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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.

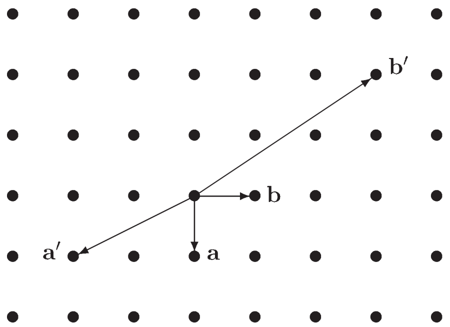

Figure 1.3.2.1
Conventional basis **a**, **b** and a non-conventional basis **a**′, **b**′ for the square lattice.

Example
The square lattice

$$\mathbf{L} = \mathbb{Z}^2 = \left\{ \begin{pmatrix} m \\ n \end{pmatrix} \mid m, n \in \mathbb{Z} \right\}$$

in $\mathbb{V}^2$ has the vectors

$$\mathbf{a} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

as its standard lattice basis. But

$$\mathbf{a}' = \begin{pmatrix} 1 \\ -2 \end{pmatrix}, \quad \mathbf{b}' = \begin{pmatrix} -2 \\ 3 \end{pmatrix}$$

is also a lattice basis of **L**: on the one hand **a**′ and **b**′ are integral linear combinations of **a**, **b** and are thus contained in **L**. On the other hand

$$-3\mathbf{a}' - 2\mathbf{b}' = \begin{pmatrix} -3 \\ 6 \end{pmatrix} + \begin{pmatrix} 4 \\ -6 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathbf{a}$$

and

$$-2\mathbf{a}' - \mathbf{b}' = \begin{pmatrix} -2 \\ 4 \end{pmatrix} + \begin{pmatrix} 2 \\ -3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \mathbf{b},$$

hence **a** and **b** are also integral linear combinations of **a**′, **b**′ and thus the two bases **a**, **b** and **a**′, **b**′ both span the same lattice (see Fig. 1.3.2.1).

The example indicates how the different lattice bases of a lattice **L** can be described. Recall that for a vector $\mathbf{v} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$ the coefficients x, y, z are called the *coordinates* and the vector $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ is called the *coordinate column* of **v** with respect to the basis **a**, **b**, **c**. The coordinate columns of the vectors in **L** with respect to a lattice basis are therefore simply columns with three integral components. In particular, if we take a second lattice basis **a**′, **b**′, **c**′ of **L**, then the coordinate columns of **a**′, **b**′, **c**′with respect to the first basis are columns of integers and thus the basis transformation $\boldsymbol{P}$ such that $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$ is an integral 3×3 matrix. But if we interchange the roles of the two bases, they are related by the inverse transformation $\boldsymbol{P}^{-1}$, *i.e.* $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = (\mathbf{a}', \mathbf{b}', \mathbf{c}')\boldsymbol{P}^{-1}$, and the argument given above asserts that $\boldsymbol{P}^{-1}$ is also an integral matrix. Now, on the one hand $\det \boldsymbol{P}$ and $\det \boldsymbol{P}^{-1}$ are both integers (being determinants of integral matrices), on the other hand $\det \boldsymbol{P}^{-1} = 1/\det \boldsymbol{P}$. This is only possible if $\det \boldsymbol{P} = \pm 1$.

Summarizing, the different lattice bases of a lattice **L** are obtained by transforming a single lattice basis **a**, **b**, **c** with integral transformation matrices $\boldsymbol{P}$ such that $\det \boldsymbol{P} = \pm 1$.

1.3.2.2. Metric properties

In the three-dimensional vector space $\mathbb{V}^3$, the *norm* or *length* of a vector $\mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}$ is (due to Pythagoras' theorem) given by

$$|\mathbf{v}| = \sqrt{v_x^2 + v_y^2 + v_z^2}.$$

From this, the *scalar product*

$$\mathbf{v} \cdot \mathbf{w} = v_x w_x + v_y w_y + v_z w_z \ \text{ for } \mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}, \mathbf{w} = \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix}$$

is derived, which allows one to express angles by

$$\cos \angle(\mathbf{v}, \mathbf{w}) = \frac{\mathbf{v} \cdot \mathbf{w}}{|\mathbf{v}|\,|\mathbf{w}|}.$$

The definition of a norm function for the vectors turns $\mathbb{V}^3$ into a *Euclidean space*. A lattice **L** that is contained in $\mathbb{V}^3$ inherits the metric properties of this space. But for the lattice, these properties are most conveniently expressed with respect to a lattice basis. It is customary to choose basis vectors **a**, **b**, **c** which define a right-handed coordinate system, *i.e.* such that the matrix with columns **a**, **b**, **c** has a positive determinant.

Definition
For a lattice $\mathbf{L} \subseteq \mathbb{V}^3$ with lattice basis **a**, **b**, **c** the *metric tensor* of **L** is the 3×3 matrix

$$\boldsymbol{G} = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix}.$$

If $\boldsymbol{A}$ is the 3×3 matrix with the vectors **a**, **b**, **c** as its columns, then the metric tensor is obtained as the matrix product $\boldsymbol{G} = \boldsymbol{A}^{\mathrm{T}} \cdot \boldsymbol{A}$. It follows immediately that the metric tensor is a symmetric matrix, *i.e.* $\boldsymbol{G}^{\mathrm{T}} = \boldsymbol{G}$.

Example
Let

$$\mathbf{a} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

be the basis of a lattice **L**. Then the metric tensor of **L** (with respect to the given basis) is

$$\boldsymbol{G} = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

With the help of the metric tensor the scalar products of arbitrary vectors, given as linear combinations of the lattice basis, can be computed from their coordinate columns as follows: If $\mathbf{v} = x_1\mathbf{a} + y_1\mathbf{b} + z_1\mathbf{c}$ and $\mathbf{w} = x_2\mathbf{a} + y_2\mathbf{b} + z_2\mathbf{c}$, then