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1.1. A general introduction to groups

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In this chapter we give a general introduction to group theory, which provides the mathematical background for considering symmetry properties. Starting from basic principles, we discuss those properties of groups that are of particular interest in crystallography. To readers interested in a more elaborate treatment of the theoretical background, the standard textbooks by Armstrong (2010), Hill (1999) or Sternberg (2008) are recommended; an account from the perspective of crystallography can also be found in Müller (2013).

1.1.1. Introduction

Crystal structures may be investigated and classified according to their symmetry properties. But in a strict sense, crystal structures in nature are never perfectly symmetric, due to impurities, structural imperfections and especially their finite extent. Therefore, symmetry considerations deal with *idealized* crystal structures that are free from impurities and structural imperfections and that extend infinitely in all directions. In the mathematical model of such an idealized crystal structure, the atoms are replaced by points in a three-dimensional point space and this model will be called a *crystal pattern*.

A symmetry operation of a crystal pattern is a transformation of three-dimensional space that preserves distances and angles and that leaves the crystal pattern as a whole unchanged. The symmetry of a crystal pattern is then understood as the collection of all symmetry operations of the pattern.

The following simple statements about the symmetry operations of a crystal pattern are almost self-evident:

(*a*) If two symmetry operations are applied successively, the crystal pattern is still invariant, thus the combination of the two operations (called their *composition*) is again a symmetry operation.

(*b*) Every symmetry operation can be reversed by simply moving every point back to its original position.

These observations (together with the fact that leaving all points in their position is also a symmetry operation) show that the symmetry operations of a crystal pattern form an algebraic structure called a *group*.

1.1.2. Basic properties of groups

Although groups occur in innumerable contexts, their basic properties are very simple and are captured by the following definition.

Definition. Let $\mathcal{G}$ be a set of elements on which a binary operation is defined which assigns to each pair (g, h) of elements the composition $g \circ h \in \mathcal{G}$. Then $\mathcal{G}$, together with the binary operation $\circ$, is called a *group* if the following hold:

(i) the binary operation is associative, *i.e.* $(g \circ h) \circ k = g \circ (h \circ k)$;

(ii) there exists a *unit element* or *identity element* $e \in \mathcal{G}$ such that $g \circ e = g$ and $e \circ g = g$ for all $g \in \mathcal{G}$;

(iii) every $g \in \mathcal{G}$ has an inverse element, denoted by g^{-1}, for which $g \circ g^{-1} = g^{-1} \circ g = e$.

In most cases, the composition of group elements is regarded as a *product* and is written as $g \cdot h$ or even gh instead of $g \circ h$. An exception is groups where the composition is addition, *e.g.* a group of translations. In such a case, the composition $\mathbf{a} \circ \mathbf{b}$ is more conveniently written as $\mathbf{a} + \mathbf{b}$.

Examples

(i) The group consisting only of the identity element e (with $e \circ e = e$) is called the *trivial group*.

(ii) The group $3m$ of all symmetries of an equilateral triangle is a group with the composition of symmetry operations as binary operation. The group contains six elements, namely three reflections, two rotations and the identity element. It is schematically displayed in Fig. 1.1.2.2.

(iii) The set $\mathbb{Z}$ of all integers forms a group with addition as operation. The identity element is 0, the inverse element for $a \in \mathbb{Z}$ is $-a$.

(iv) The set of complex numbers with absolute value 1 forms a circle in the complex plane, the *unit circle* S^1. The unit circle can be described by $S^1 = \{\exp(2\pi i\, t) \mid 0 \le t < 1\}$ and forms a group with (complex) multiplication as operation.

(v) The set of all real $n \times n$ matrices with determinant $\neq 0$ is a group with matrix multiplication as operation. This group is called the *general linear group* and denoted by $\mathrm{GL}_n(\mathbb{R})$.

If a group $\mathcal{G}$ contains finitely many elements, it is called a *finite group* and the number of its elements is called the *order* of the group, denoted by $|\mathcal{G}|$. A group with infinitely many elements is called an *infinite group*.

For a group element g, its *order* is the smallest integer $n > 0$ such that $g^n = e$ is the identity element. If there is no such integer, then g is said to be of *infinite order*.

The group operation is not required to be *commutative*, *i.e.* in general one will have $gh \neq hg$. However, a group $\mathcal{G}$ in which $gh = hg$ for all g, h is said to be a *commutative* or *abelian group*.

The inverse of the product gh of two group elements is the product of the inverses of the two elements in reversed order, *i.e.* $(gh)^{-1} = h^{-1}g^{-1}$.

A particularly simple type of groups is *cyclic groups* in which all elements are powers of a single element g. A finite cyclic group $\mathcal{C}_n$ of order n can be written as $\mathcal{C}_n = \{g, g^2, \ldots, g^{n-1}, g^n = e\}$. For example, the rotations that are symmetry operations of an equilateral triangle constitute a cyclic group of order 3.

The group $\mathbb{Z}$ of integers (with addition as operation) is an example of an infinite cyclic group in which negative powers also have to be considered, *i.e.* where $\mathcal{G} = \{\ldots, g^{-2}, g^{-1}, e = g^0, g^1, g^2, \ldots\}$.

Groups of small order may be displayed by their *multiplication table*, which is a square table with rows and columns indexed by the group elements and where the intersection of the row labelled by g and of the column labelled by h is the product gh. It follows immediately from the invertibility of the group elements that each row and column of the multiplication table contains every group element precisely once.

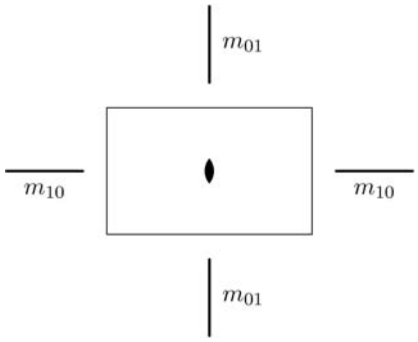

Figure 1.1.2.1
Symmetry group $2mm$ of a rectangle.

Examples

(i) A cyclic group of order 3 consists of the elements $\{g, g^2, g^3 = e\}$. Its multiplication table is

	e	g	g^2
e	e	g	g^2
g	g	g^2	e
g^2	g^2	e	g

(ii) The symmetry group $2mm$ of a rectangle (with unequal sides) consists of a twofold rotation 2, two reflections m_{10}, m_{01} with mirror lines along the coordinate axes and the identity element 1 (see Fig. 1.1.2.1; the small black lenticular symbol in the centre represents the twofold rotation point).

Note that in this and all subsequent examples of crystallographic point groups we will use the Seitz symbols (*cf.* Section 1.4.2.2) for the symmetry operations and the Hermann–Mauguin symbols (*cf.* Section 1.4.1) for the point groups.

The multiplication table of the group $2mm$ is

	1	2	m_{10}	m_{01}
1	1	2	m_{10}	m_{01}
2	2	1	m_{01}	m_{10}
m_{10}	m_{10}	m_{01}	1	2
m_{01}	m_{01}	m_{10}	2	1

The symmetry of the multiplication table (with respect to the main diagonal) shows that this is an abelian group.

(iii) The symmetry group $3m$ of an equilateral triangle consists (apart from the identity element 1) of the threefold rotations 3^+ and 3^- and the reflections m_{10}, m_{01}, m_{11} with mirror lines through a corner of the triangle and the centre of the opposite side (see Fig. 1.1.2.2; the small black triangle in the centre represents the threefold rotation point).

The multiplication table of the group $3m$ is

	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

The fact that $3^+ \cdot m_{10} = m_{11}$, but $m_{10} \cdot 3^+ = m_{01}$ shows that this group is not abelian. It is actually the smallest group (in terms of order) that is not abelian.

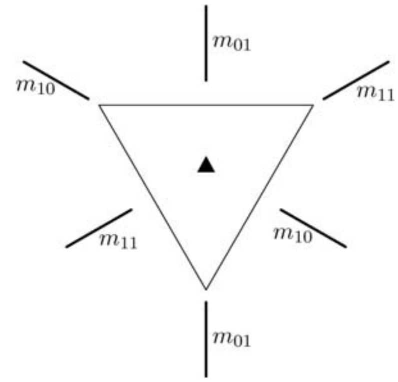

Figure 1.1.2.2
Symmetry group $3m$ of an equilateral triangle.

(iv) The symmetry group $4mm$ of the square consists of the cyclic group generated by the fourfold rotation 4^+ containing the elements $1, 4^+, 2, 4^-$ and the reflections m_{10}, m_{01}, m_{11}, $m_{1\bar{1}}$ with mirror lines along the coordinate axes and the diagonals of the square (see Fig. 1.1.2.3; the small black square in the centre represents the fourfold rotation point).

The multiplication table of the group $4mm$ is

	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
1	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
2	2	1	4^-	4^+	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
4^+	4^+	4^-	2	1	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
4^-	4^-	4^+	1	2	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	1	2	4^-	4^+
m_{01}	m_{01}	m_{10}	m_{11}	$m_{1\bar{1}}$	2	1	4^+	4^-
m_{11}	m_{11}	$m_{1\bar{1}}$	m_{10}	m_{01}	4^+	4^-	1	2
$m_{1\bar{1}}$	$m_{1\bar{1}}$	m_{11}	m_{01}	m_{10}	4^-	4^+	2	1

This group is not abelian, because for example $4^+ \cdot m_{10} = m_{11}$, but $m_{10} \cdot 4^+ = m_{1\bar{1}}$.

