

Finding Crystallographic Point Groups

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July 16, 2025

Abstract

Symmetry Groups are transformation groups acting on subsets of \mathbb{R}^3 . We study in particular two specific types of symmetry groups, namely *point groups* and *crystallographic point groups*. These groups are named so since they always keep some point $x \in \mathbb{R}^3$ fixed, under any transformation in the group! The main focus of this paper is to find and classify these point groups and crystallographic point groups.

1 Introduction

The study of crystals and crystalline structures is critical due to their significant use in modern technology. Crystals find use in microprocessors, oscillators, screens and displays, optics, and countless more. Surprisingly, mathematics (and more specifically **group theory**) can greatly aid in the characterization and study of crystals.

We can find a rationale for this connection by imagining a crystal lattice as not a physical collection of atoms and molecules but instead as mathematical lattice. More specifically, a subset of $T(3)$ (the translation group in \mathbb{R}^3) defined by

$$G = \{\alpha_1 \hat{\mathbf{b}}_1 + \alpha_2 \hat{\mathbf{b}}_2 + \alpha_3 \hat{\mathbf{b}}_3 : \alpha_i \in \mathbb{Z}; \hat{\mathbf{b}}_i \in T(3)\}$$

As it turns out, the symmetries and structures of these resulting lattices give key physical characteristics of the physical crystals they represent. It is even possible to compute and categorize all possible crystallographic structures with three dimensions (we have even found all groups up to dimension 6!).

2 Preliminaries

In this section, we cover some introductory ideas and topics in Group Theory that will allow us to construct and characterize the crystallographic groups.

Definition (Group). A group G is a collection of objects $\{g_1, g_2, \dots\}$ (not necessarily finite) in combination with a binary operation \cdot , which represents **group multiplication**. This related some pair of objects g_i, g_k with their product, $g_i g_k$. The group must meet the following properties.

1. **Identity.** There exists an element $e \in G$ such that for any element $g \in G$, the product $eg = ge = g$.
2. **Closure.** For any $g, h \in G$, the product gh is also in G .
3. **Associativity.** The equality $(ab)c = a(bc)$ is satisfied for any $a, b, c \in G$.
4. **Inverses.** For any element $g \in G$, there also exists an **inverse** g^{-1} in G such that $gg^{-1} = g^{-1}g = e$.

Additionally, the amount of elements in a group G is called the **order** of G and is denoted by $|G|$. *Note.* Notice that these groups are not necessarily commutative. That is, it is not always the case that $ab = ba$ for all elements a, b in some group. However, if a group *is* commutative, we call it **abelian**. If a group is abelian, its binary operation is usually denoted by $+$ instead of \cdot .

Definition (Subgroup). A group K is a subgroup of a group G if the set of elements of K is a subset of the elements of G , and they use the same binary operation. A group G always contains the subgroups G and $\{e\}$. These groups are called **improper subgroups**. All other subgroups are called **proper subgroups**.

Consider the following examples of groups and subgroups.

Example 1. The Integers \mathbb{Z} . The integers are a group under addition (this is our binary operation). We can show it meets the properties of a group:

1. The identity of \mathbb{Z} is 0. We have $0 + n = n$ for any integer n .
2. The integers are closed under addition, since the sum of two integers is always an integer.
3. Addition is certainly associative over the Integers.

Note. We also know that addition is also commutative over the integers, so our groups is actually Abelian!

4. The inverse of any integer n is simply $-n$ (which we know is an integer), since $n + (-n) = 0$.

One can construct infinitely many subgroups of \mathbb{Z} by considering the multiples of some integer! We denote this group by

$$n\mathbb{Z} = \{ni : i \in \mathbb{Z}\} = \{\dots, -2n, n, 0, n, \dots\}.$$

Note. If we tried to make the integers a group under multiplication instead of addition, it would fail to be a group. It fails to meet the criteria of inverses! Certainly there does not exist an integer k such that $2 \cdot k = 1$!

Example 2. Integers Modulo n . We can denote this group by \mathbb{Z}_n . This group consists of the elements $\{0, 1, \dots, n-1\}$. The binary operation, addition, outputs the sum modulus n (in other words, the remainder when the sum is divided by n). For example, $(n-1) + 1 = 0$. One could prove this is a group by a similar proof to the integers. Contrary to \mathbb{Z} , this group has finite order, which is exactly n .

There is not always a proper subgroup of \mathbb{Z}_n . If p is prime, there cannot exist a proper subgroup of \mathbb{Z}_p . However, if $n = ad$, with $d \neq 0$ then we can find subgroup of \mathbb{Z}_n by

$$d\mathbb{Z}_n = \{0, d, 2d, \dots, (a-1)d\}.$$

Example 3. General Linear Group of degree 2. Despite the fancy name, this group simply consists of all invertible matrices (non-zero determinant) under group multiplication. We can quickly show it meets the properties of a group:

1. The identity of this group is

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

2. We know this group is closed because of determinant multiplication. We have $\det(A)\det(B) = \det(AB)$, so the product of two matrices in this group will always have non-zero determinant, and thus must be in the group.
3. Group multiplication is associative.
4. We can construct inverses as shown below.

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \left(\frac{1}{ad-bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \right) = \frac{1}{ad-bc} \begin{pmatrix} ad-bc & -ab+ab \\ cd-cd & -bc+ad \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Like the integers, this group is infinite. However, it is *not* commutative:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} ae+bg & af+bh \\ ce+dg & ce+dh \end{pmatrix}$$

while

$$\begin{pmatrix} e & f \\ g & h \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} ae+fc & be+df \\ ag+ch & bg+dh \end{pmatrix}.$$

Since determinant multiplication works just like multiplication over the reals, we can use that for inspiration. One example pops up: the subgroup with of all matrices with determinant 1! This group is called the Special Linear Group.

Example 4. Permutation Groups. Permutation groups are denoted by S_n , and its elements are the permutations some set X with n objects. Here is an example of an element in S_7 :

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 6 & 2 & 4 & 5 & 3 & 7 & 1 \end{pmatrix}$$

This notation means the 1st element maps to the 6th element, the 2nd element maps to the second element, the third element maps to the 4th element, etc. We can then see the order

of S_n is $n!$: there are exactly $n!$ ways to permute n objects! Unfortunately, these groups are **non-abelian**. Here is an example to prove it (in S_4):

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 3 & 4 & 2 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 4 & 2 & 1 \end{pmatrix}$$

meanwhile

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 3 & 4 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 1 & 3 \end{pmatrix}$$

2.1 Normal Subgroups and Cosets

Definition (Coset). Let K be a subgroup of group G (denoted by $K < G$), and $g \in G$. Then, the set

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

is called the **left coset** of K . We construct the **right coset** similarly.

