

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

(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 $0, 1, 2, \dots, n - 1$. The coset with representative 0 is $\{\dots, -n, 0, n, 2n, \dots\}$, the coset with representative 1 is $\{\dots, -n + 1, 1, n + 1, 2n + 1, \dots\}$ 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 $m_{\bar{1}\bar{1}}$ are not normal because $4^+ \cdot m_{10} \cdot 4^- = m_{01} \notin \langle m_{10} \rangle$, $4^+ \cdot m_{01} \cdot 4^- = m_{10} \notin \langle m_{01} \rangle$, $4^+ \cdot m_{11} \cdot 4^- = m_{\bar{1}\bar{1}} \notin \langle m_{11} \rangle$ and $4^+ \cdot m_{\bar{1}\bar{1}} \cdot 4^- = m_{11} \notin \langle m_{\bar{1}\bar{1}} \rangle$. 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

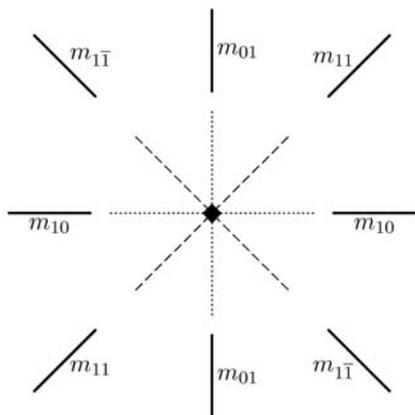


Figure 1.1.5.1
Symmetry group of an eightfold star.

$(8 + 12\mathbb{Z}) + (9 + 12\mathbb{Z}) = 17 + 12\mathbb{Z} = 5 + 12\mathbb{Z}$. 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} .