The groups that are considered in crystallography do not consist of abstract elements but of symmetry operations with a geometric meaning. In the figures illustrating the groups and also in the symbols used for the group elements, this geometric nature is taken into account. For example, the fourfold rotation 4^+ in the group $4mm$ is represented by the small black square placed at the rotation point and the reflection m_{10} by the line fixed by the reflection. To each crystallographic symmetry operation a *geometric element* is assigned which characterizes the type of the

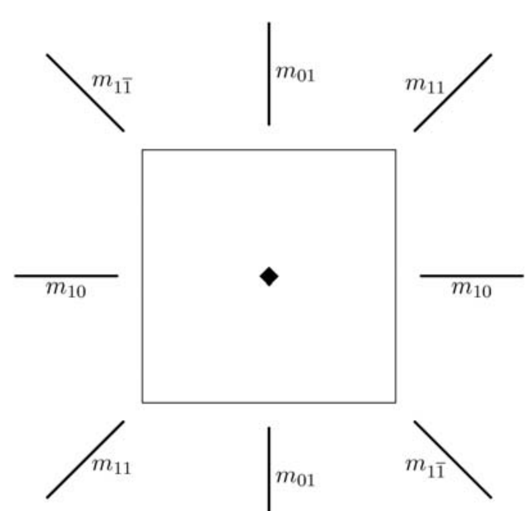

Figure 1.1.2.3
Symmetry group $4mm$ of the square.

symmetry operation. The precise definition of the geometric elements for the different types of operations is given in Section 1.2.3. For a rotation in three-dimensional space the geometric element is the line along the rotation axis and for a reflection it is the plane fixed by the reflection. Different symmetry operations may share the same geometric element, but these operations are then closely related, such as rotations around the same line. One therefore introduces the notion of a *symmetry element*, which is a geometric element together with its associated symmetry operations. In the figures for the crystallographic groups, the symbols like the little black square or the lines actually represent these symmetry elements (and not just a symmetry operation or a geometric element).

It is clear that for larger groups the multiplication table becomes unwieldy to set up and use. Fortunately, for many purposes a full list of all products in the group is actually not required. A very economic alternative of describing a group is to give only a small subset of the group elements from which all other elements can be obtained by forming products.

Definition. A subset $\mathcal{X} \subseteq \mathcal{G}$ is called a set of *generators* for $\mathcal{G}$ if every element of $\mathcal{G}$ can be obtained as a finite product of elements from $\mathcal{X}$ or their inverses. If $\mathcal{X}$ is a set of generators for $\mathcal{G}$, one writes $\mathcal{G} = \langle \mathcal{X} \rangle$.

A group which has a finite generating set is said to be *finitely generated*.

Examples

(i) Every finite group is finitely generated, since $\mathcal{X}$ is allowed to consist of all group elements.

(ii) A cyclic group is generated by a single element. In particular, the infinite cyclic group $(\mathbb{Z}, +)$ is generated by $\mathcal{X} = \{1\}$, but also by $\mathcal{X} = \{-1\}$.

(iii) The symmetry group $4mm$ of the square is generated by a fourfold rotation and any of the reflections, *e.g.* by $\{4^+, m_{10}\}$, but also by two reflections with reflection lines which are not perpendicular, *e.g.* by $\{m_{10}, m_{11}\}$.

(iv) The full symmetry group $m\bar{3}m$ of the cube consists of 48 elements. It can be generated by a fourfold rotation 4^+_{100} around the a axis, a threefold rotation 3^+_{111} around a space diagonal and the inversion $\bar{1}$. It is also possible to generate the group by only two elements, *e.g.* by the fourfold rotation 4^+_{100} and a reflection m_{110} in a plane with normal vector along one of the face diagonals of the cube.

(v) The additive group $(\mathbb{Q}, +)$ of the rational numbers is not finitely generated, because finite sums of finitely many generators $a_1/b_1, a_2/b_2, \ldots, a_n/b_n$ have denominators dividing $b_1 \cdot b_2 \cdot \ldots \cdot b_n$ and thus $1/(1 + b_1 \cdot b_2 \cdot \ldots \cdot b_n)$ is not a finite sum of these generators.

Although one usually chooses generating sets with as few elements as possible, it is sometimes convenient to actually include some redundancy. For example, it may be useful to generate the symmetry group $4mm$ of the square by $\{2, m_{10}, m_{11}\}$. The element 2 is redundant, since $2 = (m_{10}m_{11})^2$, but this generating set explicitly shows the different types of elements of order 2 in the group.

1.1.3. Subgroups

The group of symmetry operations of a crystal pattern may alter if the crystal undergoes a phase transition. Often, some symmetries are preserved, while others are lost, *i.e.* symmetry breaking takes place. The symmetry operations that are preserved form a subset of the original symmetry group which is itself a group. This gives rise to the concept of a subgroup.

Definition. A subset $\mathcal{H} \subseteq \mathcal{G}$ is called a *subgroup* of $\mathcal{G}$ if its elements form a group by themselves. This is denoted by $\mathcal{H} \leq \mathcal{G}$. If $\mathcal{H}$ is a subgroup of $\mathcal{G}$, then $\mathcal{G}$ is called a *supergroup* of $\mathcal{H}$. In order to be a subgroup, $\mathcal{H}$ is required to contain the identity element e of $\mathcal{G}$, to contain inverse elements and to be closed with respect to composition of elements. Thus, technically, every group is a subgroup of itself.

The subgroups of $\mathcal{G}$ that are not equal to $\mathcal{G}$ are called *proper subgroups* of $\mathcal{G}$. A proper subgroup $\mathcal{H}$ of $\mathcal{G}$ is called a *maximal subgroup* if it is not a proper subgroup of any proper subgroup $\mathcal{H}'$ of $\mathcal{G}$.

It is often convenient to specify a subgroup $\mathcal{H}$ of $\mathcal{G}$ by a set $\{h_1, \ldots, h_s\}$ of generators. This is denoted by $\mathcal{H} = \langle h_1, \ldots, h_s \rangle$. The order of $\mathcal{H}$ is not *a priori* obvious from the set of generators. For example, in the symmetry group $4mm$ of the square the pairs $\{m_{10}, m_{01}\}$ and $\{m_{11}, m_{1\bar{1}}\}$ both generate subgroups of order 4, whereas the pair $\{m_{10}, m_{11}\}$ generates the full group of order 8.

The subgroups of a group can be visualized in a *subgroup diagram*. In such a diagram the subgroups are arranged with subgroups of higher order above subgroups of lower order. Two subgroups are connected by a line if one is a maximal subgroup of the other. By following downward paths in this diagram, all group–subgroup relations in a group can be derived. Additional information is provided by connecting subgroups of the same order by a horizontal line if they are *conjugate* (see Section 1.1.7).

Examples

(i) The set $\{e\}$ consisting only of the identity element of $\mathcal{G}$ is a subgroup, called the *trivial subgroup* of $\mathcal{G}$.

(ii) For the group $\mathbb{Z}$ of the integers, all subgroups are cyclic and generated by some integer n, *i.e.* they are of the form $n\mathbb{Z} := \{na \mid a \in \mathbb{Z}\}$ for an integer n. Such a subgroup is maximal if n is a prime number.

(iii) For every element g of a group $\mathcal{G}$, the powers of g form a subgroup of $\mathcal{G}$ which is a cyclic group.

(iv) In $GL_n(\mathbb{R})$ the matrices of determinant 1 form a subgroup, since the determinant of the matrix product $\boldsymbol{A} \cdot \boldsymbol{B}$ is equal to the product of the determinants of $\boldsymbol{A}$ and $\boldsymbol{B}$.

(v) In the symmetry group $3m$ of an equilateral triangle the rotations form a subgroup of order 3 (see Fig. 1.1.3.1).

(vi) The symmetry group $2mm$ of a rectangle has three subgroups of order 2, generated by the reflection m_{10}, the twofold rotation 2 and the reflection m_{01}, respectively (see Fig. 1.1.3.2).

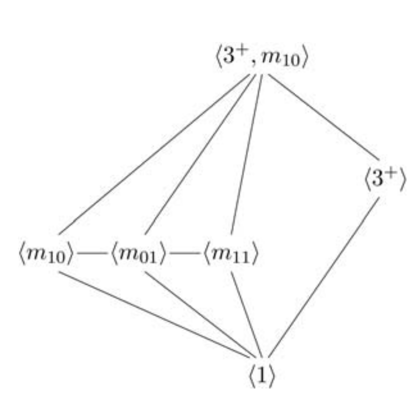

Figure 1.1.3.1
Subgroup diagram for the symmetry group $3m$ of an equilateral triangle.

