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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 $\mathrm{GL}_n(\mathbb{R})$ 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).

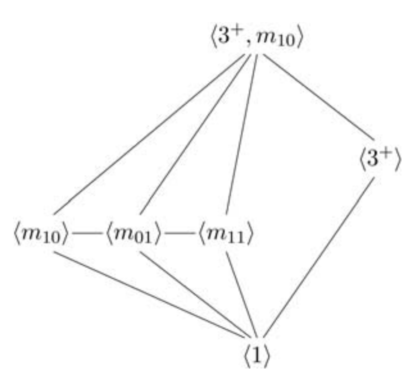

Figure 1.1.3.1
Subgroup diagram for the symmetry group $3m$ of an equilateral triangle.

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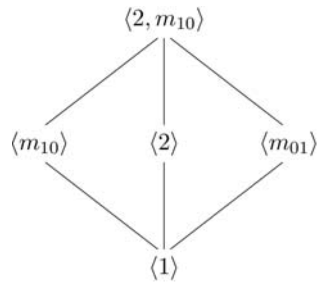

Figure 1.1.3.2
Subgroup diagram for the symmetry group $2mm$ of a rectangle.

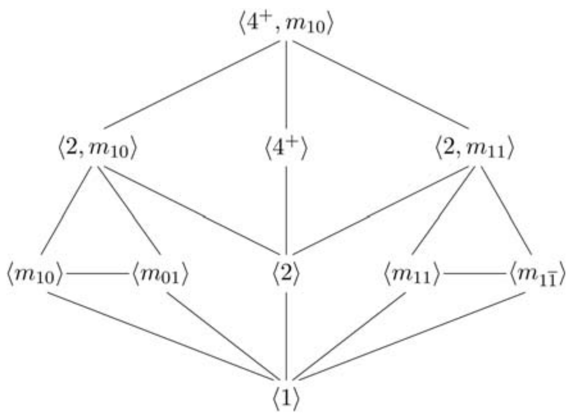

Figure 1.1.3.3
Subgroup diagram for the symmetry group $4mm$ of the square.

(vii) In the symmetry group $4mm$ 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 $4mm$ 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 $2mm$ 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

$$\mathcal{H}g := \{h_1 g, h_2 g, h_3 g, \ldots\} = \{hg \mid h \in \mathcal{H}\}.$$

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 $\mathcal{H} \leq \mathcal{G}$ 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 $g_i\mathcal{H} \neq g_j\mathcal{H}$ for $i \neq j$, 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 $\mathcal{H}g_i' \neq \mathcal{H}g_j'$ for $i \neq j$ 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 $\mathcal{G} = \{1, 3^+, 3^-\} \cup \{m_{10}, m_{01}, m_{11}\}$.

references