Note. For the rest of the paper, we shorten left coset to simply “coset”. Lets prove a few facts about cosets.

1. For every $g \in G$ there exists a coset $g'K$ such that $g \in g'K$. Since K is a subgroup, it contains e and thus $g' = g$ creates such a coset.
2. Cosets are either identical or disjoint. Consider two cosets gK and hK . Suppose they have a common element. Without loss of generality (WLOG), let $gk_1 = hk_2$. Then, $g = h(k_2k_1^{-1})$. We can then see the two cosets are identical, since for any $k \in K$ there exists $k' = k_2k_1^{-1}k$ such that $gk = gk'$.

This second fact is very useful. Consider some finite group G with n elements, with subgroup K . Since cosets are either identical or disjoint, we know there are some collection of cosets that cover G , $\{g_1K, g_2K, \dots, g_RK\}$ (the amount of distinct cosets of K is called its **index** and is denoted by $[G : K]$). Notice that the amount of elements in each coset is exactly $|K|$. If $gk_1, gk_2 \in gK$ were equal, then we must have $g^{-1}gk_1 = g^{-1}gk_2$ so $k_1 = k_2$. Thus, we get

$$\# \text{ of cosets} = \frac{|G|}{|K|}.$$

Theorem 2.1. Let G be a group of finite order, and K be a subgroup of G . Then,

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

Note. This explains why there are no subgroups of groups \mathbb{Z}_p from example 2!

The notation of cosets almost makes us want to make a group out of them, where $g_1K = g_2K$! Unfortunately, this is not always well defined. Suppose $aK = bK$ and $cK = dK$. Then, in our group, we must have $(aK)(cK) = (bK)(dK)$, or $(ac)K = (bd)K$. We have that $ak_1 = bk'_1$ and $ck_2 = dk'_2$ for any choice of $k_1, k_2 \in K$. However, in trying to prove this, we can only get to $ack = adk'$, since there is no ak to turn into bk' . However, we can fix this with a new kind of subgroup!

Definition (Normal Subgroup). A subgroup K is **normal** if for any $g \in G$ (where G is the parent group), the cosets gK and Kg are equal. An equivalent condition is that $gKg^{-1} = K$.

This fixes all our problems! We now have $ack = adk' = ak''d = bk'''d = bdk^{(4)}$. Thus, another definition.

Definition (Factor Group). Let G be a group and K a normal subgroup. Then, the group of cosets of K is called a **factor group** and is denoted by G/K .

Lets go over an example of normal subgroups and factor groups.

Example 5. Lets return to \mathbb{Z} and its subgroups $n\mathbb{Z}$. Since this group is abelian, all of subgroups are necessarily normal subgroups. Now, lets compute $\mathbb{Z}/n\mathbb{Z}$. There are exactly n cosets: $\{n\mathbb{Z}, 1+n\mathbb{Z}, \dots, n-1+n\mathbb{Z}\}$. We can see that $n+n\mathbb{Z} = n\mathbb{Z}$ since $n+na = n(a+1)$. This group then must be \mathbb{Z}_n !

3 Transformation groups

One special type of group we will study are **Transformation Groups**. They are defined as followed.

Definition (Transformation Group). The **Transformation Group** G acting on a set X consists of elements such that any $g \in G$ is a one to one mapping from X to itself. The binary operation on G is function composition (denoted by multiplication), and it must comply with the following conditions:

1. $g \circ x \in X$
2. $g_1 \circ (g_2 \circ x) = (g_1 g_2) \circ x$
3. $e \circ x = x$.

Something interesting we can note is that if X contains n elements, then any transformation group G acting on X must be a subset of S_n : certainly a one to one mapping on finite elements can be seen as a permutation.

Definition (Stabilizer). Let G be a transformation group acting on X , and let $x \in X$. Then, the **stabilizer** of x (denoted by G_x) is the set of all elements in G that map x to X . More explicitly, we can write

$$G_x = \{g \in G : g \circ x = x\}.$$

This group can also be called the isotropy subgroup at X . If a transformation g is in G_x , we say it leaves x **invariant**.

We can also define something quite similar to the stabilizer, but instead of "stabilizing" a single element, they keep some subset of X the same.

Definition (G-Symmetry). Let G be a Transformation Group on X and let $Y \subseteq X$. Then, the **G-Symmetry** on Y is all elements $g \in G$ such that $g(Y) = Y$.

Definition (G -Equivalent). Two elements $x, y \in X$ are **G -equivalent** if there exists some $g \in G$ such that $g \circ x = y$. We denote two elements are G -equivalent by $x \sim y$.

In fact, this relation is an equivalence relation! Lets quickly prove it.

Proof.

1. **Transitive.** Suppose $a \sim b$ and $b \sim c$. Then, by definition, there exists $g_1, g_2 \in G$ such that $g_1 \circ a = b$ and $g_2 \circ b = c$. Then, we have $g_2 \circ (g_1 \circ a) = c$, but this is equivalent to $(g_2 g_1) \circ a = c$. Since G is a group we have $g_2 g_1 \in G$, and $a \sim c$.
2. **Reflexive.** Since $e \in G$, and $e \circ x = x$, then for any $x \in X$ we have $x \sim x$.
3. **Symmetric.** Suppose $x \sim y$. Then, there exists a $g \in G$ such that $g \circ x = y$. Since G is a group, $g^{-1} \in G$, which certainly maps y to x , and such $y \sim x$.

□

Since this is an equivalence relation, we can find the equivalence classes of X .

Definition (Orbit). Let G be a transformation group acting on X , and let $x \in X$. The **orbit** of x (denoted by \mathcal{O}_x) is the equivalence class of x .

Now, we prove our second theorem.

Theorem 3.1. Let G be a finite transformation group on X , and let $x \in X$. Then, the following equality always holds.

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

Proof. We can prove this by creating a bijection between the left cosets of G_x and the elements in the orbit of x . Let f be a function from \mathcal{O}_x to the left cosets of G_x . Lets define $f(y)$. Let $g \in G$ be such that $g \circ x = y$. Then, we have $f(y) = gG_x$. We can see any element in gG_x must map x to y . Suppose we also have $h \in G$ such that $h \circ x = y$. Then, $g \circ x = h \circ x$ and thus $x = (g^{-1}h) \circ x$ and $g^{-1}h \in G_x$ and $h \in gG_x$.

It is easier to see this function is onto. Suppose we have some left coset kG_x . Let $k \circ x = y$. Then, $y \in \mathcal{O}_x$, and thus $f(y) = kG_x$. □

Note. We needed finiteness because the dividing orders of infinite sets doesn't make sense here

Example 6. Symmetries of the Square.

