Lecture 8

HW1 Due tonight
HW2 will be posted → due 10/2

Reminder: trying to build space groups G

(1) $T \trianglelefteq G$ T is the Bravais lattice

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

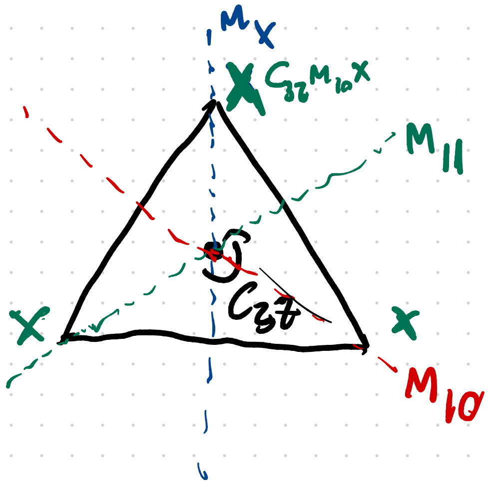
$\bar{G} = \{ R \mid \{R|\vec{d}\} \in G \} < O(3)$

(2) if R is a rotation in $\bar{G}$ then

R must be a rotation by an angle
$0, \pm\frac{\pi}{3}, \pm\frac{\pi}{2}, \pm\frac{2\pi}{3}$ or π

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

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



This group is not abelian

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

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

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

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

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

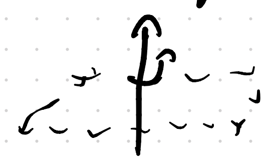
$\rightarrow$ All 3 mirror reflections are conjugate in $3m$

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

— conjugating a vertical mirror by $C_{n\hat{z}}$ rotates the mirror plane by $\frac{2\pi}{n}$

Other 22 groups:

- Horizontal mirror planes



- multiple non-parallel rotation axes (ex: D_2)

- Inversion symmetry

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

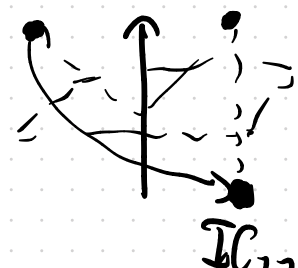
$I \in O(3)$ but not $SO(3)$

C_{nh}: 1 rotation axis, horizontal mirror

D_n: dihedral groups w/ orthogonal rotation axes

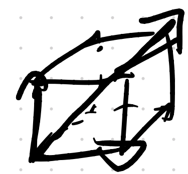
Hermann-Maugin

rotoinversions $\begin{cases} \langle I \rangle & \bar{1} \\ \langle IC_{4z} \rangle & \bar{4} \quad \text{"}-4\text{"} \end{cases}$



$$\begin{cases} \langle I C_{3z} \rangle & \bar{3} \quad \text{"-3"} \\ \langle I C_{6z} \rangle & \bar{6} \\ \langle I C_{2z} = M_z \rangle & m \end{cases}$$

Cubic groups



https://cryst.ehu.es for full pt group details

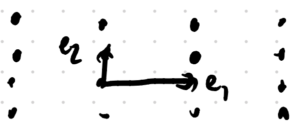
Ex: $4mm$ $\quad 4/\text{m}mm$

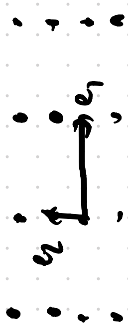
$\langle C_{4z}, M_x, M_{x+y}, M_y,$ $\quad$ $4mm \cup (4mm) M_z$

$M_{x-y}, C_{2z}, C_{4z}^{-1}, E \rangle$

$C_{2z} \cdot M_z = I$

We want to combine T and $\bar{G}$ to get G





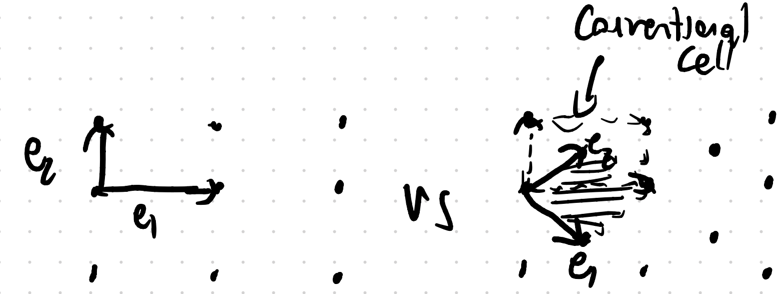
Not every choice of T is compatible w/ every $\bar{G}$

$T \trianglelefteq G$

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

6 families of Bravais lattices

→ 14 Bravais lattices



Primitive Face centered

Same point group $2mm$

One way to put $\bar{G}$ and T together:

Semidirect product

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

73 space groups can be written as semidirect products

"Symmorphic space groups"