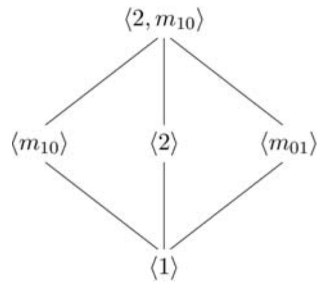

Figure 1.1.3.2
Subgroup diagram for the symmetry group 2*mm* of a rectangle.

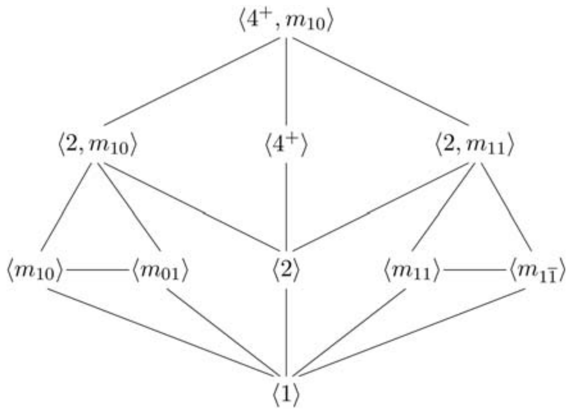

Figure 1.1.3.3
Subgroup diagram for the symmetry group 4*mm* of the square.

(vii) In the symmetry group 4*mm* of the square, the reflections m_{10} and m_{01} together with their product 2 and the identity element 1 form a subgroup of order 4. This subgroup can be recognized in the subgroup diagram of 4*mm* as the subdiagram of the subgroups of $\langle 2, m_{10}\rangle$ in the left part of Fig. 1.1.3.3 which coincides with the subgroup diagram of 2*mm* in Fig. 1.1.3.2. A different subgroup of order 4 is formed by the other pair of perpendicular reflections m_{11}, $m_{1\bar{1}}$ together with 2 and 1 and a third subgroup of order 4 is the cyclic subgroup $\langle 4^+\rangle$ generated by the fourfold rotation (see Fig. 1.1.3.3).

1.1.4. Cosets

A subgroup allows us to partition a group into disjoint subsets of the same size, called *cosets*.

Definition. Let $\mathcal{H} = \{h_1, h_2, h_3, \ldots\}$ be a subgroup of $\mathcal{G}$. Then for $g \in \mathcal{G}$ the set

$$g\mathcal{H} := \{gh_1, gh_2, gh_3, \ldots\} = \{gh \mid h \in \mathcal{H}\}$$

is called the *left coset* of $\mathcal{H}$ with *representative* g. Analogously, the *right coset* with representative g is defined as

$$\mathcal{H}g := \{h_1g, h_2g, h_3g, \ldots\} = \{hg \mid h \in \mathcal{H}\}.$$

The coset $e\mathcal{H} = \mathcal{H} = \mathcal{H}e$ is called the *trivial coset* of $\mathcal{H}$.

Remarks

(i) Since two elements gh and gh' in the same coset $g\mathcal{H}$ can only be the same if $h = h'$, the elements of $g\mathcal{H}$ are in one-to-one correspondence with the elements of $\mathcal{H}$. In particular, for a finite subgroup $\mathcal{H}$ the number of elements in each coset of $\mathcal{H}$ equals the order $|\mathcal{H}|$ of the subgroup $\mathcal{H}$.

(ii) Every element contained in $g\mathcal{H}$ may serve as representative for this coset, *i.e.* $g'\mathcal{H} = g\mathcal{H}$ for every $g' \in g\mathcal{H}$. In particular, if an element g'' is contained in the intersection $g\mathcal{H} \cap g'\mathcal{H}$ of two cosets, one has $g''\mathcal{H} = g\mathcal{H}$ and $g''\mathcal{H} = g'\mathcal{H}$. This implies that two cosets are either disjoint (*i.e.* contain no common element) or they are equal.

These two remarks have an important consequence: since an element $g \in \mathcal{G}$ is contained in the coset $g\mathcal{H}$, the cosets of $\mathcal{H}$ partition the elements of $\mathcal{G}$ into sets of the same cardinality as $\mathcal{H}$ (which is of the order of $\mathcal{H}$ in the case where this is finite).

Definition. If the number of different cosets of a subgroup $\mathcal{H} \le \mathcal{G}$ is finite, this number is called the *index* of $\mathcal{H}$ in $\mathcal{G}$, denoted by $[i]$ or $[\mathcal{G} : \mathcal{H}]$. Otherwise, $\mathcal{H}$ is said to have *infinite index* in $\mathcal{G}$.

In the case of a finite group, the partitioning of the elements of $\mathcal{G}$ into the cosets of $\mathcal{H}$ shows that both the order of $\mathcal{H}$ and the index of $\mathcal{H}$ in $\mathcal{G}$ divide the order of $\mathcal{G}$. This is summarized in the following famous result.

Lagrange's theorem

For a finite group $\mathcal{G}$ and a subgroup $\mathcal{H}$ of $\mathcal{G}$ one has

$$|\mathcal{G}| = |\mathcal{H}| \cdot [\mathcal{G} : \mathcal{H}],$$

i.e. the order of a subgroup multiplied by its index gives the order of the full group.

For example, a group of order n cannot have a proper subgroup of order larger than $n/2$.

Whether or not two cosets of a subgroup $\mathcal{H}$ are equal depends on whether the quotient of their representatives is contained in $\mathcal{H}$: for left cosets one has $g\mathcal{H} = g'\mathcal{H}$ if and only if $g^{-1}g' \in \mathcal{H}$ and for right cosets $\mathcal{H}g = \mathcal{H}g'$ if and only if $g'g^{-1} \in \mathcal{H}$.

Definition. If $\mathcal{H}$ is a subgroup of $\mathcal{G}$ and $g_1, g_2, g_3, \ldots \in \mathcal{G}$ are such that $g_i\mathcal{H} \ne g_j\mathcal{H}$ for $i \ne j$, and every $g \in \mathcal{G}$ is contained in some left coset $g_i\mathcal{H}$, then $g_1, g_2, g_3, \ldots$ is called a system of *left coset representatives* of $\mathcal{G}$ relative to $\mathcal{H}$. It is customary to choose $g_1 = e$ so that the coset $g_1\mathcal{H} = e\mathcal{H} = \mathcal{H}$ is the subgroup $\mathcal{H}$ itself. The decomposition

$$\mathcal{G} = \mathcal{H} \cup g_2\mathcal{H} \cup g_3\mathcal{H} \ldots$$

is called the *coset decomposition* of $\mathcal{G}$ into left cosets relative to $\mathcal{H}$.

Analogously, $g_1', g_2', g_3', \ldots \in \mathcal{G}$ is called a system of *right coset representatives* if $\mathcal{H}g_i' \ne \mathcal{H}g_j'$ for $i \ne j$ and every $g \in \mathcal{G}$ is contained in some right coset $\mathcal{H}g_i$. Again, one usually chooses $g_1' = e$ and the decomposition

$$\mathcal{G} = \mathcal{H} \cup \mathcal{H}g_2' \cup \mathcal{H}g_3' \ldots$$

is called the *coset decomposition* of $\mathcal{G}$ into right cosets relative to $\mathcal{H}$.

To obtain the coset decomposition one starts by choosing $\mathcal{H}$ as the first coset (with representative e). Next, an element $g_2 \in \mathcal{G}$ with $g_2 \notin \mathcal{H}$ is selected as representative for the second coset $g_2\mathcal{H}$. For the third coset, an element $g_3 \in \mathcal{G}$ with $g_3 \notin \mathcal{H}$ and $g_3 \notin g_2\mathcal{H}$ is required. If at a certain stage the cosets $\mathcal{H}, g_2\mathcal{H}, \ldots, g_m\mathcal{H}$ have been defined but do not yet exhaust $\mathcal{G}$, an element g_{m+1} not contained in the union $\mathcal{H} \cup g_2\mathcal{H} \cup \ldots \cup g_m\mathcal{H}$ is chosen as representative for the next coset.

Examples

(i) Let $\mathcal{G} = 3m$ be the symmetry group of an equilateral triangle and $\mathcal{H} = \langle 3^+\rangle$ its subgroup containing the rotations. Then for every reflection $m \in \mathcal{G}$ the elements e, m form a system of coset representatives of $\mathcal{G}$ relative to $\mathcal{H}$ and the coset decomposition is $\mathcal{G} = \{1, 3^+, 3^-\} \cup \{m_{10}, m_{01}, m_{11}\}$.

(ii) For any integer n, the set $n\mathbb{Z} := \{na \mid a \in \mathbb{Z}\}$ of multiples of n forms an infinite subgroup of index n in $\mathbb{Z}$. A system of coset representatives of $\mathbb{Z}$ relative to $n\mathbb{Z}$ is formed by the numbers $0, 1, 2, \ldots, n-1$. The coset with representative 0 is $\{\ldots, -n, 0, n, 2n, \ldots\}$, the coset with representative 1 is $\{\ldots, -n+1, 1, n+1, 2n+1, \ldots\}$ and an integer a belongs to the coset with representative k if and only if a gives remainder k upon division by n.