In this case, our set X is the points $\{(1, 1), (-1, 1), (-1, -1), (1, -1)\} \subseteq \mathbb{R}^2$, and our transformation group G is the identity, the reflections across the lines $x = 0, y = 0, y = x$, and $y = -x$. In the group is also the 3 non-trivial rotations, $90^\circ, 180^\circ$, and 270° .

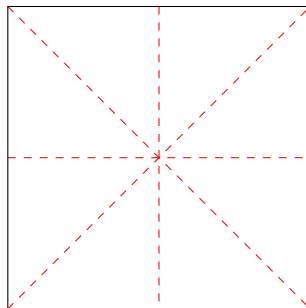


Figure 1: Square with reflections.

The stabilizer subgroup of any point $x \in X$ is exactly $\{e, f_{id}\}$, where e is the identity element and f_{id} is the i th diagonal flip (f_{1d} is reflection across $y = -x$, f_{2d} is the other flip). One can check no other elements in g fix x .

Next, we look for all G -symmetries on $Y \subseteq X$. We will only consider Y where $|Y| = 2$, $Y = \{x, y\}$. The $|Y| = 3$ case is the same as the earlier stabilizer subgroup case, since if permutation g satisfies $g \circ Y = Y$, then g also satisfies $g \circ Y^c = Y^c$ and vice versa, where Y^c is the complement of Y . We have two cases: x, y are adjacent and x, y are opposite. *Note.* Notice how for our subgroup Y the reflections/rotations in the G -symmetry must either map x onto y and vice versa or leave both points invariant.

1. x and y are adjacent. In this case, there is no rotation (other than the trivial rotation) that leaves both points invariant, and there is no rotation in general that maps x to y and vice versa. However, the reflection across the perpendicular bisector of \overline{xy} does swap the two points. Thus, the G -symmetry is $\{e, f_{im}\}$, where f_{1m} is the flip across $y = 0$ and f_{2m} is the flip across $x = 0$, and $i \in \{1, 2\}$.
2. x and y are opposite. The rotation and reflection that map x and y to themselves are e and f_{im} . Here, i is chosen such that the reflection line is coincident with x and y . There are also reflections and rotations that swap x and y , namely r_{180} (rotation by 180) and $f_{i'm}$, which is the other diagonal reflection.

There is only one orbit, since all elements can be mapped to each other via the rotations. This is expected, because of Theorem 3.1. *Note.* If we decided to include the point $O = (0, 0)$ in our set X , we would then have two orbits, since $g \circ O = O$ for all $g \in G$! This is one example of a **fixed point**, which we will define later.

4 The Orthogonal & Euclidean Groups

Our current objective in studying crystallography using group theory is to find various symmetries of objects in 3d space. In other words, we are looking at transformation groups acting on subsets of 3d space. We also want all of these transformations to preserve distances between objects: it would be inaccurate for a real solid, physical object to suddenly change size and shape upon a rotation. We can try constructing one such group ourselves.

One way to make creating such a group easier is to make it consist of only linear transformations, since we can then represent each element as a matrix. We can let v_1, v_2, v_3 represent the unit vectors along our coordinate axes, and we can thus represent any point $x \in \mathbb{R}^3$ by $x = \alpha_1 v_1 + \alpha_2 v_2 + \alpha_3 v_3$.

We then want to find all 3x3 matrices O such that they preserve distance, or $\|x\| = \|Ox\|$ for $x \in \mathbb{R}$. Since magnitude is simply the square root of the dot product $(x.x)$, we can instead assume $(Ox.Ox) = (x.x)$. By the equality

$$4(x.y) = (x + y.x + y) - (x - y.x - y)$$

we know that $(x.y) = (Ox.Oy)$. This is the case since the right hand side consists of dot products of the form $(a.a)$, and so we can act on the points using O . The elements O also preserve angle, proven by the law of cosines. We can then try to represent this equality using component form, given the fact that $Ox = \sum_i v_i \sum_j O_{ij} x_j$.

$$\begin{aligned} \sum_{i=1}^3 x_i y_i &= \sum_{i=1}^3 \left(\sum_{j=1}^3 O_{ij} x_j \right) \left(\sum_{k=1}^3 O_{ik} y_k \right) \\ &= \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 O_{ij} O_{ik} x_j y_k \\ &= \sum_{j=1}^3 \sum_{k=1}^3 \sum_{i=1}^3 O_{ij} O_{ik} x_j y_k \\ &\rightarrow \sum_{i=1}^3 O_{ij} O_{ik} = \delta_{jk} \end{aligned}$$

where δ_{jk} is the Kronecker delta. We get the implication \rightarrow since the sum must be equal to the original sum representing $(x.y)$, and thus no products $x_i y_k, i \neq k$ can appear in the sum.

We can then see that $O^t O = E_3$, where O^t is the transpose of O and E_3 is the identity element. In other words, $O^t = O^{-1}$. Now, let's show the set of all O such that $O^t = O^{-1}$ is actually a group.

1. **Identity.** We certainly have $E_3^t E_3 = E_3$, the identity.
2. **Inverses.** We have $O^t O^{tt} = O^t O = E_3$, so inverses are certainly part of the group.
3. **Associativity.** Matrix Multiplication is associative.
4. **Closure.** Consider some O_1, O_2 . Then, we must show the inverse of $O_1 O_2$ is also its transpose. But, $(O_1 O_2)^t = O_2^t O_1^t$ so and $O_2^t O_1^t O_1 O_2 = E_3$ and we are done.

This group is called the **Orthogonal Group** of degree three, or $O(3)$.

There are two types of rotations in this group: proper rotations and improper rotations. Improper rotations are the combination of the inversion $I_3 = -E_3$ and some proper

rotation O_3 . Since $\det(AB) = \det(A)\det(B)$, we can see that all proper rotations have determinant 1 and all improper rotations have determinant -1 . *Note.* You can also find a homomorphism $\phi : O(3) \rightarrow \{1, -1\}$, and see that the proper rotations are a normal subgroup. We call this group the **Special Orthogonal** group, or $SO(3)$.

One other thing to note is that for any proper rotation O , there exists a line k through the origin called the **axis of rotation** that remains invariant under O . More specifically, for any point $x \in l$, $Ox = x$. *Note.* The proof of this can be seen in [WM72].

Definition (Euclidean Group). The Euclidean group of degree three $E(3)$ is the transformation group acting on \mathbb{R}^3 that consists of **all** permutations that preserve distance. To be more precise, given any $g \in E(3)$ and points $p_1, p_2 \in \mathbb{R}^3$, the following holds:

$$\|p_1 - p_2\| = \|g \circ p_1 - g \circ p_2\|.$$

where $\|\cdot\|$ outputs the magnitude of the vector.

