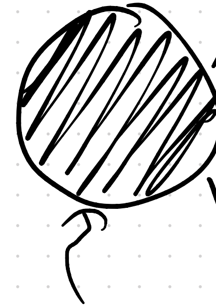
Magnetic Topological Quantum Chemistry

input: a commensurate magnetic structure



a catalogue of topologically trivial bands

easily computable topological invariants

1. Magnetic Space Groups (MSGs)
2. Representations of MSGs and electronic bands
3. Magnetic "band representations"

④ Magnetic Symmetry indicators of band topology

Overview of Terminology

1651 Shubnikov Space Groups (SSGs) (in 3D)

230 "ordinary" space groups (type I)

rotation, reflection, and translation symmetries of a crystal

230 nonmagnetic space groups (grey groups) (type II)

type-I group + time-reversal symmetry

1191 type III and IV

"Magnetic Space Groups"

type-I groups: Let G be a type-I SSG

$g \in G$ has the form $g = \{R | \vec{d}\}$

rotation or reflection

translation

$$g\vec{x} = R\vec{x} + \vec{d}$$

given $g_1 = \{R_1 | d_1\}$, $g_2 = \{\vec{R}_2 | \vec{d}_2\}$

- if $g_1 \in G$ $g_2 \in G$ then $g_1 g_2 \in G$

$$g_1 g_2 = \{R_1 | \vec{d}_1\}\{R_2 | \vec{d}_2\} = \{R_1 R_2 | R_1 \vec{d}_2 + \vec{d}_1\}$$

- Every space group contains $\{\underset{\substack{\uparrow \\ \text{identity} \\ \text{rotation}}}{E} | \underset{\substack{\nwarrow \\ \text{translation} \\ \text{by } 0}}{\emptyset}\}$

- if $g = \{R | \vec{d}\} \in G$, then we can define

$$g^{-1} = \{R^{-1} | -R^{-1} d\} \in G$$ and

$$g g^{-1} = \{E | \emptyset\}$$

Remember - electrons have spin-$\frac{1}{2}$

In quantum mechanics, we learned that if we rotate a spin-$\frac{1}{2}$ $|\chi\rangle$ by θ about an axis $\hat{n}$

$$|\chi\rangle \to e^{-\frac{i\theta}{2}\hat{n}\cdot\vec{\sigma}}|\chi$$

$\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ are Pauli matrices

$$\theta = 2\pi \quad e^{-i\frac{2\pi}{2}\hat{n}\cdot\vec{\sigma}} = \cos\pi + i\sin\pi(\hat{n}\cdot\sigma)$$

$= -1$

introduce $\{\bar{E}|\emptyset\} \in G$

$\uparrow$

2π rotation

Example: the double group 222

$$\{C_{2x}, C_{2y}, C_{2z}, E, \bar{E}\}$$

$$C_{2x}^2 = C_{2x}C_{2x} = \bar{E} = C_{2y}^2 = C_{2z}^2$$

$$C_{2x}\, C_{2y} = C_{2z} = \bar{E}\, C_{2y} C_{2x}$$

$-i\sigma_x \quad -i\sigma_y \quad -i\sigma_z$

$e^{-i\frac{\pi}{2}\sigma_x} = -i\sigma_x$

- Every type-I SSG contains a Bravais lattice of translation $T = \langle \{E|\vec{t}_1\}, \{E|\vec{t}_2\}, \{E|\vec{t}_3\} \rangle$

$T \subset G$

(14 Bravais lattices in 3D)

- If we "forget" about the translation part of every element

$$g = \{R|\vec{d}\} \longrightarrow \bar{g} = R$$

$g_1 = \{R_1 | \vec{d}_1\}$ $g_2 = \{R_2 | \vec{d}_2\}$

$g_1 g_2 = \{R_1 R_2 | R_1 \vec{d}_2 + \vec{d}_1\}$

"group homomorphism"

$g_1 \to R_1$ $g_2 \to R_2$

$g_1 g_2 \to R_1 R_2$

the group of all $\bar{g}$ is the point group $\bar{G}$ of G

$\bar{G} = G/T$ $g \to \bar{g}$ 32 point groups

The relation between G and $\bar{G}$ lets us divide space groups into 2 classes

1. Symmorphic Space groups

$$\bar{G} = \{\{R|0\} \mid R \in \bar{G}\} \subset G$$

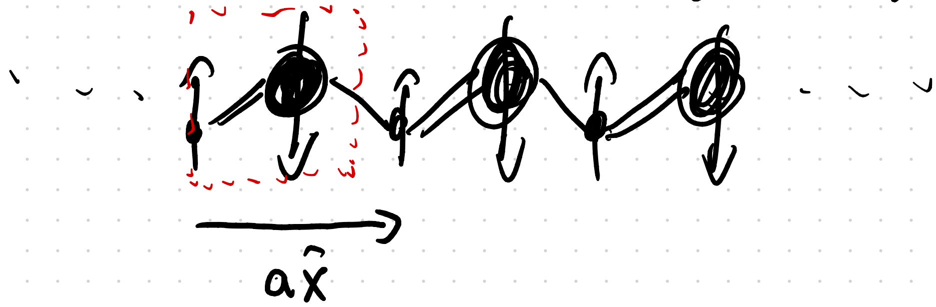
(73)

