TQC & SI for Magnetic materials. (Z.-D. Song, TMS 2024)

-. TQC for 1D system.

Seitz notation for spatial operation $g = \{p_g \mid t_g\}$ (p_g: point group op; t_g: translation)

its definition

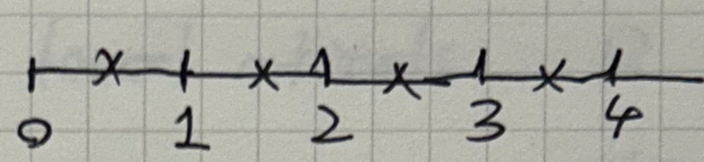
$$g \cdot r \to p_g \cdot r + t_g$$

group operation

$$g_1 g_2 = \{p_{g_1} p_{g_2} \mid p_{g_1} t_{g_2} + t_{g_1}\}$$

Consider 1D system $t_x = \{-1 \mid 100\}$ $\quad p = \{-1 \mid 000\}$

lattice in real space:



integer positions are invariant under:

$x = n$: $\{-1 \mid 2n, 0, 0\} = t_x^{2n} \cdot p$ invariant

$x = n + \frac{1}{2}$: $\{-1 \mid 2n+1, 0, 0\} = t_x^{2n+1} p$ invariant.

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* So we can decompose the unit cell as:

① $x = 0$, & its translations

~~②~~ $x = \frac{1}{2}$ & its translations

④ $(x, 1-x)$, $x \in (0, \frac{1}{2})$ & their translations.

Wyckoff pos.

→ 1a

→ 1b

→ 2c

A crystal is realized by atoms occupying the Wyckoff pos...

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* What is a band insulator:

Zak: "Band Representation" (BR)

A reducible rep of the space group induced by irreps at Wyckoff positions.

This is an opinion from chemistry: Insulators are occupied local orbitals in real space.

* But this is incorrect.

Topological insulators can be defined as violations of this statement.

But in 1D it's fine. Conter example starts in 2D.

The 1D system has four elementary BR (EBR)

Ag @ a ↓ even Au @ a ↓ odd Ag @ b ↓ even Au @ b ↓ odd.

(A BR @ 2c reduces EBR's @ a or b).

We use $|R\alpha\rangle$ to label local orbitals. $R \in \mathbb{Z}$ is unit cell

α = Ag / Au @ a / b.

The bloch basis is

$$|\phi_{k\alpha}\rangle = \frac{1}{\sqrt{N}} \cdot \sum_{R\alpha} e^{i\vec{k}\cdot(\vec{R}+\vec{t}_\alpha)} |R\alpha\rangle$$

$k=0$ & $k=\pi$ are inversion invariant.

we can use parities @ $k=0$ & π to label a band.

$$P \cdot |\phi_{k\alpha}\rangle = \frac{1}{\sqrt{N}} \cdot \sum_{R} e^{i\vec{k}\cdot(\vec{R}+\vec{t}_\alpha)} |R'\alpha\rangle \, \xi_\alpha$$

where $R' + t_\alpha = -(R + t_\alpha)$, $\xi_\alpha = \pm 1$ for Ag / Au

$R' = -R - 2t_\alpha$

$$= \frac{1}{\sqrt{N}} \cdot \sum_{R'} e^{i\vec{k}\cdot(-R'-t_\alpha)} |R'\alpha\rangle \xi_\alpha = \xi_\alpha \frac{1}{\sqrt{N}} \cdot \sum_{R'} e^{-i\vec{k}\cdot(R'+t_\alpha)} |R'\alpha\rangle$$

① if $k=0$ $\Rightarrow$ $P|\phi_{k\alpha}\rangle = \xi_\alpha |\phi_{k\alpha}\rangle$