As it turns out, $E(3)$ contains *only* translations, rotations, and products of the two. Let's prove $E(3)$ actually is a group.

Theorem 4.1. The set $E(3)$ under composition is actually a group.

Proof.

1. **Identity.** The identity is simply the trivial rotation, a rotation by 0 degrees!
2. **Inverses.** Suppose we have some element $g \in E(3)$. Then, $\|g \circ x - g \circ y\| = \|x - y\|$. Therefore, g must have an inverse, since we have a mapping from $g \circ x$ to x (remember, g itself is a bijection from \mathbb{R}^3 to itself) and distance is preserved.
3. **Associativity.** It is proven that function composition is always associative.
4. **Closure.** If $g, h \in E(3)$, then

$$\|gh \circ x - gh \circ y\| = \|g(h \circ x) - g(h \circ y)\| = \|h \circ x - h \circ y\| = \|x - y\|.$$

□

Two basic subgroups of $E(3)$ are $T(3)$ and $O(3)$, with $T(3)$ being the group of translations. We represent elements of $T(3)$ by T_a , the translation along vector a . In other words, $Tx = x + a$. In fact, the elements of $T(3)$ commute, as $T_a T_b = T_{a+b}$, so $T(3)$ is abelian and is thus a normal subgroup.

In order to find the rest of the elements in $E(3)$, we actually only need to find the elements that fix the origin Θ , since if $T\Theta = a$ for $T \in E(3)$, then $T_{-a}T$ leaves the origin invariant. We can see that $O(3)$ is certainly a subgroup of all such transformations, but it is actually group of **all** elements that fix the origin (see [Yal68]). Thus, we can represent any element T as a rotation followed by a reflection:

$$T \in E(3), \quad T = T_a O = \{a, O\} \quad O \in O(3).$$

We have that

$$\{a, O\}x = Ox + a$$

and

$$\{a_1, O_1\}\{a_2, O_2\} = \{a_1 + O_1a_2, O_1O_2\}.$$

Note. This actually means the Euclidean group is the semidirect product of the groups $T(3)$ and $O(3)$!

We can see that there are also rotations and inversions that don't fix Θ and instead fix some other line or point. Let such a transformation be called T . Now, consider $T_{-a}TT_a$. This fixes Θ and thus $T = T_aOT_{-a}$ for some $O \in O(3)$. This means for any group of transformations G that fix some point a , we can find a conjugate (and isomorphic) copy of this group that fixes Θ .

Example 7. Let a be some vector. Then, we can find the **Orthogonal Group at a** by conjugating $O(3)$ by T_a .

$$O_a(3) = T_aO(3)T_{-a} = \{T_aOT_{-a} : O \in O(3)\}$$

Lets go over all the types of elements in $E(3)$. You can find pictures of these transformations in [Tha22].

1. **Translations.** Denoted by T_a .
2. **Rotations.** $R_k(\theta)$ denotes the proper around axis k by θ radians. We can then denote any other rotation using $\{a, R_k(\theta)\}$ where a is perpendicular to k .
Note. The axis of rotation of $\{a, R_k(\theta)\}$ is parallel to k and contains the points b such that $R_k(\theta)b + a = b$.
3. **Inversions.** The inversion around point a is denoted by I_a . If $a = \Theta$, then we denote the inversion simply by I .
4. **Reflection.** Reflections are combinations of inversions and 180° rotations. For example, we can represent the reflection across the xy -plane by $R_z(180^\circ)I$. We denote reflection by F_p , where p is the plane of reflection.
5. **Screw Rotation.** This is an of the form $\{a, R_k(\theta)\}$ where a is *not* parallel to k . Then, $a = x + y$, where x is parallel to k and y is perpendicular. We then have $T_x\{y, R_k(\theta)\}$. In other words, this is a rotation followed by a translation parallel to k .
6. **Glide Reflection.** Glide reflections are reflections along with a translation parallel to that plane. The order does not matter here.

Note. We can find another normal subgroup of $E(3)$ by taking the kernel of the homomorphism $\{a, O\} \rightarrow \det(O)$. This is called the **Proper Euclidean Group** of degree three.

5 Symmetry Groups

Given any set $S \subseteq \mathbb{R}^3$, we can find the G -symmetry that acts on it! In our specific case with subsets of \mathbb{R}^3 , we simply call such a group a **Symmetry** on S . In addition, the largest symmetry group on S is called the **Complete Symmetry Group** on S .

Example 8. One example is the triangular pyramid, as shown in Figure 2 (*Note.* The complete symmetry group is different if the pyramid is also a tetrahedron). One simple symmetry group is $\{e, R_{v_3}(120^\circ), R_{v_3}(240^\circ)\}$, where the center of the base of the pyramid is Θ and the altitude is along v_3 .

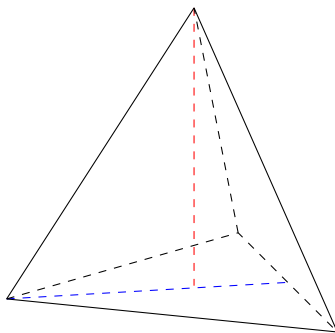


Figure 2: Triangular Pyramid

However, this is *not* the complete symmetry group. Notice there are 3 reflections that map the pyramid back to itself! They are the vertical planes containing one of the altitudes on the base (one pictured above). Thus, the complete symmetry group is

$$\{e, R_{v_3}(120^\circ), R_{v_3}(240^\circ), F_i, F_j, F_k\}$$

where i, j, k are the vertical planes mentioned previously.

The problem of finding all symmetry groups is very difficult, since it involves finding all subsets of $E(3)$! However, there are some families of these subgroups that are much easier to find. We look at one such of these families.

Definition (Discrete Symmetry Group). A discrete symmetry group G acting on $S \subseteq \mathbb{R}^3$ is a subgroup of $E(3)$ such that any for any element $x \in S$, and any open ball $B_r(a)$ (radius r , center a), the intersection $\mathcal{O}_x \cap B_r(a)$ is finite.

We can see that any finite symmetry group on S is always a discrete symmetry group, since all orbits must be finite. However, it is not the case that a discrete symmetry group be finite: consider the group of translations $\{\dots, T_{-2a}, T_{-a}, e, T_a, T_{2a}, \dots\}$.

Another helpful restriction for finding some subgroups is to require S to be of **finite extent**.

Definition (Finite Extent). A subset $S \subseteq \mathbb{R}^3$ is of **finite extent** if there exists a ball $B_r(a)$ such that $S \subseteq B_r(a)$.