2. Nonsymmorphic space groups - all the rest

(157)

$\{R|\vec{d}\} \in G$ for $\vec{d}$ a fraction of a Lattice translation

Type I SSGs are magnetic space groups



$(na\hat{x}, 0, 0)$
$n \in \mathbb{Z}$

are at
$(na + \frac{a}{2}, 0, c)$

invariant under type-I SG

P1 ← point group 1 – no nontrivial operations

primitive Bravais lattice

Type-II space groups: given any type I space group G

$$G_{II} = G \cup \mathcal{T} G$$

$\mathcal{T}$ time-reversal symmetry, commutes with all spatial symmetries

$$\mathcal{T}\{R|\vec{d}\} = \{R|\vec{d}\}\mathcal{T}$$

$\mathcal{T} \in G_{II}$ - nonmagnetic

To construct the rest, lets start with a type-I group G

"group generated by"

let $H \subset G$ ex: $G = \check{\langle} \{E|t_1\}, \{E|t_2\}, \{E|t_3\}, C_{4z} \rangle$

$H = \langle \{E|t_1\}, \{E|t_2\}, \{E|2t_3\}, C_{4z} \rangle$

we can define cosets $gH = \{gh \mid h \in H\}$

Every $g' \in G$ is in exactly one coset gH

this means that we can write

$$G = H \cup g_1 H \cup g_2 H \cdots$$

the number of cosets $[G:H]$ is called the index of H in G

$\{g_1, g_2, \ldots\}$ are called coset representatives ex: $G = \langle \{E|t_1\}, \{E|t_2\}, \{E|t_3\}, C_{4z} \rangle$ - P4

$H = \langle \{E|t_1\}, \{E|t_2\}, \{E|2t_3\}, C_{4z} \rangle$

$G = H \cup \{E|t_3\} H \qquad [G:H] = 2$

Given a type-I group G and an index-2 subgroup H

$$G = H \cup g_1 H$$

we can construct a magnetic space group M as follows

$$M = H \cup g_1 \mathcal{T} H$$

Type III - $g_1 = \{R|\vec{d}\}$ $R \neq E$

Type IV - $g_1 = \{E|\vec{d}\}$

Type 2 example

$G_{I} = \langle \vec{t}_x, \vec{t}_y, \vec{t}_z, C_{4z} \rangle$

$G_{II} = \langle \vec{t}_x, \vec{t}_y, \vec{t}_z, C_{4z}, T \rangle$

G is a group, $H \subset G$ is a subgroup

want to show: every $g' \in G$ is in exactly one coset of H

- $\{E|\emptyset\} \in H \Rightarrow g'\{E|\emptyset\} = g' \in g'H$

lets assume $g' \in g_1 H$, $g' \in g_2 H$

$g' \in g_1 H \Rightarrow g' = g_1 h_1 \quad h_1 \in H$

$g' \in g_2 H \Rightarrow g' = g_2 h_2 \quad h_2 \in H$

$\Rightarrow g_1 h_1 = g_2 h_2$

$$\Rightarrow g_2^{-1}(g_1 h_1) h_1^{-1} = g_2^{-1}(g_2 h_2) h_1^{-1}$$

$$\Rightarrow g_2^{-1} g_1 = h_2 h_1^{-1} \in H$$

$$\Rightarrow g_2^{-1} g_1 H = H$$

$$\Rightarrow g_1 H = g_2 H$$

$\Rightarrow$ every g' is in exactly one coset

$$T^2 = \bar{E}$$

II. Magnetic Space groups

Recall $M = H \cup g\mathcal{T} H$

Type-IV: $g = \{E | \vec{d}\}$

Type-III $g = \{R | \vec{d}\}$

A note on terminology

Type-I SSGs [letter denoting Bravais lattice][point group]