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

$i : \bar{G} \to G$

$i(R) = \{R | \vec{0}\}$

Notation for symmorphic space group

[letter][Hermann-Mauguin symbol for pt group]

centering of Bravais

point group

lattice

P - primitive

I - body-centered

F - face centered

⋮

Example: $P\,mm2$

point group 2mm

ordering tells us z-axis is rotation axis

primitive

primitive orthorhombic Bravais lattice

Lattice vectors

Bradley & Cracknell Table 3.1

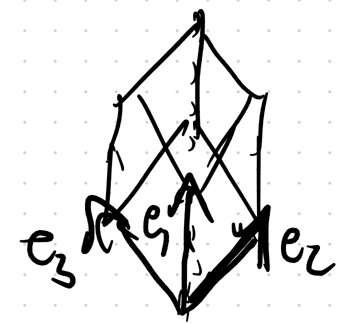
$\vec{e}_1 = (a, 0, 0)$ $\quad a \neq b \neq c$

$\vec{e}_2 = (0, b, 0)$ $\quad C_{2z}, m_x, m_y$

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

Ex: $R\bar{3}m \longrightarrow \bar{3}m = \langle C_{3z}I, I, C_{3z}, m_x \rangle$

Rhombohedral



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

$\vec{e}_2 = \frac{1}{2}(a\sqrt{3}, a, 2c)$ $\quad e_3 = \frac{1}{2}(-a\sqrt{3}, a, 2c)$

Most space groups are not symmorphic

"Nonsymmorphic" space groups $G \neq T \rtimes \bar{G}$

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

$$\bar{G} = \{E, R_1, R_2, \dots R_{n-1}\}$$

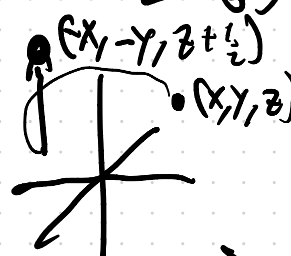
$G \neq T \rtimes \bar{G} \rightarrow$ at least one $\vec{d}_i$ must not be a Bravais lattice vector $\rightarrow$ $\vec{d}_i \notin T$ is fractional

In most cases, G is nonsymmorphic because it contains either a screw rotation or a glide reflection

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

$$2_1 \to \{C_{2z} \,|\, \tfrac{1}{2}\vec{e}_3\}$$

Ex: $\vec{e}_1 = (a, 0, 0)$
$\vec{e}_2 = (0, b, 0)$
$\vec{e}_3 = (0, 0, c)$



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

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

Denoted in Hermann Maugin notation n_l

order of the rotation

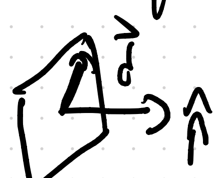
$(n_l)^n$ is a translation by l primitive lattice vectors

3_1: $\{C_{3z} | \frac{1}{3}\vec{e}_3\}$

3_2: $\{C_{3z} | \frac{2}{3}\vec{e}_3\}$

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

Glide reflection: mirror reflection + a translation within the mirror plane

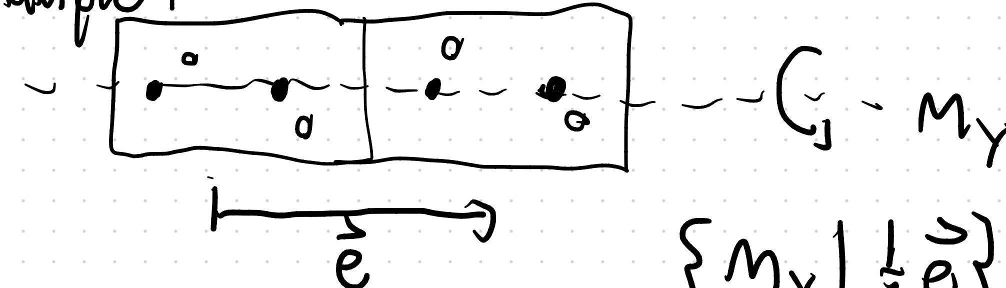


$(\{M_{\hat{n}} | \vec{d}\})$

$$\{m_r | \vec{d}\}^2 = \{E | 2\vec{d}\}$$

$\vec{d}$ - half a Bravais lattice vector

Example 1



"Pa"

$\{m_y | \frac{1}{2}\vec{e}\}$ is a symmetry

Hermann Maugin notation: m - mirror

a, b, c - translation is along a cartesian direction

n - translation along a face

Notation for nonsymmorphic space groups

[letter] [H-M for point group w/ subscripts for screw rotations alternative letters for glides]

d - translation along body diagonal

e - distinguishes between multiple glides

157 nonsymmorphic space groups
+
73 symmorphic space groups

230 space groups