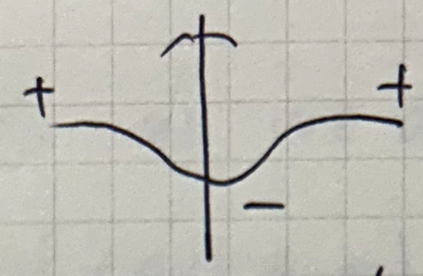
② if $k=\pi$ $\Rightarrow$ $P|\phi_{k\alpha}\rangle = \sum_R e^{i\cdot(k-2\pi)\cdot(R'+t_\alpha)} |R\alpha\rangle$

$$= \boxed{e^{-i2\pi t_\alpha}} \xi_\alpha |\phi_{k\alpha}\rangle$$

we get a phase factor

∴

	Ag @ a	Au @ a	Ag @ b	Au @ b
k = 0	+	−	+	−
k = π	+	−	−	+

So, given a band structure 

we immediately know it's real space orbital.

* in real space, we have $2 * 2 = 4$ EBRs

↓

[# irreps] × [# sites].

* in momentum space, we have $2^2 = 4$ bands (labeled by irreps)

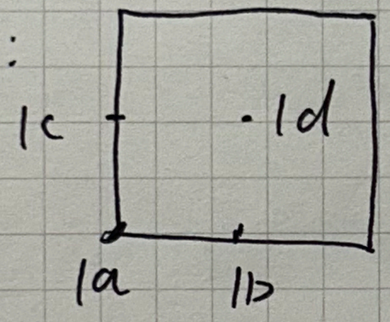
$[\#\text{ irreps}]^{\#\text{Momenta}}$.

so there is one-to-one correspondence.

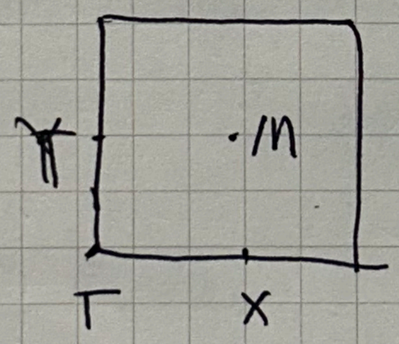
三. TQC for 2D.

The one-to-one correspondence is not true in 2D!

group generators: $t_x = \{1|100\}$ $t_y = \{1|010\}$ $P = \{-1|000\}$

Cell decomposition: 

a, b, c, d : Inversion centers.

BZ decomposition 

: Γ X Y M: Inversion invariant momenta.

#EBR = 8 = 2 × 4 ↳ 4 sites.

↓

Ag/Au

Bands (labeled by irreps) $= 2^4 = 16 <$ #EBRs.

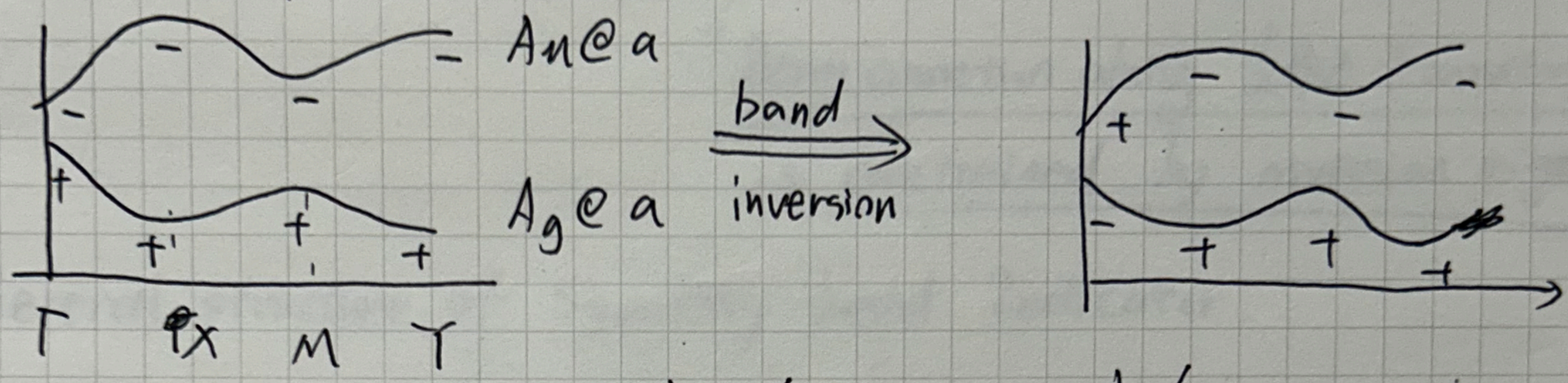
☆ : There are bands not realized by BRs.. ~~Zak's gp~~