Ex: Type-I group #99 $P\underbrace{4mm}_{\text{point group } \langle C_{4z}, M_x \rangle}$

primitive

For SSGs we will use $'$ (prime) to indicate if an operation reverses time

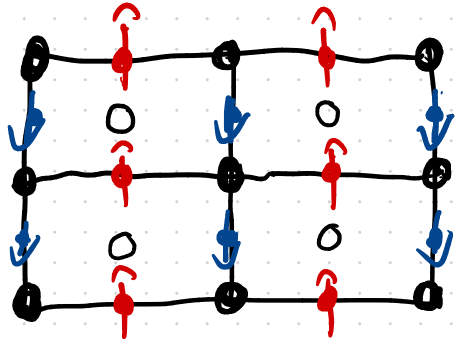
Type-II SSGs: we add $1'$ to the end of the symbol

$$P4mm1'$$

Type-III SSGs: we add $'$ to the operations that reverse time

$$P4'\underbrace{m'm}_{\langle C_{4z}\mathcal{T},\ m_x\mathcal{T},\ m_{110}\rangle}$$

primitive



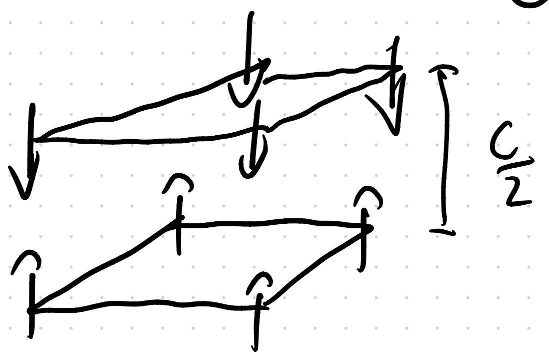
Type-IV: Two naming conventions

BNS (Belov Neronova, Smirnova) $M = H \cup \{E|\vec{d}\}\mathcal{T} H$

We use the SG symbol for H, and indicate $\{E|\vec{d}\}\mathcal{T}$ with a subscript

Ex: $P_c 4 = \langle a\hat{x}, a\hat{y}, c\hat{z}, C_{4z}, \frac{c}{2}\hat{z} \times \mathcal{T} \rangle$

(Alternative OG: use the SG symbol of
$G = H \cup \{E|\vec{d}\} H$)



- Electrons in (magnetic) solids

$$\hat{H}|\psi\rangle = \left(\frac{p^2}{2m} + V_1(x) + V_2(x, \vec{p}, \vec{\sigma})\right)|\psi\rangle = E|\psi\rangle$$

with $\hat{H}$ invariant under the symmetries of some SSG M

- every M contains a bravais lattice

$$M \supset T = \langle \vec{t}_1, \vec{t}_2, \vec{t}_3 \rangle$$

Bloch's theorem: let $U_{\vec{t}} = e^{-i\vec{p}\cdot\vec{t}/\hbar}$ generate translations by t:

$[U_{\vec{t}}, H] = 0 \Rightarrow$ we can simultaneously diagonalize

$U_{\vec{t}}$ and H

$$U_{\vec{t}}|\psi_{nk}\rangle = e^{-i\vec{k}\cdot\vec{t}}|\psi_{nk}\rangle$$

$$H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$$

$$\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$$

$$\vec{b}_i \cdot \vec{t}_j = 2\pi\delta_{ij}$$

$$k_i \in \left[-\tfrac{1}{2}, \tfrac{1}{2}\right]$$

What about $g = \{R|\vec{d}\} \in M$

U_g - implements this symmetry on Hilbert space

$$[U_g, H] = 0 \Rightarrow U_g|\psi_{nk}\rangle \text{ is an eigenstate}$$

$$\text{if } |\psi_{nk}\rangle \text{ is an eigenstate}$$

$$U_{\vec{t}}\left[U_g|\psi_{nk}\rangle\right] = U_{\{E|\vec{t}\}} U_{\{R|\vec{d}\}} |\psi_{nk}\rangle$$

$$\|$$

$$\{E|\vec{t}\}\{R|\vec{d}\} = \{R|\vec{d}+\vec{t}\}$$

$$= \{R|\vec{d}\}\{E|R^{-1}\vec{t}\}$$

$$U_g U_{\{E|R^{-1}t\}} |\psi_{nk}\rangle = U_g e^{-ik\cdot R^{-1}t} |\psi_{nk}\rangle = e^{-ik\cdot R^{-1}t} \left[U_g|\psi_{nk}\rangle\right]$$

$$k \cdot R^{-1} t = (Rk) \cdot RR^{-1} t = Rk \cdot t$$

$U_g |\psi_{nk}\rangle$ is a Bloch state with crystal momentum $R\vec{k}$

$$U_g |\psi_{nk}\rangle = \sum_m |\psi_{m\,Rk}\rangle\langle\psi_{m\,Rk}| U_g |\psi_{nk}\rangle$$

$$= \sum_m |\psi_{m\,Rk}\rangle \underbrace{B^k_{mn}(g)}_{\text{sewing matrix for } g}$$