1.1.5. Normal subgroups, factor groups

In general, the left and right cosets of a subgroup $\mathcal{H}$ differ, for example in the symmetry group $3m$ of an equilateral triangle the left coset decomposition with respect to the subgroup $\mathcal{H} = \{1, m_{10}\}$ is

$$\begin{aligned}&\{1, m_{10}\} \cup 3^+\{1, m_{10}\} \cup 3^-\{1, m_{10}\}\\ =&\{1, m_{10}\} \cup \{3^+, m_{11}\} \cup \{3^-, m_{01}\},\end{aligned}$$

whereas the right coset decomposition is

$$\begin{aligned}&\{1, m_{10}\} \cup \{1, m_{10}\}3^+ \cup \{1, m_{10}\}3^-\\ =&\{1, m_{10}\} \cup \{3^+, m_{01}\} \cup \{3^-, m_{11}\}.\end{aligned}$$

For particular subgroups, however, it turns out that the left and right cosets coincide, *i.e.* one has $g\mathcal{H} = \mathcal{H}g$ for all $g \in \mathcal{G}$. This means that for every $h \in \mathcal{H}$ and every $g \in \mathcal{G}$ the element gh is of the form $gh = h'g$ for some $h' \in \mathcal{H}$ and thus $ghg^{-1} = h' \in \mathcal{H}$. The element $h' = ghg^{-1}$ is called the *conjugate of h by g*. Note that in the definition of the conjugate element there is a choice whether the inverse element g^{-1} is placed to the left or right of h. Depending on the applications that are envisaged and on the preferences of the author, both versions ghg^{-1} and $g^{-1}hg$ are found in the literature, but in the context of crystallographic groups it is more convenient to have the inverse g^{-1} to the right of h.

An important aspect of conjugate elements is that they share many properties, such as the order or the type of symmetry operation. As a consequence, conjugate symmetry operations have the same type of geometric elements. For example, if h is a threefold rotation in three-dimensional space, its geometric element is the line along the rotation axis. The geometric element of a conjugate element ghg^{-1} is then also a line fixed by a threefold rotation, but in general this line has a different direction.

Definition. A subgroup $\mathcal{H}$ of $\mathcal{G}$ is called a *normal subgroup* if $ghg^{-1} \in \mathcal{H}$ for all $g \in \mathcal{G}$ and all $h \in \mathcal{H}$. This is denoted by $\mathcal{H} \trianglelefteq \mathcal{G}$. For a normal subgroup $\mathcal{H}$, the left and right cosets of $\mathcal{G}$ with respect to $\mathcal{H}$ coincide.

Remarks

(i) The full group $\mathcal{G}$ and the trivial subgroup $\{e\}$ are always normal subgroups of $\mathcal{G}$. These are often called the *trivial* normal subgroups of $\mathcal{G}$.

(ii) In abelian groups, every subgroup is a normal subgroup, because $gh = hg$ implies $ghg^{-1} = h \in \mathcal{H}$.

(iii) A subgroup $\mathcal{H}$ of index 2 in $\mathcal{G}$ is always a normal subgroup, since the coset decomposition relative to $\mathcal{H}$ consists of only two cosets and for any element $g \notin \mathcal{H}$ the left and right cosets $g\mathcal{H}$ and $\mathcal{H}g$ both consist precisely of those elements of $\mathcal{G}$ that are not contained in $\mathcal{H}$. Therefore, $g\mathcal{H} = \mathcal{H}g$ for $g \notin \mathcal{H}$ and for $h \in \mathcal{H}$ clearly $h\mathcal{H} = \mathcal{H} = \mathcal{H}h$ holds.

(iv) In order to check whether a subgroup $\mathcal{H}$ of $\mathcal{G}$ is a normal subgroup it is sufficient to check whether $ghg^{-1} \in \mathcal{H}$ for generators g of $\mathcal{G}$ and generators h of $\mathcal{H}$. This is due to the fact that on the one hand $(g_1g_2)\,h\,(g_1g_2)^{-1} = g_1(g_2hg_2^{-1})g_1^{-1}$ and on the other hand $g(h_1h_2)g^{-1} = (gh_1g^{-1})(gh_2g^{-1})$.

Examples

(i) In the symmetry group $3m$ of an equilateral triangle, the subgroup generated by the threefold rotation 3^+ is a normal subgroup because it is of index 2 in $3m$.
The subgroups of order 2 generated by the reflections m_{10}, m_{01} and m_{11} are not normal because $3^+ \cdot m_{10} \cdot 3^- = m_{01} \notin \langle m_{10}\rangle$, $3^+ \cdot m_{01} \cdot 3^- = m_{11} \notin \langle m_{01}\rangle$ and $3^+ \cdot m_{11} \cdot 3^- = m_{10} \notin \langle m_{11}\rangle$.

(ii) In the symmetry group $4mm$ of the square, the subgroups $\langle 2, m_{10}\rangle$, $\langle 4^+\rangle$, and $\langle 2, m_{11}\rangle$ are normal subgroups because they are subgroups of index 2.
The subgroups of order 2 generated by the reflections m_{10}, m_{01}, m_{11} and $m_{1\bar{1}}$ are not normal because $4^+ \cdot m_{10} \cdot 4^- = m_{01} \notin \langle m_{10}\rangle$, $4^+ \cdot m_{01} \cdot 4^- = m_{10} \notin \langle m_{01}\rangle$, $4^+ \cdot m_{11} \cdot 4^- = m_{1\bar{1}} \notin \langle m_{11}\rangle$ and $4^+ \cdot m_{1\bar{1}} \cdot 4^- = m_{11} \notin \langle m_{1\bar{1}}\rangle$.
The subgroup of order 2 generated by the twofold rotation 2 is normal because $4^+ \cdot 2 \cdot 4^- = 2$ and $m_{10} \cdot 2 \cdot m_{10}^{-1} = 2$.

For a subgroup $\mathcal{H}$ of $\mathcal{G}$ and an element $g \in \mathcal{G}$, the conjugates ghg^{-1} form a subgroup

$$\mathcal{H}' = g\mathcal{H}g^{-1} = \{ghg^{-1} \mid h \in \mathcal{H}\}$$

because $gh_1g^{-1} \cdot gh_2g^{-1} = gh_1h_2g^{-1}$. This subgroup is called the *conjugate subgroup* of $\mathcal{H}$ by g. As already noted, conjugation does not alter the type of symmetry operations and their geometric elements, but it is possible that the orientations of the geometric elements are changed.

Using the concept of conjugate subgroups, a normal subgroup is a subgroup $\mathcal{H}$ that coincides with all its conjugate subgroups $g\mathcal{H}g^{-1}$. This means that the set of geometric elements of a normal subgroup is not changed by conjugation; the single geometric elements may, however, be permuted by the conjugating element. In the example of the symmetry group $4mm$ discussed above, the normal subgroup $\langle 2, m_{10}\rangle$ contains the reflections m_{10} and m_{01} with the lines along the coordinate axes as geometric elements. These two lines are interchanged by the fourfold rotation 4^+, corresponding to the fact that conjugation by 4^+ interchanges m_{10} and m_{01}. The concept of conjugation will be discussed in more detail in Section 1.1.8.

One of the main motivations for studying normal subgroups is that they allow us to define a group operation on the cosets of $\mathcal{H}$ in $\mathcal{G}$. The products of any element in the coset $g\mathcal{H}$ with any element in the coset $g'\mathcal{H}$ lie in a single coset, namely in the coset $gg'\mathcal{H}$. Thus we can define the product of the two cosets $g\mathcal{H}$ and $g'\mathcal{H}$ as the coset with representative gg'.

Definition. The set $\mathcal{G}/\mathcal{H} := \{g\mathcal{H} \mid g \in \mathcal{G}\}$ together with the binary operation

$$g\mathcal{H} \circ g'\mathcal{H} := gg'\mathcal{H}$$

forms a group, called the *factor group* or *quotient group* of $\mathcal{G}$ by $\mathcal{H}$.

The identity element of the factor group $\mathcal{G}/\mathcal{H}$ is the coset $\mathcal{H}$ and the inverse element of $g\mathcal{H}$ is the coset $g^{-1}\mathcal{H}$.

A familiar example of a factor group is provided by the times on a clock. If it is 8 o'clock (in the morning) now, then we say that in nine hours it will be 5 o'clock (in the afternoon). We regard times as elements of the factor group $\mathbb{Z}/12\mathbb{Z}$ in which

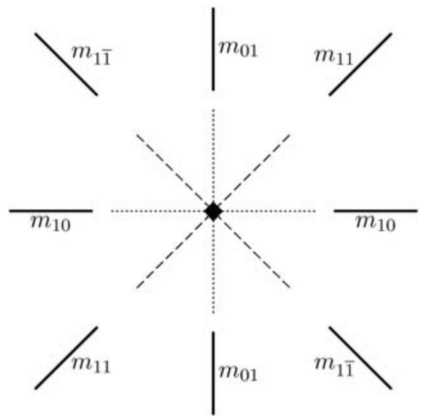

Figure 1.1.5.1
Symmetry group of an eightfold star.

$(8 + 12\mathbb{Z}) + (9 + 12\mathbb{Z}) = 17 + 12\mathbb{Z} = 5 + 12\mathbb{Z}$. In the factor group $\mathbb{Z}/12\mathbb{Z}$, the clock is imagined as a circle of circumference 12 around which the line of integers is wrapped so that integers with a difference of 12 are located at the same position on the circle.

