Lecture 9+10

Recap: Space groups

Symmorphic: $G = T \rtimes \bar{G}$

- $\bar{G} \subset G$
- 73 in 3D
- Symbols have the form [letter][pt group symbol]

Nonsymmorphic

- $\bar{G} \not\subset G$
- $G = T \cup T\{\bar{g}_1 | \vec{d}_1\} \cup T\{\bar{g}_2 | \vec{d}_2\} \ldots \cup T\{\bar{g}_{n-1} | \vec{d}_{n-1}\}$

at least one $\vec{d}_i$ must be a fractional translation

- G typically contains screw rotations or glide mirrors
- 153 in 3D
- H-M symbols have subscripts to denote screws, and letters to denote glides

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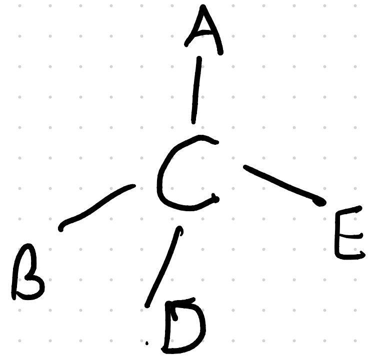
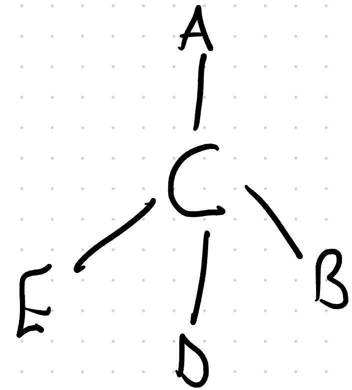
Aside: Chiral crystals

crystal structure has a handedness: given a chiral crystal, we can reverse orientation to get a different crystal

Ex:



vs



The key point: Chiral materials have no orientation-reversing symmetries

Orientation for a crystal $\vec{e}_1, \vec{e}_2, \vec{e}_3$ primitive lattice vectors

$$\operatorname{sign}\left[\vec{e}_1 \cdot (\vec{e}_2 \times \vec{e}_3)\right] = \begin{cases} +1 & \text{Right-handed coord system} \\ -1 & \text{left-handed coordinate system} \end{cases}$$

- All rotations preserve orientation

$(\hat{n}, \theta) \rightarrow R_{\hat{n}}(\theta)$ 3x3 rotation matrix

$$R_{\hat{n}}(\theta)\vec{e}_1 \cdot \left(R_{\hat{n}}(\theta)\vec{e}_2 \times R_{\hat{n}}(\theta)\vec{e}_3\right) = \det R_{\hat{n}}(\theta)\, \vec{e}_1 \cdot (\vec{e}_2 \times \vec{e}_3)$$

$\det R_{\hat{n}}(\theta) = +1$ for rotations

- spatial inversion reverses orientation $I\vec{e}_i = -\vec{e}_i$

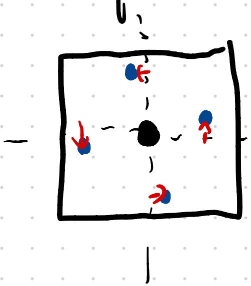
$$I\vec{e}_1 \cdot (I\vec{e}_2 \times I\vec{e}_3) = -\vec{e}_1 \cdot (\vec{e}_2 \times \vec{e}_3)$$

- mirror symmetries reverse orientation ($I \times$ twofold rotation)

⇒ Chiral materials crystallize in space groups w/ translations, rotations, and screw rotations

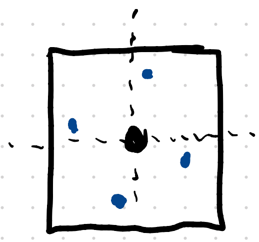
65 of these   Söncke space groups

Example in 2D



P4

chiral



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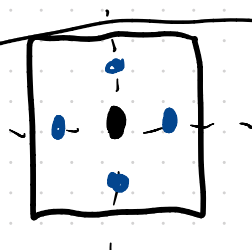


P4mm

inversion: HM symbol $\bar{1}$

rotoinversions IC_3, IC_4 IC_6

$\bar{3}$ $\bar{4}$ $\bar{6}$

(in 2D only mirrors & glides reverse orientation)