What about $\widetilde{g\int} = \{R|\vec{d}\}\widetilde{\int}$

Wigner's thm: time-reversing operations are represented by antiunitary operators $A_{g\mathcal{T}}$

$A_{g\mathcal{T}}$ is antiunitary if • $A_{g\mathcal{T}}\left(\alpha|\psi\rangle + \beta|\varphi\rangle\right)$

$= \alpha^* A_{g\mathcal{T}}|\psi\rangle + \beta^* A_{g\mathcal{T}}|\varphi\rangle$

• $\langle A_{g\mathcal{T}}\psi | A_{g\mathcal{T}}\varphi\rangle = \langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^*$

$(A_{g\mathcal{T}})^2$ is unitary [for TRS $\widetilde{\mathcal{T}}^2 = \bar{E}$]

$$U_{\vec{t}}\left[A_{g\tau}|\psi_{nk}\rangle\right] = A_{g\tau}\, U_{R^{-1}\vec{t}}\,|\psi_{nk}\rangle$$

$$= A_{g\tau}\, e^{-ik\cdot R^{-1}t}|\psi_{nk}\rangle$$

$$= e^{+ik\cdot R^{-1}t}\left[A_{g\tau}|\psi_{nk}\rangle\right]$$

$A_{g\tau}|\psi_{nk}\rangle$ has crystal momentum $-R\vec{k}$

$$A_{g\tau}|\psi_{nk}\rangle = \sum_{m} |\psi_{m\,-Rk}\rangle \underbrace{\langle\psi_{m\,-Rk}|A_{g\tau}|\psi_{nk}\rangle}_{B^{k}_{mn}(g\tau)}$$

Something special happens for $Rk \equiv k$ modulo a reciprocal lattice vector

given k, M we define $M_k = \{g \in M \mid gk \equiv k \text{ mod reciprocal lattice vector}\}$

M_k is the <u>little group</u> of k

$T \subset M_k$ for every k M_k is a SSG.

two cases: $M_k = G_k$ is a type-I group

$M_k = G_k \cup g\mathcal{T}G_k$ for G_k a type-I group

$g = \{R|d\} \in G_k$ g is a symmetry of H

$$H_{ab}(k) = \langle \psi_{ak} | H | \psi_{bk} \rangle \overset{\text{g is a symmetry of H}}{=} \langle \psi_{ak} | U_g^\dagger H U_g | \psi_{bk} \rangle$$

$$= \sum_{cd} \langle \psi_{ak} | U_g^\dagger | \psi_{ck} \rangle \langle \psi_{ck} | H | \psi_{dk} \rangle \langle \psi_{dk} | U_g | \psi_{bk} \rangle$$

$$= \left[B^{k\dagger}(g) H(k) B(g) \right]_{ab}$$

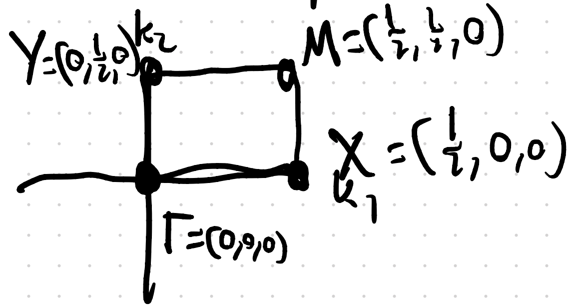
$$\Rightarrow \left[H(k), B^k(g) \right] = 0 \text{ for } g \in G_k$$

Schur's Lemma: states can be labelled by irreducible representations of G_k

Ex: type-I group $P4 = \langle a\hat{x}, a\hat{y}, c\hat{z}, C_{4z} \rangle$

recip. lattice vectors $b_1 = \frac{2\pi}{a}\hat{x}$ $b_2 = \frac{2\pi}{a}\hat{y}$, $b_3 = \frac{2\pi}{c}\hat{z}$

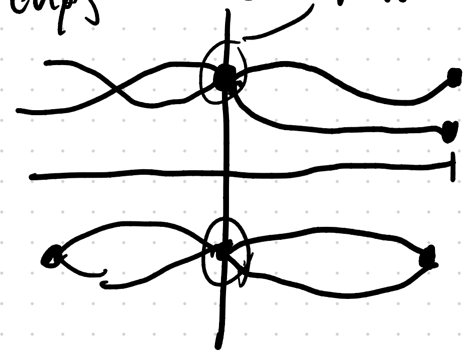
$k_3 = 0$



$G_\Gamma = P4$ $\quad G_X = P2$

$G_M = P4$ $\quad G_Y = P2$

For type I groups



What about type II–IV groups:

