Lecture 7

Reminder: HW 1 due thursday 2/13 on gradescope

Recap: Space group $G < \mathbb{E}(3)$ rigid symmetries of a crystal

$$V(\vec{x}) = V(g^{-1}\vec{x}) \text{ for all } g \in G$$

Every space group contains a Bravais lattice $T \trianglelefteq G$

$$T = \left\{ \{E \mid \textstyle\sum_i n_i \vec{e}_i\}, n_i \in \mathbb{Z} \right\}$$

$\vec{e}_1, \vec{e}_2, \vec{e}_3$ - primitive lattice vectors

Irreps of T : 1D irreps $\rho_{\vec{k}}(\{E|\vec{t}\}) = e^{-i\vec{k}\cdot\vec{t}}$

$\vec{b}_i$ – primitive reciprocal lattice vectors $\vec{b}_i \cdot \vec{e}_j = 2\pi\delta_{ij}$

$\vec{k} = \sum_i \alpha_i \vec{b}_i \quad \alpha_i \in (-\frac{1}{2}, \frac{1}{2}]$ – 1st Brillouin Zone

Schur's Lemma → Blochs theorem

$$[H, e^{-i\vec{p}\cdot\vec{t}/\hbar}] = 0 \quad \Rightarrow$$

$$H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$$ n – "band index"

$$e^{-i\vec{p}\cdot\vec{t}/\hbar}|\psi_{nk}\rangle = e^{-i\vec{k}\cdot\vec{t}}|\psi_{n\vec{k}}\rangle$$ $\hbar\vec{k}$ – "crystal momentum"

What other transformations $g = \{R|\vec{d}\} \in E(3)$ can appear in a space group

Recall: $T \trianglelefteq G$, every (pure) translation $\{E|\vec{t}\} \in G$ should be in the Bravais lattice

Suppose $g = \{R|\vec{d}\} \in G$ $\quad G \ni g^{-1} = \{R^{-1}|-R^{-1}\vec{d}\}$

$\{E|t\} \in T$ a Bravais lattice translation

$T \trianglelefteq G \Rightarrow g\{E|\vec{t}\}g^{-1} \in T$

$$\left(\{R|\vec{d}\}\{E|\vec{t}\}\right)\{R^{-1}|-R^{-1}\vec{d}\} = \{R|\vec{d}+R\vec{t}\}\{R^{-1}|-R^{-1}\vec{d}\}$$
$$= \{E|\vec{d}+R\vec{t}-\vec{d}\}$$
$$= \{E|R\vec{t}\} \in T$$

if $g = \{R|\vec{d}\} \in G$ then $R\vec{t} \in T$ for every $\vec{t} \in T$

Consider the following homomorphism

$$\varphi(\{R|\vec{d}\}) = R \in O(3) \qquad \varphi: G \to O(3)$$

$$\ker\varphi = \{\{E|\vec{t}\} \in G\} \in T$$

$O(3) > \operatorname{Im}\varphi = \{ R \mid \{R|\vec{d}\} \in G \} \underset{\substack{\uparrow \\ \text{1st isomorphism} \\ \text{theorem}}}{\cong} G/T =: \bar{G}$ ← point group of G

$\bar{G} < O(3)$ all the rotations and reflection parts of space group elements

$$R \in \bar{G} \Rightarrow R\vec{t} \in T \text{ for all } \vec{t} \in T$$

Important result: <u>Crystallographic Restriction Theorem</u>

let T be a Bravais lattice, $R \in SO(3)$ a rotation

if $R\vec{t} \in T$ for all $\vec{t} \in T$ then:

R is a rotation by either 0° 180° $\pm 120^\circ$ $\pm 90^\circ$ $\pm 60^\circ$

0 π $\pm\frac{2\pi}{3}$ $\pm\frac{\pi}{2}$ $\pm\frac{\pi}{3}$

(1-fold) (twofold) (threefold) (fourfold) (sixfold)