These bands are either { Gapless. (Zak is correct)
Gapped. (Zak is wrong, but it's a new phase).

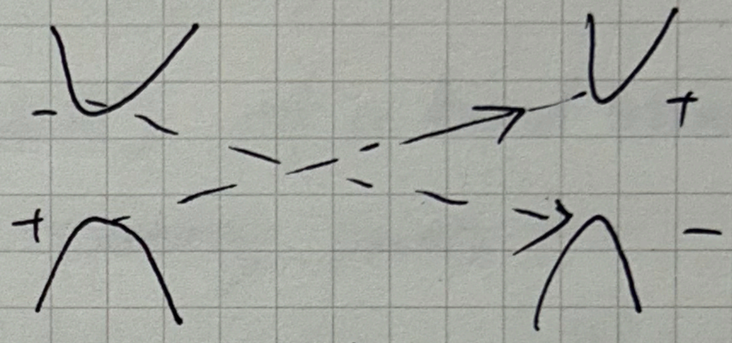
We can make a table of EBRs as we did in 1D.

	Ag@a	Au@a	Ag@b	Au@b	Ag@c	Au@c	Ag@d	Au@d
Γ	+	−	+	−	+	−	+	−
X	+	−	−	+	+	−	−	+
Y	+	−	+	−	−	+	−	+
M	+	−	−	+	−	+	+	−

The "new" phase:



Around the Γ-point



question: whether the inverted band is insulator?

We can examine this using a minimal k·p expansion

we choose $P = \sigma_z$ $\qquad P H(k) P = H(-k)$

$\therefore H(k) = m \cdot \sigma_z + d_1(k) \cdot \sigma_x + d_2(k) \cdot \sigma_y$

band inversion is realized by m changing its sign.

d_1, d_2 are odd in $\vec{k}$ due to $P = \sigma_z$.

So the simplest choice:

$$H(k) = m \cdot \sigma_z + k_x \sigma_x + k_y \sigma_y$$

$$E = \pm \sqrt{m^2 + \vec{k}^2}$$ gapped if $|m| > 0$.

Thus, Zak is wrong, and we get a new gapped phase.

The new phase

In fact, the "new phase" is Chern insulator, it has a quantized hall conductance

$$\Delta C = C(m>0) - C(m<0) = 1.$$

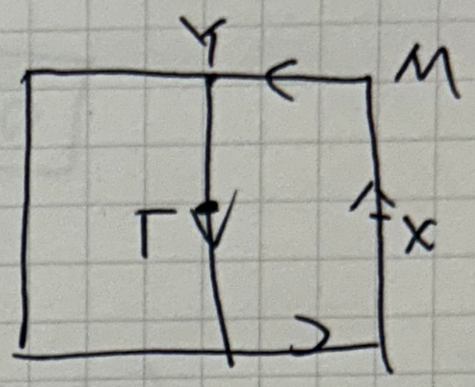
As EBR must have $C=0$, (they are product states)

there must be $\boxed{C(m>0)=1}$

In fact, one can prove ~~th~~:

$$\boxed{(-1)^C = \prod_{k} \prod_{n\in occ} \xi_{k,n}.}$$

idea:



"Berry connection along $\frac{1}{2}BZ$ boundary is constrained by inversion eigenvalues"

三. General structure of Symmetry-based Indicator.

