

1.1. GENERAL INTRODUCTION TO GROUPS

elements in the kernel of  $\varphi$  is lost after applying  $\varphi$ , 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  $\varphi$ . This observation is summarized in the following result, which is one of the most powerful theorems in group theory.

Homomorphism theorem

Let  $\varphi$  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  $g\mathcal{N} \mapsto \varphi(g)$ .

Examples

- (i) The homomorphism  $\varphi$  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  $m_{10}\mathcal{N} = \{m_{10}, m_{01}, m_{11}, m_{\bar{1}\bar{1}}\}$  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  $\varphi$  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  $\varphi$  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  $(g, \omega)$  an object  $\omega' = g(\omega)$  of  $\Omega$  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  $\Omega$ , 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  $\omega$ , i.e.  $e(\omega) = \omega$  for all  $\omega$  in  $\Omega$ .

One says that the object  $\omega$  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  $\omega$  and  $\omega'$  are regarded as equivalent if there is a group element moving  $\omega$  to  $\omega'$ . This notion of equivalence is in fact an *equivalence relation* in the strict mathematical sense:

- (a) it is *reflexive*, i.e.  $\omega$  is equivalent to itself: this is easily seen since  $e(\omega) = \omega$ ;
- (b) it is *symmetric*, i.e. if  $\omega$  is equivalent to  $\omega'$ , then  $\omega'$  is also equivalent to  $\omega$ : this holds since  $g(\omega) = \omega'$  implies  $g^{-1}(\omega') = \omega$ ;
- (c) it is *transitive*, i.e. if  $\omega$  is equivalent to  $\omega'$  and  $\omega'$  is equivalent to  $\omega''$ , then  $\omega$  is equivalent to  $\omega''$ : 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  $\Omega$  into equivalence classes, where the equivalence class of an object  $\omega \in \Omega$  consists of all objects which are equivalent to  $\omega$ .

*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  $\omega$  is called the *orbit of  $\omega$  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  $\omega$  is a subgroup of  $\mathcal{G}$  called the *stabilizer* of  $\omega$  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

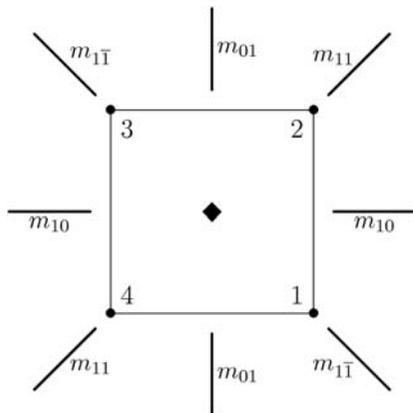
For a group  $\mathcal{G}$  acting on a set  $\Omega$  let  $\omega$  be an object in  $\Omega$  and let  $S_{\mathcal{G}}(\omega)$  be the stabilizer of  $\omega$  in  $\mathcal{G}$ .

- (i) If  $g_1S_{\mathcal{G}}(\omega) \cup g_2S_{\mathcal{G}}(\omega) \cup \dots \cup g_mS_{\mathcal{G}}(\omega)$  is the coset decomposition of  $\mathcal{G}$  relative to  $S_{\mathcal{G}}(\omega)$ , then the coset  $g_iS_{\mathcal{G}}(\omega)$  consists of precisely those elements of  $\mathcal{G}$  that move  $\omega$  to  $g_i(\omega)$ . As a consequence, the full orbit of  $\omega$  is already obtained by applying only the coset representatives to  $\omega$ , i.e.  $\mathcal{G}(\omega) = \{g_1(\omega), g_2(\omega), \dots, g_m(\omega)\}$  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  $S_{\mathcal{G}}(\omega') = gS_{\mathcal{G}}(\omega)g^{-1}$ , i.e. the stabilizer of  $\omega'$  is obtained by conjugating the stabilizer of  $\omega$  by the element  $g$  moving  $\omega$  to  $\omega'$ .

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  $\mathcal{H} = \langle m_{\bar{1}\bar{1}} \rangle$ , 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  $4mm$  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  $4mm$  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  $4mm$  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  $4mm$  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  $h \mapsto ghg^{-1}$ .

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  $\mathcal{G}$ .