With this restriction, we can see that the possible discrete symmetry groups cannot include translations, screw rotations, or glide reflections, since repeating these transformations repeatedly would eventually map S outside of $B_r(a)$. Therefore, the only possible elements in the symmetry group are rotations and rotation inversions. The following two theorems further simplifies our search.

Theorem 5.1. If G is a discrete symmetry group on $S \subseteq \mathbb{R}^3$, a nonempty set of finite extent, then there exists a point $x \in \mathbb{R}^3$ such that $g \circ x = x$ for all $g \in G$.

Proof. Consider some point $s \in S$. Since S is of finite extent, and G is discrete, the orbit \mathcal{O}_s is finite. Let its order be n . Now, consider the point

$$x = \frac{1}{n} \sum_{i=1}^n s_i,$$

where s_i is the i th element in \mathcal{O}_s . We can now act on x by some arbitrary element $g = \{a, O\}$ in G get

$$gx = O \frac{1}{n} \sum_{i=1}^n s_i + an/n = \frac{1}{n} \sum_{i=1}^n Os_i + a = \frac{1}{n} \sum_{i=1}^n gs_i.$$

However, the set $\{x_i\} = g\{x_i\}$ since g is a permutation, and thus the two sums above are equal (just re-ordered). Therefore, $gx = x$ for all $g \in G$. \square

This kind of point that is invariant under *all* transformations is called a **fixed point**. In fact, the type of group we just outlined here (finite extent + discrete) are called **point groups**, since (as we just proved), they all have some fixed point!

In addition, these point groups are also helpful since we can assume (WLOG) that the fixed point is Θ . As mentioned previously, for any point group G with fixed point Θ , we can transform it into G_a (the same group but with fixed point a) by taking the conjugate T_aGT_{-a} . The second of these two theorems narrows our search to finite groups.

Theorem 5.2. Let G be a discrete subgroup of $E(3)$ that has fixed point x . Then, G is a finite subgroup of $O_x(3)$.

Proof. First, we note that G cannot contain translations since they leave no point fixed. We can construct a unit sphere around x , and 4 non-coplanar points $\{p_1, p_2, p_3, p_4\}$ on the sphere (see *Note.*). We can then see that all elements in the orbits of the p_i are also on the sphere, as $\|gp_i - y\| = \|gp_i - gy\| = \|p_i - y\|$. Then, each transformation $g \in G$ is uniquely described by their action on the p_i . If $gx_i = g'x_i$, then the x_i are fixed by $g^{-1}g$, this product must then be the identity.

Note. We need at minimum 4 non-coplanar points. We can leave 2 points invariant with a rotation, 3 invariant with a plane reflection. With 4 points no transformation leaves all 4 invariant. \square

All that remains now to find all point groups is to find all finite subgroups of $O(3)$! We split these points into two families: point groups of the **first kind**, which contain only rotations, and point groups of the **second kind**, which also contain rotation-inversions!

6 Point Groups of the First Kind

In order to find all point groups of the first kind, we first have to define something called a **pole**.

Definition (Pole). Let G be a point group with fixed point x . We can make G act on a ball B with center x . Then, a **pole** on B is some point that is fixed under some non-trivial rotation $g \in G$. We can also define it as an element of the intersection of the axis k of g and B .

Then, for any point group G we can instead have it act on the set S of **poles** of G . We can see it is G is a symmetry group on S since if $g_1 p = p$, then $g_2 p$ is a pole of $g_2 g_1 g_2^{-1}$.

We can get a restriction on the $\#$ of orbits of poles as well as find exact values for the size of stabilizers by summing the amount of transformations that fix a pole (over all poles, **will** overcount).

Theorem 6.1. Let G be a point group, and P be the set of poles of G . Then, the amount of distinct orbits in P is either 2 or 3.

Proof. Let P be the amount of orbits in P , and $|G| = n$. Let \mathcal{O}_i be the i th orbit. Then, let n_i and p_i denote the order of the stabilizer of some element $x \in \mathcal{O}_i$ and $|\mathcal{O}_i|$ respectively (see *Note.*). Thus, the amount of (non trivial) rotations that fix any pole in \mathcal{O}_i is exactly $p_i(n_i - 1)$. From here, we can sum over all the orbits to get $\sum_{i=1}^P p_i(n_i - 1)$, the amount of rotations that leave some pole fixed.

On the other hand, all rotations leave exactly two poles fixed, so the sum must be equal to $2(n - 1)$ (again, subtract 1 to remove the trivial rotation E_3). Thus,

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

Using Theorem 3.1, ($p_i = n/n_i$), we can further reduce:

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

There are no solutions for $P = 1$, since $n \geq n_i$. Also, there are no solutions for $P \geq 4$, as $n_i \geq 2$, meaning

$$2 - \frac{4}{n} < 2 \leq 4 - \frac{1}{n_1} - \frac{1}{n_2} - \frac{1}{n_3} - \frac{1}{n_4}$$

(remember, a pole is an element fixed by a *non-trivial* rotation).

Note. The order of the stabilizers of elements in the same orbit are all the same by Theorem 3.1 □

We now list the all possible configurations orders (n_1, n_2) and (n_1, n_2, n_3) . WLOG we can let $n_1 \leq n_2 \leq n_3$.

P = 2 :

There is only one infinite family of point groups that have two orbits. Solving the equation $2 - 2/n = 2 - 1/n_1 - 1/n_2$ tells us that $n = n_1 = n_2$. There is then only one axis of rotation since there are two poles by $p_i = n/n_i$. There are n rotations around this axis, denote them $R(\theta_1), R(\theta_2), \dots, R(\theta_n)$ (we can omit the axis of rotation since there is only one). We can prove that $\theta_i = 2\pi i/n$:

WLOG we can say that $\theta_1 < \theta_2 < \dots < \theta_n$. We can then represent any $R(\theta_j)$, $2 \leq j \leq n$ by $R(\theta_1)^k + R(\phi)$, where $\phi < \theta_1$. The rotation $R(\phi)$ must then be in the group, so $\phi = 0$ and $R(\phi) = E_3$. We call such an axis with m rotations a **m-fold** axis.

We call this family of groups a cyclic group with n elements, or C_n . The physical object with complete symmetry group C_n is a pyramid with base n -gon

P = 3 :

There are more cases if $P = 3$. We can first start by assuming $n_1 = n_2$. Then,

$$2 - 2/n = 3 - 1/2 - 1/2 - 1/n_3.$$

and we get the following solution set

(a) $(n_1, n_2, n_3) = (2, 2, m)$ for $m \geq 2$, with $n = 2m$.

