Examples of groups (continued)

$SO(d)$, $O(d)$ continued

Rotation of an d-dimensional vector:

$$A'_i = \sum_{k=1}^{d} M_{ik} A_k, \quad k = 1, 2, \ldots, d$$

Rotating the coordinate system by θ_{ij} in the (x_i, x_j)-plane:

$$M = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & \cos\theta_{ij} & & \sin\theta_{ij} & & \\ & & & \ddots & & & \\ & & -\sin\theta_{ij} & & \cos\theta_{ij} & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix}$$

Any rotation can be represented as a product of rotations in planes.

$$M = M_1 M_2 \ldots M_n$$

$$\det M = 1$$

Orthogonal group in d dimensions: $O(d) = \mathcal{I} \otimes SO(d)$
What is $\mathcal{I}$ in a general case?
It is a reflection of an odd number of axes!
Reflection of an even number of axes can be achieved by consecutive rotations over π in different planes (odd # of rotations):
$x_1, x_2 :\rightarrow -x_1, -x_2 \equiv$ rotation by π in the (x_1, x_2)-plane.
$x_1, x_2, x_3, x_4 :\rightarrow -x_1, -x_2, -x_3, -x_4 \equiv x_1, x_2 :\rightarrow -x_1, -x_2,$ then $-x_2, x_3 :\rightarrow x_2, -x3$, then $x_2, x_4 :\rightarrow -x_2, -x_4$.

Reflection of the ith axis:

$$\tilde{I} = \begin{pmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & -1 & & & & \\ & & & & 1 & & & \\ & & & & & \ddots & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{pmatrix}$$

$$\det \tilde{I} = -1$$

$$\tilde{M} = \tilde{I} M = M \tilde{I}, \qquad \det \tilde{M} = -1$$

Point groups

$O(d)$ leaves the origin of co-ordinates invariant.
Any subgroup of $O(d)$ has the same property and comprises a point group.
Trivial case:
$O(d'),\ SO(d')$, where $d' = 1, 2, \ldots, d$, are subgroups of $O(d)$.
Subroups are divided into the
1st kind: containing only rotations;
2nd kind: all the others (i.e., containing $\tilde{M}$ with $\det \tilde{M} = -1$).

In what follows, we consider point groups in 3D, i.e., subgroups of $O(d)$.

The simplest case: C_n

There is a (directed) axis C in 3D. Then C_n is the group of rotations around C over angles, which are integer multiples of $2\pi/n$.
If we denote by c_n the rotation over $2\pi/n$, then

$$C_n = \{e, c_n, c_n^2, \ldots, c_n^{n-1}\}.$$

Order of this point group $= n$. C_n is cyclic.

Let $C_n \subseteq G$
Then the axis C is called an axis of the nth order.
If G contains a rotation by π around an axis perpendicular to C or a rotation around C times reflection then c_n and c_n^{-1} are conjugate.
Two axes C and C' are equivalent if c'_n is conjugate to c_n or to c_n^{-1}. This is true, if G contains an element that transforms C to C'.

D_n

This is a group that maps a right prism with an n-sided regular polygon base to itself. It has one axis C_n of the nth order and n axes u_i of the 2nd order orthogonal to C_n.
Rotation around each u_i maps C_n to itself.
c_n and c_n^{n-1} are conjugate; c_n^k and c_n^{n-k} are conjugate.

$$\text{Axes} \quad \left.\begin{array}{lllll} u_1, & u_3, & u_5, & \ldots & \text{are equivalent} \\ u_2, & u_4, & u_6, & \ldots & \text{are equivalent} \end{array}\right\} \text{by rotation around } C_n$$

