Lecture 7

Reminders: HW 1 Due Thursday 9/19

Office Hrs tomorrow 4-5pm

Recap: Introduced space group $G < \mathbb{E}(3)$ - rigid symmetries of crystals

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

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

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

$\{\vec{e}_i\}$ - primitive lattice vectors

Irreducible representations of T

1D: $e_{\vec{k}}(\{E|\vec{t}\}) = e^{-i\vec{k}\cdot\vec{t}}$ $\quad\vec{k}$ - crystal momentum

$\vec{k} = \sum_i \alpha_i \vec{b}_i \qquad \{\vec{b}_i\}$ primitive reciprocal lattice vectors $\quad \vec{b}_i \cdot \vec{e}_j = 2\pi\delta_{ij}$

$\alpha_i \in \left(-\frac{1}{2}, \frac{1}{2}\right]$

Schur's Lemma $\Rightarrow$ Bloch's theorem

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

$\rightarrow \quad H|\psi_{n\vec{k}}\rangle = E_{n\vec{k}}|\psi_{n\vec{k}}\rangle \qquad n$ - "band index"

$$e^{-i\frac{\vec{p}}{\hbar}\cdot\vec{t}}|\psi_{n\vec{k}}\rangle = e^{-i\vec{k}\cdot\vec{t}}|\psi_{n\vec{k}}\rangle$$

" $\hbar k$ is momentum "

What about other rigid transformations?

What transformations (besides $\vec{t} \in T$) can appear in a space group

Recall: $T \trianglelefteq G$ is a normal subgroup, and every translation symmetry of a space grp should be in the Bravais lattice

$$\psi_{nk}(\vec{r}) = e^{i k \cdot \vec{r}} u_{nk}(r)$$

$$u_{nk}(r + \vec{t}) = u_{nk}(\vec{r})$$

$$u_{nk}(r) = \sum_G u_{nk}(\vec{G}) e^{i \vec{G} \cdot \vec{r}}$$

$\hbar k$ momentum mod $\vec{G}$

$\vec{G}$ - reciprocal lattice vector

$$\varphi_k(r) = e^{-i \vec{k} \cdot \vec{r}}$$

$$\boxed{\psi_{nk}(r)} = \sum_G u_{nk}(\vec{G}) e^{i(\vec{k} + \vec{G}) \cdot \vec{r}}$$

$$P(p = \hbar(\vec{k} + \vec{G})) = |u_{nk}(G)|^2$$

$$g = \{R | \vec{d}\} \in E(3) \qquad g^{-1} = \{R^{-1} | -R^{-1}\vec{d}\}$$

$$\{E|\vec{t}\} \in T$$

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

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

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

if $g \in G \Rightarrow R\vec{t} \in T$ for every $\vec{t} \in T$

Consider the following homomorphism

$$\varphi(\{R|\vec{d}\}) = R \in O(3)$$

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

$$\operatorname{Im} \varphi = \{R \mid \{R|\vec{d}\} \in G\} \underbrace{\cong}_{\text{1st Isomorphism thm}} G/T = \underset{\text{point group of } G}{\bar{G}}$$

$\bar{G} < O(3)$ - all the rotation/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, and $R \in SO(3)$ be a rotation. Then if R is a symmetry of T ($R\vec{t} \in T$ for all $\vec{t} \in T$)

then R is a rotation by either

$$0^\circ \quad 180^\circ \quad \pm 120^\circ, \quad \pm 90^\circ \quad \text{or} \quad \pm 60^\circ$$

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

Pf: Lets pick a basis $\vec{e}_1, \vec{e}_2, \vec{e}_3$ of primitive lattice vectors

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

$\vec{b}_1, \vec{b}_2, \vec{b}_3$ - primitive reciprocal lattice vector

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

R_{ji} is a 3x3 matrix of integers — matrix of R expressed in the basis

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

$(\hat{x}, \hat{y}, \hat{z}) \xrightarrow{V} (\vec{e}_1, \vec{e}_2, \vec{e}_3)$

② in a basis aligned w/ the axis of rotation

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

$R_{ji} = V R V^{-1}$

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

$\Rightarrow \mathrm{tr}\, R = 1 + 2\cos\theta$ $\quad\theta$ — angle of rotation of R

① + ② $\Rightarrow$ $1 + 2\cos\theta \in \mathbb{Z}$

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

$\theta = \pm\frac{\pi}{2}, \ \pm\frac{\pi}{3}, \pm\frac{2\pi}{3} \ \ \{0, \pi\}$ $\blacksquare$

There are 32 subgroups of $O(3)$ consistent w/ this theorem [10 are actually also pt groups of 2D lattices]

