Lecture 7

Reminder: HW 1 is due 9/18 11:59pm

· Derek's office hrs tomorrow 3pm

Recap: Space groups $G < E(3)$ rigid symmetries of crystals

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

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

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

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

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

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

"crystal momentum" $\rightsquigarrow \vec{k} = \sum_i \alpha_i \vec{b}_i \quad \alpha_i \in \left(-\frac{1}{2}, \frac{1}{2}\right]$ - 1st Brillouin zone

On electronic wavefunctions $U_t = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{t}} \qquad \vec{p} = -i\frac{\partial}{\partial \vec{x}}$

Hamiltonian invariant under translations $[H, U_t] = 0$ for all $\vec{t} \in T$

So say we find $|\varphi_{\vec{k}}\rangle$, $|\phi_{\vec{k}'}\rangle$

transforming in $\rho_{\vec{k}}$ $\rho_{\vec{k}'}$

Schur's lemma: $\langle \varphi_{\vec{k}} | H | \phi_{\vec{k}'} \rangle = 0$ if k and k'

label different irreps

$\rightarrow$ We can diagonalize H by finding translation eigenstates

Bloch's Theorem
$$\begin{cases} \mathcal{U}_{\vec{t}}\,|\psi_{n\vec{k}}\rangle = e^{-i\vec{k}\cdot t}\,|\psi_{nk}\rangle \quad ① \leftarrow \text{transform in the irrep } \rho_{\vec{k}} \text{ of } T \\ H|\psi_{nk}\rangle = E_{nk}\,|\psi_{nk}\rangle \quad ② \end{cases}$$

$$\langle \vec{r}\,|\psi_{nk}\rangle = \psi_{nk}(\vec{r})$$

$$① : \langle \vec{r}\,|\mathcal{U}_{\vec{t}}\,|\psi_{nk}\rangle = \psi_{nk}(\vec{r}-\vec{t}) = e^{-i\vec{k}\cdot\vec{t}}\,\psi_{nk}(\vec{r})$$

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

$u_{nk}(\vec{r}-t) = u_{nk}(\vec{r})$ is periodic

(2) $H\psi_{nk}(r) = E_{nk}\psi_{nk}(r)$

What other transformations $g = \{R|\vec{d}\}$ can appear in G

$E(3)$

Remember $T \trianglelefteq G$ every pure translation $\{E|\vec{t}\} \in G$

should be in T

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

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

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

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

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

$\{R_1|\vec{d}_1\}\{R_2|\vec{d}_2\}$

$= \{R_1R_2|\vec{d}_1 + R_1\vec{d}_2\}$

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

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

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

$O(3) > \mathrm{Im}\,\varphi = \{ R \mid \{R|\vec{d}\} \in G \}$

1st Isomorphism theorem $\quad G/T \cong \mathrm{Im}\,\varphi = \bar{G} \leftarrow$ point group of G

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

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

Important result: Crystallographic Restriction Theorem

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

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

R is a rotation by either

$0°$,	$180°$,	$\pm 120°$,	$\pm 90°$,	$\pm 60°$
0	π,	$\pm \frac{2\pi}{3}$,	$\pm \frac{\pi}{2}$,	$\pm \frac{\pi}{3}$
1-fold	2-fold	3fold	fourfold	sixfold

Proof: let's pick primitive lattice vectors $\vec{e}_1, \vec{e}_2, \vec{e}_3$

let's pick primitive reciprocal lattice vector $\vec{b}_1, \vec{b}_2, \vec{b}_3$ $\quad \vec{b}_i \cdot \vec{e}_j = 2\pi \delta_{ij}$

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

$$n_{ji} = (\vec{b}_j \cdot R\vec{e}_i)\frac{1}{2\pi} \equiv R_{ji}$$ is a 3×3 matrix of integers

matrix elements of R in the primitive lattice basis

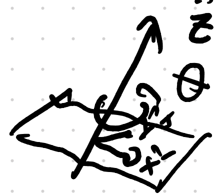
$(\hat{x},\hat{y},\hat{z}) \xrightarrow{V} (\vec{e}_1,\vec{e}_2,\vec{e}_3)$ V - change of Basis

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

$$R_{ij} = V\underbrace{[R]}_{\text{cartesian basis}}V^{-1} \rightarrow \sum_i R_{ii} = \mathrm{tr}[R]$$

