Lecture 3

14 possible Bravais lattices in 3D (T)

32 possible point groups in 3D compatible w/ these ($\bar{G}$)

Today: How do we put together T and $\bar{G}$ to get a space group G

What do we know about G? (3d)

① $G \subset \mathbb{E}(3) = \mathbb{R}^3 \rtimes O(3)$ (The space grp is a subgroup of Euclidean grp)

② $T \subset G$ (Bravais lattice is a subgroup of the space group

Some group theory background

- Let G be a group, and let $H \subset G$ be a subgroup

Lets define a <u>right coset</u> Hg $g \in G$

$$Hg = \{hg, h \in H\}$$

Given any subgroup H, the right cosets of H partition G

→ given any $g' \in G$, g' is in exactly one right coset pf: consider Hg_1, Hg_2, and assume $\exists\, \alpha \in G$ such that $\alpha \in Hg_1$, $\alpha \in Hg_2$

$\Rightarrow \alpha = h_1 g_1$ and $\alpha = h_2 g_2$

$h_1 g_1 = h_2 g_2$

$h_1 = h_2 g_2 g_1^{-1} \Rightarrow g_2 g_1^{-1} \in H$

$\Rightarrow H = H g_2 g_1^{-1} \Rightarrow Hg_1 = Hg_2$

$\rightarrow$ All right cosets are disjoint

→ $G = \overset{E}{H} \cup Hg_1 \cup Hg_2 \cup \cdots \cup Hg_{n-1}$

Coset decomposition of G

$\{g_1, g_2, \cdots g_{n-1}, E\}$ are called coset representatives

→ The number of right cosets is called the <u>index</u> of H in G $\quad |G:H|$

→ $|G:H| = |G|/|H|$ for G a finite group

Ex: $G = \mathbb{Z}$ the group of integers under addition

$H = 3\mathbb{Z}$ the group of multiples of 3 under addition

$H \subset G$

Right cosets $H\emptyset = H + \emptyset = H$

$H1 = H+1 = \{1, 4, 7, 10, \ldots, -2, -5, \ldots\}$

$H2 = H+3 = \{2, 5, 8, 11, \ldots, -1, -4, -7, \ldots\}$

$H3 = H+3 = 3\mathbb{Z} = H$

$G = \mathbb{Z} = H \cup (H+1) \cup (H+2)$

$|G : H| = 3$

Hg ← right cosets

We could repeat everything for left cosets gH

Something special happens for subgroups H where left cosets are equal to right cosets:

A subgroup $H \subset G$ is a <u>normal subgroup</u> if

$$gH = Hg \quad (\text{i.e. if } g^{-1}Hg = H)$$

conjugation

$H \triangleleft G$ - symbol for a normal subgroup

If $H \triangleleft G$, then we can define a group structure on the right cosets Hg:

Hg_1 , Hg_2 lets consider $Hg_1 Hg_2 = \{h_1 g_1 h_2 g_2, h_1, h_2 \in H\}$

if H is a normal subgroup of G

$$g_1 H = Hg_1 \Rightarrow Hg_1 Hg_2 = HHg_1 g_2 = Hg_1 g_2$$

$$G = H \cup Hg_1 \cup Hg_2 \cup \dots \cup Hg_{n-1}$$

$H \triangleleft G \Rightarrow \{H, Hg_1, Hg_2 \dots Hg_{n-1}\}$ is a group under multiplication - the quotient group G/H

Ex: $G = \mathbb{Z}$ addition is commutative $\Rightarrow n + H = H + n$ $H \triangleleft G$

$H = 3\mathbb{Z}$ consider our cosets

$$\{H,\ H+1,\ H+2\}$$

$$\begin{array}{ccc} H & H+1 & H+2 \\ \text{III} & \text{III} & \text{III} \\ \text{"}\varnothing\text{"} & \text{"}1\text{"} & \text{"}2\text{"} \end{array}$$

$$H + (H+1) = H + H + 1 = H+1$$

$$H + (H+2) = H+2$$

$$(H+1) + (H+1) = H+2$$

$$(H+1) + (H+2) = H+3 = H$$

$$G/H = \mathbb{Z}/3\mathbb{Z} \cong \text{group of integers w/ addition modulo } 3$$