A description (not complete) of a band structure is the irreps @ all high symmetry points.

$$B = [m_{k_1\rho_1}, m_{k_1\rho_2}, \cdots m_{k_2\rho_1}, m_{k_2\rho_2}, \cdots]^T$$

Here k enumerate all high symmetry points.

ρ enumerate all ~~occupied~~ irreps @ the corresponding k.

$m_{k\rho}$ is the # of occupied levels belonging to (k,ρ)

* for the 2D example $k = \Gamma, X, Y, M$

$\rho = +, -$.

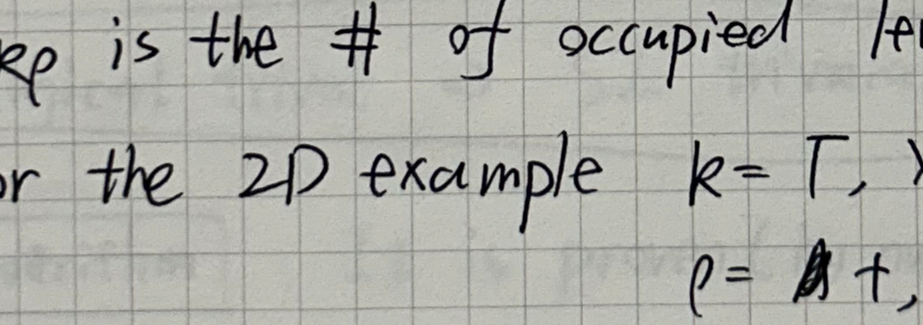
$\Rightarrow$ B is a vector of the length 8.

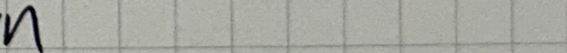
☆ For the band structure to be gapped. (along high symmetry lines)

B must satisfy some constrants.

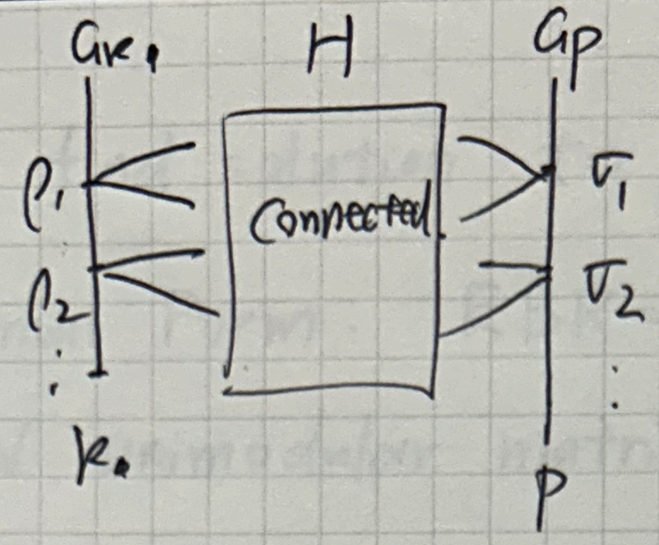
e.g.: $m_{\Gamma+} + m_{\Gamma-} = m_{X+} + m_{X-} = m_{Y+} + m_{Y-} = m_{M+} + m_{M-}$

In general





In general



$$(\rho_1+\rho_2+\cdots)\downarrow H = (\sigma_1+\sigma_2+\cdots)\downarrow H$$

All these constraints we call "Compatibilty relatims"

They form linear equations: $\boxed{C\cdot B=0}$

We define $BS=\{B\in\mathbb{Z}^N \mid C\cdot B=0\}$

↳ Abelian group. $N:=len(B)$

We define another set for B's generated by EBR's.

$$AI=\{\sum_i p_i\vec{a}_i \mid p\in\mathbb{Z}^M\}$$

$\vec{a}_i$: EBR's

M: # EBR's

Obviously, $AI \subseteq BS$.