- type II groups $M = G \cup \mathcal{J} G$: at Time-Reversal Invariant Momenta (TRIM) $k \equiv -k$ mod a recip lattice vector $\Rightarrow$ M_k is a type-II SSG otherwise M_k is a type I SSG
- Similar in type III: M_k is either a type III group

or a type I group

- in type IV: M_k is either a type IV group or a type I group, or a type III group

Lets consider a time-reversing operation $g_k \mathcal{T} \in M_k$ in the little group at some k point

$$A_{g_k \mathcal{T}} |\psi_{ak}\rangle = \sum_b |\psi_{bk}\rangle\langle\psi_{bk}| A_{g_k \mathcal{T}} |\psi_{ak}\rangle$$

$$= \sum_b |\psi_{bk}\rangle \underbrace{B^k_{ba}(g_k \mathcal{T})}_{\text{still a unitary matrix}}$$

We need to account for the fact that

$$A_{g_k \mathcal{T}}(\alpha|\psi_{ak}\rangle) = \alpha^* A_{g_k \mathcal{T}}|\psi_{ak}\rangle$$

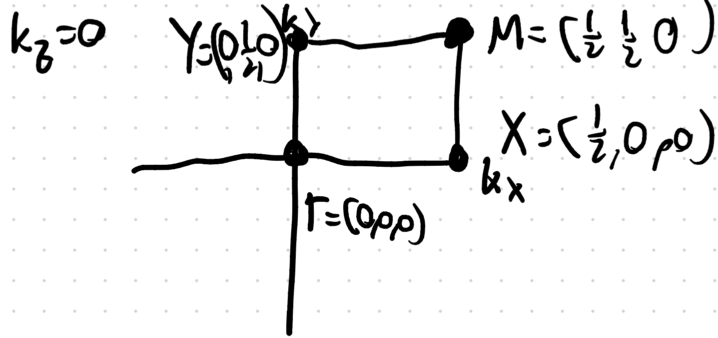
We introduce $\mathcal{K}$ - represents complex conjugation

$$A_{g_k \mathcal{T}} \to B^k(g_k \mathcal{T})\mathcal{K}$$

A set of representation matrices w/ both unitary & antiunitary operators is called a <u>co-representation</u> (corep)

Example: Type-III $P4' = (P2) \cup C_{4z}\mathcal{T}(P2)$

$$= \langle a\hat{x}, a\hat{y}, c\hat{z}, C_{4z}\mathcal{T}, C_{2z}, \bar{E}, E \rangle$$



$G_\Gamma = P4'$ - type III $\quad G_X = G_Y = P2$ - type I

$G_M = P4'$ - type III

Example: $P_c 1 = P1 \cup \{E|\frac{c}{2}\hat{z}\}\mathcal{T}\, P1 = \langle a\hat{x}, b\hat{y}, c\hat{z}, \overline{\tfrac{c}{2}\hat{z}\mathcal{T}}, \bar{E}, E\rangle$

$$\left(\{E|\tfrac{c}{2}\hat{z}\}\mathcal{T}\right)^2 = \{\bar{E}|c\hat{z}\} = \{\bar{E}|0\}\{E|c\hat{z}\}$$

Id - identity matrix

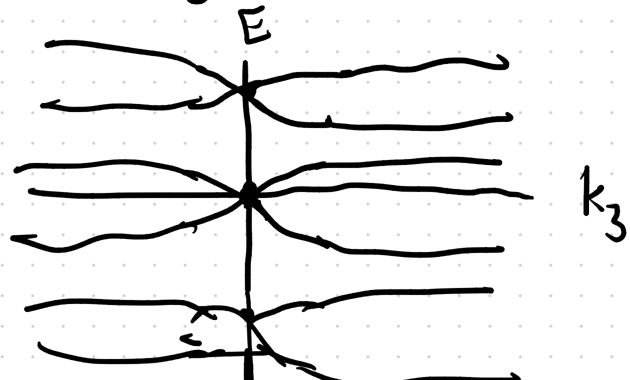
$$B^{k}(\{\bar{E}|c\hat{z}\}) = (-\mathrm{Id})e^{-ik_3 2\pi}$$

