Lecture 8

Recap: Every crystal has a Bravais lattice T

① if G is a space group, then

$$T \triangleleft G$$

the point group $\bar{G} = G/T$

$$\bar{G} = \{R \mid \{R|\vec{d}\} \in G\} \subset O(3)$$

② if $R \in \bar{G}$ then:

- R is a rotation by $0, \pm\frac{\pi}{3}, \pm\frac{2\pi}{3}, \pm\pi, \pm\frac{\pi}{2}$
- R is spatial inversion I: $(x,y,z) \to (-x,-y,-z)$

- R is the composition of $I \times$ an allowed rotation

32 allowed crystallographic point groups in 3D

$$[H, u_{\vec{t}}] = 0 \quad \forall \vec{t} \in T$$

$$H_{mk', nk} = \boxed{|\psi_{mk'}\rangle \langle \psi_{mk'}| H |\psi_{nk}\rangle \langle \psi_{nk}|}$$

$$|\psi_{nk}\rangle\langle\psi_{nk}| u_{\vec{t}} = e^{+ik\cdot\vec{t}} |\psi_{nk}\rangle\langle\psi_{nk}|$$

$$= u_t^\dagger |\psi_{nk}\rangle\langle\psi_{nk}|$$

$$u_t H_{mk', nk} = |\psi_{mk'}\rangle\langle\psi_{mk'}| u_t^\dagger H |\psi_{nk}\rangle\langle\psi_{nk}|$$

$$= |\psi_{mk'}\rangle\langle\psi_{mk'}| H U_t^\dagger |\psi_{nk}\rangle\langle\psi_{nk}|$$

$$= |\psi_{mk'}\rangle \boxed{\langle\psi_{mk'}| H |\psi_{nk}\rangle} \langle\psi_{nk}| U_t$$

$$H = \frac{p^2}{2m} + V(x)$$

$$U_L = 1 \Rightarrow k = \frac{2\pi n}{L}$$

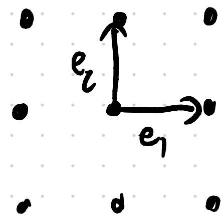
$$H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$$

$$e^{ik\cdot r} u_{nk}(r) = \psi_{nk}(r)$$

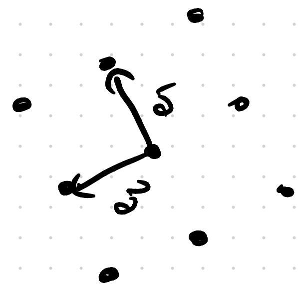
$$\left[e^{-ik\cdot r} H e^{+ik\cdot r}\right] u_{nk}(r) = E_{nk} u_{nk}(r) \leftarrow$$ k.p perturbation

$$\bar{G} = G/T$$

We wat to put $\underline{T}$ and $\underline{\bar{G}}$ together to get a G



Not every T is compatible w/ every $\bar{G}$



$$\bar{G} = G/T$$

$$R \in \bar{G} \qquad R\vec{t} \in T$$

6 families (some have different centerings)

→ 14 classes of Bravais lattice

Say we have T and a compatible pt group $\bar{G}$ $\quad \bar{G} = G/T$

$$G = T \cup T\{R_1|\vec{d}_1\} \cup T\{R_2|\vec{d}_2\} \cup \dots \cup T\{R_{n-1}|\vec{d}_{n-1}\}$$

$$\bar{G} \cong \{E, R_1, \dots, R_{n-1}\}$$

One way to put $\bar{G}$ and T together - semidirect product

$$G = T \rtimes \bar{G} = T\bar{G} = \{ \{E|\vec{t}\}\{R|\vec{0}\} \mid \vec{t} \in T, R \in \bar{G} \}$$

73 space groups that can be built as semidirect products $\rightarrow$ Symmorphic space groups

$\bar{G} < G$ for symmorphic groups

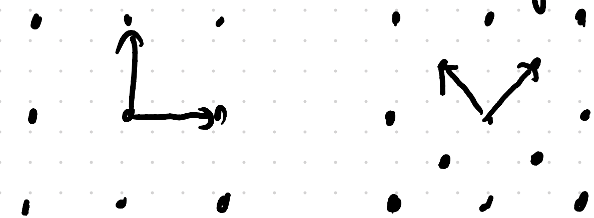
$\bar{G} \ni \{R|\vec{0}\} \in T \rtimes \bar{G}$

