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Group theory applied to crystallography

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1 Introduction

In the lessons of today we will focus on the group theoretic foundations of crystallography. As starting point we take two familiar definitions from the *International Tables for Crystallography, Vol.* **A** (ITA).

Definition 1 A *crystal pattern*[1] is a set of points in $\mathbb{R}^n$ such that the translations leaving it invariant form a (vector) lattice in $\mathbb{R}^n$.

A typical example of a 2-dimensional crystal pattern is displayed in Figure 1. Of course, the figure only displays a finite part of the pattern which is assumed to be infinite, but the continuation of the pattern should be clear from the displayed excerpt.

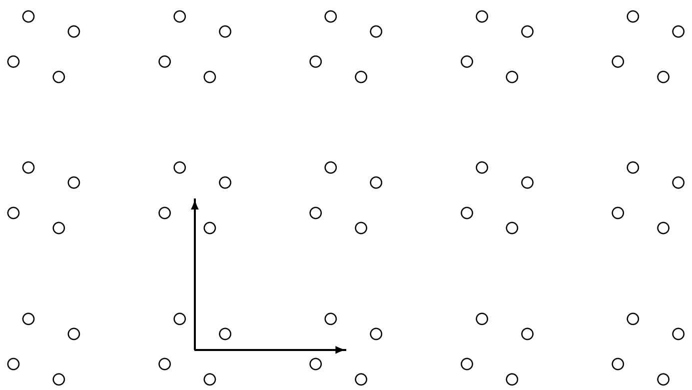


Figure 1: Crystal pattern in 2-dimensional space.

In order to get a systematic treatment of all crystal patterns, the notion of *symmetry* is exploited. Here, symmetry of a crystal pattern is understood as the collection of all isometric mappings that leave the crystal pattern as a whole unchanged.

Definition 2 A *space group*[2] is a group of isometries of $\mathbb{R}^n$ (i.e. of mappings of $\mathbb{R}^n$ preserving all distances) which leaves some crystal pattern invariant.

> The fact that the isometries that leave a crystal pattern invariant indeed form a *group* is not entirely trivial, but evident from the fact that the composition of two isometries will again result in an isometry leaving the pattern invariant.

One of the crucial roles of space groups in crystallography is that they are used to classify the different crystal patterns. The idea here is that two crystal patterns are regarded as *equivalent* if their groups of isometries are *'the same'*. In what sense two space groups are regarded as being the same will be made explicit later today.

Remark: The pattern in Figure 1 was actually obtained as the orbit of some point under a space group G which in turn is just the group of isometries of this pattern. This observation already indicates that space groups can be investigated without explicit retreat to a crystal pattern,

[1] See section 8.1.4., p. 722 of ITA, fifth edition.
[2] See section 8.1.6., p. 724 of ITA.

since a crystal pattern for which a space group is its group of isometries can always be constructed as the orbit of a (suitably chosen) point.

It is fairly obvious that the space group of the crystal pattern in Figure 1 contains translations along the indicated vectors and that it also contains fourfold rotations around the centers of each block of 4 points.

It is the purpose of today's lessons to find an appropriate description of space groups which on the one hand reflects the geometric properties of the group elements and on the other hand allows to classify space groups under various aspects.

> Although the application to 2- and 3-dimensional crystal patterns is the most interesting, it costs almost no extra effort to develop the concepts for arbitrary dimensions n. We will therefore formulate most statements for general dimension n, but will illustrate them in particular for the cases $n = 2$ and $n = 3$.

2 Elements of space groups

Before we have a closer look at the elements of space groups, we briefly review some concepts from linear algebra.

2.1 Linear mappings

Definition 3 A linear mapping g on the n-dimensional vector space $\mathbb{R}^n$ is a map that respects the sum and the scalar multiplication of vectors in $\mathbb{R}^n$, i.e. for which:

(i) $g(v+w) = g(v) + g(w)$ for all $v, w \in \mathbb{R}^n$;

(ii) $g(\alpha \cdot v) = \alpha \cdot g(v)$ for all $v \in \mathbb{R}^n$, $\alpha \in \mathbb{R}$.

Note: Since a linear mapping g respects linear combinations, it is completely determined by the images $g(v_1), \ldots, g(v_n)$ on a basis[3] $(v_1, \ldots, v_n)$:

$$g(\alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \ldots + \alpha_n \cdot v_n) = \alpha_1 \cdot g(v_1) + \alpha_2 \cdot g(v_2) + \ldots + \alpha_n \cdot g(v_n)$$

Moreover, once the images of the basis vectors are known, the image of an arbitrary linear combination $w = \alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \ldots + \alpha_n \cdot v_n$ only depends on its *coordinates* with respect to the basis.

Definition 4 Let $(v_1, \ldots, v_n)$ be a basis of $\mathbb{R}^n$ and let $w = \alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \ldots + \alpha_n \cdot v_n$ be an arbitrary vector in $\mathbb{R}^n$, written as a linear combination of the basis vectors.

Then the α_i are called the *coordinates* of w with respect to the basis $(v_1, \ldots, v_n)$ and the vector $\begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}$ is called the *coordinate vector* of w with respect to this basis.

Example: Choose $\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right)$ as basis of $\mathbb{R}^2$. Then the coordinate vector of $\begin{pmatrix} 3 \\ 4 \end{pmatrix}$ with respect to this basis is $\begin{pmatrix} -1 \\ 4 \end{pmatrix}$, since

$$\begin{pmatrix} 3 \\ 4 \end{pmatrix} = -1 \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + 4 \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} + \begin{pmatrix} 4 \\ 4 \end{pmatrix}$$

Note: If we choose the *standard basis*

$$\left(e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \ e_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \ \ldots, e_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \right)$$

for $\mathbb{R}^n$, then each column vector coincides with its coordinate vector.

[3]A *basis* of a vector space V is a set B of vectors in V such that every $v \in V$ can be uniquely written as a linear combination of the vectors in V.

However, for every basis $(v_1, \ldots, v_n)$ of $\mathbb{R}^n$, the coordinate vectors of the basis are just the vectors of the standard basis, since $v_i = 0 \cdot v_1 + \ldots + 0 \cdot v_{i-1} + 1 \cdot v_i + \ldots + 0 \cdot v_n$. It is therefore often useful to work with coordinate vectors, since that turns any given basis into the standard basis.

Since linear mappings are determined by their images on basis vectors, it is very convenient to describe them by *matrices* which provide the coordinate vectors of the images of the basis vectors.

Definition 5 Let $(v_1, \ldots, v_n)$ be a basis of $\mathbb{R}^n$ and let g be a linear mapping of $\mathbb{R}^n$. Then g can be described by the $n \times n$ matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n_2} & \ldots & a_{nn} \end{pmatrix}$$

which has as its j-th column the coordinate vector of the image $g(v_j)$ of the j-th basis vector, i.e.

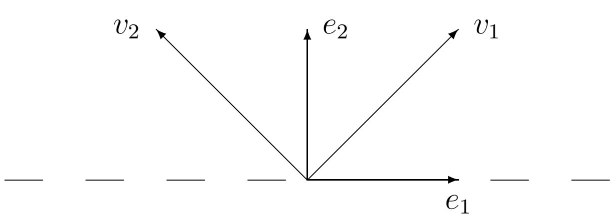
$$g(v_j) = a_{1j}v_1 + a_{2j}v_2 + \ldots + a_{nj}v_n$$

If $w = \alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \ldots + \alpha_n \cdot v_n$ is an arbitrary vector of $\mathbb{R}^n$, then the coordinate vector of its image under g is given by the *product* of the matrix A with the coordinate vector of w:

$$A \cdot \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_n \end{pmatrix} \text{ signifies that } g(w) = \beta_1 \cdot v_1 + \beta_2 \cdot v_2 + \ldots + \beta_n \cdot v_n.$$

Examples:

(1) The following figure shows two bases of $\mathbb{R}^2$, the standard basis $(e_1, e_2) = \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)$ and a different basis $(v_1, v_2) = \left(\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \end{pmatrix}\right)$.

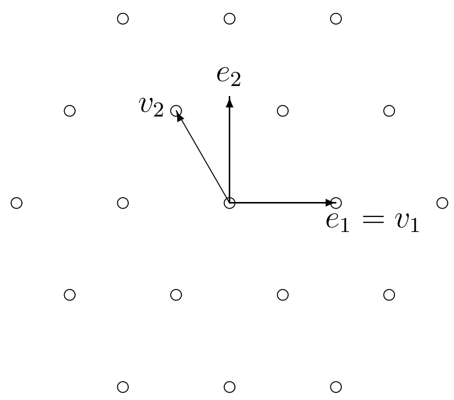


We consider the linear mapping g of $\mathbb{R}^2$ which is the reflection in the dashed line (the x-axis):

Since $e_1 \mapsto e_1$ and $e_2 \mapsto -e_2$, the matrix of g with respect to the standard basis (e_1, e_2) is $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

On the other hand, we have $v_1 \mapsto -v_2$ and $v_2 \mapsto -v_1$, hence with respect to the alternative basis (v_1, v_2), the matrix of g is $\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$.

(2) The hexagonal lattice has a threefold rotation g as symmetry operation.



With respect to the standard basis (e_1, e_2), this rotation has the matrix

$$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}.$$

However, if the symmetry adapted basis $(v_1, v_2) = \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}\right)$ is chosen, the matrix of g becomes much simpler, since $g(v_1) = v_2$ and $g(v_2) = -v_1 - v_2$. The matrix of g with respect to this basis is thus

$$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}.$$

In the context of symmetry operations, we have to make sure that a transformation can be reversed, i.e. that it has an inverse transformation such that the composition of the two mappings is the identity operation.

Definition 6 A linear mapping g on $\mathbb{R}^n$ is called *invertible* if there is a linear mapping g^{-1} such that $gg^{-1} = g^{-1}g = id$, where id denotes the identity mapping leaving every vector unchanged, i.e. $id(v) = v$ for all vectors $v \in \mathbb{R}^n$.

Lemma 7 A linear mapping g on $\mathbb{R}^n$ is invertible if and only if the images $g(v_1), \dots, g(v_n)$ of a basis $(v_1, \dots, v_n)$ of $\mathbb{R}^n$ form again a basis of $\mathbb{R}^n$.

Definition 8 The set of invertible linear mappings on $\mathbb{R}^n$ forms a group[4]. The group of corresponding $n \times n$ matrices is denoted by $GL_n(\mathbb{R})$ (for *general linear group*).

[4]A *group* G is a set of elements together with a binary operation on G, usually written as multiplication, such that (i) the operation is associative, i.e. $(g \cdot h) \cdot k = g \cdot (h \cdot k)$, (ii) G contains an identity element 1 for which $1 \cdot g = g \cdot 1 = g$ for all g and (iii) every element g of G has an inverse element g^{-1} such that $g \cdot g^{-1} = g^{-1} \cdot g = 1$.

2.2 Affine mappings

If we have a crystal pattern in n-dimensional space, there are two obvious types of operations which we might want to apply to the space in order to obtain a more suitable description of the crystal pattern:

(i) A shift of the origin[5] by a translation.

(ii) A change of basis of the underlying vector space.

Combining these two types of operations gives rise to *affine mappings*.

Definition 9 An *affine mapping* on $\mathbb{R}^n$ is the composition of a linear mapping g on $\mathbb{R}^n$ and a translation by a vector $t \in \mathbb{R}^n$.

A different motivation for the notion of affine mappings is that these are the mappings that preserve collinearity between points and ratios of distances along a line.

Notation: In the *Seitz notation*, the affine mapping which consists of the composition of the linear mapping g and the translation t is denoted by the pair $\{g \mid t\}$. One calls g the *linear part* and t the *translation part* of $\{g \mid t\}$.