$\nearrow$ $-\mathrm{Id}$ when $k_3 = 0$

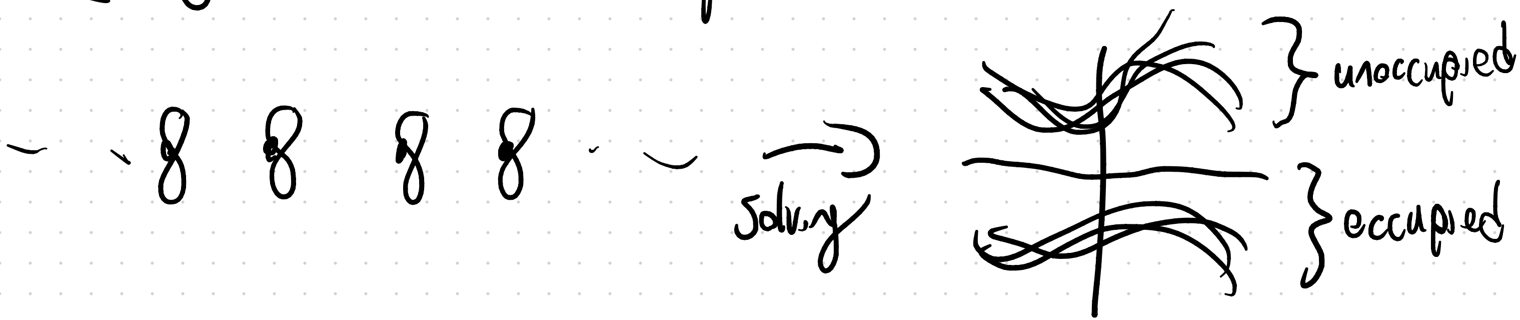
$\searrow$ $+\mathrm{Id}$

$\Gamma = (0,0,0)$; $G_\Gamma = P_c 1$: antiunitary squares to -1 $\rightarrow$ Kramers degeneracy

$Z = (0,0,\frac{1}{2})$; $G_Z = P_c 1$: antiunitary squares to $+1$ $\rightarrow$ No Kramers degeneracy



III. (Magnetic) Band representations



Can we run this in reverse?

$$\{|\psi_{nk}\rangle\} \longrightarrow |W_{nR}\rangle = \sum_{R} e^{ik\cdot R}|\psi_{nk}\rangle$$

Wannier functions $|W_{nR}\rangle$ - exponentially localized
- symmetric

An insulator can be adiabatically connected to an atomic limit if we can symmetrically move all the atoms apart w/o closing an energy gap

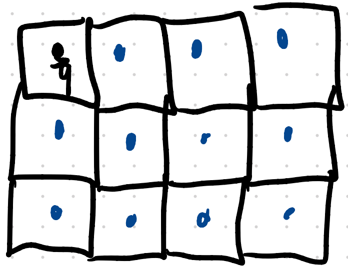
(magnetic) topological insulators <u>can't</u> be adiabatically connected to an atomic limit w/o closing a gap → no localized Wannier functions

Our goals: I. Characterize all atomic limit bands (those with exp. localized Wannier functions)
- topologically trivial bands

2. Identify invariants that tell us when a set of bands is topologically nontrivial

1. Pick a SSG G

Bravais lattice



$$G_{\vec{q}} = \{ g \in G \mid g\vec{q} = \vec{q} \}$$

$G_{\vec{q}}$ is isomorphic to a (magnetic) point group, called the site-symmetry group of $\vec{q}$.

in order to respect symmetries, orbitals @ $\vec{q}$ transform in coreps of G_q

lets say our valence orbitals $\{|W_{n00}\rangle\}$ transform in an irreducible corepresentation (corep) ρ of G_q

Translation symmetry: we have copies $|W_{n0\vec{t}}\rangle = U_{\vec{t}}|W_{n00}\rangle$

This gives me a structure invariant under

$$G_{\vec{q}} \cup \vec{t}_1 G_q \cup \vec{t}_2 G_q \cdots \underbrace{T G_q}_{\text{symmorpic SSG}} \subset G$$

- What about other elements of G?

$$G = T G_q \cup g_1 T G_q \cup \cdots \cup g_{n-1} T G_q$$

coset decomposition of G with n coset representatives $\underbrace{\{E|\emptyset\}}_{g_0}, g_1, g_2, \ldots g_{n-1}$

If we has orbitals at $\vec{q}$, it also needs to have orbitals at $g_i \vec{q}$

$\ast$ Flat band references

- Calugaru et al, Nat Phys 18, 185-189 (2022)

$\{|\underline{W_{n i \vec{t}}}\rangle\} \leftarrow$ form a corepresentation of G

For any $g \in G$ $\quad g = \{R|d\}$

$$U_g |W_{n i \vec{t}}\rangle = U_g U_{\vec{t}} U_{g_i} |W_{n00}\rangle$$

$$= U_{R\vec{t}} U_g U_{g_i} |W_{n00}\rangle$$

$$= U_{R\vec{t}} U_{g g_i} |W_{n00}\rangle$$

$$g g_i = t'_{ij} g_j h_{ij} \qquad h_{ij} \in G_q$$

$$t'_{ij} = g(g_i \vec{q}) - g_j \vec{q}$$

$$U_g |W_{ni\vec{t}}\rangle = \sum_m |W_{mj, Rt+t'_{ij}}\rangle \rho_{mn}(h_{ij})$$