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

$\langle C_{6\hat{z}} \rangle$	1	6	C_6

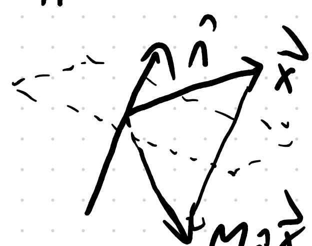
$C_{n\hat{r}}$ - rotation by angle $\frac{2\pi}{n}$ about axis $\hat{r}$

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

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

We can also add reflection symmetries (mirror symmetries)

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

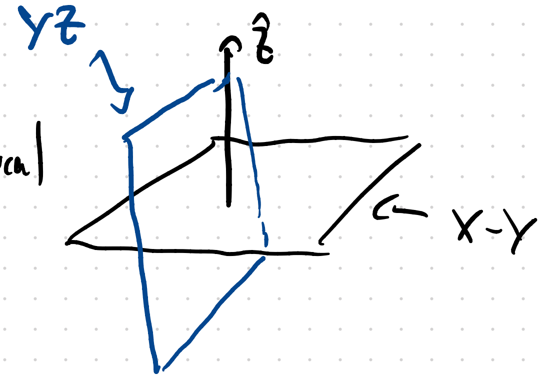


Ex: $M_x : (x, y, z) \to (-x, y, z)$

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

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

$\langle M_x \rangle$	m	C_s
$\langle C_{2\hat{z}}, M_x \rangle$	$2mm$	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 is the # of conjugacy classes of mirror reflections

$C_2 \cong C_s \cong \mathbb{Z}_2$

$\{E, C_{2\hat{z}}\}$ $\qquad$ $\{E, M_{\hat{x}}\}$

$\widehat{SO(3)}$ $\widehat{SO(3)}$

Same as abstract groups
different as subgroups of $E(3)$

Exs: 2mm and 3m

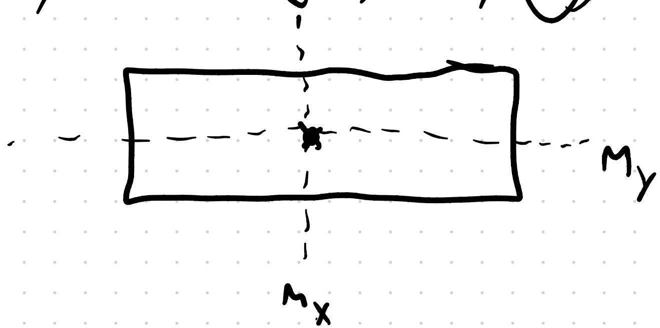
$\downarrow$

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

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

$\downarrow$

$M_y (x, y, z) = (+x, -y, z)$



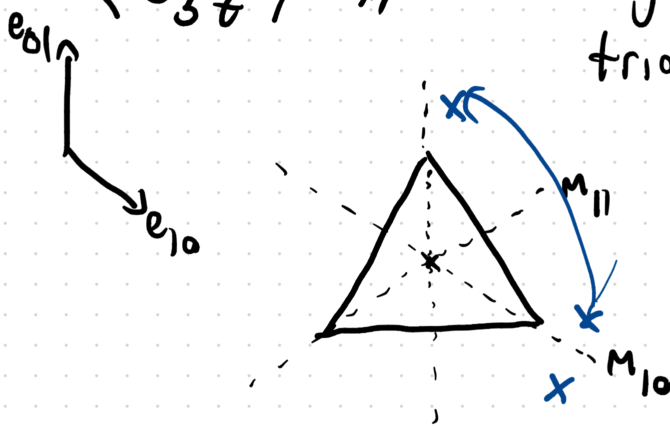
Symmetries of a rectangle

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

m_x and m_y are not conjugate

$3m$ $\langle C_{3z}, m_x \rangle$

Symmetries of an equilateral triangle



$m_x = M_{01}$

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

$$C_{3z} M_{11} = M_{01}$$

$$C_{3z} M_{01} = M_{10}$$

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

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

$C_{nz} m C_{nz}^{-1}$ rotates the mirror plane by $\frac{2\pi}{n}$

Other 22 pt groups:

- horizontal mirror planes
- multiple noncollinear rotation axes
- Inversion Symmetry

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

https://cryst.ehu.es

Bilbao Crystallographic Server

↑

Pt group tables for remaining 22 groups

↳

C_{nh}: grps w/ horizontal mirrors

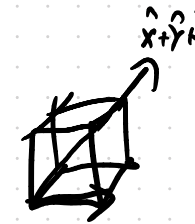
D: dihedral groups 2 orthogonal rotation axes

$\bar{4}$ - IC_{4z} - S_4

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

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

C_{2x}, $C_{3,111}$



Cubic groups

23	T	symmetries of tetrahedra
$m\bar{3}$	T_h	
$\bar{4}3m$	T_d	
432	O	symmetries of octahedra
$m\bar{3}m$	O_h	