Proposition: The Bravais lattice T of a space group G is a normal subgroup of G

pf: $\{E|\vec{t}\} \in T$ lets consider $\{\bar{g}|\vec{d}\} \in G$

$$\{\bar{g}|\vec{d}\} \equiv g$$

$$g^{-1}\{E|\vec{t}\}g$$

$$g^{-1} = \{\bar{g}^{-1}| -\bar{g}^{-1}\vec{d}\}$$

$$gg^{-1} = \{E|\vec{0}\}$$

$$= \{\bar{g}^{-1}| -\bar{g}^{-1}\vec{d}\}\{E|\vec{t}\}\{\bar{g}|\vec{d}\}$$

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

Since every pure translation in G is by assumption a Bravais lattice translation $\Rightarrow$ $g^{-1} T g = T$

(3) $T \triangleleft G$

<u>Def</u> The point group $\bar{G}$ of a space group G is isomorphic to G/T

if we look at the coset decomposition of a space grp G relative to T we get

$$G = T \cup T\{\bar{g}_1|\vec{d}_1\} \cup T\{\bar{g}_2|\vec{d}_2\} \cup \dots \cup T\{\bar{g}_{n-1}|\vec{d}_{n-1}\}$$

$G/T \cong \{E, \bar{g}_1, \bar{g}_2, \dots \bar{g}_{n-1}\}$ where we forget about the translation parts of the coset representatives -

$G/T \cong \bar{G} \subset O(3)$ one of our 32 pt groups

$$\left(\begin{aligned} &T\{\bar{g}_1|\vec{d}_1\}\, T\{\bar{g}_2|\vec{d}_2\} \\ &= T\{\bar{g}_1\bar{g}_2 \,|\, \vec{d}_1 + \bar{g}_1\vec{d}_2\} \rightarrow \{\bar{g}_i|\vec{d}_i\} = \{\bar{g}_1\bar{g}_2|\vec{d}_1 + \bar{g}_1\vec{d}_2 + T\} \end{aligned} \right)$$

What is the simplest way to get a G satisfying these properties?

take T, take a pt group $\bar{G}$ compatible with that Bravais lattice

$$G = T \cup T\{\bar{g}_1|\emptyset\} \cup T\{\bar{g}_2|\emptyset\} \cup \dots \cup \{\bar{g}_{n-1}|\emptyset\}$$

i.e. $G = T \rtimes \bar{G}$ a semidirect product

$$\{\bar{g}_i|\vec{t}\} \text{ for } \bar{g}_i \in \bar{G},\ \vec{t} \in T$$

equivalently, $G/T = \bar{G} \hookrightarrow G$ (there is an embedding of $\bar{G}$ as a subgroup of G)

$$\bar{G} \simeq \{ \{E|\emptyset\}, \{\bar{g}_1|\emptyset\}, \{\bar{g}_2|\emptyset\}, \ldots \}$$

$G = T \rtimes \bar{G}$ is a semidirect product iff

$G/T = \bar{G}$ is isomorphic to a subgroup of G

Space groups satisfying this property are called <u>symmorphic</u>

There are 73 symmorphic space groups in 3d

[letter telling us the lattice] [pt group symbol]

Ex: Space group $\underbrace{P}_{\text{Primitive}}\underbrace{mm2}_{\text{point group } mm2 \text{ orthorhombic}}$

Primitive

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

$\vec{e}_2 = (0,b,0)$

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

point group $mm2$ orthorhombic

$\{C_{2z}, m_x, m_y, E\}$

For a full list of lattice types given by letters, Table 3.1 in Bradley & Cracknell

But most space groups are not symmorphic!

$\exists$ 157 nonsymmorphic space groups

A space group is non-symmorphic if it does not have its point group as a subgroup

$$G = T \cup T\{\bar{g}_1|\vec{d}_1\} \cup T\{\bar{g}_2|\vec{d}_2\} \cup \dots \cup T\{\bar{g}_{n-1}|\vec{d}_{n-1}\}$$

if G is nonsymmorphic $\Rightarrow$ there is <u>no</u> way to choose coset representatives with all $\vec{d}_i = \emptyset$

