

1.4. THE MATHEMATICAL BACKGROUND OF THE SUBGROUP TABLES

In the mathematical model, the affine group is the automorphism group of the affine space and can be viewed as the set of all linear mappings of \mathbf{V}_{n+1} that preserve \mathbb{A}_n .

Definition 1.4.2.4.1. The *affine group* \mathcal{A}_n is the subset of the set of all linear mappings $\varphi : \mathbf{V}_{n+1} \rightarrow \mathbf{V}_{n+1}$ with $\varphi(\mathbb{A}_n) = \mathbb{A}_n$. The elements of \mathcal{A}_n are called *affine mappings*. \square

Since φ is linear, it holds that

$$\varphi(\overrightarrow{PQ}) = \varphi(Q - P) = \varphi(Q) - \varphi(P) = \overrightarrow{\varphi(P)\varphi(Q)}.$$

Hence an affine mapping also maps $\tau(\mathbb{A}_n)$ into itself.

Since the first n basis vectors of the chosen basis lie in $\tau(\mathbb{A}_n)$ and the last one in \mathbb{A}_n , it is clear that with respect to this basis the affine mappings correspond to matrices of the form

$$\mathbb{W} = \left(\begin{array}{c|c} \mathbf{W} & \mathbf{w} \\ \mathbf{o}^T & 1 \end{array} \right).$$

The linear mapping induced by φ on $\tau(\mathbb{A}_n)$ which is represented by the matrix \mathbf{W} will be referred to as the *linear part* $\overline{\varphi}$ of φ . The image $\varphi(P)$ of a point P with coordinates

$$\mathbb{x} = \left(\begin{array}{c} \mathbf{x} \\ 1 \end{array} \right) \in \mathbb{A}_n$$

can easily be found as

$$\mathbb{W}\mathbb{x} = \left(\begin{array}{c} \mathbf{W}\mathbf{x} + \mathbf{w} \\ 1 \end{array} \right).$$

If one has a way to measure lengths and angles (*i.e.* a Euclidean metric) on the underlying vector space $\tau(\mathbb{A}_n)$, one can compute the *distance* between P and $Q \in \mathbb{A}_n$ as the length of the vector \overrightarrow{PQ} and the angle determined by P, Q and $R \in \mathbb{A}_n$ with vertex Q is obtained from $\cos(P, Q, R) = \cos(\overrightarrow{QP}, \overrightarrow{QR})$. In this case, \mathbb{A}_n is the *Euclidean point space*, \mathbb{E}_n .

An affine mapping of the Euclidean point space is called an *isometry* if its linear part is an orthogonal mapping of the Euclidean vector space $\tau(\mathbb{A}_n)$. The set of all isometries in \mathcal{A}_n is called the *Euclidean group* and denoted by \mathcal{E}_n . Hence \mathcal{E}_n is the set of all distance-preserving mappings of \mathbb{E}_n onto itself. The isometries are the affine mappings with matrices of the form

$$\mathbb{W} = \left(\begin{array}{c|c} \mathbf{W} & \mathbf{w} \\ \mathbf{o}^T & 1 \end{array} \right)$$

where the linear part \mathbf{W} belongs to the orthogonal group of $\tau(\mathbb{A}_n)$.

Special isometries are the *translations*, the isometries where the linear part is \mathbf{I} , with matrix

$$\mathbb{T} = \left(\begin{array}{c|c} \mathbf{I} & \mathbf{w} \\ \mathbf{o}^T & 1 \end{array} \right).$$

The group of all translations in \mathcal{E}_n is the *translation subgroup* of \mathcal{E}_n and is denoted by \mathcal{T}_n . Note that composition of two translations means addition of the translation vectors and \mathcal{T}_n is isomorphic to the translation vector space $\tau(\mathbb{E}_n)$.

1.4.3. Groups

1.4.3.1. Groups

The affine group is only one example of the more general concept of a group. The following axiomatic definition sometimes makes it easier to examine general properties of groups.