Definition 10 The affine mapping $\{g \mid t\}$ acts on the vectors v of the vector space $\mathbb{R}^n$ by

$$\{g \mid t\}(v) := g \cdot v + t.$$

It is a fruitful exercise to compute the product of two affine mappings explicitly. For that, we apply the product of the two elements $\{g \mid t\}$ and $\{h \mid u\}$ to an arbitrary vector v:

$$\begin{aligned}(\{g \mid t\} \cdot \{h \mid u\})(v) &= \{g \mid t\}(h \cdot v + u) = g \cdot (h \cdot v + u) + t = gh \cdot v + g \cdot u + t \\ &= \{gh \mid g \cdot u + t\}(v).\end{aligned}$$

Lemma 11 The product of two affine mappings $\{g \mid t\}$ and $\{h \mid u\}$ is given by

$$\{g \mid t\} \cdot \{h \mid u\} = \{gh \mid g \cdot u + t\}.$$

The short computation above thus shows, that the linear parts of two affine mappings are simply multiplied. In contrast to that, the translation part of the product is not just the sum of the two translation parts, the translation part u of the second element is *twisted* by the action of the linear part g of the first element.

By Lemma 11 it is also easy to see which affine mappings are invertible and to derive the inverse of an invertible affine mapping: The identity element for the multiplication of affine mappings is $\{id \mid 0\}$, thus the affine mapping $\{g \mid t\}$ is invertible with inverse $\{h \mid u\}$ if and only if $h = g^{-1}$ and $g \cdot u = -t$, thus $u = -g^{-1} \cdot t$.

[5] In the *vector space* $\mathbb{R}^n$, the 0-vector plays a distinguished role as the identity element for vector addition. However, if regard $\mathbb{R}^n$ as *point space*, every point is equally valid to be chosen as origin. The other points of the point space are then obtained by translating the origin by the vectors in $\mathbb{R}^n$.

Lemma 12 The affine mapping $\{g \mid t\}$ is invertible if and only if its linear part g is an invertible linear mapping. In that case, the inverse of $\{g \mid t\}$ is given by

$$\{g \mid t\}^{-1} = \{g^{-1} \mid -g^{-1} \cdot t\}.$$

Examples:

(1) In dimension 2, a reflection in the line $x = y$ is given by

$$\{g \mid t\} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \middle| \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\}$$

which acts as

$$\left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \middle| \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} y \\ x \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} y \\ x \end{pmatrix}.$$

(2) A glide reflection with shift $\frac{1}{2}$ along the x-axis is given by

$$\{g \mid t\} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \middle| \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} \right\}$$

and acts as

$$\left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \middle| \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} \right\} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ -y \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} x + \frac{1}{2} \\ -y \end{pmatrix}.$$

(3) In 3-dimensional space, a fourfold screw rotation with a shift of $\frac{1}{4}$ around the z-axis is given by

$$\{g \mid t\} = \left\{ \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \middle| \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} \right\}$$

and acts as

$$\left\{ \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \middle| \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} \right\} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -y \\ x \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} -y \\ x \\ z + \frac{1}{4} \end{pmatrix}.$$

2.3 Affine group and Euclidean group

Since the composition of invertible affine mappings is again an invertible affine mapping, these mappings form a group, called the *affine group*.

Definition 13 The *affine group* $\mathcal{A}_n$ of degree n is the group of all affine mappings $\{g \mid t\}$ with invertible *linear part* $g \in GL_n(\mathbb{R})$.

The affine group plays a crucial role in crystallography, since all elements of n-dimensional space groups lie in the affine group $\mathcal{A}_n$. The following argument actually shows that elements from space groups have to be affine mappings with the additional property that their linear part is an isometry:

Let o be the (chosen) origin of $\mathbb{R}^n$ and let ϕ be an isometry[6] in a space group, then we denote by t the translation by the vector $\phi(o) - o$. Since a translation is an isometry, the mapping $\phi - t$ is also an isometry and by construction it fixes the origin o:

$$(\phi - t)(o) = \phi(o) - (\phi(o) - o) = o.$$

We do not need to assume that $\phi - t$ is a linear mapping, since an elementary (but not so well-known) fact just states that every isometry fixing the origin automatically has to be an invertible *linear* mapping g.

We thus conclude that the isometry ϕ is the composition of the invertible linear mapping $g = \phi - t$ and the translation t, i.e. an affine mapping $\{g \mid t\}$. Moreover, the linear part g has to be an isometry.

Lemma 14 Each element of a space group is an affine mapping $\{g \mid t\}$ for which the linear part g is an isometry.

The distance between two points x and y in $\mathbb{R}^n$ is defined as the length of the vector translating x to y. The usual way to express lengths (and angles) in $\mathbb{R}^n$ is via the *dot product*.

Definition 15 For two vectors $v = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$ and $w = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$ the *dot product* $v \circ w$ is given by

$$v \circ w := v^{tr} \cdot w = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = x_1 y_1 + x_2 y_2 + \ldots + x_n y_n = \sum_{i=1}^{n} x_i y_i.$$

In terms of the dot product, the length of a vector $v \in \mathbb{R}^n$ is given by

$$\|v\| := \sqrt{v \circ v}$$

and the angle α between two vectors v and w is determined by the relation

$$\cos(\alpha) = \frac{v \circ w}{\|v\| \cdot \|w\|}.$$

Using the dot product, the property of a linear mapping g to be an isometry can now be restated by saying that g preserves the dot product.

Definition 16 A linear mapping g on $\mathbb{R}^n$ is an isometry if

$$g(v) \circ g(w) = v \circ w \text{ for all } v, w \in \mathbb{R}^n.$$

We now assume that g is written with respect to the standard basis $(e_1, e_2, \ldots, e_n)$ of $\mathbb{R}^n$. For the standard basis, the dot products are given by

$$e_i \circ e_j = \begin{cases} 1 & \text{if } i = j; \\ 0 & \text{if } i \neq j. \end{cases}$$

[6] A mapping ϕ is an isometry if it preserves distances, i.e. if $\|\phi(x) - \phi(y)\| = \|x - y\|$ for all x and y.

For an isometry g this means that $g(e_i)^{tr} \cdot g(e_i) = 1$ and $g(e_i)^{tr} \cdot g(e_j) = 0$ for $i \neq j$. But $g(e_i)$ is just the i-th column of the matrix g, hence $g(e_i)^{tr} \cdot g(e_j)$ is the i-j-entry of $g^{tr} \cdot g$. Hence, g is an isometry if and only if $g^{tr} \cdot g$ is the identity matrix. Matrices with this property are called *orthogonal matrices*.

Lemma 17 A linear mapping g, written as a matrix with respect to the standard basis, is an isometry if and only if g is an orthogonal matrix, i.e. if $g^{tr} \cdot g = id$ or, equivalently, $g^{tr} = g^{-1}$.

By now we have seen that space group elements are affine mappings with orthogonal linear part. Since $(g \cdot h)^{tr} = h^{tr} \cdot g^{tr} = h^{-1} \cdot g^{-1} = (g \cdot h)^{-1}$, the product of two orthogonal matrices is again orthogonal, hence the affine mappings with orthogonal linear part form a subgroup[7] of the affine group, called the *Euclidean group*.

Definition 18 The group $\mathcal{E}_n := \{\{g \mid t\} \in \mathcal{A}_n \mid g^{tr} = g^{-1}\}$ of affine mappings with orthogonal linear part is called the *Euclidean group*.

In particular, every space group consists of elements of the Euclidean group and is thus a subgroup of the Euclidean group.

An important way to investigate subgroups of the affine group (e.g. the Euclidean group or a space group) hinges on the fact that the linear parts are just multiplied when two affine mappings are multiplied. This means that forgetting about the translation part results in a homomorphism[8] from the affine group to the matrix group $GL_n(\mathbb{R})$.

Theorem 19 Let Π be the mapping $\Pi : \mathcal{A}_n \to GL_n(\mathbb{R}) : \{g \mid t\} \mapsto g$ which forgets about the translation part of an affine mapping.

(i) The mapping Π is a group homomorphism from $\mathcal{A}_n$ onto $GL_n(\mathbb{R})$. The kernel[9] of Π is $\mathcal{T} := \{\{id \mid t\} \mid t \in \mathbb{R}^n\}$ and its image is $GL_n(\mathbb{R})$. In particular, $\mathcal{T}$ is a normal subgroup[10] of $\mathcal{A}_n$.

(ii) $\mathcal{A}_n$ contains a subgroup isomorphic to the image $GL_n(\mathbb{R})$ of Π, namely the group $\mathcal{G} = \{\{g \mid 0\} \mid g \in GL_n(\mathbb{R})\}$ of elements with trivial translation part.

(iii) Every element $\{g \mid t\}$ can be written as $\{g \mid t\} = \{id \mid t\} \cdot \{g \mid 0\}$, thus $\mathcal{A}_n = \mathcal{T} \cdot \mathcal{G}$. Since the intersection $\mathcal{T} \cap \mathcal{G}$ consists only of the identity element $\{id \mid 0\}$, this decomposition is unique and hence the affine group $\mathcal{A}_n$ is a semidirect product[11] $\mathcal{T} \rtimes GL_n(\mathbb{R})$ of $\mathcal{T}$ and $GL_n(\mathbb{R})$.

[7] A subset H of a group G that forms itself a group is called a *subgroup* of G. Since H inherits the operation from G, one only has to check that H is closed under the group operation and under taking inverses.

[8] A *homomorphism* φ between two groups G and H is a mapping that preserves the multiplication structure, i.e. for which $\varphi(gh) = \varphi(g)\varphi(h)$.

[9] The *kernel* of a group homomorphism $G \to H$ is the set of those elements of G which are mapped to the identity element 1 of H. The kernel always forms a normal subgroup of the group G.

[10] A *normal subgroup* N of G (notation $N \trianglelefteq G$) is a subgroup which is closed under conjugation, i.e. for which $g^{-1} \cdot n \cdot g \in N$ for all $n \in N$ and $g \in G$. For a normal subgroup N, the cosets $Ng = \{n \cdot g \mid n \in N\}$ form a group with multiplication defined by the representatives, i.e. $(Ng) \cdot (Nh) = N(g \cdot h)$. This group is called the *factor group* or *quotient group* of G by N.

[11] A group G is a *semidirect product* if G contains a normal subgroup N and a subgroup H such that every element g of G can be uniquely written as $g = n \cdot h$ with $n \in N$ and $h \in H$. In the case that $n \cdot h = h \cdot n$ for all $n \in N$ and $h \in H$, G is the *direct product* of N and H.

The homomorphism Π can be applied to every subgroup $G \leq \mathcal{A}_n$ of the affine group, it has the group of linear parts as its image and the normal subgroup of translations in G as its kernel. The homomorphism Π therefore allows to split a space group G into two parts.

Definition 20 Let G be a space group and let Π be the homomorphism defined in Theorem 19.

(i) The translation subgroup $T := \{\{id \mid t\} \in G\}$ is the kernel of the restriction of Π to G.

(ii) The group $P := \Pi(G)$ of linear parts in G is called the *point group*[12] of G. It is isomorphic to the factor group G/T.

Note: In general, a subgroup $G \leq \mathcal{A}_n$ is not the semidirect product of its translation subgroup and its point group. For space groups, only the *symmorphic* groups are semidirect products, whereas groups containing e.g. glide reflections with a glide not contained in their translation subgroup do not contain their point group as a subgroup.

Exercise 1.
In general, the product of affine mappings is not commutative, i.e. one usually has $\mathfrak{g} \cdot \mathfrak{h} \neq \mathfrak{h} \cdot \mathfrak{g}$. Prove that two affine mappings $\{g \mid t\}$ and $\{h \mid u\}$ commute if and only if

(i) the linear parts g and h commute;

(ii) the translation parts fulfill $(g - id) \cdot u = (h - id) \cdot t$.