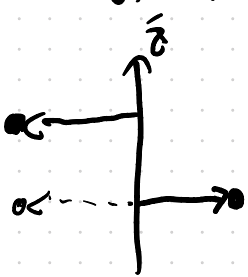
$\Rightarrow$ some of the $\vec{d}_i$ must be <u>fractions</u> of a Bravais lattice translation

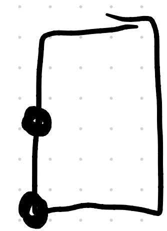
Two types of operations $\{\bar{g}|\vec{d}\}$ immediately tell us a space group has to be nonsymmorphic screw rotations and glide mirrors

a rotation followed by a fractional translation along the axis of rotation

$\left\{ C_{2z} \middle| \frac{\hat{z}}{2} c \right\}$ with

bravais lattice $\langle \{ E | c\hat{z} \} \rangle$





$$\{C_{2z} | \tfrac{\hat{z}}{2}c\}^2 = \{C_{2z} | \tfrac{\hat{z}}{2}c\}\{C_{2z} | \tfrac{\hat{z}}{2}c\} = \{E | c\hat{z}\} \in T$$

$$G = T \cup T\{C_{2z} | \tfrac{\hat{z}}{2}c\}$$

$G/T = \bar{G} = \{E, C_{2z}\}$ but there is no group operation isomorphic to $\{C_{2z} | \emptyset\}$

$$\{C_{m\hat{n}} | \vec{d}\} \qquad \vec{d} \not\perp \hat{n}$$

$\{C_{m\hat{n}} | \vec{d}\}^m = \{E | l\vec{t}\}$ l is an integer s

$$\vec{d} = \frac{l}{m}\vec{t}$$

M_ℓ $\qquad$ $\{C_{2z} \mid \frac{\hat{z}}{2}c\} \rightarrow 2_1$

$3_1, 3_2$

$4_1, 4_2, 4_3$

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

ex: 3_1: $\{C_{3\hat{z}} \mid \frac{c\hat{z}}{3}\}$.

$$\{C_{3\hat{z}} \mid \frac{c\hat{z}}{3}\}^3 = \{E \mid c\hat{z}\}$$

3_2: $\{C_{3\hat{z}} \mid \frac{2c\hat{z}}{3}\}$.

$$\{C_{3\hat{z}} \mid \frac{2c\hat{z}}{3}\}^3 = \{E \mid 2c\hat{z}\}$$

Glide mirror: a mirror reflection across a plane, followed by a translation in the plane

$g = \{M_z \mid \frac{a}{2}\hat{x}\}$; $(x, y, z) \rightarrow (x + \frac{a}{2}, y, -z)$

$g^2 = \{E \mid a\hat{x}\}$

a, b, c glides along a cartesian direction

n - glides along a face diagonal

d - glide along a body diagonal

e - when there multiple glides w/ the same mirror plane

Ex: $P2_13$

Primitive cubic → P

$\underbrace{2_1 3}$ — 23 is the point group - cubic

the twofold rotation is a 2_1 screw

$$\left(\{m \mid \vec{d}\}\right)^2 = \{m^2 \mid \vec{d} + m\vec{d}\}$$

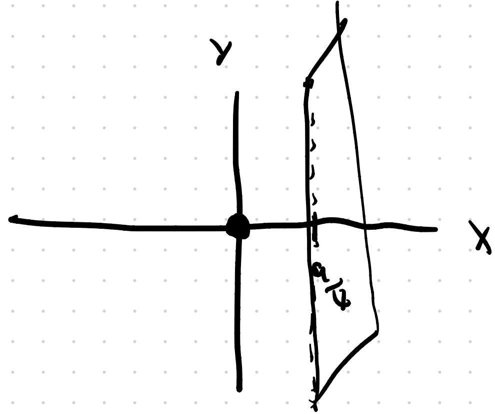
if $m\vec{d} = \vec{d}$

$$= \{E \mid 2\vec{d}\} \in T$$

$\Rightarrow$ $2\vec{d}$ a Bravais lattice translation

$$\left(\{M_x \mid \tfrac{a\hat{x}}{2} \boxed{+\tfrac{\hat{y}}{2}}\}\right)^2$$

$$\{E \mid \hat{y}\}$$



$\{M_x | \frac{a\hat{x}}{2}\} : (x, y, z) \to (\frac{a}{2} - x, y, z)$

$(\frac{a}{4}, y, z)$