There are no other point groups with $n_2 = 2$, so we try the next case, $n_2 = 3$. We get the following solutions:

(b) $(n_1, n_2, n_3) = (2, 3, 3)$, with $n = 12$

(c) $(n_1, n_2, n_3) = (2, 3, 4)$ with $n = 24$

(d) $(n_1, n_2, n_3) = (2, 3, 5)$ with $n = 60$

There are no more solutions of this form (try to solve the equation for $n_3 = 6$). If we try $n_2 = 4$, then we get $2 - 2/n < 2 \leq 3 - 1/2 - 1/4 - 1/n_i$. If we try $n_1 = 3$, we run into a similar issue. So, these represent all possible point groups of type one. We now must calculate them.

(a). We can see there exists an m -fold axis l since $n_3 = m$. We also know there are m 2 fold axis (see *Note.*). Since the poles of the l are in the same orbit, we know all of the two fold axis $\{\tau_i\}$ are perpendicular l . A rotation by $2\pi/m$ maps the τ_i to themselves, and the angle difference between two adjacent τ_i is π/m (since a rotation about some two fold axis must also map the τ_i to themselves).

We call this family of groups D_m , the dihedral group of order $2m$. The corresponding object is a prism with base n -gon.

Note. We get the number of axis of m -fold by counting the number of poles in the corresponding orbit and dividing by two.

(b). There are 3 3 fold axis and 4 three fold axis. Consider the poles $\{p_1, p_2, p_3, p_4\}$ in one of the orbits with 4 elements. Now, consider the stabilizer C_3 of p_1 . A non-trivial element g in this stabilizer must permute all p_j , $2 \leq j \leq 4$ to a *different* pole, since otherwise $g^2 = E$ a contradiction (proper rotations fix at most 2 poles). So, the distance from p_1 to any of the other poles is equal. We can repeat this for the rest of the p_i . Thus, the poles are spread evenly on the sphere, and the symmetry group is a subgroup the symmetries of the tetrahedron. However, the two groups have the same order and are thus equal!

We call this group the tetrahedral group and denote it by T .

(c). There are 3 four fold axis, 6 two fold axis, and 4 three fold axis. We can repeat a similar process as in (b) on the poles of the four fold axis to show that the for poles not lying on the same axis, the distance between them is always equal. Thus, the 3 four fold axis are orthogonal. We can then see these 6 poles form an octahedron, and thus our group is a subset of the symmetry group on the octahedron. But once again, the order of these two groups is equal! This group is represented by O .

Note. The symmetries of the octahedron are also the symmetries of the cube.

(d). We know there are 10 three fold axis, 15 two fold axis, and 6 five fold axis. We can take inspiration from previous examples here. These last 2 examples were symmetries of a platonic solid, so lets try checking those to see if they fit our description. The icosahedron also has 10 three fold axis (about centers of faces), 6 five fold axis (through opposite vertices) and 15 two fold axis (through midpoints of opposite edges). This is decent evidence that our symmetry group is exactly that of the icosahedron, and it is! We denote it by Y .

Note. One can prove this more rigorously by considering the set of poles of the five fold axis, dividing them up into hemispheres. From here, we can show each pole has 5 close neighbors of at equal distance. We can then construct an icosahedron using these poles are vertices.

7 Point Groups of the Second Kind

Fortunately, we did most of the heavy lifting finding all of the point groups of type one due to the following theorem.

Theorem 7.1. Let G be a point group and K be a subgroup consisting of only proper rotations. Then, G is exactly one of the following:

1. $G = K$
2. $G = K \cup IK$
3. $G \cong K \cup IK^c$

Proof. Lets consider a point group of the second kind. Suppose that $I \in G$. We know that $|K| = |K^c|$ and $I \notin K$, so it must be the case that $G = IK$.

Now, suppose $I \notin G$. Then, we can let $K^+ = IK^c$. We can see this is a set of proper rotations, and is disjoint from K . Now, we want to show an isomorphism from G to $G^+ = K \cup K^+$. We have

$$\phi(g) = \begin{cases} g & g \in SO(3) \\ Ig & g \notin SO(3). \end{cases}$$

This is clearly a homomorphism since I commutes with all elements. It also must be an isomorphism since if $Ig = Ig'$ then $g = g'$ and any element in G^+ can be mapped to. \square

We can now find the rest of the point groups!

1. $C_n \cup IC_n$
2. $D_n \cup ID_n$
3. $T \cup IT = T_d$
4. $O \cup IO = O_d$
5. $Y \cup IY = Y_h$

We can find the groups from case 3 by looking at point groups of type one that have a normal subgroup with half the total order.

6. $G^+ = C_{2n}$ and $K = C_n$
7. $G^+ = D_n$ and $K = C_n$
8. $G^+ = D_{2n}$ and $K = D_n$
9. $G^+ = O$ and $K = T$

We can use **Schonflies Notation** to classify these groups.

9. This is the complete symmetry group of the tetrahedron, denoted by T_d .
7. This is the symmetry group C_n with vertical reflections through two fold axis added, denoted by C_{nv} .
- 1 + 6. We take the odd n case from 1. and the even n case from 6. This is the symmetry group generated by the rotation reflection $F_K R(\pi/m)$, where K is the plane perpendicular to the vertical axis. This set of group is denoted by S_{2n} .
- 6 + 1. We take odd n from case 6 and even n from case 1. Then, the resulting group is simply C_n in addition to a horizontal reflection perpendicular to the rotation axis. This group is called C_{nh} .

- 2 + 8. We take even/odd parity in the same order as the previous examples. This is actually the complete symmetry group on the prism. We denote it by D_{nh} . It contains C_{nh} as a subgroup.
- 8 + 2. These groups are the complete symmetry groups on twisted prisms, where the top base of a prism is rotated π/m radians from the bottom. We call these D_{nd}

8 Crystallographic Point Groups

In order to define a crystallographic point group, we must first define what they act on: lattices in \mathbb{R}^3 .

Definition (Lattice). A lattice $L \subseteq \mathbb{R}^3$ is a collection of points of the form

$$\{\alpha_1 v_1 + \alpha_2 v_2 + \alpha_3 v_3 : \alpha_i \in \mathbb{Z}; v_i \in T(3)\},$$

where v_i is linearly independent.

Note. This set can also be seen as the orbit of some point x under the translation group generated by T_{v_i} .

Definition (Crystallographic Point Group). A subgroup of $E(3)$ with fixed point x acting on a lattice L is called a **Crystallographic Point Group**. The largest such group on L at x is called the **Holohedry** of L at x .