Conclude that an arbitrary affine mapping $\{g \mid t\}$ commutes with a translation $\{id \mid u\}$ if and only if u is fixed under g, i.e. if $g \cdot u = u$.

2.4 Matrix notation

A very convenient way of representing affine mappings are the so-called *augmented matrices* which allow to apply affine mappings by usual matrix multiplication (i.e. just like ordinary linear mappings).

Definition 21 The *augmented matrix* of an affine mapping $\{g \mid t\}$ with linear part $g \in GL_n(\mathbb{R})$ and translation part $t \in \mathbb{R}^n$ is the $(n+1) \times (n+1)$ matrix

$$\left(\begin{array}{c|c} g & t \\ \hline 0 \ldots 0 & 1 \end{array}\right).$$

In order to apply such an augmented matrix to a vector $v \in \mathbb{R}^n$, the vector is also augmented by an additional component of value 1. The usual left-multiplication of a vector by a matrix now gives

$$\left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array}\right) \cdot \left(\begin{array}{c} v \\ \hline 1 \end{array}\right) = \left(\begin{array}{c} g \cdot v + t \\ \hline 1 \end{array}\right)$$

and ignoring the additional component yields the desired result.

[12] See section 8.1.6., p. 725 of ITA.

We explicitly check that the product of the augmented matrices coincides with the product of affine mappings as given in Lemma 11. By usual matrix multiplication we get:

$$\left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array}\right) \cdot \left(\begin{array}{c|c} h & u \\ \hline 0 & 1 \end{array}\right) = \left(\begin{array}{c|c} gh & g \cdot u + t \\ \hline 0 & 1 \end{array}\right),$$

thus the linear part of the product is gh and the translation part is $g \cdot u + t$, as required.

Note: In view of the representation of affine mappings by augmented matrices, the homomorphism Π defined in Theorem 19 becomes very natural: It just picks the upper left $n \times n$ submatrix of an $(n+1) \times (n+1)$ augmented matrix.

Examples:

(1) `p4mm`
If we take as crystal pattern the lattice points of a common square lattice, the group of isometries of this pattern is the group generated by a fourfold rotation, the reflection in the x-axis and the two unit translations along the x- and y-axis. These four elements are given by the matrices

$$\left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right).$$

(2) `c2mm`
If the crystal pattern consists of the lattice points of a rectangular lattice and the centers of the rectangles, the space group of this pattern is generated by two reflections in the x- and y-axis and translations to the centers of two adjacent rectangles. These generators are given by the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & -\frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right).$$

(3) $\mathtt{P}4_1$
In this example a 3-dimensional crystal pattern is assumed that in addition to the translations only allows a fourfold screw rotation which after 4 applications results in a unit translation along the z-axis. This space group is generated by the matrices

$$\left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{4} \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \left(\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

Exercise 2.
Two space group elements are given by the following transformations:

$$\mathfrak{g} : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} z + \frac{1}{2} \\ x + \frac{1}{2} \\ -y \end{pmatrix}, \quad \mathfrak{h} : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} -y \\ x + \frac{1}{2} \\ z + \frac{1}{2} \end{pmatrix}.$$

Determine the augmented matrices for $\mathfrak{g}$ and $\mathfrak{h}$ and compute the products $\mathfrak{g} \cdot \mathfrak{h}$ and $\mathfrak{h} \cdot \mathfrak{g}$.

3 Analysis of space groups

We have already noted that every space group is a subgroup of the Euclidean group $\mathcal{E}_n$ and that it can be split into its translation subgroup T and its point group P via the homomorphism Π. We will now deduce some fundamental properties of these ingredients and their interplay.

3.1 Lattices

Definition 22 A *lattice* in $\mathbb{R}^n$ is the set

$$L := \{x_1 v_1 + x_2 v_2 + \ldots + x_n v_n \mid x_i \in \mathbb{Z} \text{ for } 1 \leq i \leq n\}$$

of all *integral* linear combinations of a basis $B = (v_1, \ldots, v_n)$ of $\mathbb{R}^n$. The basis B is called a *lattice basis* of L.

It is inherent in the definition of a crystal pattern that the translation vectors of the translations leaving the pattern invariant form a lattice, since the translation vectors are required to have positive minimal length.

Definition 23 Let G be a space group with translation subgroup T. Then the set

$$L = \{v \in \mathbb{R}^n \mid \{id \mid v\} \in T\}$$

of translation vectors in T is called the *translation lattice* or *vector lattice* of G.

> The distinction between the translation subgroup T of a space group and its translation lattice L may seem somewhat artificial, since the two groups are clearly isomorphic via the homomorphism $\{id \mid t\} \to t$. However, since we multiply space group elements, but add lattice vectors, it is good practice to keep the two notions apart.

By definition, a lattice is determined by a lattice basis. Note however, that every lattice has infinitely many bases.

Example: For the standard 2-dimensional lattice $\mathbb{Z}^2 = \left\{ \begin{pmatrix} x \\ y \end{pmatrix} \mid x, y \in \mathbb{Z} \right\}$ every pair of vectors $\left(\begin{pmatrix} a \\ b \end{pmatrix}, \begin{pmatrix} c \\ d \end{pmatrix} \right)$ with $a, b, c, d \in \mathbb{Z}$ such that $\det \begin{pmatrix} a & c \\ b & d \end{pmatrix} = \pm 1$ is a lattice basis of $\mathbb{Z}^2$:

It is clear that the two basis vectors are elements of $\mathbb{Z}^2$. By inverting the matrix with the two vectors as its columns, one sees that

$$\begin{pmatrix} d & -c \\ -b & a \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} = (ad - bc) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} d & -c \\ -b & a \end{pmatrix} \cdot \begin{pmatrix} c \\ d \end{pmatrix} = (ad - bc) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and hence the vectors e_1 and e_2 of the standard basis of $\mathbb{Z}^2$ are integral linear combinations of the two basis vectors.

The example indicates how the different lattice bases of a lattice L can be described quite elegantly. Assume that $B = (v_1, \ldots, v_n)$ is a lattice basis of L, then the coordinate vectors of the vectors in L with respect to this basis are simply the vectors with integral components. In particular, if we take a second lattice basis $B' = (w_1, \ldots, w_n)$ of L, then the coordinate vectors of B' with respect to B are integral vectors and thus the basis transformation from B to B' is an integral matrix X.

But we could just as well have started with the basis B', then the coordinate vectors of the vectors in B also have integral coordinates with respect to the basis B'. Thus, also the basis transformation from B' to B, i.e. the inverse of the matrix X is an integral matrix.

Lemma 24 Let L be a lattice in $\mathbb{R}^n$ with lattice basis $B = (v_1, \ldots, v_n)$. Then every other lattice basis $B' = (w_1, \ldots, w_n)$ is of the form $B' = (X \cdot v_1, \ldots, X \cdot v_n)$ with $X \in GL_n(\mathbb{Z})$, i.e. the basis transformation from B to B' is an invertible integral matrix.

Metric tensors

The geometry of a lattice is usually captured by the *metric tensor* of its lattice basis, which contains the dot products of the basis vectors.

Definition 25 For a basis $B = (v_1, \ldots, v_n)$ the *metric tensor* of B is the matrix $F \in \mathbb{R}^{n\times n}$ of dot products of the basis vectors, i.e. $F_{ij} = v_i \circ v_j$.

If X is the $n \times n$ matrix with v_i as i-th column, then the metric tensor is obtained as $F = X^{tr} \cdot X$.

For a lattice L with lattice basis B, the metric tensor of B is often also called the metric tensor of L (with respect to B).

Since the metric tensor of a lattice depends on the lattice basis, it is useful to know how the metric tensor transforms under basis transformations. This is one of the many instances where the coordinate vectors play an important role.

One first observes that for the vectors of the lattice basis $(v_1, \ldots, v_n)$ one has

$$v_i \circ v_j = F_{ij} = e_i^{tr} \cdot F \cdot e_j.$$

This means that the dot product of v_i and v_j is obtained by multiplying the metric tensor from the left by the transposed coordinate vector of v_i and from the right by the coordinate vector of v_j. But since the dot product is linear in both arguments, this property immediately extends to arbitrary vectors.

Lemma 26 Let $B = (v_1, \ldots, v_n)$ be a lattice basis of the lattice L with metric tensor F. Let $v, w \in \mathbb{R}^n$ be vectors with coordinate vectors $\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$ and $\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$ with respect to B. Then

$$v \circ w = (x_1 \ \cdots \ x_n) \cdot F \cdot \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}.$$

From the previous lemma we can immediately deduce how the metric tensor transforms under basis transformations.

Lemma 27 Let $B = (v_1, \ldots, v_n)$ be a lattice basis of the lattice L with metric tensor F. Let $B' = (v_1', \ldots, v_n')$ be another lattice basis of L and denote by X the basis transformation from

B to B', i.e. X is the integral matrix with the coordinate vector of v_i' with respect to B as its i-th column. Then the metric tensor of B' is

$$F' = X^{tr} \cdot F \cdot X.$$

Via the metric tensor it can also be decided whether two lattices L_1 and L_2 are *isometric*, i.e. whether there exists a distance-preserving isomorphism from L_1 to L_2.

Lemma 28 Two lattices L_1 and L_2 in $\mathbb{R}^n$ are *isometric* if and only if there exist lattice bases $B_1 = (v_1, \dots, v_n)$ of L_1 and $B_2 = (w_1, \dots, w_n)$ of L_2 such that the metric tensors of B_1 and B_2 are the same.

Although a lattice has infinitely many different lattice bases, it is a finite problem to check whether two lattices are isometric. The idea is to fix a lattice basis B_1 for the first lattice. Then, among the *finitely many* vectors in L_2 which have the same lengths as vectors in the basis B_1, a subset of n vectors has to be found which have the correct dot products.

Fundamental domains

A lattice L can be used to subdivide $\mathbb{R}^n$ into congruent cells of finite volume. The idea is to define a suitable subset C of $\mathbb{R}^n$ such that the translates of C by the vectors in L cover $\mathbb{R}^n$ without overlapping. Such a subset C is called a *fundamental domain* of $\mathbb{R}^n$ with respect to L. Two standard constructions for such fundamental domains are the *unit cell* and the *Voronoï*[13] or *Dirichlet*[14] *cell*.

Definition 29 Let L be a lattice in $\mathbb{R}^n$ with lattice basis $B = (v_1, \dots, v_n)$.

(i) The set $C := \{x_1v_1 + x_2v_2 + \ldots + x_nv_n \mid 0 \le x_i < 1 \text{ for } 1 \le i \le n\}$ is called the *unit cell* of L with respect to the basis B.

(ii) The set $C := \{w \in \mathbb{R}^n \mid \|w\| \le \|w - v\| \text{ for all } v \in L\}$ is called the *Voronoï cell* or *Dirichlet cell* of L (around the origin).

The unit cell is simply the parallelepiped spanned by the basis vectors of the (chosen) lattice basis.

The construction of the Dirichlet cell is independent of the basis of L. It consists of those points of $\mathbb{R}^n$ which are closer to the origin than to any other lattice point of L. Note that the boundaries of the Dirichlet cells overlap, thus in order do get a proper fundamental domain, part of the boundary has to be deleted from the Dirichlet cell.

Primitive lattices and centred lattices

Although it is natural to describe a lattice by a lattice basis, it has turned out useful in crystallography to use particularly simple bases with nice properties and to describe lattices with respect to these bases even if they are no lattice basis.