The clock example is a special case of factor groups of the integers. We have already seen that the set $n\mathbb{Z} = \{na \mid a \in \mathbb{Z}\}$ of multiples of a natural number n forms a subgroup of index n in $\mathbb{Z}$. This is a normal subgroup, since $\mathbb{Z}$ is an abelian group. The factor group $\mathbb{Z}/n\mathbb{Z}$ represents the addition of integers *modulo n*.

Examples

(i) If we take $\mathcal{G}$ to be the symmetry group $4mm$ of the square and choose as normal subgroup the subgroup $\mathcal{H} = \langle 4^+ \rangle$ generated by the fourfold rotation, we obtain a factor group $\mathcal{G}/\mathcal{H}$ with two elements, namely the cosets $\mathcal{H} = \{1, 2, 4^+, 4^-\}$ and $m_{10}\mathcal{H} = \{m_{10}, m_{01}, m_{11}, m_{1\bar{1}}\}$. The trivial coset $\mathcal{H}$ is the identity element in the factor group $\mathcal{G}/\mathcal{H}$ and contains the rotations in $4mm$. The other element $m_{10}\mathcal{H}$ in the factor group $\mathcal{G}/\mathcal{H}$ consists of the reflections in $4mm$.

In this example, the separation of the rotations and reflections in $4mm$ into the two cosets $\mathcal{H}$ and $m_{10}\mathcal{H}$ makes it easy to see that the product of two cosets is independent of the chosen representative of the coset: the product of two rotations is again a rotation, hence $\mathcal{H} \cdot \mathcal{H} = \mathcal{H}$, the product of a rotation and a reflection is a reflection, hence $\mathcal{H} \cdot m_{10}\mathcal{H} = m_{10}\mathcal{H} \cdot \mathcal{H} = m_{10}\mathcal{H}$, and finally the product of two reflections is a rotation, hence $m_{10}\mathcal{H} \cdot m_{10}\mathcal{H} = \mathcal{H}$. The multiplication table of the factor group is thus

	$\mathcal{H}$	$m_{10}\mathcal{H}$
$\mathcal{H}$	$\mathcal{H}$	$m_{10}\mathcal{H}$
$m_{10}\mathcal{H}$	$m_{10}\mathcal{H}$	$\mathcal{H}$

(ii) The symmetry group of a square is the same as the symmetry group of an eightfold star, as shown in Fig. 1.1.5.1. If we regard the star as being built from four lines (two dotted and two dashed), then the twofold rotation does not move any of the lines, it only interchanges the points within each line (symmetric with respect to the centre). Regarding the lines as sets of points, the twofold rotation thus does not change anything. The effects of the different symmetry operations on the lines of the eightfold star are then precisely given by the factor group $\mathcal{G}/\mathcal{H}$, where $\mathcal{G}$ is the symmetry group $4mm$ of the square and $\mathcal{H}$ is the normal subgroup generated by the twofold rotation 2: the cosets relative to $\mathcal{H}$ are $\{1, 2\}$, $\{4^+, 4^-\}$, $\{m_{10}, m_{01}\}$, $\{m_{11}, m_{1\bar{1}}\}$, and these cosets collect together the elements of $4mm$ that have the same effect on the lines of the eightfold star. For example, both 4^+ and 4^- interchange both the two dotted and the two dashed lines, m_{10} and m_{01} both interchange the two dashed lines but fix the two dotted lines and m_{11} and $m_{1\bar{1}}$ both interchange the two dotted lines but fix the two dashed lines. Owing to the fact that $\mathcal{H}$ is a normal subgroup, the product of elements from two cosets always lies in the same coset, independent of which elements are chosen from the two cosets. For example, the product of an element from the coset $\{4^+, 4^-\}$ with an element of the coset $\{m_{10}, m_{01}\}$ always gives an element of the coset $\{m_{11}, m_{1\bar{1}}\}$. Working out the products for all pairs of cosets, one obtains the following multiplication table for the factor group $\mathcal{G}/\mathcal{H}$:

	$\{1, 2\}$	$\{4^+, 4^-\}$	$\{m_{10}, m_{01}\}$	$\{m_{11}, m_{1\bar{1}}\}$
$\{1, 2\}$	$\{1, 2\}$	$\{4^+, 4^-\}$	$\{m_{10}, m_{01}\}$	$\{m_{11}, m_{1\bar{1}}\}$
$\{4^+, 4^-\}$	$\{4^+, 4^-\}$	$\{1, 2\}$	$\{m_{11}, m_{1\bar{1}}\}$	$\{m_{10}, m_{01}\}$
$\{m_{10}, m_{01}\}$	$\{m_{10}, m_{01}\}$	$\{m_{11}, m_{1\bar{1}}\}$	$\{1, 2\}$	$\{4^+, 4^-\}$
$\{m_{11}, m_{1\bar{1}}\}$	$\{m_{11}, m_{1\bar{1}}\}$	$\{m_{10}, m_{01}\}$	$\{4^+, 4^-\}$	$\{1, 2\}$

(iii) If one takes cosets with respect to a subgroup that is not normal, the products of elements from two cosets do not lie in a single coset. As we have seen, the left cosets of the group $3m$ of an equilateral triangle with respect to the non-normal subgroup $\mathcal{H} = \{1, m_{10}\}$ are $\{1, m_{10}\}$, $\{3^+, m_{11}\}$ and $\{3^-, m_{01}\}$. Taking products from elements of the first and second coset, we get $1 \cdot 3^+ = 3^+$ and $1 \cdot m_{11} = m_{11}$, which are both in the second coset, but $m_{10} \cdot 3^+ = m_{01}$ and $m_{10} \cdot m_{11} = 3^-$, which are both in the third coset.

1.1.6. Homomorphisms, isomorphisms

In order to relate two groups, mappings between the groups that are compatible with the group operations are very useful.

Recall that a *mapping* φ from a set A to a set B associates to each $a \in A$ an element $b \in B$, denoted by $\varphi(a)$ and called the *image* of a (under φ).

Definition. For two groups $\mathcal{G}$ and $\mathcal{H}$, a mapping φ from $\mathcal{G}$ to $\mathcal{H}$ is called a *group homomorphism* or *homomorphism* for short, if it is compatible with the group operations in $\mathcal{G}$ and $\mathcal{H}$, *i.e.* if

$$\varphi(gg') = \varphi(g)\varphi(g') \text{ for all } g, g' \text{ in } \mathcal{G}.$$

The compatibility with the group operation is captured in the phrase

The image of the product is equal to the product of the images.

Fig. 1.1.6.1 gives a schematic description of the definition of a homomorphism. For φ to be a homomorphism, the two curved arrows are required to give the same result, *i.e.* first multiplying two elements in $\mathcal{G}$ and then mapping the product to $\mathcal{H}$ must be the same as first mapping the elements to $\mathcal{H}$ and then multiplying them.

It follows from the definition of a homomorphism that the identity element of $\mathcal{G}$ must be mapped to the identity element of $\mathcal{H}$ and that the inverse g^{-1} of an element $g \in \mathcal{G}$ must be mapped to the inverse of the image of g, *i.e.* that $\varphi(g^{-1}) = \varphi(g)^{-1}$. In general, however, other elements than the identity element may also be mapped to the identity element of $\mathcal{H}$.

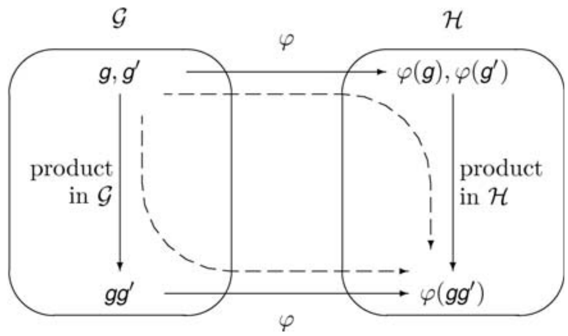

Figure 1.1.6.1
Schematic description of a homomorphism.

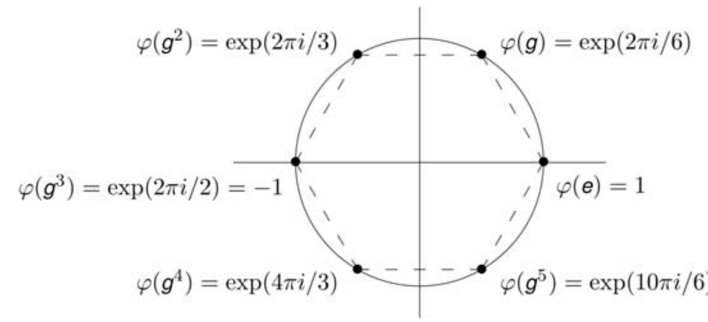

Figure 1.1.6.2
Cyclic group of order 6 embedded in the group of the unit circle.

Definition. Let φ be a group homomorphism from $\mathcal{G}$ to $\mathcal{H}$.

(i) The set $\{g \in \mathcal{G} \mid \varphi(g) = e\}$ of elements mapped to the identity element of $\mathcal{H}$ is called the *kernel* of φ, denoted by $\ker \varphi$.