$\boxed{\text{Quotient group} = \frac{BS}{AI} \quad \text{defines SI}}$

$\boxed{\text{SI nontrival} \Rightarrow \text{topological nontrivial}}$

$\boxed{\text{topological trival} \Rightarrow \text{SI trivial}}$ definition.

1D Inv: $\mathbb{Z}_1$

2D Inv: $\mathbb{Z}_2$

$\boxed{\text{* Algorithm}}$: It is proven (by numerical enumeration) that

$$\dim[BS]=\dim[AI].$$

$\therefore \forall B\in BS, \exists p\in\mathbb{Z}^M$, s.t. $B=\sum_i p_i\vec{a}_i$

The question is: whether p_i is necessarily $\boxed{\text{fractional}}$

If not, B is SI-trivial.

To calculate this, we introduce the EBR matrix

$$EBR=[\vec{a}_1, \vec{a}_2, \cdots]$$

We try to find solution to $B = EBR \cdot p$

Smith Normal Form: $EBR = L \cdot \Lambda \cdot R$

L: $N \times N$ unimodular matrix, it's integer, L^{-1} is also integer

R: $M \times M$ unimodular matrix.

Λ: $N \times M$, diagonal matrix with integer elements.

$$B = EBR \cdot p = L \cdot \Lambda \cdot [R \cdot p] = L \cdot \Lambda \cdot q$$
$$= q$$

The question becomes: whether q is necessarily fractional.

$\Leftrightarrow$ whether Λ has diagonal elements > 1.

if $\Lambda' s$ $= \begin{bmatrix} 1 & & \\ & 1 & \\ & & \ddots \end{bmatrix}$ then $q = \Lambda^{-1} \cdot L^{-1} \cdot B$

Λ^{-1} pseude inverse is always integral.

On the other hand, if $\Lambda_{ii} > 1$

then $q_i = \frac{1}{\Lambda_{ii}}$ can generate an integral $|B\rangle$

it must be a TI.

$\Rightarrow$ **SI classification $= \mathbb{Z}_{\Lambda_{11}} \times \mathbb{Z}_{\Lambda_{22}} \times \cdots \mathbb{Z}_{\Lambda_{rr}}$**

$r = \text{rank}(\Lambda)$

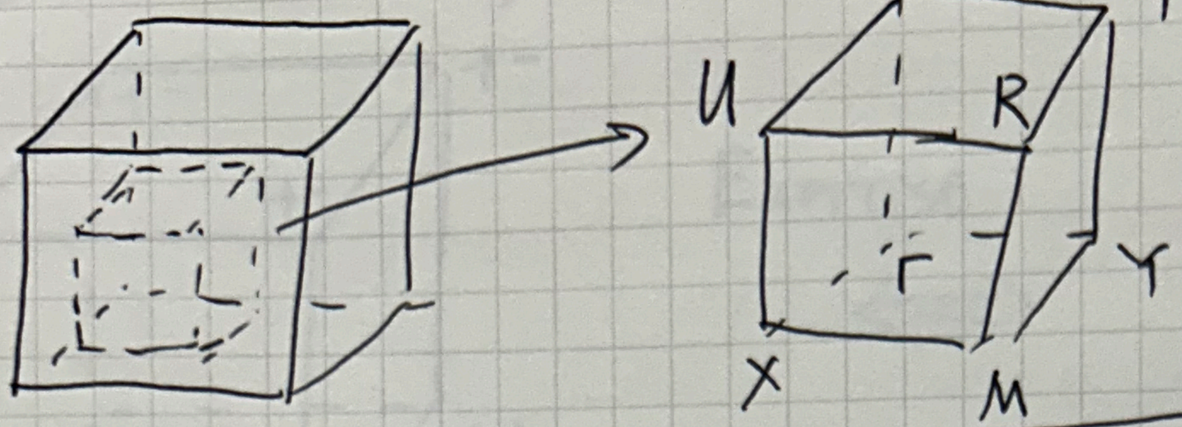
III. TQC for 3D system with inversion symmetry (magnetic)

(i) 1D $SI = \mathbb{Z}_1$ (trivial)

(ii) 2D $SI = \mathbb{Z}_2$ (parity of Chern #)

(iii) 3D $SI = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$.