[13] Georgii Fedoseevich Voronoï, 1868 - 1908
[14] Johann Peter Gustav Lejeune Dirichlet, 1805 - 1859

Definition 30 In a *primitive lattice* all vectors are integral linear combinations of a given basis, which thus is a lattice basis.

A *centred lattice* is a lattice obtained as the union of a primitive lattice L and one or more translates of L by centring vectors.

Example: The easiest example of a centred lattice is the *centred rectangular* or *rhombic* lattice in 2-dimensional space. As a basis the lattice basis $\left(\begin{pmatrix} a \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ b \end{pmatrix}\right)$ of a rectangular lattice R is chosen. The centring vector $v_c = \begin{pmatrix} \frac{a}{2} \\ \frac{b}{2} \end{pmatrix}$ is the center of the unit cell of R and the centred rectangular lattice R_c is given by

$$R_c := R \cup (v_c + R).$$

The name *centred lattice* reflects the fact that the centring vectors are usually the centers of unit cells or faces of unit cells.

3.2 Point groups

So far, we have only seen that the point group P of a space group G is a group of matrices in $GL_n(\mathbb{R})$. However, much more can be said about P, in particular it is a *finite group* of *integral matrices* if the space group G is written with respect to a lattice basis of its translation lattice L.

We will now show how these crucial properties of a point group are derived and even include some proofs (because they are very short).

Theorem 31 Let G be a space group, let $P = \Pi(G)$ be its point group and L its translation lattice.

Then P *acts*[15] *on the lattice* L, i.e. for $v \in L$ and $g \in P$ one has $g \cdot v \in L$.

Proof: Since T is a normal subgroup of G, conjugating the element $\left(\begin{array}{c|c} id & v \\ \hline 0 & 1 \end{array}\right)$ by an element $\left(\begin{array}{c|c} g^{-1} & t \\ \hline 0 & 1 \end{array}\right) \in G$ gives again an element of T. Working out this conjugation explicitly gives:

$$\begin{aligned} \left(\begin{array}{c|c} g^{-1} & t \\ \hline 0 & 1 \end{array}\right)^{-1} \left(\begin{array}{c|c} id & v \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} g^{-1} & t \\ \hline 0 & 1 \end{array}\right) &= \left(\begin{array}{c|c} g & -g \cdot t \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} g^{-1} & t + v \\ \hline 0 & 1 \end{array}\right) \\ &= \left(\begin{array}{c|c} id & g \cdot v \\ \hline 0 & 1 \end{array}\right) \in T. \end{aligned}$$

This shows that indeed $g \cdot v \in L$ and hence the point group P acts on the lattice L. ♦

By now we have worked out that the point group P of G is a group of isometries and that it acts on the lattice L of translations in G. This means that P is a subgroup of the full symmetry group

$$Aut(L) := \{g \in GL_n(\mathbb{R}) \mid g^{tr} = g^{-1},\ g(L) = L\}$$

of L. From this fact we now can prove that P is a finite group.

[15] A group G acts on a set Ω if for every $g \in G$ and $\omega \in \Omega$ an element $g \cdot \omega \in \Omega$ (the image of ω under g) is defined such that $1 \cdot \omega = \omega$ for all $\omega \in \Omega$ and $(gh) \cdot \omega = g \cdot (h \cdot \omega)$.

Theorem 32 The point group P of a space group G is finite.

Proof: We fix some lattice basis $(v_1, \dots, v_n)$ of L and assume that v_n is the longest of these basis vectors (they may of course all have the same length). Since L is a lattice, it is in particular discrete, hence it contains only finitely many vectors of length at most $\|v_n\|$. Since a symmetry operation of L preserves lengths, it can only permute vectors of the same length. But for a finite set of m elements there are at most $m! = 1 \cdot 2 \cdot \ldots \cdot (m-1) \cdot m$ permutations, and since every element of P is determined by its action on the lattice basis, there are only finitely many possibilities for the elements of P. ♦

From Theorem 32 we conclude that with respect to the standard basis of $\mathbb{R}^n$, the point group P of G is a finite group of orthogonal matrices. However, Theorem 31 states that the point group acts on the translation lattice L of G. Therefore it is natural to write G and also P with respect to a lattice basis of L. This results in the elements of P being integral matrices which are no longer orthogonal but fix the metric tensor of L.

Theorem 33 If a space group G is written with respect to a basis $(v_1, \dots, v_n)$ of $\mathbb{R}^n$, then the metric tensor F of this basis is invariant under transformations from the point group P of G, i.e.

$$g^{tr} F g = F \text{ for each } g \in P.$$

In particular, if G is written with respect to a lattice basis of its translation lattice, the point group elements are integral matrices which fix the metric tensor of the lattice basis, i.e.

$$P \subseteq \{g \in GL_n(\mathbb{Z}) \mid g^{tr} F g = F\}.$$

Proof: Let $g \in P$ be an element from the point group of G written with respect to the basis $(v_1, \dots, v_n)$ and denote by g' the same element written with respect to the *standard basis* of $\mathbb{R}^n$. Let X be the matrix of the basis transformation from the standard basis to the new basis, i.e. the matrix with v_i as i-th column. Then the rules for basis transformations state that $g = X^{-1} g' X$ and $g' = X g X^{-1}$.

For the orthogonal matrix g' we know that $g'^{tr} g' = id$ and replacing g' by $X g X^{-1}$ gives

$$g^{tr} g' = id \Rightarrow X^{-tr} g^{tr} X^{tr} X g X^{-1} = id \Rightarrow g^{tr} X^{tr} X g = X^{tr} X.$$

The metric tensor $F = X^{tr} X$ of the basis $(v_1, \dots, v_n)$ is thus preserved by g.

In the case that $(v_1, \dots, v_n)$ is a lattice basis of L, the columns of an element $g \in P$ are the coordinate vectors of a lattice vector with respect to a lattice basis and thus have integral entries. ♦

Example: The space group p3 has as translation lattice a hexagonal lattice L and its point group P is generated by a threefold rotation. With respect to the standard basis of $\mathbb{R}^2$ a generator of P is given by the matrix

$$g' = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

and one checks that g is indeed an orthogonal matrix, i.e. that $g^{tr} \cdot g = id$.

A lattice basis of the hexagonal lattice L is

$$(v_1, v_2) = \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \right) \text{ with metric tensor } F = \begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{pmatrix}.$$

If we transform the matrix g' to the lattice basis, we obtain

$$g = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$$

and this matrix indeed fixes the metric tensor, since

$$\begin{aligned} g^{tr} F g &= \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & 1 \\ -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{pmatrix} = F. \end{aligned}$$

Exercise 3.
The point group P (in the geometric class $\overline{3}\texttt{m1}$) is generated by the matrices

$$g = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \ h = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

(i) Check that P fixes the metric tensor $F = \begin{pmatrix} 2a & -a & 0 \\ -a & 2a & 0 \\ 0 & 0 & b \end{pmatrix}$. It thus acts on a hexagonal lattice.

(ii) P also acts on a rhombohedral lattice, which is obtained from the above hexagonal lattice by the basis transformation

$$X = \frac{1}{3} \begin{pmatrix} -1 & 2 & -1 \\ -2 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \text{ with inverse transformation } X^{-1} = \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \end{pmatrix}$$

Transform the metric tensor F of the hexagonal lattice to the metric tensor of the rhombohedral lattice (with the columns of X as lattice basis).

(iii) Transform P to the rhombohedral lattice (thus obtaining a point group P' in the arithmetic class $\overline{3}\texttt{mR}$) and check that the so obtained point group fixes the metric tensor computed in (ii).

3.3 Transformation to a lattice basis

The observation that the point group P acts on the translation lattice L gives rise to a change of perspective:

New point of view: Instead of writing all vectors and matrices (and hence the augmented matrices) with respect to the standard basis of $\mathbb{R}^n$ it is convenient to transform the elements of a space group to a lattice basis of its translation lattice.

Since this point of view slightly differs from the perspective of traditional crystallography, we discuss it in some detail, arguing that the (very useful) conventions taken in 2- and 3-dimensional space do not carry over to higher dimensions.

Discussion: The transformation to a lattice basis is not the standard point of view taken in traditional crystallography (dealing with $\mathbb{R}^2$ and $\mathbb{R}^3$).

- As already mentioned in Section 3.1, one often distinguishes between *primitive lattices*, where the chosen *conventional basis* is actually a lattice basis and *centred lattices*, where the *conventional cell* spanned by the vectors of the conventional basis contains more than one lattice point.

  In a centred lattice, not all vectors have integral coordinates with respect to the conventional basis and the lattice thus is actually larger than the lattice generated by the chosen conventional basis.

- From the perspective of traditional crystallography, always transforming to a lattice basis may look like we are only dealing with primitive lattices and not with centred lattices. However, this is not true because in our approach simply all lattices are what traditionally is called primitive.

- The fundamental reason for our point of view is that there is no reasonable general concept in n-dimensional space that allows to distinguish between primitive and centred lattices.

- The reason for the distinction between primitive and centred lattices is that it is often useful to work with bases which have especially nice and simple properties.

  In dimensions 2 and 3 it is indeed the case that for families of lattices which are contained in each other (like the cubic lattice and its centrings), one of these lattices has a particularly nice basis (such as the standard basis for the cubic lattice).

- In dimensions 2 and 3 the primitive lattices always have symmetry groups which are the same or larger than those of their centrings. More precisely, the only case where a centring has a smaller symmetry group is the rhombohedral lattice which has a symmetry group of order[16] 12, whereas its corresponding primitive lattice, the hexagonal lattice, has a symmetry group of order 24.

  This means that in 2- and 3-dimensional space the point groups for the centred lattices remain integral when they are written with respect to a lattice basis of the corresponding primitive lattice.

- However, the situation changes if one proceeds to dimensions beyond 3. There it is often impossible to distinguish one of the lattices in a family as primitive lattice, since none of the lattices may have a basis with particular nice geometric properties.

- Moreover, the automorphism groups of the lattices in one family may differ substantially, and not always the most simple one has the largest symmetry group. Two examples may illustrate this:

  – In dimension 4, the standard lattice $\mathbb{Z}^4$ generated by the standard basis has a symmetry group of order 384. It has a sublattice of index 2 which has a symmetry group of order 1152, i.e. larger by a factor of 3. (This sublattice is the so-called root lattice of type F_4 and has the corners of the regular polytope called the 24-cell as vectors of minimal length.)

[16] The *order* of a group G is the number of elements in G and is denoted by $|G|$. If the number of elements is not finite, one says that G has infinite order.

– In dimension 8 the situation is even more intriguing: The root lattice of type E_8 might be regarded as a centring of the 8-dimensional checkerboard lattice D_8, which in turn is the sublattice of all vectors with even coordinate sum in the standard lattice $\mathbb{Z}^8$. Both the standard lattice and the checkerboard lattice have a symmetry group of order $10\,321\,920$, whereas the E_8 lattice has a much larger symmetry group of order $696\,729\,600$.

- The example with the lattices $\mathbb{Z}^8$ and E_8 in 8-dimensional space also gives rise to a more fundamental problem. Although the symmetry group of the E_8 lattice is much larger than that of $\mathbb{Z}^8$, it does not contain the full symmetry group of $\mathbb{Z}^8$, but only a proper subgroup of it. This means that there is no basis of $\mathbb{R}^n$ with respect to which both the symmetries of the E_8 lattice and those of the standard lattice $\mathbb{Z}^8$ could be written as integral matrices. This means that there is no sensible choice for a conventional basis in this case!

- Finally, we will see that for the interplay between the translation subgroup and the point group of a space group it is extremely convenient to use the property that the translations are integral vectors.

