

1. SPACE GROUPS AND THEIR SUBGROUPS

tuple of n vectors $\mathbf{B} := (\mathbf{a}_1, \dots, \mathbf{a}_n)$ such that every vector of \mathbf{V} can be written uniquely as a linear combination of the basis vectors: $\mathbf{V} = \{\mathbf{x} = x_1\mathbf{a}_1 + \dots + x_n\mathbf{a}_n \mid x_1, \dots, x_n \in \mathbb{R}\}$. Whereas a vector space has many different bases, the number n of vectors of a basis is uniquely determined and is called the *dimension* of \mathbf{V} . The isomorphism (see Section 1.4.3.4 for a definition of isomorphism) $\varphi_{\mathbf{B}}$ between \mathbf{V} and \mathbf{V}_n maps the vector $\mathbf{x} = x_1\mathbf{a}_1 + \dots + x_n\mathbf{a}_n \in \mathbf{V}$ to its coefficient column

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in \mathbf{V}_n$$

with respect to the chosen basis \mathbf{B} . The mapping $\varphi_{\mathbf{B}}$ respects addition of vectors and multiplication of vectors with real numbers. Moreover, $\varphi_{\mathbf{B}}$ is a bijective mapping, which means that for any coefficient column $\mathbf{x} \in \mathbf{V}_n$ there is a unique vector $\mathbf{x} \in \mathbf{V}$ with $\varphi_{\mathbf{B}}(\mathbf{x}) = \mathbf{x}$. Therefore one can perform all calculations using the coefficient columns.

An important concept in mathematics is the *automorphism group* of an object. In general, if one has an object (here the vector space \mathbf{V}) together with a structure (here the addition of vectors and the multiplication of vectors with real numbers), its automorphism group is the set of all one-to-one mappings of the object onto itself that preserve the structure.

A bijective mapping $\varphi : \mathbf{V} \rightarrow \mathbf{V}$ of the vector space \mathbf{V} into itself satisfying $\varphi(\mathbf{v} + \mathbf{w}) = \varphi(\mathbf{v}) + \varphi(\mathbf{w})$ for all $\mathbf{v}, \mathbf{w} \in \mathbf{V}$ and $\varphi(x\mathbf{v}) = x\varphi(\mathbf{v})$ for all real numbers $x \in \mathbb{R}$ and all vectors $\mathbf{v} \in \mathbf{V}$ is called a *linear mapping* and the set of all these linear mappings is the *linear group* of \mathbf{V} . To know the image of $\mathbf{x} = x_1\mathbf{a}_1 + \dots + x_n\mathbf{a}_n$ under a linear mapping φ it suffices to know the images of the basis vectors $\mathbf{a}_1, \dots, \mathbf{a}_n$ under φ , since $\varphi(\mathbf{x}) = x_1\varphi(\mathbf{a}_1) + \dots + x_n\varphi(\mathbf{a}_n)$. Writing the coefficient columns of the images of the basis vectors as columns of a matrix \mathbf{A} [i.e. $\varphi(\mathbf{a}_i) = \sum_{j=1}^n \mathbf{a}_j A_{ji}$, $i = 1, \dots, n$], then the coefficient column of $\varphi(\mathbf{x})$ with respect to the chosen basis \mathbf{B} is just $\mathbf{A}\mathbf{x}$. Note that the matrix of a linear mapping depends on the basis \mathbf{B} of \mathbf{V} . The matrix that corresponds to the composition of two linear mappings is the product of the two corresponding matrices. We have thus seen that the linear group of a vector space \mathbf{V} of dimension n is isomorphic to the group of all invertible $(n \times n)$ matrices *via* the isomorphism $\varphi_{\mathbf{B}}$ that associates to a linear mapping its corresponding matrix (with respect to the basis \mathbf{B}). This means that one can perform all calculations with linear mappings using matrix calculations.

In crystallography, the translation-vector space has an additional structure: one can measure lengths and angles between vectors. An n -dimensional real vector space with such an additional structure is called a *Euclidean vector space*, \mathbf{E}_n . Its automorphism group is the set of all (bijective) linear mappings of \mathbf{E}_n onto itself that preserve lengths and angles and is called the *orthogonal group* \mathcal{O}_n of \mathbf{E}_n . If one chooses the basis $\mathbf{B} = (\mathbf{e}_1, \dots, \mathbf{e}_n)$ to be the unit vectors (which are orthogonal vectors of length 1), then the isomorphism $\varphi_{\mathbf{B}}$ above maps the orthogonal group \mathcal{O}_n onto the set of all $(n \times n)$ matrices \mathbf{A} with $\mathbf{A}^T\mathbf{A} = \mathbf{I}$, the $(n \times n)$ unit matrix. T denotes the transposition operator, which maps columns to rows and rows to columns.

1.4.2.3. The affine space

In this section we build up a model for the ‘point space’. Let us first assume $n = 2$. Then the affine space \mathbb{A}_2 may be imagined as an infinite sheet of paper parallel, let us say, to the (\mathbf{a}, \mathbf{b}) plane

and cutting the \mathbf{c} axis at $x_3 = 1$ in crystallographic notation. The points of \mathbb{A}_2 have coordinates

$$\begin{pmatrix} x_1 \\ x_2 \\ 1 \end{pmatrix},$$

which are the coefficients of the vector from the origin to the point.

This observation is generalized by the following:

Definition 1.4.2.3.1.

$$\mathbb{A}_n := \left\{ \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 1 \end{pmatrix} \mid x_i \in \mathbb{R} \right\}$$

is an n -dimensional *affine space*. □

If

$$P = \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 1 \end{pmatrix} \text{ and } Q = \begin{pmatrix} y_1 \\ \vdots \\ y_n \\ 1 \end{pmatrix} \in \mathbb{A}_n,$$

then the vector \overrightarrow{PQ} is defined as the difference

$$Q - P = \begin{pmatrix} y_1 - x_1 \\ \vdots \\ y_n - x_n \\ 0 \end{pmatrix}$$

(computed in the vector space \mathbf{V}_{n+1}). The set of all \overrightarrow{PQ} with $P, Q \in \mathbb{A}_n$ forms an n -dimensional vector space which is called the *underlying vector space* $\tau(\mathbb{A}_n)$. Omitting the last coefficient, we can identify

$$\tau(\mathbb{A}_n) = \left\{ \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 0 \end{pmatrix} \mid x_1, \dots, x_n \in \mathbb{R} \right\}$$

with \mathbf{V}_n . As the coordinates already indicate, the sets \mathbb{A}_n as well as $\tau(\mathbb{A}_n)$ can be viewed as subsets of \mathbf{V}_{n+1} . Computed in \mathbf{V}_{n+1} , the sum of two elements in $\tau(\mathbb{A}_n)$ is again in $\tau(\mathbb{A}_n)$, since the last coefficient of the sum is $0 + 0 = 0$ and the sum of a point $P \in \mathbb{A}_n$ and a vector $\mathbf{v} \in \mathbf{V}_n$ is again a point in \mathbb{A}_n (since the last coordinate is $1 + 0 = 1$), but the sum of two points does not make sense.

1.4.2.4. The affine group

The affine group of geometry is the set of all mappings of the point space which fulfil the conditions

- (1) parallel straight lines are mapped onto parallel straight lines;
- (2) collinear points are mapped onto collinear points and the ratio of distances between them remains constant.