3D BZ:



& inversion-invariant momenta.

The three $\mathbb{Z}_2$ factors: $\boxed{z_{2I,i} = \sum_{K, K_i=\pi} n_K^- \mod 2.}$ $i = x, y, z$

The $\mathbb{Z}_4$ factor: $\boxed{\eta_{4z} = \sum_K n_K^- \mod 4}$

~~① $\eta_{4I} = \sum_K$~~

① $\eta_{4z} \mod 2$

$$= \left(\sum_{K=\Gamma X Y M} n_K^- - \sum_{K=ZURT} n_K^- \right) \mod 2$$

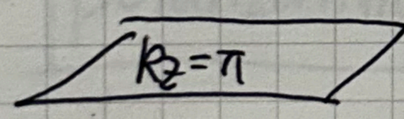
$$= \underline{\left(C_{k_z=0} - C_{k_z=\pi} \right) \mod 2}.$$

∴ if $\eta_{4z} = 1, 3$. the system is a WSM.

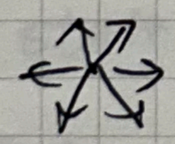
Model: $H = m(k_z)\sigma_z + k_x\sigma_x + k_y\sigma_y$

m @ $k_z = 0, \pi$ have different signs.

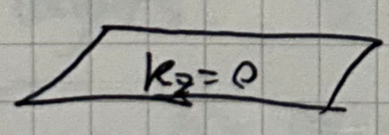
$m(k_z) = 0$ defines the Weyl points.



$C = 1$



a monopole in momentum space.



$C = 0$

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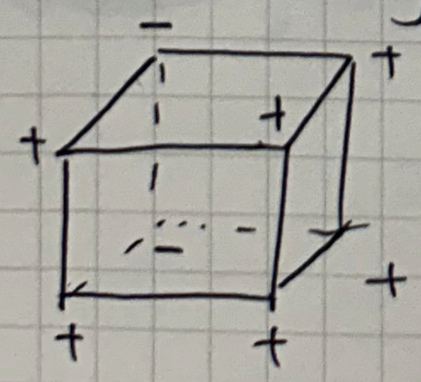
② All the other SZ's can be realized by insulators.

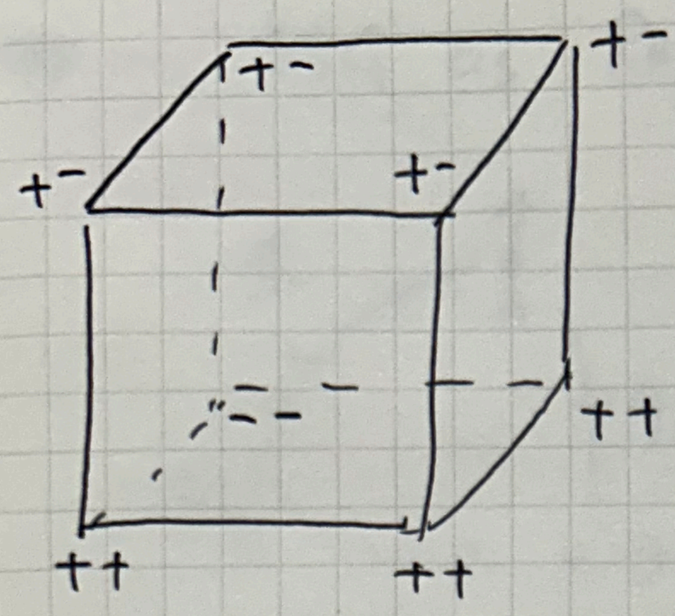
e.g. $z_{2I,x}$, z_{2Iy} z_{2Iz} $\eta_{4z} = (0, 0, 1, 0)$