Lemma 34 Let G be a space group written with respect to some basis B of $\mathbb{R}^n$ (e.g. the standard basis). Let X be the matrix of a basis transformation to a new basis B' of $\mathbb{R}^n$, i.e. the columns of X are the coordinate vectors of the vectors in B' with respect to the basis B.

Then writing out the conjugation by the basis transformation explicitly

$$\left(\begin{array}{c|c} X^{-1} & 0 \\ \hline 0 & 1 \end{array}\right)\left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array}\right)\left(\begin{array}{c|c} X & 0 \\ \hline 0 & 1 \end{array}\right) = \left(\begin{array}{c|c} X^{-1}gX & X^{-1}\cdot t \\ \hline 0 & 1 \end{array}\right)$$

shows that with respect to the new basis B' the element $\{g \mid t\}$ of G is transformed to the element

$$\{g' \mid t'\} = \{X^{-1}gX \mid X^{-1}\cdot t\}.$$

In particular, if $(v_1,\dots,v_n)$ is a lattice basis of the translation lattice of G and X is the transformation matrix to this lattice basis, then the translation $\{id \mid v_i\}$ is transformed to

$$\{id \mid X^{-1}\cdot v_i\} = \{id \mid e_i\}$$

where e_i is the i-th vector of the standard basis of $\mathbb{R}^n$.

Writing a space group G with respect to a lattice basis $(v_1,\dots,v_n)$ of its translation lattice L thus has the following consequences:

- All vectors $v\in\mathbb{R}^n$ are given as *coordinate vectors* with respect to the basis $(v_1,\dots,v_n)$, i.e. the coordinate vector $\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$ denotes the vector $v = x_1v_1 + \ldots + x_nv_n$.

- In particular, the translation lattice L becomes $L=\mathbb{Z}^n$, since the lattice vectors are precisely the integral linear combinations of a lattice basis.

- The translation subgroup T of G becomes $T = \{\{id \mid t\} \mid t\in\mathbb{Z}^n\}$.

- The point group P becomes a subgroup of $GL_n(\mathbb{Z})$, since the images of the vectors in the lattice basis are again lattice vectors and thus integral linear combinations of the lattice basis.

Example: In the examples above we gave the space group `c2mm` of the centred rectangular lattice with respect to a basis of the rectangular lattice. This resulted in translations with nonintegral coordinates. If we transform this group to the lattice basis $\left(\begin{pmatrix}\frac{a}{2}\\ \frac{b}{2}\end{pmatrix}, \begin{pmatrix}\frac{a}{2}\\ -\frac{b}{2}\end{pmatrix}\right)$, the generators given above are transformed to

$$\left(\begin{array}{cc|c} 0 & 1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 0 & -1 & 0 \\ -1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right).$$

Written with respect to the lattice basis, the point group fixes the metric tensor

$$\frac{1}{4}\begin{pmatrix} a^2+b^2 & a^2-b^2 \\ a^2-b^2 & a^2+b^2 \end{pmatrix}.$$

3.4 Systems of nonprimitive translations

We already remarked that in general a space group G is not a semidirect product of its translation subgroup T and its point group P, since G does not necessarily contain a subgroup which is isomorphic to P.

Example: The smallest example for a space group that is not a semidirect product is the space group G with point group of order 2 acting on a rectangular lattice such that the nontrivial element of the point group is induced by a glide reflection $\mathfrak{g}$:

$$\mathfrak{g} = \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right).$$

Any product of $\mathfrak{g}$ with a translation has a translation component along the x-axis of the form $\frac{1}{2}+k$ with $k \in \mathbb{Z}$ and $\mathfrak{g}^2 = \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right)$ is itself also a translation. Hence the space group G has besides the identity element no elements of finite order and in particular no subgroup of order 2, isomorphic to its point group.

Although the point group P may not be found as a subgroup, it still plays an important role for the description of the elements of G, since P is isomorphic to the factor group G/T.

Definition 35 For a subgroup $T \leq G$, a *(right) coset* of T is a set of the form

$$T\mathfrak{g} = \{t\mathfrak{g} \mid t \in T\} \text{ for some } \mathfrak{g} \in G.$$

Two cosets are either equal or disjoint.

A set $\{\mathfrak{g}_1, \ldots, \mathfrak{g}_r\}$ of elements in G is called a set of *coset representatives* or *transversal* for T in G if G is the disjoint union of the cosets $T\mathfrak{g}_1, T\mathfrak{g}_2, \ldots, T\mathfrak{g}_r$, i.e. if

$$G = T\mathfrak{g}_1 \,\dot{\cup}\, T\mathfrak{g}_2 \,\dot{\cup} \ldots \dot{\cup}\, T\mathfrak{g}_r.$$

In the case of space groups, one has $\{id \mid v\} \cdot \{g \mid t\} = \{g \mid t + v\}$, hence all elements in a coset of T have the same linear part. This implies that every transversal of T in G has to contain each linear part of P precisely once.

Lemma 36 Every transversal of the translation subgroup T in a space group G with point group P contains precisely one element for each element g in the point group and is thus of the form

$$\{\{g \mid t_g\} \mid g \in P\}.$$

Remark: A transversal of T in G is quite useful to construct (a reasonable part of) an orbit of G on $\mathbb{R}^n$ which in general will be a crystal pattern having G as its space group.

For that, choose a point $x \in \mathbb{R}^n$ and apply all elements of the transversal to x. If not all of the so obtained points are different or if two of these points differ by a lattice vector, the point x is in *special position*[17] and its orbit may have a space group differing from G. Otherwise, the point x is in *general position* and the full orbit of x under G is obtained by translating the $|P|$ points constructed via the transversal by lattice vectors. The space group of the orbit of a point in general position is precisely G.

Example: Figure 2 below displays an orbit of the space group $G =$ p2gg for which a transversal with respect to its translation subgroup T (corresponding to a rectangular lattice) is

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right).$$

It is convenient to plot an asymmetric symbol at the positions of the orbit points instead of a point, since this allows to recognize reflections and rotations more easily.

As point x for which the orbit is calculated, we choose the point $x = \begin{pmatrix} 0.2 \\ 0.15 \end{pmatrix}$ and we plot the symbol ϕ at each position in the appropriate orientation (the point x has the symbol $\bullet$). The dashed box contains the four points obtained from the transversal and it is obvious that translating this box by the lattice vectors results in the full orbit.

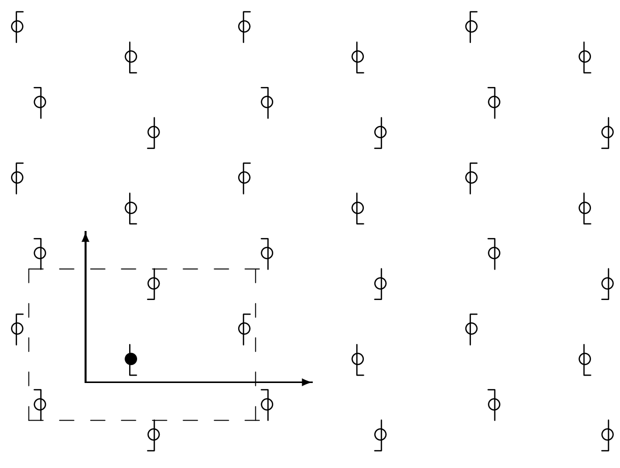


Figure 2: Orbit of a point in general position under space group p2gg.

[17] The precise definitions for *special* and *general positions* will be given in Section 6.

Definition 37 Let $\{\{g \mid t_g\} \mid g \in P\}$ be a transversal of T in G. Then the set $\{t_g \mid g \in P\}$ of translation parts in this transversal is called a *system of nonprimitive translations* or *translation vector system* which we will abbreviate as SNoT.

Of course, the transversal and thus the SNoT is by no means unique, since each t_g may be altered by a vector from the translation lattice. This means in particular that an element t_g which lies in the translation lattice L can be replaced by the 0-vector.

This also explains the term 'nonprimitive translation', since one may assume that the elements of the SNoT lie inside the unit cell of the lattice, and are therefore vectors with non-integral coordinates (or 0).

From the multiplication rule of affine mappings we can deduce an important property of a SNoT.

Theorem 38 The product $\{g \mid t_g\} \cdot \{h \mid t_h\} = \{gh \mid g \cdot t_h + t_g\}$ lies in the same coset of T as the element $\{gh \mid t_{gh}\}$, therefore the elements of a SNoT conform with

$$t_{gh} = g \cdot t_h + t_g + t \text{ for some } t \in L$$

which we call the *product condition*, abbreviated as

$$t_{gh} \equiv g \cdot t_h + t_g \mod L.$$

In particular, a SNoT is completely determined by its values on generators of the point group, since the value on products follows via the product condition.

If we assume that a space group is written with respect to a lattice basis, we can assume that the elements of its SNoT have coordinates $0 \leq x_i < 1$, since adjusting them by lattice vectors means to alter their coordinates by values in $\mathbb{Z}$. This actually makes the SNoT unique.

Definition 39 A space group G that is written with respect to a lattice basis of its translation lattice is determined by:

- the metric tensor F of the lattice basis;
- a finite group $P \leq GL_n(\mathbb{Z})$ fixing the metric tensor F;
- a SNoT $\{t_g \mid t \in P\}$ with coordinates in the interval $[0, 1)$.

The space group can then be written as:

$$G = \left\{ \left(\begin{array}{c|c} g & t_g + t \\ \hline 0 & 1 \end{array} \right) \mid g \in P, t \in \mathbb{Z}^n \right\}.$$

A space group in this form is said to be given in *standard form*.

Exercise 4.
A space group G is generated by the elements

$$\mathfrak{g} = \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{4} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \ \mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & \frac{3}{2} \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array} \right), \ \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array} \right).$$

The point group P of G has 4 elements, the identity element and the linear parts of $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{g} \cdot \mathfrak{h}$.

(i) Determine the translation lattice of G (which is not the standard lattice), transform G to a lattice basis of its translation lattice and write G in standard form. (Hint: $\mathfrak{g}^2$ and $\mathfrak{h}^2$ are translations.)

(ii) The elements $\mathfrak{g} \cdot \mathfrak{h}$ and $\mathfrak{h} \cdot \mathfrak{g}$ have the same linear part. Check that their translation part only differs by a lattice vector of the translation lattice.

4 Construction of space groups

So far we have analyzed what a space group G looks like. We have seen that G contains a translation subgroup T as a normal subgroup and that the factor group by this normal subgroup is (isomorphic to) the group of linear parts of the space group, and is a finite group called the point group P. The way in which G is built from T and P is controlled by a system of nonprimitive translations.

We will now investigate the converse problem, how for a given translation lattice L and a point group P acting on L, a space group G can be built that has translation subgroup $T \cong L$ and point group $P \cong G/T$ and what the different possibilities are.

We will always assume that we write a space group with respect to a lattice basis of its translation lattice, hence in terms of coordinate vectors we have $L = \mathbb{Z}^n$ and $P \leq GL_n(\mathbb{Z})$.

Since we have seen that a space group is completely determined by its translation subgroup T, its point group P and a SNoT, the question boils down to finding the different possible SNoTs for a point group $P \leq GL_n(\mathbb{Z})$.

One possible solution to our question always exists, namely the trivial SNoT which has $t_g = 0$ for all $g \in P$.

Definition 40 For a given point group $P \leq GL_n(\mathbb{Z})$, the space group

$$G = \left\{ \left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array} \right) \mid g \in P, t \in \mathbb{Z}^n \right\}$$

with trivial SNoT is called the *symmorphic* space group with point group P. It is a semidirect product of $\mathbb{Z}^n$ and P.

4.1 Shift of origin

Before we address the question how nontrivial SNoTs can be found, we first note a slight complication.