Notation for symmorphic groups:

[Letter][Hermann - Maugin symbol for pt group]

tells us
Bravais lattice
centering

Example of centering:



Primitive Face centered

Ex: Pmm2

Primitive

orthorhombic

point group 2mm
ordered to show us
that the twofold rotation
axis is along z

$$mm2 = \{E, C_{2z}, M_x, M_y\}$$

$\vec{e}_1 = (a, 0, 0)$

$\vec{e}_2 = (0, b, 0)$ $\qquad a \neq b \neq c$

$\vec{e}_3 = (0, 0, c)$

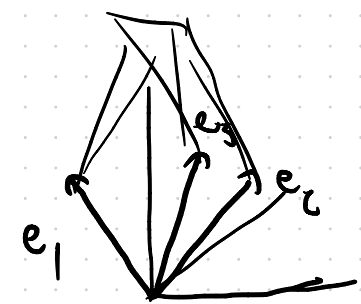
Ex: $R\bar{3}m$ — point group $\bar{3}m = \langle C_{3\hat{z}}, M_x, I \rangle$

rhombohedral

$\vec{e}_1 = (0, -a, c)$

$\vec{e}_2 = \frac{1}{2}(a\sqrt{3}, a, 2c)$

$\vec{e}_3 = \frac{1}{2}(-a\sqrt{3}, a, 2c)$



Symmorphic space groups: $G = \underset{\substack{\uparrow \\ \text{translations}}}{T} \rtimes \bar{G}$ ← rotations/reflections

Most space groups are not symmorphic

Nonsymmorphic space groups: $G = T \not\rtimes \bar{G}$

What does this mean

$$G = T \cup T\{R_1|\vec{d}_1\} \cup T\{R_2|\vec{d}_2\} \cup \dots T\{R_{n-1}|\vec{d}_{n-1}\}$$

$$\bar{G} = \{E, R_1, \dots, R_{n-1}\}$$

if G is not symmorphic at least one $\vec{d}_i$ has to be a <u>fractional translation</u>.

In most cases: G is nonsymmorphic b/c it contains <u>screw rotation</u> or <u>glide reflection</u>

Screw rotation: $\{C_{n\hat{r}} | \vec{d}\}$ where $\vec{d}$ has a component along $\vec{r}$ that's a fraction of a lattice vector

$\vec{d} \cdot \hat{r} = \frac{l}{n} \vec{e}$

denoted n_l

$(n_l)^n$ - a translation by l primitive lattice vectors along $\hat{r}$ $l < n$

$\vec{e}_3 = (0,0,c)$

Ex:

$2_1 \quad \{C_{2z} \mid \tfrac{1}{2}\vec{e}_3\} \qquad \{C_{2z} \mid \tfrac{1}{2}e_3\}^2 = \{E \mid \vec{e}_3\}$

$$(x,y,z) \to (-x,-y,z+\tfrac{1}{2})$$

$3_1 = \{C_{3z} \mid \tfrac{1}{3}\vec{e}_3\} \qquad (3_1)^3 = \{E \mid \vec{e}_3\}$

$3_2 = \{C_{3z} \mid \tfrac{2}{3}\vec{e}_3\} \qquad (3_2)^3 = \{E \mid 2\vec{e}_3\}$

$4_1, 4_2, 4_3, \quad 6_1, 6_2, 6_3, 6_4, 6_5$

$$2_3 = \{C_{2z} | \tfrac{3}{2}\vec{e}_3\} = \{E|\vec{e}_3\}\{C_{2z}|\tfrac{1}{2}\vec{e}_3\}$$

$$= \{E|\vec{e}_3\}(2_1)$$

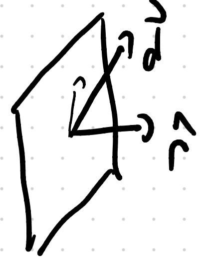
$$\text{"}2_2\text{"} = \{C_{2z}|\vec{e}_3\}$$

