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Euclidean group and its subgroups

All possible symmetry operations (space groups) in a crystal can be composed of symmetry operations from the translation group T and one of the so-called crystallographic point groups.

- Define the following terms within the context of crystallography:
  symmetry operation, symmetry element, symmetry group
  Solution:

  Symmetry operation A geometric operation that leaves the crystal unchanged or in other words, a transformation that converts the crystal in itself.
  Example: Rotation by 180° about a two-fold axis.

  Symmetry element The geometric object that is associated with a symmetry operation. It contains all points that stay unchanged during the transformation.
  Example: A mirror plane during a reflection or an axis during a rotation about that axis.

  Symmetry group The group of all transformations under which an object is invariant, i. e. for a tetrahedron it's the tetrahedron group.

- What is the Euclidean group $\mathrm{E}(n)$ and how is it related to the orthogonal group $\mathrm{O}(n)$?
  Solution:
  The elements of $\mathrm{E}(n)$ comprise all distance-preserving transformations in Euclidean space and n dimensions and essentially contain translations, rotations and reflections as well as any combinations of those. The said distance between two points is called Euclidean norm and defined by

$$d(\boldsymbol{p}, \boldsymbol{q}) = \sqrt{\sum_{i=1}^{3}(q_i - p_i)^2} = \|\boldsymbol{q} - \boldsymbol{p}\| \,. \tag{1}$$

  The Euclidean group contains the subgroups T(n) and O(n), which are the translational group and the orthogonal group, and is itself a subgroup of the group of affine transformations (which additionally includes scaling and shearing).

  Mathematically, this can be expressed by a so-called semi-direct product (indicating that translations and orthogonal transformations are not independent) (left) or equivalently as factor group (right),

$$\mathrm{E}(n) \cong \mathrm{T}(n) \rtimes \mathrm{O}(n) \quad \Leftrightarrow \quad \mathrm{O}(n) \cong \mathrm{E}(n)/\mathrm{T}(n) \,. \tag{2}$$

  By excluding reflections (i. e. transformations that do not preserve handedness or orientation), the special Euclidean group $\mathrm{SE}(n)$ or $\mathrm{E}^+(n)$ can be identified as a subgroup. Again decomposing into translational and rotational subgroups yields

$$\mathrm{SE}(n) \cong \mathrm{T}(n) \rtimes \mathrm{SO}(n) \quad \Leftrightarrow \quad \mathrm{SO}(n) \cong \mathrm{SE}(n)/\mathrm{T}(n) \,, \tag{3}$$

  where $\mathrm{SO}(n)$ or $\mathrm{O}^+(n)$ denotes the special orthogonal group, whose elements are the proper or pure rotations, i. e. rotations without reflections. Naturally, $\mathrm{SO}(n)$ is a subgroup of $\mathrm{O}(n)$,

$$\mathrm{O}(n) \cong \mathrm{SO}(n) \times \mathrm{C}_2 \quad \Leftrightarrow \quad \mathrm{SO}(n) \cong \mathrm{O}(n)/\mathrm{C}_2 \,. \tag{4}$$

  with $\mathrm{C}_2 = \{\mathbb{1}, -\mathbb{1}\}$ being the cyclic group of order 2, which consists of the identity and the reflection matrix. In 3 dimensions, SO(3) is also known as the rotation group whose elements are isomorphic to the orthogonal 3x3 matrices with determinant 1,

$$\mathrm{O}(3) = \{A \in M_{3x3} \mid A^\intercal = A^{-1}\} \,, \quad \mathrm{SO}(3) = \{A \in \mathrm{O}(3) \mid \det(A) = 1\} \,. \tag{5}$$

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- Give examples for elements of the rotation group $\mathrm{SO}(3) = \mathrm{O}^+(3)$ and the inversion group $\mathrm{C_i}$ (a. k. a. cyclic group of order 2, $\mathrm{C_2}$). Determine their determinant. Fill the Cayley table for $\mathrm{C_i}$. Show that both symmetry operations commute.

  Solution:

  SO(3) is the special orthogonal group. Its elements are so called "proper rotations", i. e. rotations that preserve the orientation (in contrast to reflections).

  Example: Counter-clockwise rotation by φ around the z-axis in a right-handed Cartesian coordinate system:

$$R(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \det(R(\varphi)) = \cos^2\varphi + \sin^2\varphi = 1\,. \tag{6}$$

  A general rotation of a vector $\boldsymbol{x}$ about an arbitrary axis $\boldsymbol{n}$ (with $\boldsymbol{n}\cdot\boldsymbol{n} = 1$) can be written as

$$R(\varphi\boldsymbol{n})\,\boldsymbol{x} = \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x}) + (\boldsymbol{n}\times\boldsymbol{x})\sin(\varphi) - \boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x})\cos(\varphi)\,, \tag{7}$$

  which is known as the Rodrigues formula. Setting $\varphi = 0$ should yield the initial vector $\boldsymbol{x}$,

$$\begin{aligned} R(0\boldsymbol{n})\,\boldsymbol{x} &= \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x}) - \boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x}) && (8)\\ &= \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x}) - [\boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x}) - \boldsymbol{x}(\boldsymbol{n}\cdot\boldsymbol{n})] && (9)\\ &= \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x}) - \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x}) + \boldsymbol{x} && (10)\\ &= \boldsymbol{x}\,, \qquad \checkmark && (11) \end{aligned}$$

  where the Graßmann formula (a. k. a. "bac-cab" rule),

$$\boldsymbol{a}\times(\boldsymbol{b}\times\boldsymbol{c}) = \boldsymbol{b}(\boldsymbol{a}\cdot\boldsymbol{c}) - \boldsymbol{c}(\boldsymbol{a}\cdot\boldsymbol{b})\,, \tag{12}$$

  has been used.