(ii) The set $\varphi(\mathcal{G}) := \{\varphi(g) \mid g \in \mathcal{G}\}$ is called the *image of $\mathcal{G}$ under φ*.

In the case where only the identity element of $\mathcal{G}$ lies in the kernel of φ, one can conclude that $\varphi(g) = \varphi(g')$ implies $g = g'$ and φ is called an *injective homomorphism*. In this situation no information about the group $\mathcal{G}$ is lost and the homomorphism φ can be regarded as an *embedding* of $\mathcal{G}$ into $\mathcal{H}$.

The image $\varphi(\mathcal{G})$ of any homomorphism from $\mathcal{G}$ to $\mathcal{H}$ forms not just a subset, but a subgroup of $\mathcal{H}$. It is not required that $\varphi(\mathcal{G})$ is all of $\mathcal{H}$, but if this happens to be the case, φ is called a *surjective homomorphism*.

Examples

(i) For the symmetry group $4mm$ of the square a homomorphism φ to a cyclic group $\mathcal{C}_2 = \{e, g\}$ of two elements is given by $\varphi(1) = \varphi(4^+) = \varphi(2) = \varphi(4^-) = e$ and $\varphi(m_{10}) = \varphi(m_{01}) = \varphi(m_{11}) = \varphi(m_{1\bar{1}}) = g$, *i.e.* by mapping the rotations in $4mm$ to the identity element of $\mathcal{C}_2$ and the reflections to the non-trivial element.
Since every element of $\mathcal{C}_2$ is the image of some element of $4mm$, φ is a surjective homomorphism, but it is not injective because the kernel consists of all rotations in $4mm$ and not only of the identity element.

(ii) The cyclic group $\mathcal{C}_n = \{e, g, g^2, \ldots, g^{n-1}\}$ of order n is mapped into the (multiplicative) group S^1 of the unit circle in the complex plane by mapping g^k to $\exp(2\pi ik/n)$. As displayed in Fig. 1.1.6.2, the image of $\mathcal{C}_n$ under this homomorphism are points on the unit circle which form the corners of a regular n-gon.
This is an injective homomorphism because the smallest $k > 0$ with $\exp(2\pi ik/n) = 1$ is $k = n$ and $g^n = e$ in $\mathcal{C}_n$, thus by this homomorphism $\mathcal{C}_n$ can be regarded as a subgroup of S^1. It is clear that φ cannot be surjective, because S^1 is an infinite group and the image $\varphi(\mathcal{C}_n)$ consists of only finitely many elements.

(iii) For the additive group $(\mathbb{Z}, +)$ of integers and a cyclic group $\mathcal{C}_n = \{e, g, g^2, \ldots, g^{n-1}\}$, for every integer q a homomorphism φ is defined by mapping $1 \in \mathbb{Z}$ to g^q, which gives $\varphi(a) = g^{qa}$ for $a \in \mathbb{Z}$. This is never an injective homomorphism, because $n\mathbb{Z} = \{na \mid a \in \mathbb{Z}\}$ is contained in the kernel of φ. Whether or not φ is surjective depends on whether g^q is a generator of $\mathcal{C}_n$. This is the case if and only if n and q have no non-trivial common divisors.

Definition. A homomorphism φ from $\mathcal{G}$ to $\mathcal{H}$ is called an *isomorphism* if $\ker \varphi = \{e\}$ and $\varphi(\mathcal{G}) = \mathcal{H}$, *i.e.* if φ is both injective and surjective. An isomorphism is thus a one-to-one mapping between the elements of $\mathcal{G}$ and $\mathcal{H}$ which is also a homomorphism.

Groups $\mathcal{G}$ and $\mathcal{H}$ between which an isomorphism exist are called *isomorphic groups*, this is denoted by $\mathcal{G} \cong \mathcal{H}$.

Isomorphic groups may differ in the way they are realized, but they coincide in their structure. In essence, one can regard isomorphic groups as the same group with different names or labels for the group elements. For example, isomorphic groups have the same multiplication table if the elements are relabelled according to the isomorphism identifying the elements of the first group with those of the second. If one wants to stress that a certain property of a group $\mathcal{G}$ will be the same for all groups which are isomorphic to $\mathcal{G}$, one speaks of $\mathcal{G}$ as an *abstract group*.

Examples

(i) The symmetry group $3m$ of an equilateral triangle is isomorphic to the group S_3 of all permutations of $\{1, 2, 3\}$. This can be seen as follows: labelling the corners of the triangle by $1, 2, 3$, each element of $3m$ gives rise to a permutation of the labels and mapping an element to the corresponding permutation is a homomorphism. The only element fixing all three corners of the triangle is the identity element of $3m$, thus the homomorphism is injective. On the other hand, the groups $3m$ and S_3 both have 6 elements, hence the homomorphism is also surjective, and thus it is an isomorphism.

(ii) For the symmetry group $\mathcal{G} = 4mm$ of the square and its normal subgroup $\mathcal{H}$ generated by the fourfold rotation, the factor group $\mathcal{G}/\mathcal{H}$ is isomorphic to a cyclic group $\mathcal{C}_2 = \{e, g\}$ of order 2. The trivial coset (containing the rotations in $4mm$) corresponds to the identity element e, the other coset (containing the reflections) corresponds to g.

(iii) The real numbers $\mathbb{R}$ form a group with addition as operation and the positive real numbers $\mathbb{R}_{>0} = \{x \in \mathbb{R} \mid x > 0\}$ form a group with multiplication as operation. The exponential mapping $x \mapsto \exp(x)$ is a homomorphism from $(\mathbb{R}, +)$ to $(\mathbb{R}_{>0}, \cdot)$ because $\exp(x + y) = \exp(x) \cdot \exp(y)$. It is an injective homomorphisms because $\exp(x) = 1$ only for $x = 0$ [which is the identity element in $(\mathbb{R}, +)$] and it is a surjective homomorphism because for any $y > 0$ there is an $x \in \mathbb{R}$ with $\exp(x) = y$, namely $x = \log(y)$. The exponential mapping therefore provides an isomorphism from $(\mathbb{R}, +)$ to $(\mathbb{R}_{>0}, \cdot)$.

The kernel of a homomorphism φ is always a normal subgroup, since for $h \in \ker \varphi$ and $g \in \mathcal{G}$ one has $\varphi(ghg^{-1}) = \varphi(g)\varphi(h)\varphi(g^{-1}) = \varphi(g)\varphi(g^{-1}) = e$. The information about the elements in the kernel of φ is lost after applying φ, because they are all mapped to the identity element of $\mathcal{H}$. More precisely, if $\mathcal{N} = \ker\varphi$, then all elements from the coset $g\mathcal{N}$ are mapped to the same element $\varphi(g)$ in $\mathcal{H}$, since for $n \in \mathcal{N}$ one has $\varphi(gn) = \varphi(g)\varphi(n) = \varphi(g)$. Conversely, if elements are mapped to the same element, they have to lie in the same coset, since $\varphi(g) = \varphi(g')$ implies $\varphi(g^{-1}g') = e$, thus $g^{-1}g' \in \mathcal{N}$ and thus $g^{-1}g'\mathcal{N} = \mathcal{N}$, *i.e.* $g\mathcal{N} = g'\mathcal{N}$. The cosets of $\mathcal{N}$ therefore partition the elements of $\mathcal{G}$ according to their images under φ. This observation is summarized in the following result, which is one of the most powerful theorems in group theory.

Homomorphism theorem

Let φ be a homomorphism from $\mathcal{G}$ to $\mathcal{H}$ with kernel $\ker\varphi = \mathcal{N} \trianglelefteq \mathcal{G}$. Then the factor group $\mathcal{G}/\mathcal{N}$ is isomorphic to the image $\varphi(\mathcal{G})$ *via* the isomorphism $g\mathcal{N} \longmapsto \varphi(g)$.

Examples

(i) The homomorphism φ from $4mm$ to $\mathcal{C}_2 = \{e, g\}$ sending the rotations in $4mm$ to $e \in \mathcal{C}_2$ and the reflections to $g \in \mathcal{C}_2$ has the group $\mathcal{N} = \langle 4 \rangle$ of rotations in $4mm$ as its kernel. The factor group $4mm/\mathcal{N}$ has the cosets $\mathcal{N} = \{1, 4^+, 2, 4^-\}$ and $m_{10}\mathcal{N} = \{m_{10}, m_{01}, m_{11}, m_{1\bar{1}}\}$ as its elements and the homomorphism theorem confirms that mapping $\mathcal{N}$ to $e \in \mathcal{C}_2$ and $m_{10}\mathcal{N}$ to $g \in \mathcal{C}_2$ is an isomorphism from $4mm/\mathcal{N}$ to $\mathcal{C}_2$.

(ii) The homomorphism φ from the additive group $(\mathbb{Z}, +)$ of integers to the cyclic group $\mathcal{C}_n = \langle g \rangle$ mapping k to g^k has $\mathcal{N} = n\mathbb{Z} = \{na \mid a \in \mathbb{Z}\}$ as its kernel. Since φ is a surjective homomorphism, the homomorphism theorem states that the factor group $\mathbb{Z}/n\mathbb{Z}$ is isomorphic to the cyclic group $\mathcal{C}_n$. The operation in the factor group $\mathbb{Z}/n\mathbb{Z}$ is 'addition *modulo n*'.