$$\{C_{nz}|\alpha\hat{z}\}^n = \{E|n\alpha\hat{z}\}$$

$$n\alpha\hat{z} \in T$$

Glide reflections: mirror reflections + a translation not orthogonal to the mirror plane

$$\{m_{\hat{n}}|\vec{d}\}$$



$\vec{d} \times \hat{r} \neq 0$

$$\{M_{\hat{r}} | \vec{d}\}^2 = \{E | \vec{d} + M_{\hat{r}} \vec{d}\} \in T$$

$\vec{e}_1 = (a, 0, 0)$

Component of $\vec{d}$ in the mirror plane is half a lattice vector

$$g = \{M_{\hat{z}} | \tfrac{1}{2}\vec{e}_1\}$$

$$g: (x, y, z) \to (x + \tfrac{a}{2}, y, -z)$$

$$g^2 = \{E | \vec{e}_1\}$$

Symbol for glide symmetry

M - mirror (not a glide)

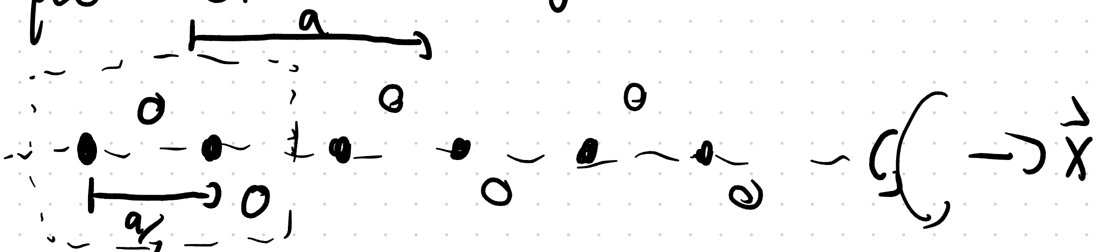
a, b, c - glide w/ translation along cartesian direction

n - glide w/ translation along face

d - glide w/ translation along diagonal

e - multiple glides w/ same mirror plane

Example: Quasi-1D system

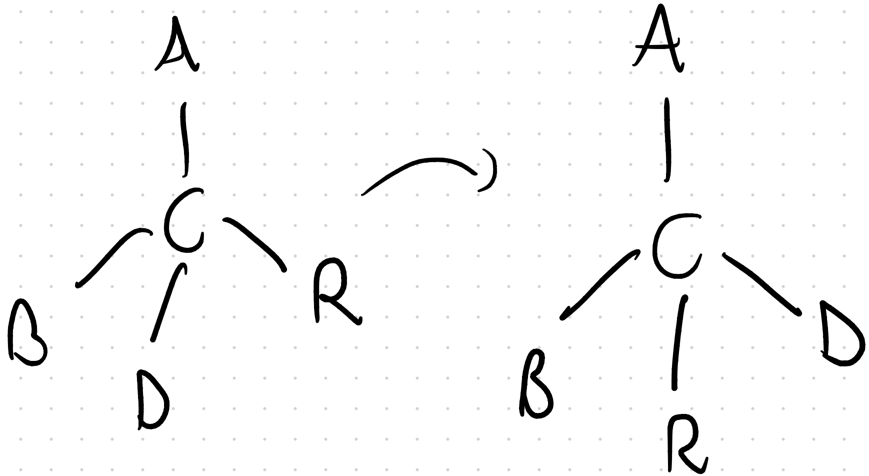


$$T = \{\{E \mid n a \hat{x}\} \mid n \in \mathbb{Z}\}$$

$\{M_y \mid \frac{a}{2}\hat{x}\}$ - "a" type glide

$$G = T \cup T\{M_y \mid \tfrac{a}{2}\hat{x}\} = Pa$$

157 nonsymmorphic space groups
+
73 symmorphic $\rightarrow$ 230 space groups



Base

$$G/T = \bar{G}$$

Face centered orthorhombic

$$\vec{e}_1 = \frac{1}{2}(a, b, 0)$$
$$\vec{e}_2 = \frac{1}{2}(a, -b, 0)$$
$$\vec{e}_3 = (0, 0, c)$$

$a = b = c$