WLOG we can let the origin Θ be the fixed point going forwards. While we did find all *possible* crystallographic point groups (must be a subset of the point groups by Theorem 5.2), it is not the case that there exists a corresponding lattice for every point group. We know this because of the following theorem.

Theorem 8.1 (The Crystallographic Restriction). If G is a crystallographic point group acting on lattice L , then its rotations and rotation inversions are all of order 2, 3, 4 or 6.

Proof. Let the basic vectors of L be v_1, v_2, v_3 . Then, for $g \in G$, we have

$$gb_i = \sum_{j=1}^3 O_{ji} b_j.$$

Since the b_i are basic vectors, all the O_{ji} must be integers. Importantly, the **trace** of C must be an integer. However, the trace is also independent of basis. So, we can use change of basis on O to transform the rotation matrix O into

$$O' = I^k \begin{pmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

where $k \in \{1, -1\}$ and θ is the size of the rotation. Then, the trace of O' is $\pm(2\cos(\theta) + 1)$. Since this is integral, the only possible values for θ are $0, \pi/3, \pi/2, 2\pi/3, \pi$ corresponding to rotations with degree 2, 3, 4, and 6 (along with the inversion around the fixed point). \square

We then have all possible crystallographic point groups:

$$C_1, C_2, C_3, C_4, C_6, C_{1h}, C_{2h}, C_{3h}, C_{4h}, C_{6h}, C_{2v}, C_{3v}, C_{4v}, C_{6v}, \\ D_2, D_3, D_4, D_6, D_{2h}, D_{3h}, D_{4h}, D_{6h}, S_2, S_4, S_6, D_{2d}, D_{3d}, T, T_d, T_h, O, O_h.$$

These then must be the 32 possible crystallographic point groups. We can show all of these are actually crystallographic point groups by constructing the holohedries and their corresponding lattices, called **bravais lattices**. The following theorems show us there are only 7 possible lattices.

Theorem 8.2. If L is a lattice, the holohedry F on L must include the inversion I .

Proof. Let v_i be the basis vectors. Then, consider arbitrary point $x \in L$. Thus, $x = x_1v_1 + x_2v_2 + x_3v_3$, where $x_i \in \mathbb{Z}$. Then $Ix = -x_1v_1 - x_2v_2 - x_3v_3$. Negating an integer results in an integer, so $Ix \in L$. \square

We can now limit our search to point groups of type 2, corresponding to option 2. in theorem 7.1.

Theorem 8.3. If holohedry F contains subgroup C_n , for $n \in \{3, 4, 6\}$, it also contains subgroup C_{nv} .

Proof. Let l be the n -fold axis. Then, we simply must show there exists a reflection plane through l , since the rotations will generate C_{nv} . Let C be a rotation through axis l by angle $2\pi/n$. We can see that for any lattice point $y \in L$, the point $Cy - y \in P$ where P is the plane perpendicular to l through the origin. Then, there must exist a vector in $L \cap Q$ of minimal length, call it b_1 .

We can then create a new basis for our lattice with b_1, b_2, b_3 where $b_2 = Cb_1$. We know this is the case since b_1 and b_2 are linearly independent and there is no smaller vector a in the parallelogram made by b_1, b_2 (if there was, you could find a vector smaller than b_1).

For our third basis vector b_3 , we can define it as $b_3 = p + t$, where p is a vector in Q and t is a vector parallel to l (p, t not necessarily lattice points). When we act on b_3 with C we get

$$Cb_3 = C(p + t) = Cp + Ct = Cp + t = \alpha_1 b_1 + \alpha_2 b_2 + t$$

subtracting b_3 from both sides and rewriting b_2 yields

$$Cb_3 - b_3 = Cp - p = a_1 b_1 + a_2 Cb_1$$

We can then multiply this equation by C^{-1} and subtract to get

$$Cp + C^{-1}p - 2p = (a_1 - a_2)b_1 + a_2 Cb_1 - a_1 C^{-1}b_1$$

We can prove via trigonometry that $Cp + C^{-1}p = 2 \cos(2\pi/n)p$ (any the same for any point in Q). Therefore,

$$(2 \cos(2\pi/n) - 2)p = (a_1 + a_2)b_2 + (a_1 - a_2 - 2a_1 \cos(2\pi/n))b_1 \quad (1)$$

Now, let K be the plane through l and perpendicular to b_1 . The flip is then F_K . We can see that $F_K b_1 = -b_1$. If $n = 3$, then $F_K b_2 = b_2 + b_1$, if $n = 4$ then $F_K = b_2$ and if $n = 6$ then $F_K = b_2 - b_1$.

To show $F_K b_3 \in L$ is harder. First, remember that $b_3 = p + t$, and $F_K t = t$ since $t \in K$. Then, $F_K b_3 = t + F_K p$. We now split into our three cases.

$n = 6$ We use equation (1) to help all cases. The left hand side becomes $-p$, and we get the following equations.

$$\begin{aligned} p &= -(a_1 + a_2)b_2 + a_2b_1 \\ F_K p &= -(a_1 + a_2)(b_2 - b_1) - a_2b_1 = -(a_1 + a_2)b_2 + a_1b_1 \end{aligned}$$

We can then combine to get $F_K p = v + (a_1 - a_2)b_1$ and thus

$$F_K b_3 = u + v + (a_1 - a_2)b_1 = b_3 + (a_1 - a_2)b_1 \in L.$$

$n = 4$ The left hand side of (1) becomes $-2p$ in this case. Thus,

$$\begin{aligned} p &= -\frac{1}{2}(a_1 + a_2)b_2 - \frac{1}{2}(a_1 - a_2)b_1 \\ F_K p &= -\frac{1}{2}(a_1 + a_2)b_2 + \frac{1}{2}(a_1 - a_2)b_1. \end{aligned}$$

Once again, we get $F_K p = v + (a_1 - a_2)b_1$ and $F_K b_3 = b_3 + (a_1 - a_2)b_1 \in L$.

$n = 3$ The left hand side of (1) is now $-3p$. Then,

$$\begin{aligned} p &= -\frac{1}{3}(a_1 + a_2)b_2 - \frac{1}{3}(2a_1 - a_2)b_1 \\ F_K p &= -\frac{1}{3}(a_1 + a_2)(b_2 + b_1) + \frac{1}{3}(2a_1 - a_2)b_1 = -\frac{1}{3}(a_1 + a_2)b_2 + \frac{1}{3}(a_1 - 2a_2)b_2. \end{aligned}$$

We again get reach the same formula for $F_K b_3$.

□

This finally narrows the crystallographic point groups to exactly the 7 holohedries:

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

9 Bravais Lattices

We conclude with finding the 7 corresponding families of lattices. These are called the **Bravais Lattices**.

