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

\[ E(d) \text{ Euclidean group} \]

\[ \{E(1d)\} \{R1\|0\} = \{R1\|0\} \quad , \quad R \in O(d) \text{ orthogonal transformation} \]

\[ E(d) = \mathbb{R}^d \times O(d) \text{ semidirect product} \]

\[ \{R_1\|d_1\} \{R_2\|0\} = \{R_1R_2 \| R_1d_2 + d_1\} \]

We want to start looking @ symmetries of crystals
$G$-space group - Symmetry group of some crystal

$G \subset \Gamma(d)$

1. Crystals have discrete translation symmetry
   - Every space group $G$ contains a Bravais lattice

   \[
   \{ \{ (v_1 e_1 + v_2 e_2 + \ldots + v_d e_d) \mid v_1, v_2, \ldots, v_d \in \mathbb{Z} \} \}
   \]

   Any set of $d$ linearly independent vectors $e_1, e_2, \ldots, e_d$
   generates a Bravais lattice
Let's say we have a space group \( G \) and a Bravais lattice \( \mathbb{Z}^d \).

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 (\( g \in \text{SO}(d) \) for \( d = 2, 3 \)).
Then \( g \) is a rotation by \( 0, \frac{2\pi}{6}, \frac{2\pi}{4}, \frac{2\pi}{3}, \frac{2\pi}{1} \) 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 \( A \parallel \hat{n} \)
$B$ is a lattice point if $g$ is a symmetry of my lattice, then $B'$ is also a lattice point.

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

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

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

$$\theta \geq \frac{2\pi}{6}$$
If $\theta \neq \frac{2\pi}{n}$ and $n \in \mathbb{Z}$, 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 $\frac{2\pi}{11}, \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}$.

$SO(4) = SO(3) \times SO(3)$. 

\[ 1 \quad 1 \quad 1 \quad 1 \]

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Let's look at all of the possible subgroups of $O(d)$ \([d=2,3]\) that could be symmetries of a Bravais lattice.

2d: 10 possible groups

<table>
<thead>
<tr>
<th>Group</th>
<th>Hemmann-Mauguin Notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trivial group - no extra symmetries</td>
<td>1</td>
</tr>
<tr>
<td>$\langle C_{2z} \rangle = {E, C_{2z}, C_{2z}^2 = E}$</td>
<td>2</td>
</tr>
<tr>
<td>$\langle C_{3z} \rangle$</td>
<td>3</td>
</tr>
<tr>
<td>$\langle C_{4z} \rangle$</td>
<td>4</td>
</tr>
<tr>
<td>$\langle C_{6z} \rangle$</td>
<td>6</td>
</tr>
</tbody>
</table>

C1, C2, C3, C4, C6
We can also have reflections in addition to rotation mirrors.

\[ M \hat{\alpha} \]

\[ M_x \]

\[ C_{2z} M_x (x, y) = C_{2z} (-x, y) = (x, y) = M_y (x, y) \]

This gives us 5 more groups:

\[ \langle M \rangle \]

\[ \langle C_{2z}, M_x \rangle \]

\[ \langle C_{3z}, M_x \rangle \]

\[ \langle C_{4z}, M_x \rangle \]

\[ \begin{array}{c|c|c}
M & C_{s} & C_{2zv} \\
2mm & C_{3v} & C_{3v} \\
3m & C_{3v} & C_{4v} \\
4mm & C_{4v} & C_{4v} \\
\end{array} \]
These are the crystallographic point groups in 2D:

\[ \left\{ C_{n_z} \mid \vec{d} \right\} \]

\[ C_{n_z} \overset{\vec{d}}{\rightarrow} C_{n_z} \vec{d} \]

This is an \( n \)-fold rotation about the point \( \vec{d} \).
Ex: 4mm

$C_{4z}, M_x, C_{4z} M_x = M_{11}$

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

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

In 2d, there are 5 Bravais lattices:
- Monoclinic
- Maonoclinic
- Centered rectangular

We can classify 2D Bravais lattices based on which of these pt group symmetries they can have.
What about 3D? There are 22 additional groups.

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

<table>
<thead>
<tr>
<th>$&lt;I&gt;$</th>
<th>$&lt;I, C_{2v}&gt;$</th>
<th>$&lt;I, C_{4v}&gt;$</th>
<th>$&lt;IC_{4v}&gt;$</th>
<th>$&lt;I, C_{3v}&gt;$</th>
<th>$&lt;I, C_{6v}&gt;$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$</td>
<td>$2/m$</td>
<td>$C_i, C_{2i}$</td>
<td>$S_4$</td>
<td>$C_3$</td>
<td>$C_6$</td>
</tr>
<tr>
<td>$4/m$</td>
<td>$C_{2i}$</td>
<td>$C_{2i}$</td>
<td>$S_4$</td>
<td>$C_3$</td>
<td>$C_6$</td>
</tr>
<tr>
<td>$4$</td>
<td>$C_{2i}$</td>
<td>$C_{2i}$</td>
<td>$S_4$</td>
<td>$C_3$</td>
<td>$C_6$</td>
</tr>
<tr>
<td>$3$</td>
<td>$C_3$</td>
<td>$C_3$</td>
<td>$S_4$</td>
<td>$C_3$</td>
<td>$C_6$</td>
</tr>
<tr>
<td>$6/m$</td>
<td>$C_{6i}$</td>
<td>$C_{6i}$</td>
<td>$S_4$</td>
<td>$C_3$</td>
<td>$C_6$</td>
</tr>
</tbody>
</table>

$<I, C_{2v}> \{ E, I, C_{2v}, I_{C2v}=M_2 \}$

$<IC_{4v}> \{ E, IC_{4v}, C_{2v}, (IC_{4v})^3=(IC_{4v})^2 \}$
\[ \langle I, C_{6z} \rangle \quad \frac{\bar{3}}{\text{M} \text{M} \text{M}} \quad \langle I, C_{3z} \rangle \quad \frac{3\text{m}}{\text{D}_{3d}} \]

11 more pt groups come from heavy multiple rotation axes.

\[ \langle C_{2x}, C_{2y} \rangle \quad \frac{222}{\text{D}_{2}} \]
we have 32 pt groups
we have 14 Bravais lattices
we want to put a point group together
w/ a compatible Bravais lattice to get a space group G
\( \{ \mathcal{g} \} \) \( \geq \rho + \text{grp } \mathcal{G} \)
\( \mathcal{G} \) is Bravais lattice \( \mathcal{T} \)
\( \mathcal{G} = \mathcal{T} \times \mathcal{G} \) - space groups w/ this structure are called symmorphic

\( \overline{\mathcal{G}} \subset \mathcal{G} \) iff \( \mathcal{G} \) is symmorphic