Crystallographic Point Groups

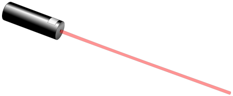
H. Chan

July 16, 2025

Table Of Contents

Rationale

Crystals find countless uses in modern technology.



Groups

Definition (Group)

A group is a set X along with a binary operation $*$ that adheres to the following properties:

(i) There exists an element e in X such that $e \cdot x = x \cdot e = x$ for all $x \in X$

(ii) For any $x \in X$, there exists another element $x^{-1} \in X$ such that $xx^{-1} = x^{-1}x = e$.

(iii) For any $x, y, z \in X$, the equality $(xy)z = x(yz)$ holds.

(iv) For any $x, y \in X$, the product xy is also in X.

Lets look at a few examples:

Examples

The Integers $(\mathbb{Z}, +)$

General Linear Group $GL(n, R)$.

Groups (cont.)

Definition (Cosets)

Given a subgroup K of G and $g \in G$, then we define the **left coset** gK to be

$$gK = \{gk : k \in K\}.$$

Theorem

Let G be a group of finite order and K be a subgroup. Then, the order of K is a factor of the order of G.

Corollary

If G is a group of finite order, and K is a subgroup then the following always holds:

$$[G : K] = \frac{|G|}{|K|}.$$

Transformation Groups

Definition (Transformation Group)

A **Transformation Group** G acting on X is a group that consists of permutations of X. For $x \in X$, we denote the element x gets permuted to by element $g \in G$ by $g \circ x$.

The **stabilizer subgroup** of an element x is the set of all $g \in G$ such that $g \circ x = x$. We denote the stabilizer by G_x.

The **orbit** $\mathcal{O}_x$ of x are all elements $y \in X$ such that there exists a $g \in G$ such that $g \circ x = y$.

The Euclidean Group

Definition (Euclidean Group)

The **Euclidean Group** on three dimensions $E(3)$ is the group of all rotations on $\mathbb{R}^3$ that preserve distance. These include both **translations** and **rotations**.

Theorem

Let S be a set of finite extent and G a discrete symmetry group on S. Then, there exists a point $y \in \mathbb{R}^3$ such that for all $g \in G$, $g \circ y = y$.

Theorem

If G is a discrete subgroup of $E(3)$ with fixed point y, then G is a finite subgroup of $O(3)$.

Computing Point Groups

Theorem

There exists a one to one correspondence between the left cosets of G_x and the elements in $\mathcal{O}_x$. Thus,

$$|\mathcal{O}_x| = \frac{|G|}{|G_x|}.$$

Proof Idea

(i) Define a function $f : \mathcal{O}_x \to G/G_x$ by $f(y) = g_y G_x$, where $g_y \circ x = y$.

(ii) Show that this function is a bijection, and is well-defined.

Computing Point Groups (cont.)

Let P denote the amount of orbits (of poles), $n = |G|$, and n_i and p_i denote the size and size of the stabilizer of the ith orbit respectively.

Then, the number of rotations that fix any pole in some orbit is exactly $n_i(p_i - 1)$. We can then sum this over all of the orbits to get $\sum_{i=1}^{P} n_i(p_i - 1)$.

On the other hand, every rotation fixes exactly two poles, so the sum must also be $2(n-1)$. Thus,

$$2(n-1) = \sum_{i=1}^{P} n_i(p_i - 1).$$

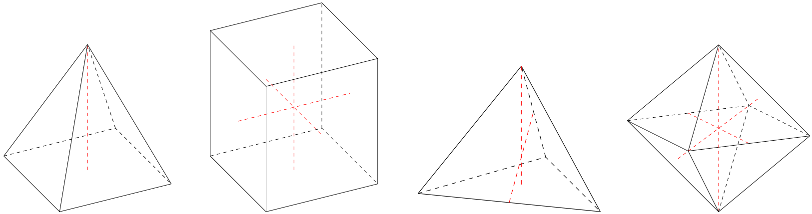
Reducing using previous theorems, we get

$$2\left(1 - \frac{1}{n}\right) = \sum_{i=1}^{P}\left(1 - \frac{1}{p_i}\right)$$

Computing Point Groups (cont.)

There are only solutions to the previous equations when $P = 2, 3$. We get the following symmetries.

C_n: This family is given by $(n_1, n_2) = n$, $n = 2, 3, \ldots$.
D_n: This family is given by $(n_1, n_2, n_3) = (2, 2, m), m = 2, 3, \ldots$.
T: This is the symmetry group of the Tetrahedron. $(n_1, n_2, n_3) = (2, 3, 3)$.
O: Symmetry group of the Octahedron/Cube, $(n_1, n_2, n_3) = (2, 3, 4)$.
I: Symmetry group of the Icosahedron, $(n_1, n_2, n_3) = (2, 3, 5)$.



A Different type of Point Group

Theorem

Let G be a finite subgroup of $O(3)$ and let K be a subset of G containing only proper rotations. Then, one of the following is true:

(i) $G = K$,

(ii) $G = K \cup IK$,

(iii) $G \cong K \cup I\overline{K}$, $G \neq K$, *and* $\overline{K} = \{g \in G : g \notin K\}$.

Some new Groups!

$$C_{nv},\ D_{nh},\ T_h,\ S_{2m},\ O_h,\ I_h$$

Lattices

Crystallographic Point Groups are Point groups that act on **Lattices**.

Definition (Lattice)

A 3 dimensional lattice is defined as a set L such that

$$L = \{\alpha_1 \hat{v}_1 + \alpha_2 \hat{v}_2 + \alpha_3 \hat{v}_3 : \alpha_i \in \mathbb{Z}\}.$$

where $\{\hat{v}_i\}$ is linearly independent. We define the **unit cell** to be the parallelepiped with minimal area with edges of length $|\hat{v}_i|$.

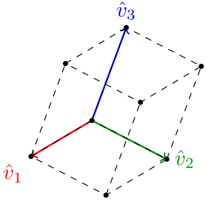


Figure: Basis Vectors and a unit cell.

Theorem (The Crystallographic Restriction)

Let G be a crystallographic point group. Then, all rotations and rotation-inversions in G are of order $2, 3, 4$ or 6.

Proof Idea

(i) Show that the **Trace** of any element $g \in G$ must be integral.
(ii) Use change of basis to map the rotation axis $\hat{k}$ to a basis vector, and find the resulting rotation matrix.
(iii) Show that the only values of θ that result in integral trace are $2, 3, 4$ and 6.

Holohedries and Bravais Lattices

Definition (Holohedry)

For some lattice L, the **Holohedry** of L is the *maximal* crystallographic group on L.

There are exactly 7 Holohedries, and they are the following

$$S_2, C_{2h}, D_{2h}, D_{4h}, D_{3h}, D_{6h}, O_h.$$

Bravais Lattices are the 7 families of lattices that the Holohedries above.

Questions?

Any Questions?

Thanks to Simon Rubinstein and Lucy Vuong for all the help!