Fourier transform: $|a_{nik}\rangle = \sum_t e^{ik\cdot\vec{t}} |W_{ni\vec{t}}\rangle$

$$U_g |a_{nik}\rangle = \sum_{mj} |a_{mjRk}\rangle B^k_{mj,ni}(g)$$

$$\rightarrow B^k_{mj,ni}(g) = e^{-iRk\cdot t'_{ij}} \rho_{mn}(h_{ij})$$

"Band representation"

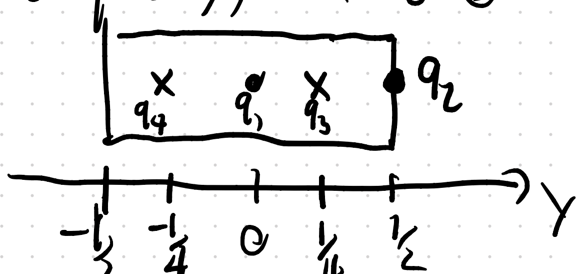
- MBANDREP tool on Bilbao Crystallographic Server

Points $\vec{q}$ and their site-symmetry groups are classified into <u>Wyckoff positions</u>

- MWYCKPOS on Bilbao Server

Example: $P_b m$ - type $\underline{\text{IV}}$ = $\langle t_x, t_y, t_z, m_y, \tfrac{1}{2}t_y \cdot \mathcal{T} \rangle$

for simplicity, $x = z = 0$



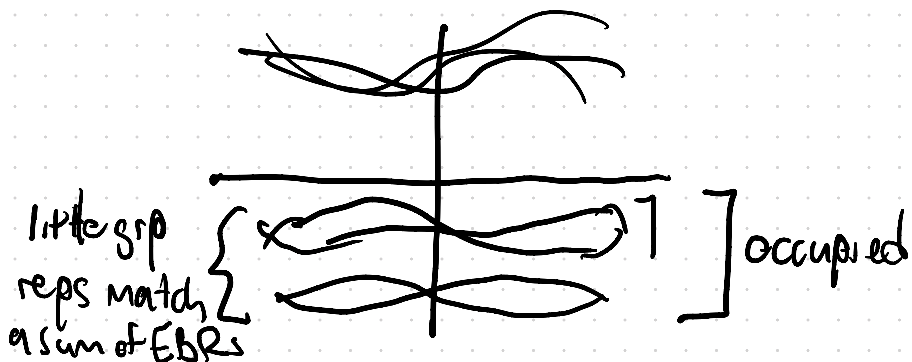
$$G_{q_1} = \langle m_y \rangle = m$$

$$G_{q_2} = \langle \{m_y | t_y\} \rangle \cong m$$

$G_{q_3} = \langle \{ \tfrac{1}{2}\hat{t}_y \mid m_y \} \rangle \simeq m'$

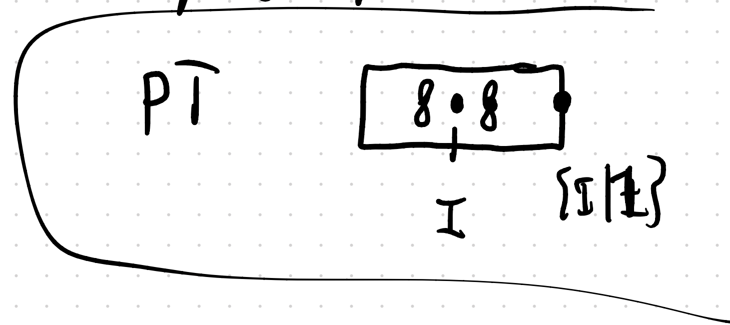
$G_{q_4} \simeq m'$

Any band structure that can be built from an atomic limit (i.e. w/ exponentially localized, symmetric Wannier functions) can be built from a sum of EBRS



if trivial

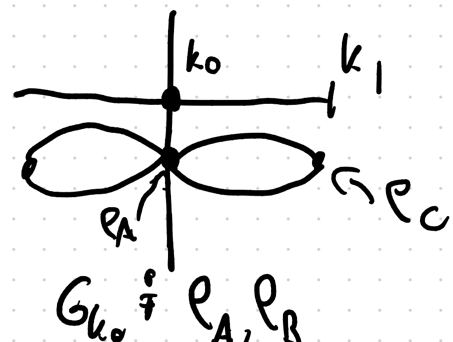
If the little group coreps of the occupied bands <u>do not</u> match a sum of EBRs, then the occupied bands <u>must</u> be topologically nontrivial