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

② if we go to a basis aligned w/ the axis of rotation



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

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

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

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

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

$0 \to \theta = \pm\frac{\pi}{2}$; $\pm\frac{1}{2} \to \pm\frac{\pi}{6}$ or $\pm\frac{2\pi}{3}$

$\rightarrow$ There are only 32 subgroups of $O(3)$ consistent w/ this theorem [10 are point groups of 2-D lattices]

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

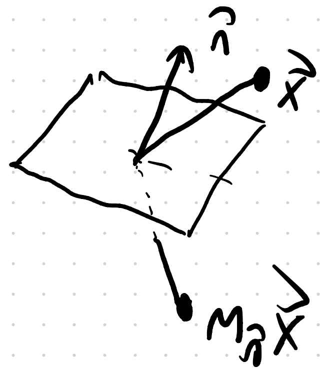
$C_{n\hat{r}}$ - rotation by angle $\frac{2\pi}{n}$ about axis $\hat{r}$

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

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

We can also look at groups w/ reflection symmetries (mirror)

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



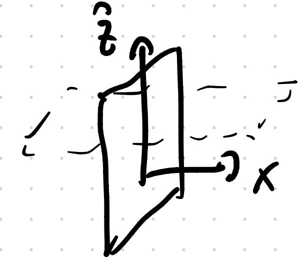
$M_x : (x, y, z) \to (-x, y, z)$

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

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

$\langle M_x \rangle$	M	C_s

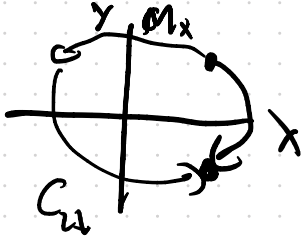
$\langle C_{2z}, M_x \rangle$	$2mm$	C_{2v}	"vertical"
$\langle C_{3z}, M_x \rangle$	$3m$	C_{3v}	
$\langle C_{4z}, M_x \rangle$	$4mm$	C_{4v}	
$\langle C_{6z}, M_x \rangle$	$6mm$	C_{6v}	

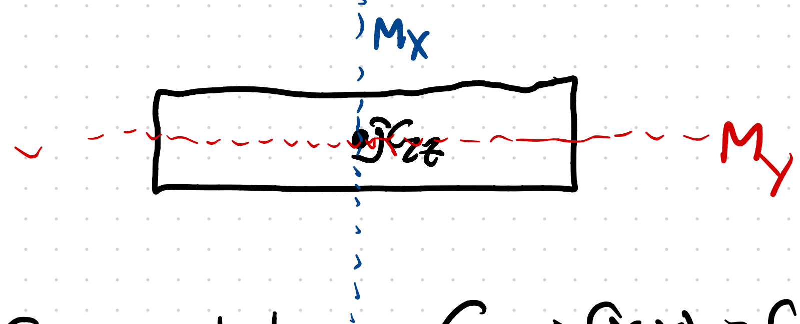


#'s of m's : # of conjugacy classes of reflections

Ex: $2mm$ and $3m$

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





$C_{2z} = M_x M_y$

Group is abelian

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

$M_y = C_{2z} M_x$

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

$M_x = C_{2z} M_y$

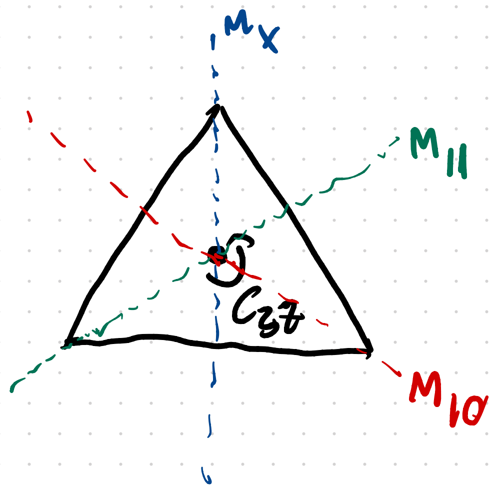
$M_y: (x,y) \to (x,-y)$

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

$M_x M_y M_x^{-1} = M_y$

M_x and M_y are not conjugate to each other in 2mm

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



This group is **not** abelian