Pf: Pick a basis $\underbrace{\vec{e}_1, \vec{e}_2, \vec{e}_3}_{\in T}$ of primitive lattice vectors

$$R\vec{e}_i = \sum_j \vec{e}_j n_{ji} \in T \qquad n_{ji} \in \mathbb{Z}$$

$\vec{b}_1, \vec{b}_2, \vec{b}_3$ be primitive reciprocal lattice vectors

$$R_{ji} = \frac{1}{2\pi} \vec{b}_j \cdot (R\vec{e}_j) = n_{ji}$$

R_{ji} is a 3×3 matrix of integers

Matrix elements of R in the basis of primitive lattice vectors

$$(\hat{x}, \hat{y}, \hat{z}) \xrightarrow{V} (\vec{e}_1, e_2, e_3)$$

$$(\hat{x}, \hat{y}, \hat{z}) \xrightarrow{V^{-1}} (\vec{b}_1, \vec{b}_2, \vec{b}_3) \frac{1}{2\pi}$$

$$R_{ij} = VRV^{-1}$$

1. $\mathrm{tr}\, R = \sum_i R_{ii} = \sum_i n_{ii} \in \mathbb{Z}$

2. in a basis aligned with the axis of rotation

$$[R] = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

θ is the angle of rotation of R

$$\operatorname{tr} R = 1 + 2\cos\theta$$

$\Rightarrow$ $1 + 2\cos\theta \in \mathbb{Z}$ must be an integer

$\Rightarrow$ $2\cos\theta \in \mathbb{Z}$

$\cos\theta = 0, \pm\frac{1}{2}, \pm 1$

$$\boxed{\theta = \pm\frac{\pi}{2},\ \pm\frac{\pi}{3} \text{ or } \pm\frac{2\pi}{3},\ 0,\ \pi}$$

crystallographic point groups

There are only 32 subgroups of $O(3)$ consistent with this theorem [10 are also pt groups of

2D lattices]

Group	Hermann-Maugin notation	Schönflies notation
trivial group $\{E\}$	1	C_1
$\langle C_{2z} \rangle$	2	C_2
$\langle C_{3\hat{z}} \rangle$	3	C_3
$\langle C_{4\hat{z}} \rangle$	4	C_4
$\langle C_{6\hat{z}} \rangle$	6	C_6

$C_{n\hat{r}}$ - rotation by angle $\frac{2\pi}{n}$ about axis $\hat{r}$

$$(C_{n\hat{r}})^n = E$$

$\langle \ldots \rangle$ - group generated by ...

we can also look @ point groups w/ reflection symmetries (mirror symmetries)

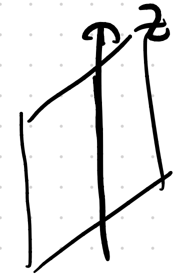
$M_{\hat{n}}$ - reflection about a plane normal to $\hat{n}$

Ex: $M_x : (x,y,z) \to (-x,y,z)$

$M_y : (x,y,z) \to (x,-y,z)$

$M_z : (x,y,z) \to (x,y,-z)$

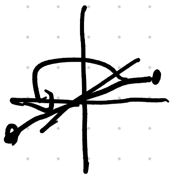
$\langle M_x \rangle$	m	C_s
$\langle C_{2z}, M_x \rangle$	$2mm$	C_{2v} ← 'vertical'
$\langle C_{3z}, M_x \rangle$	$3m$	C_{3v}
$\langle C_{4z}, M_x \rangle$	$4mm$	C_{4v}
$\langle C_{6z}, M_x \rangle$	$6mm$	C_{6v}