Lets use space groups to study band structure

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

Bloch's theorem

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

What about other symmetries $\{\bar{g}|\vec{d}\} \in G$

let $U_{\{\bar{g}|\vec{d}\}}$ be the unitary operator that implements $\{\bar{g}|\vec{d}\}$ on our Hilbert space

$$[U_{\{\bar{g}|\vec{d}\}}, H] = 0$$

consider $\{E|\vec{t}\}\{\bar{g}|\vec{d}\} = \{\bar{g}|\vec{t}+\vec{d}\}$

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

$$U_{\vec{t}}\, U_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle = U_{\{\bar{g}|\vec{d}\}} U_{\{E|\bar{g}^{-1}\vec{t}\}} |\psi_{n\vec{k}}\rangle$$

$$= U_{\{\bar{g}|\vec{d}\}}\left(e^{-i\vec{k}\cdot(\bar{g}^{-1}\vec{t})}\right)|\psi_{n\vec{k}}\rangle$$

$$= e^{-i\vec{k}\cdot(\bar{g}^{-1}\vec{t})}\, \underline{U_{\{\bar{g}|\vec{d}\}}}|\psi_{n\vec{k}}\rangle$$

$$\boxed{\begin{aligned} \{\bar{g}|\vec{d}\}\vec{x} &= \bar{g}\vec{x}+\vec{d} \\ \{\bar{g}|\vec{d}\}\vec{k} &= \bar{g}\vec{k} \end{aligned}}$$

$$\vec{k}\cdot(\bar{g}^{-1}\vec{t}) = (\bar{g}k)\cdot(\bar{g}\bar{g}^{-1}\vec{t})$$

$$= (\bar{g}k) \cdot \vec{t}$$

$$U_{\vec{t}}\left[U_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle\right] = e^{-i\bar{g}k\cdot\vec{t}}\left[U_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle\right]$$

$\Rightarrow \quad U_{\{\bar{g}|\vec{d}\}}|\psi_{n\vec{k}}\rangle$ transforms in the $\vec{\bar{g}k}$ representation of T

$$U_{\{\bar{g}|\vec{d}\}}|\psi_{n\vec{k}}\rangle = \sum_{m}|\psi_{m\bar{g}k}\rangle\langle\psi_{m\bar{g}k}|U_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle$$

$$\boxed{\{|\psi_{nk}\rangle\} \to \{|\psi_{m\bar{g}\vec{k}}\rangle\}} \equiv \sum_m |\psi_{m\bar{g}k}\rangle B^{\vec{k}}_{mn}(\{\bar{g}|\vec{d}\})$$

"Sewing matrix" for the symmetry $\{\bar{g}|\vec{d}\}$

If $\bar{g}\vec{k} = \vec{k} + \vec{b}$ for $\vec{b}$ a reciprocal lattice vector

then $e^{-i\bar{g}\vec{k}\cdot\vec{t}} = e^{-i(\vec{k}+\vec{b})\cdot t} = e^{-i\vec{k}\cdot\vec{t}}\, e^{-i\underline{\vec{b}\cdot\vec{t}}}$

$= e^{-i\vec{k}\cdot\vec{t}}\, \cancel{e^{-2\pi i n}}^{\,1}$

Then $B^{k}_{mn}(\{\bar{g}|\vec{d}\})$ is a map between states at the <u>same</u> $\vec{k}$

Given $\vec{k}$ we can define

$$G_{\vec{k}} = \left\{ \{\bar{g}|\vec{d}\} \in G \;\middle|\; \bar{g}\vec{k} \equiv \vec{k} \text{ (modulo reciprocal lattice vectors)} \right\}$$

$G_{\vec{k}}$ is called the little group of $\vec{k}$

$\{ B^{k}_{mn}(g_k) \,|\, g_k \in G_k \}$ form a representation of the little group

Schur's lemma: states $\{|\psi_{nk}\rangle\}$ transform in representations of G_k and states in the same irrep of G_k are degenerate.

Lets look at an example: $\underbrace{P}_{\text{primitive cubic Bravais lattice}}\underbrace{432}_{\text{octahedral pt group}}$

$$\vec{e}_1 = a\hat{x} \qquad \vec{b}_1 = \frac{2\pi}{a}\hat{x}$$
$$\vec{e}_2 = a\hat{y} \quad \xrightarrow{\text{reciprocal lattice vectors}} \quad \vec{b}_2 = \frac{2\pi}{a}\hat{y}$$
$$\vec{e}_3 = a\hat{z} \qquad \vec{b}_3 = 2\pi/a\,\hat{z}$$

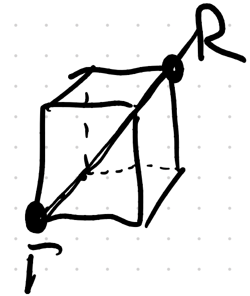
1. lets take $\vec{k} = \vec{0}$ (known as Γ)

if $\{\bar{g}|\vec{d}\} \in G \quad \bar{g}\vec{k} = \vec{k} = 0$

every element of G leaves Γ invariant

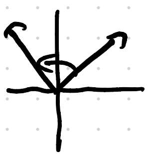
$$G_\Gamma \cong G$$

② $\vec{k} = \frac{1}{2}\vec{b}_1 + \frac{1}{2}\vec{b}_2 + \frac{1}{2}\vec{b}_3 \rightarrow \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = R$



$$P432 = \langle T, C_{4z}, C_{3,111} \rangle$$

C_{4z}:



$x \to y$

$y \to -x$

$z \to z$

$$C_{3,111}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$

$$C_{4z}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right) = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) - \vec{b}_2$$

$$G_R \cong G$$

3 $\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$ $k_1 \neq k_2 \neq k_3$ each random irrational numbers