If n is odd, then all $u_1, u_2, u_3, u_4, \ldots$ are equivalent.
Classes: <u>n even</u>

$$\{e\}, \{c_1, c_n^{n-1}\}, \ldots, \{c_n^{n/2-1}, c_n^{n/2+1}\}, \{c_n^{n/2}\}, \{u_1, u_3, \ldots\}, \{u_2, u_4, \ldots\}$$

$$q(D_n) = \tfrac{1}{2}n + 3$$

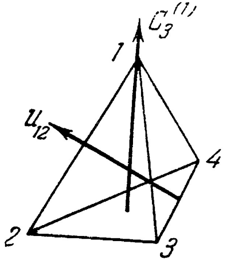
<u>n odd</u>

$$\{e\}, \{c_1, c_n^{n-1}\}, \ldots, \{c_n^{(n-1)/2}, c_n^{(n+1)/2}\}, \{u_1, u_2, u_3, u_4, \ldots\}$$

$$q(D_n) = \tfrac{1}{2}(n + 3)$$

T

The tetrahedral group is a rotational symmetry group of the regular tetrahedron.   Order = 12.

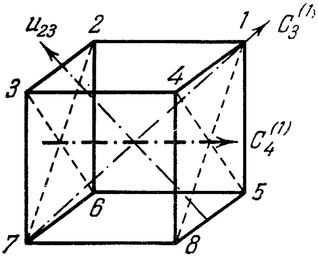


Axes $C_3^{(i)}$, $i = 1, 2, 3, 4$, are equivalent, but unidirectional.
2nd-order axes u_{ik} are equivalent.
Four classes:
$\{e\}, \{c_3^{(1)}, \ldots, c_3^{(1)}\}, \{c_3^{(1)\,2}, \ldots, c_3^{(1)\,2}\}, \{u_{12}, u_{13}, u_{23}\}$

O

The octahedral group is a rotational symmetry group of the cube.

Order = 24. O is isomorphic to S_4.



$$\left.\begin{array}{ll} C_3^{(i)}, & i = 1, 2, 3, 4 \\ C_4^{(i)}, & i = 1, 2, 3 \end{array}\right\} \text{two} - \text{directional}$$

2nd-order axes: $u_{12}, u_{23}, u_{34}, u_{41}, u_{26}, u_{37}$

Classes:

$$\{e\}, \{c_4^{(i)}, c_4^{(i)\,3}\}, \{c_4^{(i)\,2}\}, \{c_3^{(i)}, c_3^{(i)\,2}\}, \{u_{ik}\}$$

I (alternative notation: Y)

The icosahedral group is the rotational symmetry group of both the regular dodecahedron and the regular icosahedron.
Order = 60
Classes:

$$\{e\}, \{c_5^{(i)}, c_5^{(i)\,4}\}, \{c_5^{(i)\,2}, c_5^{(i)\,3}\}, \{c_3^{(j)}, c_3^{(j)\,2}\}, \{c_2^{(k)}\}$$

$$i = 1, \ldots 6; \quad j = 1, \ldots 10; \quad k = 1, \ldots 15$$

This is a full list of the finite point groups of the 1st kind.

Limit $n \to \infty$

C_∞ – trivial (rotations in 2D);
$D_\infty = C_n \otimes U$, where U is a group or rotations around a 2nd-order axis $u \perp C_\infty$

Finite point groups of the 1st kind: Summary

Group	Order	# of classes
C_n	n	n
D_n	$2n$	$\frac{n}{2}+3, \quad n=2k$ $\frac{n+3}{2}, \quad n=2k+1$
T	12	4
O	24	5
Y	60	5

Point groups of the 2nd kind

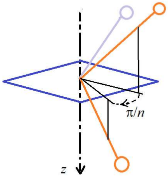
$\mathcal{S}_{2n}$

$2n$-fold rotation-reflection symmetry group (not to be confused with the group of permutations!)

$\mathcal{S}_{2n}$ is a cyclic group of order $2n$:

$e,\ s_{2n},\ s_{2n}^2,\ \ldots,\ s_{2n}^{2n-1}.$

$\{e,\ s_{2n}^2,\ s_{2n}^4,\ \ldots,\ s_{2n}^{2n-2}\} = C_n \subset \mathcal{S}_{2n}$



C_{nh}

Rotations and rotation-reflections over angles (integer) $\times\, 2\pi/n$

Order = 12. Elements:
$c_n^k,\quad \sigma_h c_n^k = s(2\pi k/n), \qquad k = 0, 1, \ldots, n-1,$
σ_h is the reflection in the horizontal ($\perp C_n$) plane.
Each class consists of only one element.