Example: The 1-dimensional example of the space group generated by the 'glide-reflection' $\mathfrak{g} = \left(\begin{array}{c|c} -1 & \frac{1}{2} \\ \hline 0 & 1 \end{array} \right)$ and the translation $\left(\begin{array}{c|c} 1 & 1 \\ \hline 0 & 1 \end{array} \right)$ is a space group in standard form, since $\mathfrak{g}^2 = \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & 1 \end{array} \right)$. But of course, there is nothing like a glide-reflection in 1-dimensional space, there are only two space groups, one with trivial point group and the other with a point group of order 2 and both are symmorphic.

If we check how $\mathfrak{g}$ acts, we see that 0 is mapped to $\frac{1}{2}$ and $\frac{1}{2}$ is mapped to 0, but $\frac{1}{4}$ remains fixed. We therefore have a reflection in the point $\frac{1}{4}$ which means that our space group is indeed symmorphic, but that the origin is not chosen in a clever way.

What the above example tells us is that a shift of the origin alters the SNoT of a space group. We can actually compute quite easily how the SNoT is changed by a shift of the origin by a vector

v. To compute how the matrices change, we have to conjugate with the matrix $\left(\begin{array}{c|c} id & v \\ \hline 0 & 1 \end{array}\right)$:

$$\left(\begin{array}{c|c} id & -v \\ \hline 0 & 1 \end{array}\right)\left(\begin{array}{c|c} g & t_g \\ \hline 0 & 1 \end{array}\right)\left(\begin{array}{c|c} id & v \\ \hline 0 & 1 \end{array}\right) = \left(\begin{array}{c|c} id & -v \\ \hline 0 & 1 \end{array}\right)\left(\begin{array}{c|c} g & g\cdot v + t_g \\ \hline 0 & 1 \end{array}\right)$$
$$= \left(\begin{array}{c|c} g & g\cdot v + t_g - v \\ \hline 0 & 1 \end{array}\right) = \left(\begin{array}{c|c} g & t_g + (g-id)\cdot v \\ \hline 0 & 1 \end{array}\right).$$

The translation part t_g from the SNoT is thus changed by $(g - id) \cdot v$.

Definition 41 A SNoT of the form $\{(g - id) \cdot v \mid g \in P\}$ for some vector $v \in \mathbb{R}^n$ is called an *inner derivation*.

The strange term 'inner derivation' has its origin in differential geometry and is commonly used in cohomology theory. We only remark that a SNoT can actually be regarded as an element of a cohomology group.

Note: Inner derivations can be added in an obvious way: For $t_g = (g - id) \cdot v$ and $t'_g = (g - id) \cdot v'$ we have $t_g + t'_g = (g - id) \cdot (v + v')$.

Theorem 42 A space group with SNoT $\{t_g \mid g \in P\}$ is symmorphic if and only if each t_g is of the form $t_g = (g - id) \cdot v$ for some fixed vector $v \in \mathbb{R}^n$, i.e. if the SNoT is an inner derivation.

More generally, assume that two space groups G and G' with the same point group P have SNoTs $\{t_g \mid g \in P\}$ and $\{t'_g \mid g \in P\}$ which differ by an inner derivation, i.e.

$$t_g - t'_g = (g - id) \cdot v \text{ for some vector } v.$$

Then G and G' actually are the same space group, only written with respect to different origins differing by the vector v.

Example: Let P be the point group `2mm` generated by

$$g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ h = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

For a vector $v = \begin{pmatrix} x \\ y \end{pmatrix}$ we get $(g - id) \cdot v = \begin{pmatrix} 0 \\ -2y \end{pmatrix}$ and $(h - id) \cdot v = \begin{pmatrix} -2x \\ 0 \end{pmatrix}$ as inner derivations.

An arbitrary SNoT $\{t_g = \begin{pmatrix} a \\ b \end{pmatrix}, t_h = \begin{pmatrix} c \\ d \end{pmatrix}\}$ can thus be changed to $\{t'_g = \begin{pmatrix} a \\ 0 \end{pmatrix}, t'_h = \begin{pmatrix} 0 \\ d \end{pmatrix}\}$ by an inner derivation by choosing $v = \frac{1}{2}\begin{pmatrix} c \\ b \end{pmatrix}$.

Exercise 5.
Show that an inner derivation $\{t_g = (g - id) \cdot v \mid g \in P\}$ fulfills the product condition $t_{gh} \equiv g \cdot t_h + t_g \bmod L$ by showing that even the equality $t_{gh} = g \cdot t_h + t_g$ holds.

The following theorem (which is not hard to prove) states that by an appropriate shift of the origin, the coordinates of a SNoT become rational numbers with denominators at most the order $|P|$ of the point group. This immediately shows that there are only finitely many different space groups for a given point group and lattice, since there are only finitely many rational numbers $0 \le \frac{p}{q} < 1$ with denominator at most $|P|$.

Theorem 43 Let $\{t_g \mid g \in P\}$ be the SNoT of a space group. If the origin is shifted by the vector

$$v = \frac{1}{|P|} \sum_{g \in P} t_g,$$

then the SNoT $\{t'_g \mid g \in P\}$ with respect to the new origin has the property that $t'_g \in \frac{1}{|P|}\mathbb{Z}^n$. This means that the coordinates of the t'_g are rational numbers with denominators dividing $|P|$ (and thus in particular bounded by $|P|$).

4.2 Determining systems of nonprimitive translations

We have seen that the different possible space groups built from T and P are determined by the different SNoTs modulo inner derivations. The possible SNoTs are restricted by:

(1) the product condition $t_{gh} \equiv g \cdot t_h + t_g \bmod \mathbb{Z}^n$;

(2) the translation part t of $\{id \mid t\}$ has to be an integral vector, i.e. $t \in \mathbb{Z}^n$.

The product condition reduces the determination of the SNoT to generators of the point group P. But even then the second restriction - although appearing fairly innocent - amounts in a seemingly infinite task:

Problem: If an arbitrary product in the generators of P gives the identity element of P, then the translation part of the corresponding product in the space group has to be an integral vector. In principle these are infinitely many different products which one would have to check.

Fortunately, the question of describing all products in the generators of a group which result in the identity is a classical problem in group theory and actually was one of the first problems to be addressed computationally. The idea is to use a *presentation* of the point group by *abstract generators* and *defining relators*.

Definition 44 A group $P = \langle g_1, \ldots, g_s \rangle$ has the *presentation*[18]

$$\langle x_1, \ldots, x_s \mid r_1, \ldots, r_t \rangle$$

with *abstract generators* x_i and *defining relators* $r_j = r_j(x_1, \ldots, x_s)$ which are products in the x_i and their inverses x_i^{-1}, if the following hold:

- Substituting g_i for x_i in the relators yields the identity element of P.
- All products of the g_i giving the identity can be derived from the relators r_j by the following transformations:
  - insertion or deletion of a relator in a product;
  - conjugation with a generator x_i or its inverse x_i^{-1};
  - insertion or deletion of subterms of the form xx^{-1} and $x^{-1}x$.

[18] An equivalent but more abstract definition of the presentation of a group uses the concept of a *free group*. In that context the group P is obtained as the factor group of a free group by the smallest normal subgroup containing the relators.

Examples:

(1) The cyclic group C_n of order n has the presentation $\langle x \mid x^n \rangle$.

(2) The symmetry group D_n of a regular n-gon has the presentation

$$\langle x, y \mid x^n, y^2, (xy)^2 \rangle$$

where x represents a rotation of order n and y a reflection.

The first two relators allow to reduce the powers of x and y by n and 2, respectively. The third relator can be read as $xy = yx^{-1}$ and allows to collect all powers of x to the left and all y to the right. The relators thus allow to reduce every product in x and y to one of the $2n$ products $x^i y^j$ with $0 \leq i < n$ and $0 \leq j < 2$. These $2n$ products correspond to the $2n$ elements of D_n.

(3) The symmetric group S_4 of all permutations of 4 symbols has the presentation

$$\langle x, y, z \mid x^2, y^2, z^2, (xy)^3, (yz)^3, (xz)^2 \rangle$$

where x, y, z represent the permutations $(1,2)$, $(2,3)$, $(3,4)$, respectively. In this example it is slightly harder to check that the given relators are actually sufficient.

(4) The symmetry group O_h of the cube has generators

$$g = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \; h = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

A presentation for this group with x and y representing g and h is given by

$$\langle x, y \mid x^6, y^4, (xyx)^2, (xy^{-1})^2 \rangle.$$

Remarks:

(1) For a finite group it is always possible to find defining relators. For small groups this can usually be done by hand, but often it is more convenient to use standard tools from computer algebra packages.

(2) The opposite problem, to identify a group given by a presentation is much harder. In general, it is even impossible to decide whether a product in a group given by abstract generators and defining relators is the identity element of the group.

The application of group presentations to the problem of determining SNoTs is based on the following observation.

Theorem 45 Let $g_1, \ldots, g_s$ be generators of a point group P and let $\langle x_1, \ldots, x_s \mid r_1, \ldots, r_t \rangle$ be a presentation of P.

Assume further that $\mathfrak{g}_i = \left(\begin{array}{c|c} g_i & t_i \\ \hline 0 & 1 \end{array} \right)$ are augmented matrices for $1 \leq i \leq s$ such that substituting x_i by $\mathfrak{g}_i$ in the relators of P gives translations with translation vector in $\mathbb{Z}^n$.

Then all products in the $\mathfrak{g}_i$ which have the identity of P as linear part have translation parts in $\mathbb{Z}^n$.

This theorem is proved by checking that the transformations given in Definition 44 by which the products evaluating to the identity may be manipulated do not change the property of having a translation part in $\mathbb{Z}^n$.

Corollary 46 Let P be a point group with presentation as above and let $\mathfrak{g}_i$ be augmented matrices such that the relators of P evaluate to translations with translation vectors in $\mathbb{Z}^n$.

Then, extending the translations t_i for the generators of P to all elements of P via the product condition $t_{gh} = g \cdot t_h + t_g$ gives a SNoT for P.

We are thus reduced to the problem of choosing translation parts for the generators of P such that evaluating the relators of P on these elements gives translations with integral coordinates. But this means just to solve a (finite) system of linear congruences modulo $\mathbb{Z}$, which are called the *Frobenius*[19] *congruences*.

Definition 47 Let $g_1, \ldots, g_s$ be generators of a point group P and let $\langle x_1, \ldots, x_s \mid r_1, \ldots, r_t \rangle$ be a presentation of P.

Let $\mathfrak{g}_i = \left(\begin{array}{c|c} g_i & t_i \\ \hline 0 & 1 \end{array}\right)$ be augmented matrices for $1 \leq i \leq s$ where the coordinates of the translation vectors t_i are *indeterminates*.

Then evaluating the relators of P in the augmented matrices $\mathfrak{g}_i$ and equating the result with $0 \bmod \mathbb{Z}$ gives rise to a system of linear congruences which are called the *Frobenius congruences*.

Every solution of the Frobenius congruences gives rise to a SNoT for P. Since we already know that SNoTs differing only by an inner derivation represent the same space group with respect to a different origin, in order to determine the different space groups with point group P and translation lattice $\mathbb{Z}^n$, we only have to consider representatives of the solutions of the Frobenius congruences up to inner derivations.

> **To whom it may concern:** We are by now heavily busy with cohomology theory. The solutions of the Frobenius congruences modulo inner derivations are nothing but the first cohomology group $H^1(P, \mathbb{R}^n/\mathbb{Z}^n)$ which is isomorphic to the second cohomology group $H^2(P, \mathbb{Z}^n)$.

Example: We consider the point group `2mm` generated by

$$g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ h = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

which has presentation $\langle x, y \mid x^2, y^2, (xy)^2 \rangle$.