Definition 1.4.3.1.1. A *group* (\mathcal{G}, \cdot) is a set \mathcal{G} with a mapping $\mathcal{G} \times \mathcal{G} \rightarrow \mathcal{G}; (g, h) \mapsto g \cdot h$, called the *composition law* or *multiplication* of \mathcal{G} , satisfying the following three axioms:

- (i) $(g \cdot h) \cdot k = g \cdot (h \cdot k)$ for all $g, h, k \in \mathcal{G}$ (associative law).
- (ii) There is an element $e \in \mathcal{G}$ called the *unit element* of \mathcal{G} with $e \cdot g = g \cdot e = g$ for all $g \in \mathcal{G}$.
- (iii) For all $g \in \mathcal{G}$, there is an element $g^{-1} \in \mathcal{G}$, called the *inverse* of g , with $g \cdot g^{-1} = g^{-1} \cdot g = e$. \square

Normally the symbol \cdot is omitted, hence the product $g \cdot h$ is just written as gh and the set \mathcal{G} is called a *group*.

One should note that in particular property (i), the associative law, of a group is something very natural if one thinks of group elements as mappings. Clearly the composition of mappings is associative. In general, one can think of groups as groups of mappings as explained in Section 1.4.3.2.

A subset of elements of a group \mathcal{G} which themselves form a group is called a *subgroup*:

Definition 1.4.3.1.2. A non-empty subset $\emptyset \neq \mathcal{U} \subseteq \mathcal{G}$ is called a *subgroup* of \mathcal{G} (abbreviated as $\mathcal{U} \leq \mathcal{G}$) if $g \cdot h^{-1} \in \mathcal{U}$ for all $g, h \in \mathcal{U}$. \square

The affine group is an example of a group where \cdot is given by the composition of mappings. The unit element $e \in \mathcal{A}_n$ is the identity mapping given by the matrix

$$\mathbb{I} = \left(\begin{array}{c|c} \mathbf{I} & \mathbf{o} \\ \mathbf{o}^T & 1 \end{array} \right),$$

which also represents the translation by the vector \mathbf{o} . The composition of two affine mappings is again an affine mapping and the inverse of an affine mapping \mathbb{W} has matrix

$$\mathbb{W}^{-1} = \left(\begin{array}{c|c} \mathbf{W}^{-1} & -\mathbf{W}^{-1}\mathbf{w} \\ \mathbf{o}^T & 1 \end{array} \right).$$

Since the inverse of an isometry and the composition of two isometries are again isometries, the set of isometries \mathcal{E}_n is a subgroup of the affine group \mathcal{A}_n . The translation subgroup \mathcal{T}_n is a subgroup of \mathcal{E}_n .

Any vector space \mathbf{V}_n is a group with the usual vector addition as composition law. Therefore $\tau(\mathbb{A}_n)$ is also a group.

Remarks

- (i) For every group \mathcal{G} , the set $\{e\}$ consisting only of the unit element of \mathcal{G} is a subgroup of \mathcal{G} called the *trivial subgroup* $\mathcal{I} = \{e\}$.
- (ii) If \mathcal{U} is a subgroup of \mathcal{V} and \mathcal{V} is a subgroup of the group \mathcal{G} , then \mathcal{U} is a subgroup of \mathcal{G} .
- (iii) If \mathcal{U} and \mathcal{V} are subgroups of the group \mathcal{G} , then the intersection $\mathcal{U} \cap \mathcal{V}$ is also a subgroup of \mathcal{G} .
- (iv) If $S \subseteq \mathcal{G}$ is a subset of the group \mathcal{G} , then the smallest subgroup of \mathcal{G} containing S is denoted by

$$\langle S \rangle := \bigcap \{ \mathcal{U} \leq \mathcal{G} \mid S \subseteq \mathcal{U} \}$$

1. SPACE GROUPS AND THEIR SUBGROUPS

and is called the *subgroup generated by S* . The elements of S are called the *generators* of this group. It is convenient not to list all the elements of a group \mathcal{G} but just to give generators of \mathcal{G} (this also applies to finite groups).