$G_{\vec{k}} = T$ labelled as GP (general position)

All info can be found in KVEC on the Bilbao Server

Representations of little groups:

$T \triangleleft G_k$ for every k → little groups are isomorphic to space groups

Two cases

1. G_k is a symmorphic space group
2. G_k is a nonsymmorphic space group

$\overline{G}_k$

$\to$ Easy $\quad g_k \in G_k$ can be written $g_k = \{E|\vec{t}\}\{\bar{g}|0\}$

if ρ is a representation of G_k

$$\rho(g_k) = \rho(\{E|\vec{t}\})\rho(\{\bar{g}|0\}) \qquad \rho(\{E|\vec{t}\}) = e^{-ik\cdot\vec{t}}$$
$$= e^{-i\vec{k}\cdot\vec{t}}\rho(\{\bar{g}|0\})$$

given a representation ρ of G_k we get a representation η of $\overline{G}_k = G_k/T$

$$\boxed{\eta(\bar{g})} = \rho(\{\bar{g}|0\})$$

given a representation η of $\bar{G}_k$ we can construct a representation ρ of G_k

For symmorphic little groups G_k, representations of G_k are determined by point group representations of $\bar{G}_k = G_k/T$ (little cogroup)

2) G_k nonsymmorphic $\leftarrow \{\bar{g}_i|\vec{d}_i\}$ where $\vec{d}_i$ is a fractional lattice translation

$$\{\bar{g}_1|\vec{d}_1\}\{\bar{g}_2|\vec{d}_2\} = \{E|\vec{t}\}\{\bar{g}_3|\vec{d}_3\} \qquad \bar{g}_1\bar{g}_2 = \bar{g}_3$$

$$\left(\text{Ex: } \{C_{2z}|\tfrac{1}{2}\hat{z}\}\{C_{2z}|\tfrac{1}{2}\hat{z}\} = \{E|\hat{z}\}\right)$$

if ρ is a representation of G_k

$$\rho(\{\bar{g}_1|\vec{d}_1\})\rho(\{\bar{g}_2|\vec{d}_2\}) = e^{-i\vec{k}\cdot\vec{t}}\rho(\{\bar{g}_3|\vec{d}_3\})$$

this defines
- a representation of an extension of $\bar{G}_k$ by $e^{-i\vec{k}\cdot\vec{t}}$
- a projective representation of $\bar{G}_k$

Example: $P2_1$ $\quad \vec{e}_1 \quad \vec{e}_2 \quad \vec{b}_1 \quad \vec{b}_2$

$\vec{e}_3 = c\hat{z}$ $\qquad$ $\vec{b}_3$

$\{C_{2z} | \tfrac{1}{2}\vec{e}_3\}$

① Γ point: $\vec{k} = 0$ $\qquad$ $G_\Gamma = P2_1$

if ρ_Γ is an irrep of G_Γ $\quad \rho_\Gamma(\{E|\vec{t}\}) = e^{-i 0\cdot\vec{t}} = 1$

$$\rho_\Gamma(\{C_{2z}|\tfrac{1}{2}\vec{e}_3\})\,\rho_\Gamma(\{C_{2z}|\tfrac{1}{2}\vec{e}_3\}) = \rho_\Gamma(\{E|\vec{e}_3\})$$
$$= 1$$
$$= \rho_\Gamma(\{E|\vec{0}\})$$

→ at Γ, irreps of the little group can always be determined from $\overline{G}$

ρ_Γ	E	C_2
Γ_1	1	1
Γ_2	1	-1

$$\rho_{\Gamma_2}\left(\{C_{2z} | \tfrac{1}{2}\vec{e}_3\}\right) = -1$$

What about $\vec{k} = \frac{1}{2}\vec{b}_3$ reduced coordinates $(0, 0, \frac{1}{2})$ $[Z]$

$$G_Z = G \qquad \rho_Z\left(\{E|\vec{t}\}\right) = e^{-i\frac{1}{2}\vec{b}_3\cdot\vec{t}} = e^{-i\pi t_3}$$

where $\vec{t} = t_1\vec{e}_1 + t_2\vec{e}_2 + t_3\vec{e}_3$

$$\rho_Z\left(\{C_{2z}|\tfrac{1}{2}e_3\}\right)^2 = \rho_Z\left(\{E|\vec{e}_3\}\right) = -1 \ (= e^{-i\pi})$$

$\frac{1}{2}b_3\cdot\vec{e}_3 = \frac{1}{2}(2\pi) = \pi$

ρ	E	$\{E\|\vec{t}\}$	$\{C_{2z}\|\frac{1}{2}\vec{e}_3\}$
Z_1	$+1$	$e^{-i\pi t_3}$	$+i$
Z_2	$+1$	$e^{-i\pi t_3}$	$-i$

Extended group $\quad E, C_2, X$

$X^2 = E$

$C_2^2 = X$