Evaluating the relators on the augmented matrices

$$\mathfrak{g} = \left(\begin{array}{cc|c} 1 & 0 & a \\ 0 & -1 & b \\ \hline 0 & 0 & 1 \end{array}\right), \ \mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & c \\ 0 & 1 & d \\ \hline 0 & 0 & 1 \end{array}\right)$$

[19] Georg Frobenius, 1849 - 1917, introduced this approach in 1911. It was reintroduced in mathematical crystallography by Johann Jakob Burckhardt, 1903 - 2006, in the 1930's.

gives the three matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 2a \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 2d \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right).$$

The Frobenius congruences are thus

$$2a \equiv 0 \bmod \mathbb{Z} \quad \text{and} \quad 2d \equiv 0 \bmod \mathbb{Z}.$$

We have already seen that the inner derivations for this group allow to set $b = 0$ and $c = 0$, and it is indeed a good idea to first compute the inner derivations and eliminate as many of the indeterminates as there are linearly independent inner derivations before evaluating the relators.

Thus, modulo the inner derivations we have the possible solutions $a \in \{0, \frac{1}{2}\}$ and $d \in \{0, \frac{1}{2}\}$ which give rise to the following four SNoTs:

(1) $t_g = t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$: this is the symmorphic space group.

(2) $t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \ t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$: the space group has a glide reflection along the x-axis and an ordinary reflection along the y-axis.

(3) $t_g = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \ t_h = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$: the space group has an ordinary reflection along the x-axis and a glide reflection along the y-axis.

(4) $t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \ t_h = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$: the space group has glide reflections along the x- and y-axis.

Exercise 6.
Compute the inner derivations and the solutions of the Frobenius congruences modulo the inner derivations for the following point groups P:

(1) P is generated by

$$g = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ h = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^2, y^2, (xy)^2 \rangle$.

(2) P is generated by

$$g = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \ h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^4, y^2, (xy)^2 \rangle$.

Example: In order to show that the concept of finding SNoTs via Frobenius congruences carries over to higher dimensions, we consider a 4-dimensional example.

The symmetry group of a regular octagon is the dihedral group of order 16, which is generated by the matrices

$$g = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \ h = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^8, y^2, (xy)^2 \rangle$. Note that representing the group by 2×2 matrices is possible, but involves irrational numbers like $\sqrt{2}$ and thus results in a non-crystallographic group.

We first determine the inner derivations. Since $g - id$ is an invertible matrix, letting v run over $\mathbb{R}^4$ results in $(g - id) \cdot v$ running over all vectors of $\mathbb{R}^4$. Thus the translation part of g can be chosen as the 0-vector and only the translation part of h has to be considered in indeterminates.

The first relator is now superfluous. Evaluating the other two relators on the matrices

$$\mathfrak{g} = \left(\begin{array}{cccc|c} 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \end{array}\right), \ \mathfrak{h} = \left(\begin{array}{cccc|c} 0 & 0 & 0 & 1 & a \\ 0 & 0 & 1 & 0 & b \\ 0 & 1 & 0 & 0 & c \\ 1 & 0 & 0 & 0 & d \\ \hline 0 & 0 & 0 & 0 & 1 \end{array}\right)$$

gives the two matrices

$$\mathfrak{h}^2 = \left(\begin{array}{cccc|c} 1 & 0 & 0 & 0 & a+d \\ 0 & 1 & 0 & 0 & b+c \\ 0 & 0 & 1 & 0 & b+c \\ 0 & 0 & 0 & 1 & a+d \\ \hline 0 & 0 & 0 & 0 & 1 \end{array}\right), \ (\mathfrak{g}\mathfrak{h})^2 = \left(\begin{array}{cccc|c} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & a+c \\ 0 & 0 & 1 & 0 & 2b \\ 0 & 0 & 0 & 1 & a+c \\ \hline 0 & 0 & 0 & 0 & 1 \end{array}\right)$$

The Frobenius congruences are thus:

$$a + d \equiv 0 \bmod \mathbb{Z},\ b + c \equiv 0 \bmod \mathbb{Z},\ a + c \equiv 0 \bmod \mathbb{Z},\ 2b \equiv 0 \bmod \mathbb{Z}$$

We either have $b = 0$ which implies $c = 0$, $a = 0$, $d = 0$ or $b = \frac{1}{2}$ which implies $c = \frac{1}{2}$, $a = \frac{1}{2}$, $d = \frac{1}{2}$.

The only nontrivial SNoT is thus given by

$$t_g = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \ t_h = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

4.3 Normalizer action

There is still one issue we have to consider in order to arrive at truly different space groups. So far, we have regarded the point group P as the set of linear parts of the space group G. However, these elements can be permuted by an (abstract) automorphism of the point group. Applying an automorphism means to *relabel* the elements without changing their role in the group.

Example: The cyclic group C_4 of order 4 has an automorphism which interchanges the two elements of order 4 in the group. The element of order 2 is fixed by the automorphism since it plays a unique role in the group (being the only element of order 2).

Since we are dealing with space groups, we can only apply such automorphisms which respect that the space group has translation lattice $\mathbb{Z}^n$. In particular, an automorphism has to map the standard basis of $\mathbb{Z}^n$ to another lattice basis of $\mathbb{Z}^n$ and therefore must be given by conjugation with an element of $GL_n(\mathbb{Z})$.

Definition 48 For a point group $P \leq GL_n(\mathbb{Z})$ the group

$$N := N_{GL_n(\mathbb{Z})}(P) := \{a \in GL_n(\mathbb{Z}) \mid a^{-1}ga \in P \text{ for all } g \in P\}$$

is called the *integral normalizer* of P.

It is the group of automorphisms of P which additionally map the lattice $\mathbb{Z}^n$ to itself.

Remark: It can in general be a fairly difficult task to determine the integral normalizer of a point group P. However, in low dimensions the point groups are well-known groups and also their automorphisms can be computed easily. It then remains to check whether an abstract automorphism is induced by conjugation with an integral matrix.

Examples:

(1) The group $P = \{id, -id\}$ has $N = GL_n(\mathbb{Z})$ as its integral normalizer, since $\pm id$ commutes with any matrix. This shows that the integral normalizer is not necessarily a finite group. However, since the finite group P has only finitely many different automorphisms, there are only finitely many different conjugation actions on P. The subgroup of N which fixes P elementwise, i.e. for which $a^{-1}ga = g$ holds for all $g \in P$ is called the *integral centralizer* of P. It is a subgroup of finite index in the integral normalizer.

(2) The point group P generated by the matrices

$$g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ h = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

has an integral normalizer which is generated by g, h and the additional element

$$a = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which interchanges the two basis vectors.

Note that the group P has an abstract automorphism φ of order 3 which cyclically interchanges the elements g, h and gh. But since gh has trace -2, whereas g and h have trace 0, an automorphism which is given by matrix conjugation has to fix gh and can only interchange g and h, since the trace is invariant under matrix conjugation.

(3) The full symmetry group P of the square lattice generated by the matrices

$$g = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \ h = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

has an abstract automorphism which interchanges the two types of reflections (reflections in x- and y-axis vs. diagonal reflections). This automorphism is induced by conjugation with the matrix

$$a = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

which is an element of $GL_n(\mathbb{Q})$ but not of $GL_n(\mathbb{Z})$ and thus is not contained in the integral normalizer of P. The integral normalizer $N_{GL_2(\mathbb{Z})}(P)$ is thus just P itself.

Lemma 49 Assume that $a \in N_{GL_n(\mathbb{Z})}(P)$ and that $\{g \mid t_g\} \in G$. The action of a on $\{g \mid t_g\}$ is given by

$$\left(\begin{array}{c|c} a^{-1} & 0 \\ \hline 0 & 1 \end{array}\right) \cdot \left(\begin{array}{c|c} g & t_g \\ \hline 0 & 1 \end{array}\right) \cdot \left(\begin{array}{c|c} a & 0 \\ \hline 0 & 1 \end{array}\right) = \left(\begin{array}{c|c} a^{-1}ga & a^{-1} \cdot t_g \\ \hline 0 & 1 \end{array}\right).$$

In particular, if $g' \in P$ such that $g = a^{-1}g'a$, then conjugation by a maps $\{g \mid t_g\}$ to $\{g \mid a^{-1} \cdot t_{g'}\}$.

The element t_g of a SNoT is thus changed by the action of a, namely according to

$$t_g \mapsto a^{-1} \cdot t_{aga^{-1}}.$$

We have just seen that transforming a space group with an element from the integral normalizer will in general change the SNoT. However, since an automorphism is applied, the space group obtained via the action of the integral normalizer is not a different space group but rather a relabeling of the elements of the same space group.

Important note: The integral normalizer reveals an *inherent ambiguity* in the geometric situation. In example (2) above we have seen that the integral normalizer of the group P generated by

$$g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ h = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

contains the transformation which interchanges the two basis vectors. This means that after interchanging the basis vectors, the group P remains the same. But this means, that the two reflections are *geometrically indistinguishable*. The crucial point is that g and h are reflections in two perpendicular lines, but none of these lines can be distinguished geometrically as belonging to the first basis vector.

Example: We have already computed that there are four SNoTs modulo inner derivations for the point group $P = 2\mathtt{mm}$ generated by

$$g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ h = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}:$$

(1) $t_g = \begin{pmatrix} 0 \\ 0 \end{pmatrix},\ t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$; (2) $t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix},\ t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$;

(3) $t_g = \begin{pmatrix} 0 \\ 0 \end{pmatrix},\ t_h = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$; (4) $t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix},\ t_h = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$.

Since the normalizer element $a = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ interchanges g and h, its action on the SNoTs can be seen immediately.

Applying a to the SNoTs (1) and (4) does not change them, but for the SNoT (2) with $t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix},\ t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ we get

$$t_g \mapsto a^{-1} \cdot t_{aga^{-1}} = a \cdot t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad t_h \mapsto a^{-1} \cdot t_{aha^{-1}} = a \cdot t_g = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$$

and this is precisely the SNoT (3).

The two SNoTs (2) and (3) are thus interchanged by the integral normalizer and give rise to the same space group.

Discussion: It is worthwhile to discuss this example in full detail: The point group `2mm` is the symmetry group of a rectangular lattice. It fixes a metric tensor of the form

$$F = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \; a, b > 0, a \neq b.$$

However, from the point group it can not be concluded whether $a < b$ or $a > b$, i.e. whether the first or the second basis vector is the short one. If we thus have a space group with a reflection along one of the axes and a glide reflection along the other one, we can not tell whether the glide is along the short or the long side. Thus, the two space groups with either a glide along the first or a glide along the second basis vector are regarded as equivalent.

Note: The algorithm consisting of:

- finding the inner derivations;
- setting up and solving the Frobenius congruences;
- finding orbit representatives for the action of the integral normalizer modulo the inner derivations

was described by Zassenhaus[20] in 1948 and is therefore often called the *Zassenhaus algorithm*.

Exercise 7.
A certain point group P (known as $\mathtt{m}\bar{3}$) is generated by

$$g = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \; h = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and has presentation $\langle x, y \mid x^6, y^2, (xy)^3, (x^3y)^2 \rangle$.

Since $g - id$ is invertible, $(g - id) \cdot v$ runs over all vectors in $\mathbb{R}^3$, hence by a shift of origin the translation part of g may be assumed to be 0.

The integral normalizer of P contains the matrix $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ which interchanges the second and third basis vector.

Determine the solutions of the Frobenius congruences for P (assuming that $t_g = 0$) and check which of the resulting SNoTs lie in one orbit under the integral normalizer of P.

[20]Hans Zassenhaus, 1912-1991

5 Space group classification

In this section we will consider various aspects under which space groups may be grouped together. We will start with the finest notion of equivalence, which are the *space group types* and will end with the coarsest, the classification into *crystal families*.