Example 1.4.3.1.3

A well known group is the addition group of integers $\mathbb{Z} = \{0, 1, -1, 2, -2, \dots\}$ where \cdot is normally denoted by $+$ and the unit element $e \in \mathbb{Z}$ is 0. The group \mathbb{Z} is generated by $\{1\}$. Other generating sets are for example $\{-1\}$ or $\{2, 3\}$. Taking two integers $a, b \in \mathbb{Z}$ which are divisible by some fixed integer $p \in \mathbb{Z}$, then the sum $a + b$ and the negatives $-a$ and $-b$ are again divisible by p . Hence the set $p\mathbb{Z}$ of all integers divisible by p is a subgroup of \mathbb{Z} . It is generated by $\{p\}$.

Definition 1.4.3.1.4. The *order* $|\mathcal{G}|$ of a group \mathcal{G} is the number of elements in the set \mathcal{G} . \square

Most of the groups \mathcal{G} in crystallography, for example $\mathbb{Z}, \mathbf{V}_n, \mathcal{A}_n$, have infinite order.

Groups that are generated by one element are called *cyclic*. The cyclic group of order n is called Cyc_n . (We prefer to use three letters to denote the mathematical names of frequently occurring groups, since the more common symbol C_n could possibly cause confusion with the Schoenflies symbol C_n .)

The group \mathbf{V}_n is not generated by a finite set.

These two groups \mathbb{Z} and \mathbf{V}_n have the property that for all elements g and h in the group it holds that $g \cdot h = h \cdot g$. Hence these two groups are Abelian in the sense of the following:

Definition 1.4.3.1.5. The group (\mathcal{G}, \cdot) is called *Abelian* if $g \cdot h = h \cdot g$ for all $g, h \in \mathcal{G}$. \square

1.4.3.2. Actions of groups on sets

The affine group \mathcal{A}_n is defined *via* its action on the affine space \mathbb{A}_n . In general, the greatest significance of groups is that they act on sets.

Definition 1.4.3.2.1. Let \mathcal{G} be a group. A non-empty set M is called a (*left*) \mathcal{G} -set if there is a mapping $\mathcal{G} \times M \rightarrow M$ satisfying the following conditions:

- (i) $(gh) \cdot m = g \cdot (h \cdot m)$ for all $g, h \in \mathcal{G}$ and $m \in M$.
- (ii) $e \cdot m = m$ for all $m \in M$.

If M is a \mathcal{G} -set, one also says that \mathcal{G} acts on M . \square

Example 1.4.3.2.2

- (a) The affine space \mathbb{A}_n is a \mathcal{G} -set for the affine group $\mathcal{G} = \mathcal{A}_n$.
- (b) $\tau(\mathbb{A}_n)$ is an \mathcal{A}_n -set, where \mathcal{A}_n acts *via* the linear parts.
- (c) $\tau(\mathbb{A}_n)$ is also a group and acts on \mathbb{A}_n by translations $\mathbf{v} \cdot P := P + \mathbf{v}$ for $\mathbf{v} \in \tau(\mathbb{A}_n), P \in \mathbb{A}_n$.
- (d) If $\mathcal{U} \leq \mathcal{G}$ is a subgroup of the group \mathcal{G} , then \mathcal{G} is a \mathcal{U} -set where $\cdot : \mathcal{U} \times \mathcal{G} \rightarrow \mathcal{G}$ is the usual composition law. In particular, each group \mathcal{G} is a \mathcal{G} -set and hence every group \mathcal{G} can be viewed as a group of mappings from \mathcal{G} onto \mathcal{G} .

Definition 1.4.3.2.3. Let \mathcal{G} be a group and M a \mathcal{G} -set. If $m \in M$, then the set $\mathcal{G} \cdot m := \{g \cdot m | g \in \mathcal{G}\}$ is called the *orbit* of m under \mathcal{G} .

The \mathcal{G} -set M is called *transitive* if $M = \mathcal{G} \cdot m$ for any $m \in M$ consists of a single orbit under \mathcal{G} .

If $m \in M$ then the *stabilizer of m in \mathcal{G}* is $\text{Stab}_{\mathcal{G}}(m) := \{g \in \mathcal{G} | g \cdot m = m\}$.

For a space group \mathcal{G} and a point P in the point space, the stabilizer $\text{Stab}_{\mathcal{G}}(P)$ is called the *site-symmetry group* of P with respect to \mathcal{G} .