1.1.7. Group actions

The concept of a group is the essence of an abstraction process which distils the common features of various examples of groups. On the other hand, although abstract groups are important and interesting objects in their own right, they are particularly useful because the group elements *act* on something, *i.e.* they can be applied to certain objects. For example, symmetry groups act on the points in space, but they also act on lines or planes. Groups of permutations act on the symbols themselves, but also on ordered and unordered pairs. Groups of matrices act on the vectors of a vector space, but also on the subspaces. All these different actions can be described in a uniform manner and common concepts can be developed.

Definition. A *group action* of a group $\mathcal{G}$ on a set $\Omega = \{\omega \mid \omega \in \Omega\}$ assigns to each pair (g, ω) an object $\omega' = g(\omega)$ of Ω such that the following hold:

(i) applying two group elements g and g' consecutively has the same effect as applying the product $g'g$, *i.e.* $g'(g(\omega)) = (g'g)(\omega)$ (note that since the group elements act *from the left* on the objects in Ω, the elements in a product of two (or more) group elements are applied right-to-left);

(ii) applying the identity element e of $\mathcal{G}$ has no effect on ω, *i.e.* $e(\omega) = \omega$ for all ω in Ω.

One says that the object ω is *moved* to $g(\omega)$ by g.

Example

The abstract group $\mathcal{C}_2 = \{e, g\}$ occurs as symmetry group in three-dimensional space with three different actions of g:

(i) If g is a reflection, then the points fixed by g form a two-dimensional plane.

(ii) If g is a twofold rotation, then the fixed points of g form a one-dimensional line.

(iii) If g is an inversion, then only a single point is fixed by g.

Often, two objects ω and ω' are regarded as equivalent if there is a group element moving ω to ω'. This notion of equivalence is in fact an *equivalence relation* in the strict mathematical sense:

(*a*) it is *reflexive*, *i.e.* ω is equivalent to itself: this is easily seen since $e(\omega) = \omega$;

(*b*) it is *symmetric*, *i.e.* if ω is equivalent to ω', then ω' is also equivalent to ω: this holds since $g(\omega) = \omega'$ implies $g^{-1}(\omega') = \omega$;

(*c*) it is *transitive*, *i.e.* if ω is equivalent to ω' and ω' is equivalent to ω'', then ω is equivalent to ω'': this is true because $g(\omega) = \omega'$ and $g'(\omega') = \omega''$ implies $g'g(\omega) = \omega''$.

Via this equivalence relation, the action of $\mathcal{G}$ partitions the objects in Ω into equivalence classes, where the equivalence class of an object $\omega \in \Omega$ consists of all objects which are equivalent to ω.

Definition. Two objects $\omega, \omega' \in \Omega$ lie in the same *orbit* under $\mathcal{G}$ if there exists $g \in \mathcal{G}$ such that $\omega' = g(\omega)$.

The set $\mathcal{G}(\omega) := \{g(\omega) \mid g \in \mathcal{G}\}$ of all objects in the orbit of ω is called the *orbit of ω under $\mathcal{G}$*.

The set $S_{\mathcal{G}}(\omega) := \{g \in \mathcal{G} \mid g(\omega) = \omega\}$ of group elements that do not move the object ω is a subgroup of $\mathcal{G}$ called the *stabilizer* of ω in $\mathcal{G}$.

If the orbit of a group action is finite, the length of the orbit is equal to the index of the stabilizer and thus in particular a divisor of the group order (in the case of a finite group). Actually, the objects in an orbit are in a very explicit one-to-one correspondence with the cosets relative to the stabilizer, as is summarized in the *orbit–stabilizer theorem*.

Orbit–stabilizer theorem

For a group $\mathcal{G}$ acting on a set Ω let ω be an object in Ω and let $S_{\mathcal{G}}(\omega)$ be the stabilizer of ω in $\mathcal{G}$.

(i) If $g_1 S_{\mathcal{G}}(\omega) \cup g_2 S_{\mathcal{G}}(\omega) \cup \ldots \cup g_m S_{\mathcal{G}}(\omega)$ is the coset decomposition of $\mathcal{G}$ relative to $S_{\mathcal{G}}(\omega)$, then the coset $g_i S_{\mathcal{G}}(\omega)$ consists of precisely those elements of $\mathcal{G}$ that move ω to $g_i(\omega)$. As a consequence, the full orbit of ω is already obtained by applying only the coset representatives to ω, *i.e.* $\mathcal{G}(\omega) = \{g_1(\omega), g_2(\omega), \ldots, g_m(\omega)\}$ and the number of cosets equals the length of the orbit.

(ii) For objects in the same orbit under $\mathcal{G}$, the stabilizers are *conjugate subgroups* of $\mathcal{G}$ (*cf.* Section 1.1.5). If $\omega' = g(\omega)$, then $S_{\mathcal{G}}(\omega') = g S_{\mathcal{G}}(\omega) g^{-1}$, *i.e.* the stabilizer of ω' is obtained by conjugating the stabilizer of ω by the element g moving ω to ω'.

Example

The symmetry group $\mathcal{G} = 4mm$ of the square acts on the corners of a square as displayed in Fig. 1.1.7.1. All four points lie in a single orbit under $\mathcal{G}$ and the stabilizer of the point 1 is $\mathcal{H} = \langle m_{1\bar{1}} \rangle$, *i.e.* a subgroup of index 4, as required by the orbit–stabilizer theorem. The stabilizers of the other points are conjugate to $\mathcal{H}$: The stabilizer of corner 3 equals $\mathcal{H}$ and the stabilizer of both the corners 2 and 4 is $\langle m_{11} \rangle$, which is conjugate to $\mathcal{H}$ by the fourfold rotation 4^+ which moves corner 1 to corner 2.

An n-dimensional space group $\mathcal{G}$ acts on the points of the n-dimensional space $\mathbb{R}^n$. The stabilizer of a point $P \in \mathbb{R}^n$ is called

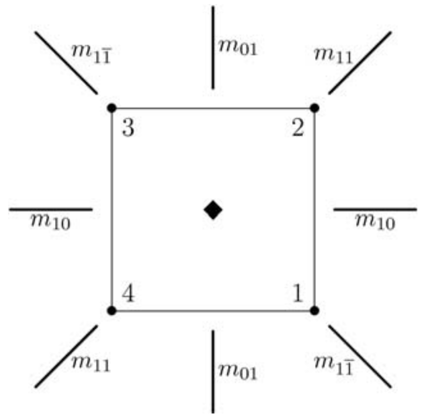

Figure 1.1.7.1
Stabilizers in the symmetry group 4*mm* of the square.

the *site-symmetry group* of P (in $\mathcal{G}$). These site-symmetry groups play a crucial role in the classification of positions in crystal structures. If the site-symmetry group of a point P consists only of the identity element of $\mathcal{G}$, P is called a point in *general position*, points with non-trivial site-symmetry groups are called points in *special position*.

According to the orbit–stabilizer theorem, points that are in the same orbit under the space group and which are thus symmetry equivalent have site-symmetry groups that are conjugate subgroups of $\mathcal{G}$. This gives rise to the concept of *Wyckoff positions*: points with site-symmetry groups that are conjugate subgroups of $\mathcal{G}$ belong to the same Wyckoff position. As a consequence, points in the same orbit under $\mathcal{G}$ certainly belong to the same Wyckoff position, but points may have the same site-symmetry group without being symmetry equivalent. The Wyckoff position of a point P consists of the union of the orbits of all points Q that have the same site-symmetry group as P. For a detailed discussion of the crucial notion of Wyckoff positions we refer to Section 1.4.4.

Example

In the symmetry group 4*mm* of the square the points $x, 0$ lying on the geometric element of m_{01} (*i.e.* the reflection line) are clearly stabilized by m_{01}. The origin $0, 0$ has the full group 4*mm* as its site-symmetry group, for all other points $x, 0$ with $x \neq 0$ the site-symmetry group is the group $\langle m_{01} \rangle$ generated by the reflection m_{01}.

The orbit of a point $P = x, 0$ with $x \neq 0$ is the four points $x, 0,\ \ 0, x,\ \ -x, 0,\ \ 0, -x$, where both $x, 0$ and $-x, 0$ have site-symmetry group $\langle m_{01} \rangle$ and $0, x$ and $0, -x$ have the conjugate site-symmetry group $\langle m_{10} \rangle$. This means that the Wyckoff position of *e.g.* the point $P = \frac{1}{2}, 0$ consists of the set of all points $x, 0$ and $0, x$ with arbitrary $x \neq 0$, *i.e.* of the union of the geometric elements of m_{01} and m_{10} with the exception of their intersection $0, 0$. A complete description of the distribution of points among the Wyckoff positions of the group 4*mm* is given in Table 3.2.3.1.

1.1.8. Conjugation, normalizers

In this section we focus on two group actions which are of particular importance for describing intrinsic properties of a group, namely the conjugation of group elements and the conjugation of subgroups. These actions were mentioned earlier in Section 1.1.5 when we introduced normal subgroups.