To find the Bravais Lattices, we can take a look at some of the specific elements they contain. Other than S_2 , all of these groups have an n -fold axis l where $n \in \{2, 4, 6\}$ and a reflection F_K where K is perpendicular to l . We now find the possible basis vectors for every option of n .

$n = 2$ For each of these cases, we can employ similar strategies as we did to prove theorem 8.3. We retrace our steps, but we call the plane K instead of Q . In this case we *can't* let $b_2 = Cb_1$, since $Cb_1 = -b_1$ (the rotation C is the rotation on the 2 fold axis). However, we *can* find two linearly independent vectors in K by taking $a + F_K a$ on some vectors. Thus, we have $b_1, b_2 \in K$.

Again, we can find b_3 by splitting it into p and t (defined as before). Then, $Cb_3 - b_3 = Cp - p = a_1b_1 + a_2b_2$. Since $Cp = -p$ we have $p = \frac{1}{2}a_1b_1 + \frac{1}{2}a_2b_2$. Thus, $b_3 = t + \frac{1}{2}a_1b_1 + \frac{1}{2}a_2b_2$, with $a_1, a_2 \in \{0, 1\}$ since we can add or subtract multiples of b_1 and b_2 .

$n = 4$ This follows exactly from Theorem 8.3. We have $b_3 = t - \frac{1}{2}(a_1 - a_2)b_1 - \frac{1}{2}(a_1 + a_2)b_2$. $a_1 + a_2$ and $a_1 - a_2$ are either both even or both odd, so we have either

$$b_3 = t \quad \text{or} \quad b_3 = t + \frac{1}{2}b_1 + \frac{1}{2}b_2$$

$n = 6$ This also follows from Theorem 8.3. We instead get $b_3 = t + a_2b_1 - (a_1 + a_2)b_2$. These are both integral, and as such we can repeatedly add or subtract b_1 and b_2 , so $b_3 = t$. This is the only case where b_3 **must** be orthogonal to b_1 and b_2 .

Now we can make the holohedries.

1. **Cubic Holohedry** O_h . Our axis l is one of the three 4 axis. We will only case (1). Thus, we have b_1, b_2 have equal length, b_3 is on l , and they are all orthogonal to each other. O_h has 4 axis of rotations on the plane K , so one must be between vectors b_1 and b_2 . Let this be called l_1 . It is *not* a rotation by $\pi/2$ radians since this would map b_1 and b_2 onto points not in L . Thus, l_1 is a rotation by π . We also need l_1 to make an angle of $\pi/4$ with b_1 and b_2 , since otherwise they would map to elements not in L .

From here, it must be the case that there is an axis of rotation on b_1 and b_2 , and they must be of order 4. A rotation by $\pi/4$ around axis b_2 must map b_3 to either b_1 or b_2 , and thus all basis vectors have the same magnitude. We can see that the resulting lattice has a cube as a primitive cell.

The other possible lattices are the **body centered** or **face centered** variations, which include lattice points in the center of the cube or on all the faces of the cube. In these cases, the primitive cell is *not* the cube. For the rest of the computations for other cases, or visualizations of these lattices see [WM72] and [Tha22] respectively. Refer to these for diagrams and calculations of non-basic variations.

2. **Hexagonal Holohedry** D_{6h} From our previous theorems, we know that b_1, b_2 are in the reflection plane K and are the same length and have angle $\pi/3$. We also know that b_3 is on l , and is thus perpendicular to b_1, b_2 . With our basis vectors found, it is simple to see that D_{6h} is actually a symmetry group on it. There are no variations. It is uniquely determined by $\|b_1\|$ and $\|b_3\|$.

3. **Rhombohedral** D_{3d} . Using the same process as we did to prove Theorem 8.3, we can find b_3 in terms of b_1 , b_2 , and some vector perpendicular to them both, t . We get $b_3 = t + \frac{1}{3}(b_1 - b_2)$ (the case where $b_3 = t$ results in the Hexagonal Holohedry). We know that the 3 twofold rotations must be in K . Again, they are evenly spaced. There must exist a reflection between b_1 and b_3 (inclusive). If it was between the b_1 and b_2 (or b_2 and b_3), then the axis must be halfway between the two vectors. However, this would map $b_3 = t + \frac{1}{3}(b_1 - b_2)$ to $-t + \frac{1}{3}(b_2 - b_1)$, which is impossible. Therefore, all two fold axis must be on basis vectors. Using similar reasoning, the reflection planes must bisect the angles between the two fold axis. These lattices are uniquely determined by $\|b_1\|$ and $\|t\|$.
4. **Tetragonal Holohedry** D_{4h} . Let l be the 4 fold axis. We once again establish basis vectors b_1 and b_2 (of equal length) and get possible values of b_3 from our above case-work. So, we assume $b_3 = t$. We can then see that D_{4h} is indeed a symmetry group on this lattice: two fold rotations (and their corresponding reflections) are through b_1 and b_2 as well as through the angle bisector of (b_1, b_2) and $(b_2, -b_1)$. However, in order for D_{4h} to be the holohedry, we must have $\|b_1\| \neq \|b_3\|$, since otherwise, it would have the hexagonal holohedry.

There is one variation, the body centered variation.

5. **Orthorhombic Holohedry** D_{2h} We have 3 2 fold axis (all orthogonal), as well as the vertical reflection through them. We must have one two fold rotation through t , and it is thus orthogonal to both b_1 and b_2 . So, the other 2 two fold axis are in the plane K . There are two cases here: either the two fold axis are on b_1 and b_2 or they are between b_1 and b_2 . Case two is handled in [WM72]. In the first case, it must be true that the b_i are mutually orthogonal since the two fold axis of D_{2h} are orthogonal. Thus, these are uniquely determined by $\|b_1\|, \|b_2\|, \|b_3\|$.

They have 3 variations stemming from case (2), body and face centered but also **base centered**, where there are lattice points on the centers of the bottom and top face of the cell.

6. **Monoclinic Holohedry** C_{2h} We again have basis vectors b_1 and b_2 . We consider the case $b = p$. We can see that C_{2h} is definitely a symmetry group on this lattice: a rotation around l maps $b_1 \rightarrow -b_1$ and $b_2 \rightarrow -b_2$. The reflection maps $b_3 \rightarrow -b_3$. This is only a holohedry if the angle between b_1 and b_2 and the lengths $\|b_1\|, \|b_2\|, \|b_3\|$ don't overlap with a previously seen lattice.

There is one variation, the base centered variation.

7. **Triclinic Holohedry** S_2 We have $S_2 = \{E_3, I_3\}$, so every lattice not in an above classification must be a Triclinic Holohedry.

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