To identify these lets rephrase everything as a linear algebra problem

lets collect all the little group irreps at high symmetry k points into $\vec{r}$ - "symmetry data vector"

$1 \times N_{irrep}$



EBR table: $E: N_{\text{irrep}} \times N_{\text{EBR}}$

$\vec{B}: 1 \times N_{\text{EBR}}$ - non-negative integers

$\vec{V} = \vec{E} \cdot \vec{B}$ gives the symmetry data vector for an atomic limit band structure

non-negative integers

$G_{k_1}: \rho_C \; \rho_D$

$$\vec{v} = (\underset{\rho_A}{1}, \underset{\rho_B}{0}, \underset{\rho_C}{1}, \underset{\rho_D}{0})$$

Are there allowed $\vec{v}$ that cannot take this form?

integer valued

Smith Decomposition: $E = L^{-1} \Lambda R$

L, R are integer valued AND their inverses are integer valued

$$\Lambda = \begin{pmatrix} a_1 & & & & & & \\ & a_2 & & & & & \\ & & a_3 & & & & \\ & & & \ddots & & & \\ & & & & 0 & & \\ & & & & & 0 & \\ & & & & & & 0 \end{pmatrix}$$ diagonal $a_i \geq 0$

$$\vec{v} = L^{-1} \Lambda R \vec{B}$$

$$L\vec{v} = \vec{v}'$$

$$R\vec{B} = \vec{B}'$$

$$L\vec{v} = \Lambda (R\vec{B})$$

$$\vec{v}' = \Lambda \vec{B}'$$

$$\begin{pmatrix} v_1' \\ v_2' \\ v_3' \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 & & & \\ & a_2 & & \\ & & a_3 & \\ & & & \ddots \end{pmatrix} \begin{pmatrix} B_1' \\ B_2' \\ B_3' \\ \vdots \end{pmatrix}$$

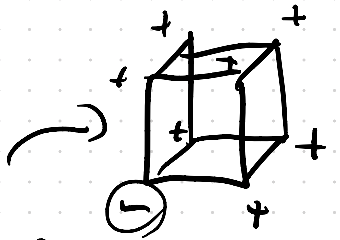
for any $a_i > 1$, we get a $\vec{v}$ that <u>cannot</u> come from an integer linear combination of EBRs this defines a <u>symmetry indicator group</u>

$$\mathbb{Z}_{a_1} \oplus \mathbb{Z}_{a_2} \oplus \cdots \oplus \mathbb{Z}_{a_n}$$ of topologically nontrivial bands

Ex: Type-I $P\bar{1}$ $\quad \underbrace{\mathbb{Z}_2 \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2}_{\text{Chern \# in planes of the BZ}} \oplus \underbrace{\mathbb{Z}_4}_{\text{strong invariant}}$

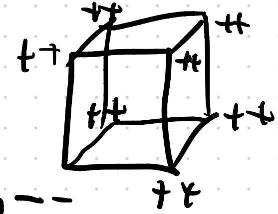
The columns of L^{-1} give us the sets of irreps corresponding to our nontrivial bands

$\mathbb{Z}_4=1$



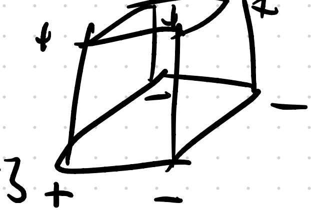
- Weyl Semimetal

$\mathbb{Z}_4=2$



Higher order topological insulator (magnetic axion insulator)

$\mathbb{Z}_4=3$



Weyl Semimetal

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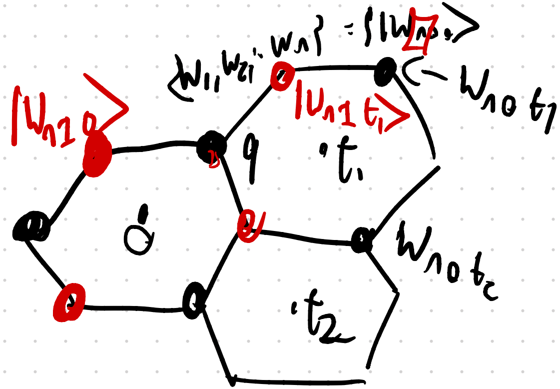

$\{w_1, w_2, \ldots w_n\} = \{|w_{n\circ}\rangle$
$|W_{n1}\, 0\rangle$
$|W_{n1}\, t_1\rangle$
$W_{n0}\, t_1$
$W_{n0}\, t_2$
t_1
t_2