\# of m's = \# of conjugacy classes of mirror reflections

Ex: $2mm$ and $3m$

$2mm: \langle C_{2z}, M_x \rangle = \{E, C_{2z}, M_x, C_{2z}M_x = M_y\}$



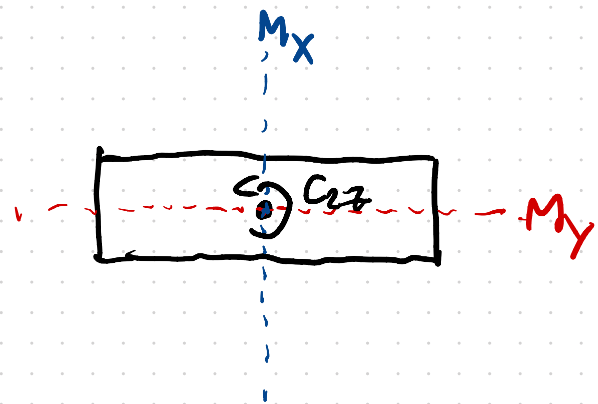
$C_{2z}: (x,y) \to (-x,-y)$

$M_x: (x,y) \to (-x,y)$

$C_{2z}M_x: (x,y) \to (x,-y)$

$\quad = M_y$

Symmetry of a rectangle



$M_x M_y = C_{2z}$

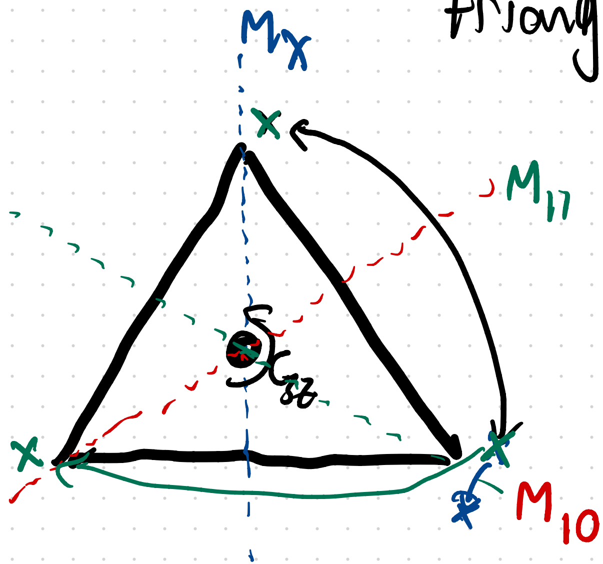
$C_{2z} M_x C_{2z}^{-1} = M_x$

$C_{2z} M_y C_{2z}^{-1} = M_y$

$M_x M_y = M_y M_x$

So M_x and M_y are not conjugate in $2mm$

$3m$: $\langle C_{3z}, M_x \rangle$ - Symmetry group of an equilateral triangle



$$C_{3z} M_{10} = M_{11}$$

$$C_{3z} M_{11} = M_x$$

$$C_{3z} M_x = M_{10}$$

$$C_{3z} M_{10} C_{3z}^{-1} = M_{11} C_{3z}^{-1} = M_x$$

$C_{3z} M_x C_{3z}^{-1} = M_{11}$ $\rightarrow$ all 3 mirror reflections are conjugate in 3_m

Heuristic: multiplying a vertical mirror by $C_{n\hat{z}}$ rotates the mirror plane by $\frac{\pi}{n}$

conjugating rotates mirror plane by $\frac{2\pi}{n}$

Other 22 pt groups in 3D:

- horizontal mirror planes
- multiple noncollinear rotation axes (D_2)
- Inversion symmetry

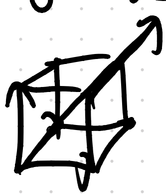
$I: (x, y, z) \to (-x, -y, -z)$

$I \in O(3)$ but not $SO(3)$

C_{nh}: groups w/ horizontal mirrors

D_n: dihedral - grps w/ orthogonal rotation axes

Cubic symmetry groups



$C_{3,(1)}$

$\bar{1} - \langle I \rangle$

$\bar{4} - \langle IC_{4z} \rangle$

$\bar{3} - \langle IC_{3z} \rangle$

$\bar{6} - \langle IC_{6z} \rangle$

https://cryst.ehu.es for full detail on all 22 groups

$$\{E, C_{5z}, C_{5z}^2, C_{5z}^3, C_{5z}^4\}$$