Lecture 2 | Recap: Rigid transformations of space (isometries)

$\mathbb{E}(d)$ Euclidean group

$\cap$

$\{E|\vec{d}\}\{R|\vec{0}\} = \{R|\vec{d}\}$, $R \in O(d)$ orthogonal transformation

$\vec{d} \in \mathbb{R}^d$ translation

$\mathbb{E}(d) = \mathbb{R}^d \rtimes O(d)$ semidirect product

$$\{R_1|\vec{d}_1\}\{R_2|\vec{d}_2\} = \{R_1R_2 | R_1\vec{d}_2 + \vec{d}_1\}$$

We want to start looking @ symmetries of crystals

G - space group - symmetry grp of some xtal

$G \subset \mathbb{E}(d)$

① Crystals have discrete translation symmetry

→ Every space group G contains a Bravais lattice

$$\{\{E \mid n_1\vec{e}_1 + n_2\vec{e}_2 + \dots n_d\vec{e}_d\},\ n_1, n_2, \dots n_d \in \mathbb{Z}\}$$

Any set of d linearly independent vectors $\vec{e}_1, \vec{e}_2, \dots \vec{e}_d$ generate a Bravais lattice

Lets say we have a space group G and a Bravais lattice $\mathbb{Z}^d \subset G$

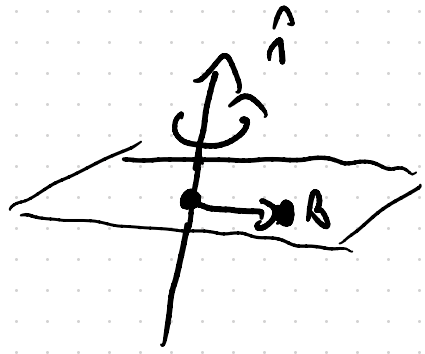
Q: What other symmetries can be in G?

Thm: Crystallographic Restriction Theorem

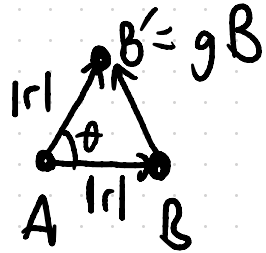
Suppose we have a Bravais lattice in 2 or 3 dimensions, and suppose that g is a rotational symmetry of the lattice ($g \in SO(d)$ $d=2,3$)

Then g is a rotation by $0, \frac{2\pi}{6}, \frac{2\pi}{4}, \frac{2\pi}{3}$, or π radians

pf: first, note that g is specified by an axis $\hat{n}$ of rotation, and so it leaves invariant planes $\perp \hat{n}$



let A be a pt on the rotation axis
let B be the closest lattice point to A $\perp \hat{n}$



$\vec{B}' - \vec{B}$ B is a lattice point

if g is a symmetry of my lattice, then B' is also a lattice point

$\Rightarrow$ $\vec{B}' - \vec{B}$ is a lattice translation in the plane

$$|\vec{B}' - \vec{B}| = \sqrt{2|r|^2(1-\cos\theta)} = |r|\sqrt{2(1-\cos\theta)} \geq |r|$$

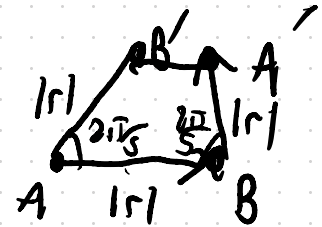
$$\cos\theta \leq \tfrac{1}{2}$$

$$\theta \geq \frac{2\pi}{6}$$

if $\theta \neq \frac{2\pi}{n}$ $n \in \mathbb{Z}$ then g^M is a rotation by an angle smaller than $\frac{2\pi}{6}$

$\Rightarrow$ g is a rotation by $\frac{2\pi}{n}$ $n \leq 6$

We can rule out $n=5$



$\Rightarrow$ g is a rotation by $\frac{2\pi}{1}, \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}$

$$\boxed{SO(4) \text{ "=" } SO(3) \times SO(3)}$$

Lets look at all of the possible subgroups of $O(d)$ $[d=2,3]$ that <u>could</u> be symmetries of a Bravais lattice

2d: 10 possible groups

lies in x-y plane
$\hat{z}$ is the rotation axis

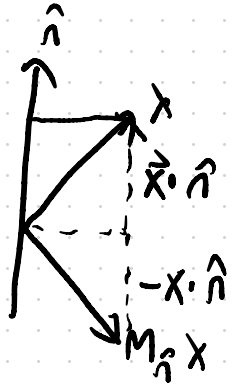
Group	Hermann-Mauguin notation	Schönflies Notation
• trivial group → no extra symmetries	1	C_1
• $\langle C_{2z} \rangle = \{E, C_{2z}, C_{2z}^2 = E\}$	2	C_2
• $\langle C_{3z} \rangle$	3	C_3
• $\langle C_{4z} \rangle$	4	C_4
$\langle C_{6z} \rangle$	6	C_6