$\Rightarrow$ 3D Chern insulator

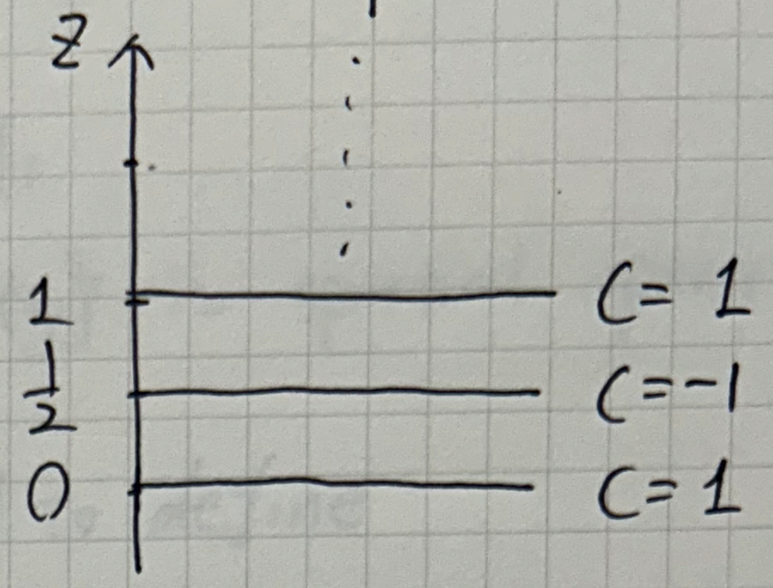
with $C_x = C_y = 0$ $C_z = 1 \pmod 2$

e.g. $(Z_{22,x}, Z_{22,y}, Z_{22,z}, \not{Z}\, y_{42}) = (0,0,0,2)$



Exercise: $\Longleftrightarrow$

real space.

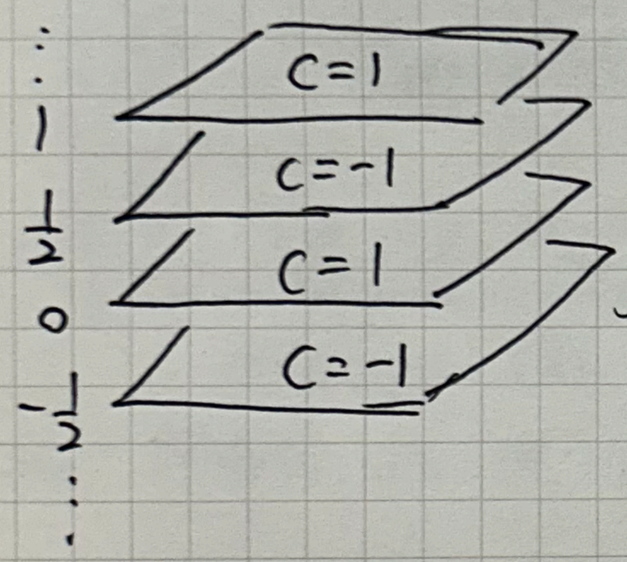


it's not a 3D Chern insulator.

What's it?

two aspects: (1) bulk response (2) boundary state.

(1) magneto electric effect. $P = \frac{\theta}{2\pi} B$



(i) even layers.

(ii) assuming boundary is fully gapped.

streda formula: $\frac{\partial \rho}{\partial t} = C \cdot \frac{\partial B}{\partial t}$

↑ Chern #

$\therefore \rho_l = (-1)^{2l} \cdot B$

$(l = 0, \pm\frac{1}{2}, \cdots)$

$\therefore$ **polarization $= \frac{1}{2}B$** $\qquad$ **$\theta = \pi$**

(2) boundary state:

odd layers. s.t. inversion is respected.

(d-2)-dimensional boundary state at the equator

symmetric deformation cannot remove it.

$\therefore$ Axion Insulator is a "higher order" TI