The *kernel \mathcal{K} of the action* of \mathcal{G} on M is the intersection of the stabilizers of all elements in M ,

$$\mathcal{K} := \{g \in \mathcal{G} | g \cdot m = m \text{ for all } m \in M\}.$$

M is called a *faithful \mathcal{G} -set* and the action of \mathcal{G} on M is also called *faithful* if the kernel of the action is trivial, $\mathcal{K} = \{e\}$. \square

Note that any space group \mathcal{R} acts faithfully on the point space.

Remarks

- (i) If $m_1, m_2 \in M$, then their orbits are either equal or disjoint. For if there is an element $g_1 \cdot m_1 = g_2 \cdot m_2$, then by the axioms of \mathcal{G} -sets $m_1 = e m_1 = (g_1^{-1} g_1) \cdot m_1 = g_1^{-1} \cdot (g_1 \cdot m_1) = g_1^{-1} \cdot (g_2 \cdot m_2) = (g_1^{-1} g_2) \cdot m_2$, hence every element $g \cdot m_1$ in the orbit of m_1 is of the form $g \cdot (g_1^{-1} g_2 \cdot m_2) = (g g_1^{-1} g_2) \cdot m_2$ and therefore lies in the orbit of m_2 . Hence the set of orbits gives a partition of M into disjoint sets. If M is a finite set, then its order is the sum of the lengths of the different orbits.
- (ii) $\text{Stab}_{\mathcal{G}}(m)$ is a subgroup of \mathcal{G} , since for $g_1, g_2 \in \text{Stab}_{\mathcal{G}}(m)$, the product $(g_1 g_2^{-1}) \cdot m = g_1 \cdot (g_2^{-1} \cdot m) = g_1 \cdot m = m$.
- (iii) If $m_1 = g \cdot m_2$, then $\text{Stab}_{\mathcal{G}}(m_1) = g \text{Stab}_{\mathcal{G}}(m_2) g^{-1} = \{g h g^{-1} | h \in \text{Stab}_{\mathcal{G}}(m_2)\}$.

Example 1.4.3.2.4 (Example 1.4.3.2.2 continued)

- (a) \mathbb{A}_n is a transitive \mathcal{A}_n -set. This is a mathematical expression of the fact that in point space no point is distinguished.
- (b) The \mathcal{A}_n -set $\tau(\mathbb{A}_n)$ decomposes into two orbits $\{\mathbf{o}\}$ and $\{\mathbf{v} \in \tau(\mathbb{A}_n) | \mathbf{v} \neq \mathbf{o}\}$. The kernel of the action of \mathcal{A}_n on $\tau(\mathbb{A}_n)$ is the translation subgroup \mathcal{T}_n .
- (c) $\tau(\mathbb{A}_n)$ acts transitively on \mathbb{A}_n . The kernel of the action only consists of the zero vector \mathbf{o} .

We now introduce some terminology for groups which is nicely formulated using \mathcal{G} -sets.

Definition 1.4.3.2.5. The orbit of $g \in \mathcal{G}$ under the action of the subgroup $\mathcal{U} \leq \mathcal{G}$ is the *right coset* $\mathcal{U}g = \{ug | u \in \mathcal{U}\}$ (cf. IT A, Section 8.1.5). Analogously one defines a *left coset* as

$$g\mathcal{U} = \{gu | u \in \mathcal{U}\}$$

and denotes the set of left cosets by \mathcal{G}/\mathcal{U} .

If the number of left cosets (which is always equal to the number of right cosets) of \mathcal{U} in \mathcal{G} is finite, then this number is called the *index* $[\mathcal{G} : \mathcal{U}]$ of \mathcal{U} in \mathcal{G} . If this number is infinite, one says that the index of \mathcal{U} in \mathcal{G} is infinite. \square

Example 1.4.3.2.6

\mathbb{A}_n is a coset of \mathbf{V}_n in \mathbf{V}_{n+1} , namely

$$\mathbb{A}_n = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} + \mathbf{V}_n.$$

If one thinks of \mathbb{A}_2 as an infinite sheet of paper and puts uncountably many such sheets of paper (one for each real number) one onto the other, one gets the whole 3-space \mathbf{V}_3 .