  Inversion is the reflection at the center of a reference system. It can be represented by the orthogonal matrix

$$I = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{with} \quad \det(I) = (-1)^3 = -1, \tag{13}$$

  and produces the same Cayley table as $\mathrm{C_2}$ since both groups are isomorphic to each other:

$$\begin{array}{c|cc} \mathrm{C_i} & E & I \\ \hline E & E & I \\ I & I & E \end{array} \tag{14}$$

  Let I be the operator corresponding to inversion, i. e. $I\boldsymbol{x} = -\boldsymbol{x}$ and $R(\boldsymbol{\varphi})$ be the same for the rotation, i. e. $R(\boldsymbol{\varphi})\boldsymbol{x} = \boldsymbol{x}'$. Here, $\boldsymbol{\varphi}$ is a vector whose direction is equal to the rotation axis and whose magnitude is equal to the angle which is rotated by. Both operators are obviously linear. We can show:

$$R(\boldsymbol{\varphi})(I\boldsymbol{x}) = R(\boldsymbol{\varphi})(-\boldsymbol{x}) = -R(\boldsymbol{\varphi})\boldsymbol{x} = I(R(\boldsymbol{\varphi})\boldsymbol{x}) \quad \Rightarrow \quad RI = IR\,, \tag{15}$$

  hence both operations (inversion and rotation) do indeed commute.

- What are improper rotations? What is the difference between a roto-inversion and a roto-reflection? Proof that they can be converted into each other. What about their determinant?

  Solution:

  Improper rotations are combinations of a rotation about an axis followed by a reflection on a plane perpendicular to that very axis. More specifically, there are two types of improper rotations that must be distinguished: the roto-reflection, which obeys the initial definition, and the roto-inversion, which is a composition of a rotation about an axis followed by an inversion. However, both can be converted into each other:

  Let $R(\varphi \boldsymbol{n})$ be a rotation by φ about the unit vector $\boldsymbol{n} = \boldsymbol{\varphi}/\varphi$. First we note, that a rotation by 180° followed by an inversion is equal to a reflection on a mirror plane which the rotation axis is perpendicular to (cf. Fig. 1).

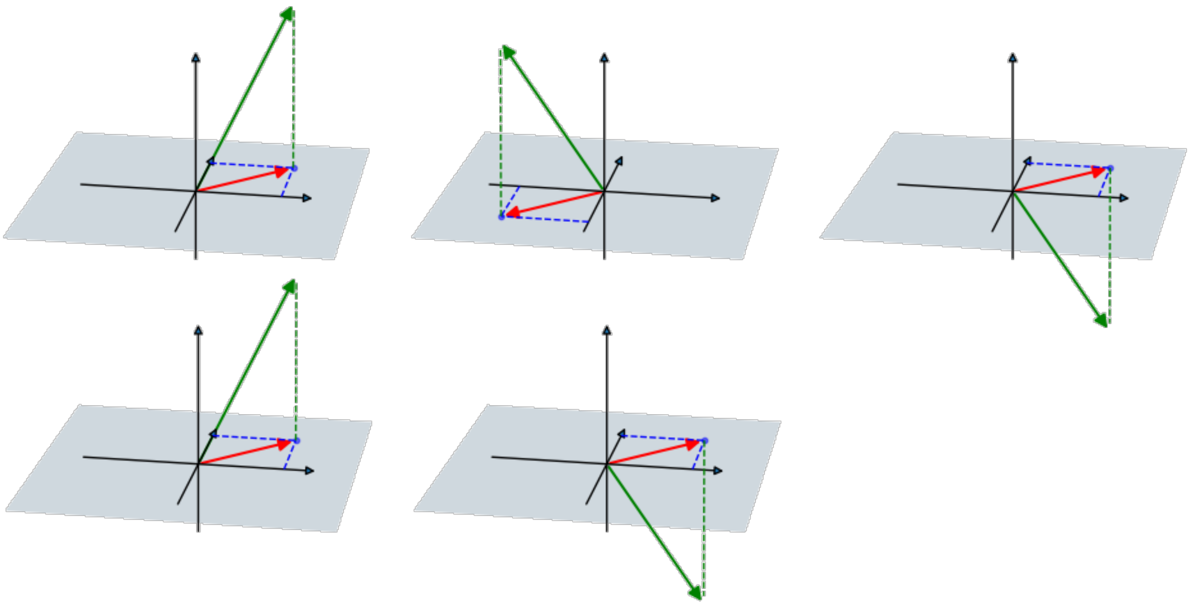

Figure 1: Reflection = Rotation by 180° + Inversion
1st row: initial view → rotation 180° → inversion
2nd row: initial view → reflection

