1.3. A general introduction to space groups

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1.3.1. Introduction

We recall from Chapter 1.2 that an *isometry* is a mapping of the point space $\mathbb{E}^n$ which preserves distances and angles. From the mathematical viewpoint, $\mathbb{E}^n$ is an *affine space* in which two points differ by a unique vector in the underlying *vector space* $\mathbb{V}^n$. The crucial difference between these two types of spaces is that in an affine space no point is distinguished, whereas in a vector space the zero vector plays a special role, namely as the identity element for the addition of vectors. After choosing an origin O, the points of the affine space $\mathbb{E}^n$ are in one-to-one correspondence with the vectors of $\mathbb{V}^n$ by identifying a point P with the difference vector $\overrightarrow{OP}$.

A *crystallographic space-group operation* is an isometry that maps a crystal pattern onto itself. Since isometries are invertible and the composition of two isometries leaves a crystal pattern invariant as a whole if the two single isometries do so, the space-group operations form a group $\mathcal{G}$, called a *crystallographic space group*.

As a mapping of points in an affine space, a space-group operation is an affine mapping and is thus composed of a linear mapping of the underlying vector space and a translation. Once a coordinate system has been chosen, space-group operations are conveniently represented as *matrix–column pairs* $(\boldsymbol{W}, \boldsymbol{w})$, where $\boldsymbol{W}$ is the *linear part* and $\boldsymbol{w}$ the *translation part* and a point with coordinates $\boldsymbol{x}$ is mapped to $\boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ (*cf.* Section 1.2.2).

A translation is a matrix–column pair of the form $(\boldsymbol{I}, \boldsymbol{w})$, where $\boldsymbol{I}$ is the unit matrix and all translations taken together form the *translation subgroup* $\mathcal{T}$ of $\mathcal{G}$. The translation subgroup is an infinite group that forms an abelian normal subgroup of $\mathcal{G}$. The factor group $\mathcal{G}/\mathcal{T}$ is a finite group that can be identified with the group of linear parts of $\mathcal{G}$ *via* the mapping $(\boldsymbol{W}, \boldsymbol{w}) \longmapsto \boldsymbol{W}$, which simply forgets about the translation part. The group $\mathcal{P} = \{\boldsymbol{W} \mid (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}\}$ of linear parts occurring in $\mathcal{G}$ is called the *point group* $\mathcal{P}$ of $\mathcal{G}$.

The representation of space-group operations as matrix–column pairs is clearly adapted to the fact that space groups can be built from these two parts, the translation subgroup and the point group. This viewpoint will be discussed in detail in Section 1.3.3. It allows one to treat space groups in many aspects analogously to finite groups, although, due to the infinite translation subgroup, they are of course infinite groups.

1.3.2. Lattices

A crystal pattern is defined to be periodic in three linearly independent directions, which means that it is invariant under translations in three linearly independent directions. This periodicity implies that the crystal pattern extends infinitely in all directions. Since the atoms of a crystal form a discrete pattern in which two different points have a certain minimal distance, the translations that fix the crystal pattern as a whole cannot have arbitrarily small lengths. If $\mathbf{v}$ is a vector such that the crystal pattern is invariant under a translation by $\mathbf{v}$, the periodicity implies that the pattern is invariant under a translation by $m\mathbf{v}$ for every integer m. Furthermore, if a crystal pattern is invariant under translations by $\mathbf{v}$ and $\mathbf{w}$, it is also invariant by the composition of these two translations, which is the translation by $\mathbf{v} + \mathbf{w}$. This shows that the set of vectors by which the translations in a space group move the crystal pattern is closed under taking integral linear combinations. This property is formalized by the mathematical concept of a *lattice* and the translation subgroups of space groups are best understood by studying their corresponding lattices. These lattices capture the periodic nature of the underlying crystal patterns and reflect their geometric properties.

1.3.2.1. Basic properties of lattices

The two-dimensional vector space $\mathbb{V}^2$ is the space of columns $\begin{pmatrix} x \\ y \end{pmatrix}$ with two real components $x, y \in \mathbb{R}$ and the three-dimensional vector space $\mathbb{V}^3$ is the space of columns $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ with three real components $x, y, z \in \mathbb{R}$. Analogously, the n-dimensional vector space $\mathbb{V}^n$ is the space of columns $\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$ with n real components.

For the sake of clarity we will restrict our discussions to three-dimensional (and occasionally two-dimensional) space. The generalization to n-dimensional space is straightforward and only requires dealing with columns of n instead of three components and with bases consisting of n instead of three basis vectors.

Definition

For vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ forming a basis of the three-dimensional vector space $\mathbb{V}^3$, the set

$$\mathbf{L} := \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$$

of all *integral* linear combinations of $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a *lattice* in $\mathbb{V}^3$ and the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are called a *lattice basis* of $\mathbf{L}$.

It is inherent in the definition of a crystal pattern that the translation vectors of the translations leaving the pattern invariant are closed under taking integral linear combinations. Since the crystal pattern is assumed to be discrete, it follows that all translation vectors can be written as integral linear combinations of a finite generating set. The fundamental theorem on finitely generated abelian groups (see *e.g.* Chapter 21 in Armstrong, 1997) asserts that in this situation a set of three translation vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ can be found such that all translation vectors are integral linear combinations of these three vectors. This shows that the translation vectors of a crystal pattern form a lattice with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ in the sense of the definition above.

By definition, a lattice is determined by a lattice basis. Note, however, that every two- or three-dimensional lattice has infinitely many bases.