$\langle \cdot \rangle$ group generated by

We can also have reflections in addition to rotations

mirrors

$M_{\hat{n}}$



Ex: $M_{\hat{x}} : (x,y) \to (-x,y)$

$C_{2z}M_x(x,y)$
$= C_{2z}(-x,y) = (x,-y)$
$= M_y(x,y)$

This gives us 5 more groups

$\langle M_x \rangle$	M	C_s
$\langle C_{2z}, M_x \rangle$	$2mm$	C_{2v}
$\langle C_{3z}, M_x \rangle$	$3m$	C_{3v}
$\langle C_{4z}, M_x \rangle$	$4mm$	C_{4v}

$\langle C_{6z}, m_x \rangle$ | 6mm | C_{6v}

These are the crystallographic point groups in 2D

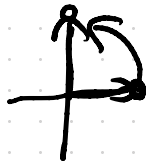
$$\{E|\vec{d}\}\{C_{nz}|\vec{0}\}\{E|-\vec{d}\}(\vec{d}) = \vec{d}$$

$$\{C_{nz}|\vec{d}\} = \{C_{nz}|\vec{d} - C_{nz}\vec{d}\}$$

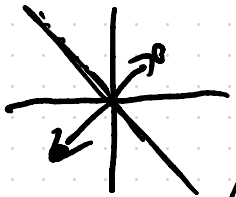
this is an $n$fold rotation about the point $\vec{d}$

Ex: $4mm$ $\quad C_{4z}, M_x, C_{4z}M_x = M_{11}$

$C_{4z}: (x,y) \to (-y,x)$



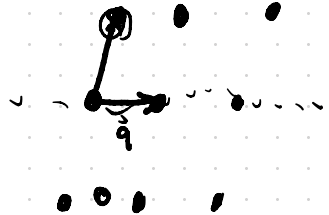
$C_{4z}M_x(x,y) \to C_{4z}(-x,y) \to (-y,-x)$



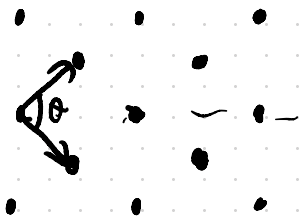
We can classify 2d Bravais lattices based on which of these pt group symmetries they can have

In 2d $\exists$ 5 Bravais lattices

Monoclinic



Monoclinic



Centered rectangular

What about 3D? There are 22 additional groups

① Inversion symmetry $I: (x,y,z) \to (-x,-y,z)$

$\langle I \rangle$	T	C_i
$\langle I, C_{2z} \rangle$	$2/m$	C_{2h}
$\langle I, C_{4z} \rangle$	$4/m$	C_{4h}
$\langle IC_{4z} \rangle$	$\bar{4}$	S_4
$\langle I, C_{3z} \rangle$	$\bar{3}$	C_{3i}
$\langle I, C_{6z} \rangle$	$6/m$	C_{6h}

$\langle I, C_{2z} \rangle = \{E, I, C_{2z}, IC_{2z} = M_z\}$

$\langle IC_{4z} \rangle = \{E, IC_{4z}, C_{2z}, (IC_{4z})^2 = (IC_{4z})^{-1}\}$

$\langle I C_{6z} \rangle$	$\bar{6}$	C_{3h}
$\langle I, C_{2z}, M_x \rangle$	mmm	D_{2h}
$\langle I, C_{2/z}, M_x \rangle$	$4/mmm$	D_{4h}
$\langle I, C_{6z}, M_x \rangle$	$6/mmm$	D_{6h}
$\langle I, C_{3z}, M_x \rangle$	$\bar{3}m$	D_{3d}

11 more pt groups come from having multiple rotation axes

$\langle C_{2x}, C_{2y} \rangle$	222	D_2

we have 32 pt groups
we have 14 Bravais lattices

we want to put a point grp together w/ a compatible Bravais lattice to get a space group G

$\{\bar{g} \mid \vec{t}\}$ $\quad$ $\bar{g} \in$ pt grp $\bar{G}$

$\vec{t} \in$ bravais lattice T

$G = T \rtimes \bar{G}$ - space grps w/ this structure are called symmorphic

$\bar{G} \subset G$ iff G is symmorphic