C_{nv}

Group of symmetry of a regular n-gonal pyramid.

n odd $\qquad$ n even

One rotation axis of the order n and n "vertical" (i.e., containing this axis) reflection planes.
C_{nv} and D_n are isomorphous:

$$c_n^k \leftrightarrow c_n^k, \quad \sigma_{k+1} \leftrightarrow u_{k+1}, \qquad k = 0, 1, 2, \ldots, n-1.$$

Isomorphism $\Rightarrow$ the same number of classes,

$$q(C_{nv}) = \frac{n}{2} + 3, \quad n \text{ even}; \qquad q(C_{nv}) = \frac{n+3}{2}, \quad n \text{ odd}$$

D_{nh}

Group of symmetry of a regular n-sided prism.

$4n$ elements: $2n$ elements of C_{nh};

n horizontal 2nd-order axes $u_1, u_2, \dots, u_n$;

n vertical reflection planes $\sigma_1, \sigma_2, \dots, \sigma_n$.

The axis C_n is two-directional. Therefore, the rotations are distributed into classes in the same way as in the group C_{nv}. The same is true for rotation-reflections $\sigma_h c_n^k$.

Other classes:

n even:

$$\{\sigma_1, \sigma_3, \dots, \sigma_{n-1}\},\ \{\sigma_2, \sigma_4, \dots, \sigma_n\},$$

$$\{u_1, u_3, \dots, u_{n-1}\},\ \{u_2, u_4, \dots, u_n\}.$$

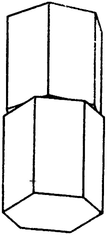
n even:

$$\{\sigma_1, \sigma_2, \sigma_3, \dots, \sigma_{n-1}, \sigma_n\},\ \{u_1, u_2, u_3, \dots, u_{n-1}, u_n\}.$$

Classes in total:

$$q(D_{nh}) = n + 10, \quad n \text{ even}; \qquad q(D_{nh}) = n + 5, \quad n \text{ odd}$$

D_{nd}



Group of symmetry of two regular n-sided prisms, put on top of each other and rotated by π/n with respect to each other.

$4n$ elements: $2n$ elements of $\mathcal{S}_{2n}$;

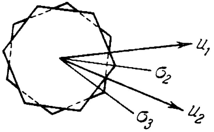
n horizontal 2nd-order axes $u_1, u_2, \ldots, u_n$;

n vertical reflection planes $\sigma_1, \sigma_2, \ldots, \sigma_n$, see the bottom figure.

Classes:

$\{e\}, \{s_{2n}, s_{2n}^{2n-1}\}, \ldots, \{s_{2n}^{n-1}, s_{2n}^{n+1}\}, \{s_{2n}^{n}\},$

$\{u_1, u_2, \ldots, u_n\}, \{\sigma_1, \sigma_2, \ldots, \sigma_n\}$

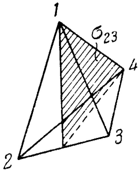


$$q(D_{nd}) = n + 3$$

T_d

Group of symmetry of a tetrahedron.

All edges have the same length



24 elements: 12 elements of the group T;

6 reflections w. resp. to planes

$\sigma_{12}, \sigma_{13}, \sigma_{14}, \sigma_{23}, \sigma_{24}, \sigma_{34}$;

$2 \times 3 = 6$ rotation-reflections

s_4, s_4^3 around each of the

three 2nd-order axes.

<u>Five</u> classes:

$$\{e\},\ \{c_3^{(i)}, c_3^{(i)\,2}\},\ \{u_{ik}\},\ \{s_4^{(ik)}, s_4^{(ik)\,3}\},\ \{\sigma_{ik}\},$$

# of elements	$\{e\}$		$\{c_3^{(i)}, c_3^{(i)\,2}\}$		$\{u_{ik}\}$		$\{s_4^{(ik)}, s_4^{(ik)\,3}\}$		$\{\sigma_{ik}\}$	
	1	+	8	+	3	+	6	+	6	= 24

with all relevant i, k within a class.

