ ~ pure imag $\therefore$ prod ~ real }

<u>$m\neq n$:</u>

$$E_n\langle u_m|\partial_\gamma u_n\rangle = \langle u_m|\big(\partial_\gamma(\mathcal{H}|u_n\rangle)\big) - \langle u_m|\cancel{(\partial_\gamma E_n)}|u_n\rangle$$

$\because \langle u_m|u_n\rangle = 0$

$$= \langle u_m|(\partial_\gamma \mathcal{H})|u_n\rangle + \langle u_m|\mathcal{H}|\partial_\gamma u_n\rangle$$

$$\therefore \langle u_m|(\partial_\gamma \mathcal{H})|u_n\rangle = (E_n - E_m)\langle u_m|\partial_\gamma u_n\rangle$$

$$\text{llly}\quad \langle u_n|(\partial_\beta \mathcal{H})|u_m\rangle = (E_n - E_m)\langle \partial_\beta u_n|u_m\rangle$$

$$\therefore \Omega^{(n)}_\alpha(\vec{k}) = \mathrm{Im}\; \epsilon_{\alpha\beta\gamma}\sum_{m\neq n} \frac{\langle u_n|(\partial_\beta\mathcal{H})|u_m\rangle\langle u_m|\underbrace{(\partial_\gamma\mathcal{H})}_{\text{velocity operator} \sim \text{current}}|u_n\rangle}{(E_n - E_m)^2}$$

Ω ~ related to Hall conductivity (via Kubo formula)

* For Spin in $\vec{h}$ field, with $\mathcal{H} = -\vec{h}\cdot\vec{\sigma}$:

$$u_- = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix};\quad u_+ = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi}\end{pmatrix}$$

Consider 'parameters' $\equiv (h_x, h_y, h_z)$

$\vec{\nabla}\mathcal{H} = -\vec{\sigma}$; Let us work near $(0,0,h) \Rightarrow |+\rangle = \begin{pmatrix}0\\-1\end{pmatrix};\ |-\rangle = \begin{pmatrix}1\\0\end{pmatrix}$

$$\therefore \Omega = \mathrm{Im}(1/4h^2)\left(\langle -|\sigma_x|+\rangle\langle +|\sigma_y|-\rangle - \langle -|\sigma_y|+\rangle\langle +|\sigma_x|-\rangle\right) = \underbrace{-\tfrac{1}{2}(1/h^2)}_{\sim\text{monopole}}$$

* Edge theory:

$$\mathcal{H}(m\sim 0,\ \vec{k}\sim 0) \approx (-k_x\sigma_1 - k_y\sigma_2 + m\sigma_3)$$

Consider boundary at $y=0$ between topological & trivial

$y>0$ Topological $(m>0)$ $\quad \Psi_>(x,y) \overset{?}{=} e^{-\alpha y} e^{ik_x x}\,\Phi_>$

$\cdots \longrightarrow x$

$y<0$ Trivial $(m\to-\infty)$ $\quad (\Psi_< = 0$ outside$)$

$$\mathcal{H}_>\Psi_> = (i\partial_x\sigma_1 + i\partial_y\sigma_2 + m\sigma_3)\, e^{-\alpha y} e^{ik_x x}\,\Phi_>$$

$$= e^{-\alpha y} e^{ik_x x}(k_x\sigma_1 - i\alpha\sigma_2 + m\sigma_3)\,\Phi_>$$

$$\mathcal{H}_>\Psi_> = \varepsilon\, e^{-\alpha y} e^{ik_x x}\,\Phi_>$$

$$\Rightarrow (k_x\sigma_1 - i\alpha\sigma_2 + m\sigma_3)\,\Phi_> = \varepsilon\,\Phi_>$$

Let $\sigma_1\Phi_> = \pm\Phi_>$ $\quad \therefore \Phi_> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ or $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$

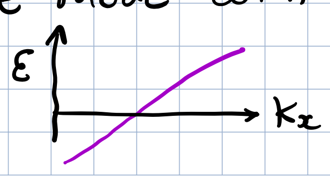
$$(-i\alpha\sigma_2 + m\sigma_3)\,\Phi_> = \alpha\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\Phi_> + m\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\Phi_>$$

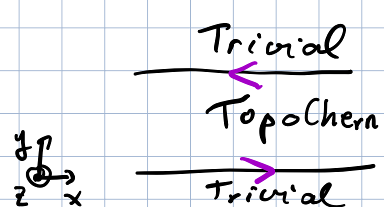
$$= \begin{cases} \frac{\alpha}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix} + m\begin{pmatrix}1\\-1\end{pmatrix} & \oplus \\ \frac{\alpha}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} + m\begin{pmatrix}1\\1\end{pmatrix} & \ominus \end{cases}$$

$\because m>0 \Rightarrow$ only $\oplus$ solution survives with $\alpha = m$

$\therefore \Psi_> = \frac{1}{\sqrt{2}} e^{-my} e^{ik_x x}\begin{pmatrix}1\\1\end{pmatrix}$ & $\varepsilon = k_x \Rightarrow v_x = \frac{\partial\varepsilon}{\partial k_x} > 0$

Chiral edge mode with $v_x > 0$





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

* Superconducting variant of SSH chain → Kitaev chain
* Variants of 2D Chern insulator:

  ↗ Time reversal invariant analogue ~ 2D QSH → 3D Topological Insulators

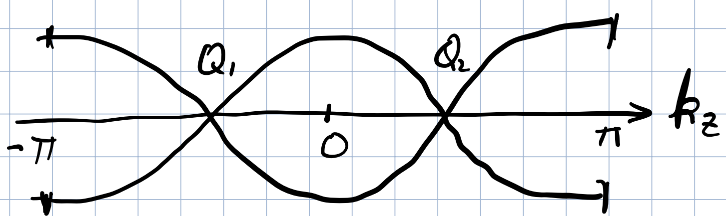
  ↘ Stacked CI ⇒ 3D Weyl semimetal (gapless)

* <u>Weyl semimetal as stacked CI</u> / "Bulk boundary" in momentum space

$$H = -\sum_k \begin{pmatrix} c_{k\uparrow}^\dagger & c_{k\downarrow}^\dagger \end{pmatrix} \left[\sin k_x \sigma_1 + \sin k_y \sigma_2 + (2 - \cos k_x - \cos k_y - m)\sigma_3 \right] \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix}$$

Generalizing to 3D, let $m \equiv m(k_z) = \cos k_z$

$$\left.\begin{array}{l} \text{when } k_z = \pm\pi,\ m = -1 \Rightarrow \text{2D trivial insulator} \\ \text{when } k_z = 0,\ m = +1 \Rightarrow \text{2D Chern insulator} \end{array}\right\}$$



gap closing at $k_z = \pm\frac{\pi}{2}$
Weyl nodes

* Counting DOF: $\vec{h}(\vec{k})\cdot\vec{\sigma} \Rightarrow \text{gap} = 2|h(\vec{k})|$

  closing gap ⇒ tuning 3 components → 0 ⇒ 3D accidental

* Hall effect: $\sigma_{xy}^{3D} = \frac{e^2}{h}\Delta Q$ *

* Surface Fermi arcs ⇒ version of edge states of QH