  We will assign the following symbol for reflections:

$$\sigma_{\boldsymbol{n}} \equiv \sigma(\boldsymbol{n}) = IR(\pi \boldsymbol{n})\,. \tag{16}$$

  Now assume a rotation by an arbitrary angle φ instead of 180°. Using the latter geometric identity, we further proof that a roto-reflection (rotation followed by a reflection on the plane perpendicular to the rotation axis) about φ is equal to a roto-inversion (rotation followed by an inversion) about $\pi + \varphi$ (cf. Fig. 2):

$$\sigma(\boldsymbol{n})R(\varphi \boldsymbol{n}) = IR(\pi \boldsymbol{n})R(\varphi \boldsymbol{n}) = IR((\pi + \varphi)\boldsymbol{n})\,. \tag{17}$$

  For roto-reflections, we assign the symbol

$$S_{\boldsymbol{n}}(\varphi) \equiv S(\varphi \boldsymbol{n}) = \sigma(\boldsymbol{n})R(\varphi \boldsymbol{n}) \tag{18}$$

  The determinant of such an improper rotation is always -1 since

$$\det(IR(\alpha \boldsymbol{n})) = \det(I)\det(R(\alpha \boldsymbol{n})) \tag{19}$$

$$= \det(I)\det(R(\alpha_1 \boldsymbol{e}_1))\det(R(\alpha_2 \boldsymbol{e}_2))\det(R(\alpha_3 \boldsymbol{e}_3)) \tag{20}$$

$$= (-1)\cdot 1 \cdot 1 \cdot 1 = -1\,. \tag{21}$$

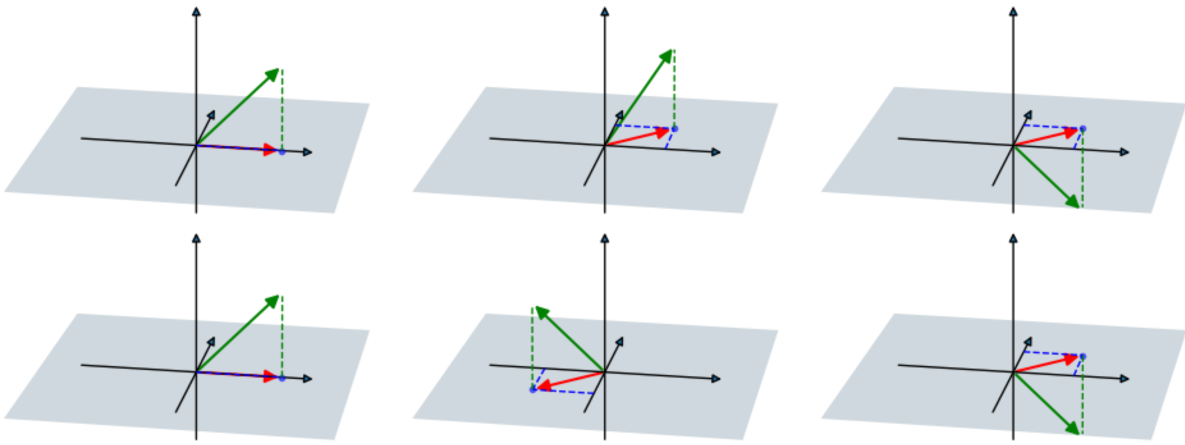

Figure 2: Roto-reflection by φ = Roto-inversion by $\varphi + 180°$
1st row: initial view - rotation φ - reflection
2nd row: initial view - rotation $\varphi + 180°$ - inversion

Example: The roto-reflection $S(\frac{2\pi}{n}\boldsymbol{e}_z)$ is a composition of the two basic operations

i) reflection on the x-y plane σ_z,

ii) n-fold rotation about the z-axis, C_n.

We can immediately construct the corresponding matrix

$$S_z = \sigma_z C_n = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \cos(\frac{2\pi}{n}) & -\sin(\frac{2\pi}{n}) & 0 \\ \sin(\frac{2\pi}{n}) & \cos(\frac{2\pi}{n}) & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos(\frac{2\pi}{n}) & -\sin(\frac{2\pi}{n}) & 0 \\ \sin(\frac{2\pi}{n}) & \cos(\frac{2\pi}{n}) & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{22}$$

with determinant

$$\det(S_z) = -\cos^2\left(\frac{2\pi}{n}\right) - \sin^2\left(\frac{2\pi}{n}\right) = -1\,. \tag{23}$$

Note: S_x, S_y and S_z are usually used to abbreviate $S_{\boldsymbol{n}}$ with $\boldsymbol{n} = \boldsymbol{e}_1, \boldsymbol{e}_2$ or $\boldsymbol{e}_3$, respectively, and similarly for $\sigma_{\boldsymbol{n}}$.