A group $\mathcal{G}$ acts on its elements *via* $g(h) := ghg^{-1}$, *i.e.* by conjugation. Note that the inverse element g^{-1} is required on the right-hand side of h in order to fulfil the rule $g(g'(h)) = (gg')(h)$ for a group action.

The orbits for this action are called the *conjugacy classes of elements* of $\mathcal{G}$ or simply *conjugacy classes* of $\mathcal{G}$; the conjugacy class of an element h consists of all its conjugates ghg^{-1} with g running over all elements of $\mathcal{G}$. Elements in one conjugacy class have *e.g.* the same order, and in the case of groups of symmetry operations they also share geometric properties such as being a reflection, rotation or rotoinversion. In particular, conjugate elements have the same type of geometric element.

The connection between conjugate symmetry operations and their geometric elements is even more explicit by the orbit–stabilizer theorem: If h and h' are conjugate by g, *i.e.* $h' = ghg^{-1}$, then g maps the geometric element of h to the geometric element of h'.

Example

The rotation group of a cube contains six fourfold rotations and if the cube is in standard orientation with the origin in its centre, the fourfold rotations 4^+_{100}, 4^+_{010} and 4^+_{001} and their inverses have the lines along the coordinate axes

$$\left\{ \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix} \mid x \in \mathbb{R} \right\}, \left\{ \begin{pmatrix} 0 \\ y \\ 0 \end{pmatrix} \mid y \in \mathbb{R} \right\} \text{ and } \left\{ \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix} \mid z \in \mathbb{R} \right\}$$

as their geometric elements, respectively. The twofold rotation 2_{110} around the line

$$\left\{ \begin{pmatrix} x \\ x \\ 0 \end{pmatrix} \mid x \in \mathbb{R} \right\}$$

maps the *a* axis to the *b* axis and *vice versa*, therefore the symmetry operation 2_{110} conjugates 4^+_{100} to a fourfold rotation with the line along the *b* axis as geometric element. Since the positive part of the *a* axis is mapped to the positive part of the *b* axis and conjugation also preserves the handedness of a rotation, 4^+_{100} is conjugated to 4^+_{010} and not to the inverse element 4^-_{010}. The line along the *c* axis is fixed by 2_{110}, but its orientation is reversed, *i.e.* the positive and negative parts of the *c* axis are interchanged. Therefore, 4^+_{001} is conjugated to its inverse 4^-_{001} by 2_{110}.

For the conjugation action, the stabilizer of an element h is called the *centralizer* $\mathcal{C}_{\mathcal{G}}(h)$ of h in $\mathcal{G}$, consisting of all elements in $\mathcal{G}$ that commute with h, *i.e.* $\mathcal{C}_{\mathcal{G}}(h) = \{g \in \mathcal{G} \mid gh = hg\}$.

Elements that form a conjugacy class on their own commute with all elements of $\mathcal{G}$ and thus have the full group as their centralizer. The collection of all these elements forms a normal subgroup of $\mathcal{G}$ which is called the *centre* of $\mathcal{G}$.

A group $\mathcal{G}$ acts on its subgroups *via* $g(\mathcal{H}) := g\mathcal{H}g^{-1} = \{ghg^{-1} \mid h \in \mathcal{H}\}$, *i.e.* by conjugating all elements of the subgroup. The orbits are called *conjugacy classes of subgroups* of $\mathcal{G}$. Considering the conjugation action of $\mathcal{G}$ on its subgroups is often convenient, because conjugate subgroups are in particular isomorphic: an isomorphism from $\mathcal{H}$ to $g\mathcal{H}g^{-1}$ is provided by the mapping $h \longmapsto ghg^{-1}$.

The stabilizer of a subgroup $\mathcal{H}$ of $\mathcal{G}$ under this conjugation action is called the *normalizer* $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of $\mathcal{H}$ in $\mathcal{G}$. The normalizer of a subgroup $\mathcal{H}$ of $\mathcal{G}$ is the largest subgroup $\mathcal{N}$ of $\mathcal{G}$ such that $\mathcal{H}$ is a normal subgroup of $\mathcal{N}$. In particular, a subgroup is a normal subgroup of $\mathcal{G}$ if and only if its normalizer is the full group $\mathcal{G}$.

The number of conjugate subgroups of $\mathcal{H}$ in $\mathcal{G}$ is equal to the index of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ in $\mathcal{G}$. According to the orbit–stabilizer theorem, the different conjugate subgroups of $\mathcal{H}$ are obtained by conjugating $\mathcal{H}$ with coset representatives for the cosets of $\mathcal{G}$ relative to $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$.

Examples

(i) In an abelian group $\mathcal{G}$, every element is only conjugate with itself, since $ghg^{-1} = h$ for all g, h in $\mathcal{G}$. Therefore each conjugacy class consists of just a single element.
Also, every subgroup $\mathcal{H}$ of an abelian group $\mathcal{G}$ is a normal subgroup, thus its normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ is $\mathcal{G}$ itself and $\mathcal{H}$ is only conjugate to itself.

(ii) The conjugacy classes of the symmetry group $3m$ of an equilateral triangle are $\{1\}$, $\{m_{10}, m_{01}, m_{11}\}$ and $\{3^+, 3^-\}$. The centralizer of m_{10} is just the group $\langle m_{10}\rangle$ generated by m_{10}, *i.e.* 1 and m_{10} are the only elements of $3m$ commuting with m_{10}. Analogously, one sees that the centralizer $\mathcal{C}_{\mathcal{G}}(h) = \langle h\rangle$ for each element h in $3m$, except for $h = 1$.
The subgroups $\langle m_{10}\rangle$, $\langle m_{01}\rangle$ and $\langle m_{11}\rangle$ are conjugate subgroups (with conjugating elements 3^+ and 3^-). These subgroups coincide with their normalizers, since they have index 3 in the full group.

(iii) The conjugacy classes of the symmetry group $4mm$ of a square are $\{1\}$, $\{2\}$, $\{m_{10}, m_{01}\}$, $\{m_{11}, m_{1\bar{1}}\}$ and $\{4^+, 4^-\}$. Since 2 forms a conjugacy class on its own, this is an element in the centre of $4mm$ and its centralizer is the full group. The centralizer of m_{10} is $\langle m_{10}, m_{01}\rangle$, which is also the centralizer of m_{01} (note that m_{10} and m_{01} are reflections with normal vectors perpendicular to each other, and thus commute). Analogously, $\langle m_{11}, m_{1\bar{1}}\rangle$ is the centralizer of both m_{11} and $m_{1\bar{1}}$. Finally, 4^+ only commutes with the rotations in $4mm$, therefore its centralizer is $\langle 4^+\rangle$.
The five subgroups of order 2 in $4mm$ fall into three conjugacy classes, namely the normal subgroup $\langle 2\rangle$ and the two pairs $\{\langle m_{10}\rangle, \langle m_{01}\rangle\}$ and $\{\langle m_{11}\rangle, \langle m_{1\bar{1}}\rangle\}$. The normalizer of both $\langle m_{10}\rangle$ and $\langle m_{01}\rangle$ is $\langle 2, m_{10}\rangle$ and the normalizer of both $\langle m_{11}\rangle$ and $\langle m_{1\bar{1}}\rangle$ is $\langle 2, m_{11}\rangle$.

In the context of crystallographic groups, conjugate subgroups are not only isomorphic, but have the same types of geometric elements, possibly with different directions. In many situations it is therefore sufficient to restrict attention to representatives of the conjugacy classes of subgroups. Furthermore, conjugation with elements from the normalizer of a group $\mathcal{H}$ permutes the geometric elements of the symmetry operations of $\mathcal{H}$. The role of the normalizer may in this situation be expressed by the phrase

The normalizer describes the *symmetry of the symmetries*.

Thus, the normalizer reflects an intrinsic ambiguity between different but equivalent descriptions of an object by its symmetries.

Example

The subgroup $\mathcal{H} = \langle 2, m_{10}\rangle$ is a normal subgroup of the symmetry group $\mathcal{G} = 4mm$ of the square, and thus $\mathcal{G}$ is the normalizer of $\mathcal{H}$ in $\mathcal{G}$. As can be seen in the diagram in Fig. 1.1.7.1, the fourfold rotation 4^+ maps the geometric element of the reflection m_{10} to the geometric element of m_{01} and *vice versa*, and fixes the geometric element of the rotation 4^+. Consequently, conjugation by 4^+ fixes $\mathcal{H}$ as a set, but interchanges the reflections m_{10} and m_{01}. These two reflections are geometrically indistinguishable, since their geometric elements are both lines through the centres of opposite edges of the square.
Analogously, 4^+ interchanges the geometric elements of the reflections m_{11} and $m_{1\bar{1}}$ of the subgroup $\mathcal{H}' = \langle 2, m_{11}\rangle$. These are the two reflection lines through opposite corners of the square.
In contrast to that, $\mathcal{G}$ does not contain an element mapping the geometric element of m_{10} to that of m_{11}. Note that an eightfold rotation would be such an element, but this is, however, not a symmetry of the square. The reflections m_{10} and m_{11} are thus geometrically different symmetry operations of the square.

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