T_h

$T_h = \mathcal{I} \otimes T$, where $\mathcal{I}$ is the group of inversion.

24 elements: 12 elements of the group T;
1 inversion;
8 rotations-reflections

$$\mathcal{I} c_3^{(i)} = s_6^{(i)\,5}, \quad \mathcal{I} c_3^{(i)\,2} = s_6^{(i)}, \qquad i = 1, 2, 3, 4;$$

6 reflections

$$\mathcal{I} u_{ik} = \sigma_{ik}, \quad u_{ik} \perp \sigma_{ik}, \qquad \{ik\} = \{12\}, \{13\}, \{14\}.$$

Eight classes:

$$\{e\},\ \{c_3^{(i)}\},\ \{c_3^{(i)\,2}\},\ \{u_{ik}\},\ \{\mathcal{I}\},\ \{s_6^{(i)}\},\ \{s_6^{(i)\,5}\},\ \{\sigma_{ik}\},$$

# of elem. 1 + 4 + 4 + 3 + 1 + 4 + 4 + 3 = 24

with all relevant i, k within a class.

O_h

Group of symmetry of a cube.

48 elements: 24 elements of the group O;

1 inversion;

3 reflections w. resp. to three planes parallel to the sides;

6 reflections w. resp. to planes containing diagonals of opposite sides;

8 rotation-reflections by $\pm\pi/3$ around the four 3rd-order axes;

6 rotation-reflections by $\pm\pi/4$ around the four 4th-order axes.

Six classes are the same as in O; another six classes are obtained from the previous ones by applying inversion.

In total $q(O_h) = 12$

I_h (alternative notation: Y_h)

Group of symmetry of a dodecahedron (Platonic solid with 12 regular pentagonal sides).

$$I_h = \mathcal{I} \otimes I$$

Order $= 120$; $\qquad q(I_h) = 10$

This is a full list of the finite point groups of the 2nd kind.

Limit $n \to \infty$

$$\lim_{n\to\infty} C_{nh} \equiv C_{\infty h}, \qquad \lim_{n\to\infty} C_{nv} \equiv C_{\infty v},$$

$$\lim_{n\to\infty} D_{nh} = \lim_{n\to\infty} D_{nd} \equiv D_{\infty h}$$

Finite point groups of the 2nd kind: Summary

Group	Order	# of classes
S_{2n}	$2n$	$2n$
C_{nh}	$2n$	$2n$
C_{nv}	$2n$	$\frac{n}{2}+3$ . . $n=2k$ $\frac{n+3}{2}$ . . $n=2k+1$
D_{nh}	$4n$	$n+10$ . . $n=2k$ $n+5$ . . $n=2k+1$
D_{nd}	$4n$	$n+3$
T_d	24	5
T_h	24	8
O_h	48	12
I_h	120	10

Crystallographic restriction theorem

Rotational symmetries of a crystal are limited to 2-fold, 3-fold, 4-fold, and 6-fold.

(This does not apply to quasicrystals).

Consider two points, A and B of a crystalline lattice. $\mathbf{r} = \vec{AB}$.

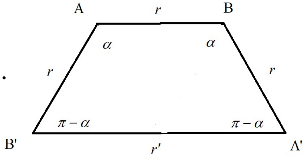
Let α be an angle of rotation leaving the structure invariant.

Rotation by α around A: B $\to$ B$'$.

Rotation by α around B: A $\to$ A$'$.

r$' = \vec{A'B'} = m$r, where m is integer.

Points A, B, B$'$, A$'$ are vertices of a trapezium.



Three sides with a length r, the side A$'$B$'$ is of the length r'.

$$r' = r + 2r\cos(\pi - \alpha) = r - 2r\cos\alpha$$

$$\cos\alpha = -\frac{m-1}{2} = \frac{M}{2}, \qquad M \text{ integer}$$

$|\cos\alpha| \leq 1 \Rightarrow M = 0, \pm 1, \pm 2 \Rightarrow \alpha = 0,\ \pi/3,\ \pi/2,\ 2\pi/3,\ \pi$

Either no rotational symmetry or $C_2,\ C_3,\ C_4,\ C_6$.