5.1 Space group types

By the approach via translation lattices and point groups which are glued together to a space group via a SNoT, we can (in principle) determine all space groups in n-dimensional space up to isomorphism, provided the possible lattices and point groups are known.

By a famous theorem of Bieberbach (1911) isomorphism of space groups is the same as affine equivalence.

Theorem 50 Two space groups in n-dimensional space are isomorphic if and only if they are conjugate[21] by an affine mapping from $\mathcal{A}_n$.

In crystallography, usually a notion of equivalence slightly different from affine equivalence is used. Since crystals occur in physical space and physical space can only be transformed by orientation preserving mappings, space groups are only regarded as equivalent if they are conjugate by an *orientation preserving* affine mapping, i.e. by an affine mapping that has linear part with positive determinant.

Definition 51 Two space groups are said to belong to the same *space group type* if they are conjugate under an orientation preserving affine mapping.

Example: The two space groups $\mathtt{P4}_1$ and $\mathtt{P4}_3$ generated by fourfold screw rotations in opposite directions are clearly *isomorphic*, but they belong to *different space group types*. The affine mapping transforming them into each other (reflection in $x = y$ plane) is *not orientation preserving*.

However, groups that differ only by their orientation are closely related to each other and share many properties. One addresses this phenomenon by the concept of *enantiomorphism*.

Definition 52 Two space groups G and G' are said to form an *enantiomorphic pair* if they are conjugate under an affine mapping, but not under an orientation preserving affine mapping.

If G is the full group of isometries of some crystal pattern, then its enantiomorphic counterpart G' is the group of isometries of the mirror image of this crystal pattern.

The number of space group types is thus the number of isomorphism classes plus the number of enantiomorphic pairs. For dimensions up to 6, these numbers are displayed in Table 1.

dimension	1	2	3	4	5	6
isomorphism classes	2	17	219	4783	222018	28927922
enantiomorphic pairs	0	0	11	111	79	7052
space group types	2	17	230	4894	222097	28934974

Table 1: Number of space group types in dimensions up to 6.

[21] Two groups G and H are said to be *conjugate* by an element x if $H = \{x^{-1}gx \mid g \in G\}$. Obviously this requires that multiplication of the elements of G and H with x is well-defined. Usually, x is an element of a larger group K containing both G and H as subgroups. One then also says that G and H are conjugate subgroups of K.

5.2 Arithmetic classes

Starting from the space groups, it is natural to collect those space groups together which only differ by their SNoTs. Assuming that the space groups are given in standard form, i.e. with respect to a lattice basis of their translation subgroups, this means that two groups are regarded as equivalent if they only differ by the choice of the lattice basis. But that means that the point groups are conjugate by an integral matrix.

Definition 53 Two space groups (written with respect to lattice bases of their translation subgroups) lie in the same *arithmetic class* if their point groups P and P' are conjugate by an integral basis transformation, i.e. if $P' = \{X^{-1}gX \mid g \in P\}$ for some $X \in GL_n(\mathbb{Z})$.

We will also say that two point groups $P, P' \leq GL_n(\mathbb{Z})$ lie in the same arithmetic class if they are conjugate by a matrix in $GL_n(\mathbb{Z})$.

Point groups in the same arithmetic class act on the same lattice and differ only by the choice of the lattice basis.

Since for each point group and each lattice there is one distinguished SNoT, namely the trivial SNoT giving rise to the symmorphic space group, it is evident that the number of arithmetic classes of space groups is the same as the number of symmorphic space group types.

Example: The space groups $\mathtt{Pm}\overline{\mathtt{3}}\mathtt{m}$, $\mathtt{Pn}\overline{\mathtt{3}}\mathtt{n}$, $\mathtt{Pm}\overline{\mathtt{3}}\mathtt{n}$ and $\mathtt{Pn}\overline{\mathtt{3}}\mathtt{m}$ all belong to the same arithmetic class that may be represented by the symmorphic group $\mathtt{Pm}\overline{\mathtt{3}}\mathtt{m}$. This arithmetic class is different from the arithmetic classes of the symmorphic space groups $\mathtt{Fm}\overline{\mathtt{3}}\mathtt{m}$ and $\mathtt{Im}\overline{\mathtt{3}}\mathtt{m}$, since there the point groups act on different (centred) lattices.

In Table 2, these numbers of arithmetic classes of space groups are given for dimensions up to 6.

dimension	1	2	3	4	5	6
arithmetic classes	2	13	73	710	6079	85311

Table 2: Number of arithmetic classes in dimensions up to 6.

We have seen that the point group P of a space group G is a subgroup of the full symmetry group $Aut(L)$ of the translation lattice L of G. But $Aut(L)$ is a finite subgroup of $GL_n(\mathbb{Z})$, hence it is a point group itself, namely of the symmorphic space group with point group $Aut(L)$ and translation lattice L.

This shows that some of the arithmetic classes are distinguished, because their groups are full symmetry groups of their lattices, while others are proper subgroups.

Definition 54 Let P be a point group acting on a lattice L such that P is the full symmetry group of L. Then the arithmetic class containing P is called a *Bravais*[22] *class*.

Since the groups in one Bravais class act on the same lattice, but groups from different Bravais classes act on different lattices, the Bravais classes correspond to the different *Bravais types of lattices* or *lattice types* for short.

There are now two obvious directions in which arithmetic classes can be merged into larger classes. The word 'direction' can be taken literally, if groups are considered to be positioned in

[22] Auguste Bravais, 1811-1863, described the different types of lattices in 2- and 3-dimensional space in 1850.

a plane, where groups of the same order are on the same horizontal level and subgroups thus lie below their supergroups.

Vertically: Starting with a group P from a Bravais class, we can join the arithmetic class of P with the arithmetic classes of its subgroups. However, since P acts on a particular lattice, we will only consider those subgroups of P which do not act on a *more general* lattice, i.e. on a lattice which has a smaller symmetry group than P.

This direction of joining arithmetic classes leads to the notion of *Bravais flocks*.

Horizontally: Suppose that P is a point group acting on some lattice L. Then P also acts on other lattices than L, obvious examples are scalings like $2L$, $3L$, or $\frac{1}{2}L$. The interesting cases are those lattices L' which lie between L and one of its scalings, these are just the *centrings* of L.

In general, the action of P on L' gives rise to a point group P' which does not lie in the same arithmetic class as P, but is isomorphic with P' and it is worthwhile to join the arithmetic classes of P and P'.

This direction of joining arithmetic classes leads to the notion of *geometric classes* which are also known as *point group types*.

5.3 Bravais flocks

We have already seen that a lattice can be characterized by its metric tensor containing the dot products of a lattice basis. If a point group P acts on a lattice L, it fixes the metric tensor of L. However, a point group in general fixes not only a single metric tensor (or multiples thereof), but it actually fixes all metric tensors from a certain vector space.

Definition 55 Let $P \leq GL_n(\mathbb{Z})$ be a finite integral matrix group. Then

$$\mathcal{F}(P) := \{F \in \mathbb{R}^{n\times n} \mid F = F^{tr},\ g^{tr}Fg = F \text{ for all } g \in P\}$$

is called the *space of metric tensors* of P.

The dimension of $\mathcal{F}(P)$ is called the *number of parameters* for the metric tensors of P.

Note: The metric tensor of a lattice basis is a *positive definite*[23] matrix. It is clear that not all matrices in $\mathcal{F}(P)$ are positive definite (e.g. for $F \in \mathcal{F}(P)$ positive definite, $-F$ is certainly not positive definite), but the positive definite matrices in $\mathcal{F}(P)$ form what is called an *open cone*. This open cone contains a basis of $\mathcal{F}(P)$ consisting of positive definite metric tensors. The metric tensors in the open cone of $\mathcal{F}(P)$ thus represent the different geometries of lattices on which P acts.

If P is generated by the matrices $g_1, \ldots, g_r$, the space $\mathcal{F}(P)$ of metric tensors can be computed as the space of solutions of a system of linear equations in the entries of F, namely

$$g_i^{tr}Fg_i - F = 0,\ 1 \leq i \leq r.$$

[23] A symmetric matrix F is *positive definite* if $v^{tr}Fv > 0$ for $v \neq 0$.

Examples:

(1) Let $P = \mathtt{2mm}$ be the group generated by

$$g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \; h = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

and let $F = \begin{pmatrix} a & c \\ c & b \end{pmatrix}$. Then

$$g^{tr} F g - F = \begin{pmatrix} a & -c \\ -c & b \end{pmatrix} - \begin{pmatrix} a & c \\ c & b \end{pmatrix} = \begin{pmatrix} 0 & -2c \\ -2c & 0 \end{pmatrix},$$

$$h^{tr} F h - F = \begin{pmatrix} a & -c \\ -c & b \end{pmatrix} - \begin{pmatrix} a & c \\ c & b \end{pmatrix} = \begin{pmatrix} 0 & -2c \\ -2c & 0 \end{pmatrix},$$

hence $c = 0$ and a and b are arbitrary, thus the number of parameters is 2 and

$$\mathcal{F}(P) = \left\{ \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \mid a, b \in \mathbb{R} \right\}.$$

This space of metric tensors characterizes the rectangular lattice.

(2) Let $P = \mathsf{4}$ be the group generated by $g = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and let $F = \begin{pmatrix} a & c \\ c & b \end{pmatrix}$. Then

$$g^{tr} F g - F = \begin{pmatrix} b & -c \\ -c & a \end{pmatrix} - \begin{pmatrix} a & c \\ c & b \end{pmatrix} = \begin{pmatrix} b-a & -2c \\ -2c & b-a \end{pmatrix},$$

hence $c = 0$ and $a = b$ is arbitrary, thus the number of parameters is 1 and

$$\mathcal{F}(P) = \left\{ \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \mid a \in \mathbb{R} \right\}.$$

This space of metric tensors characterizes the square lattice.

The space of metric tensors is useful to decide whether a subgroup of some point group P acts on a more general lattice than P. For example, the group 4 from example (2) above has the same space of metric tensors as the full symmetry group 4mm of the square lattice. However, the subgroup 2 of 4 (generated by g^2) has a space of metric tensors of dimension 3. It acts on the oblique lattice, which is more general than the square lattice.

Definition 56 Let P be a point group from a Bravais class. Then the *Bravais flock* of P consists of the arithmetic classes of subgroups of P, which have the same space of metric tensors as P.

The Bravais flocks collect together those arithmetic classes which genuinely act on the same lattice. They are thus in correspondence with the lattice types and Bravais classes, since each Bravais flock contains exactly one Bravais class.

Example: The symmorphic space groups for the centred tetragonal lattice are $\mathtt{I4}$, $\mathtt{I\bar{4}}$, $\mathtt{I4/m}$, $\mathtt{I422}$, $\mathtt{I4mm}$, $\mathtt{I\bar{4}m2}$, $\mathtt{I\bar{4}2m}$ and $\mathtt{I4/mmm}$. The arithmetic classes of these groups are joined into the Bravais flock of the *centred tetragonal lattice*. The point groups of all groups in this Bravais flock have the same spaces of metric tensors as the groups in the arithmetic class $\mathtt{4/mmmI}$ (which have 2 parameters).

The numbers of Bravais flocks, and thus also of Bravais classes and lattice types are given in Table 3.

dimension	1	2	3	4	5	6
lattice types	1	5	14	64	189	841

Table 3: Number of lattice types in dimensions up to 6.

5.4 Geometric classes

Let P be a point group acting on a lattice L and written with respect to a lattice basis of L. Assume that P also acts on a lattice L' which is different from L and let X be the transformation matrix from the lattice basis of L to a lattice basis of L'. Written with respect to that basis of L' the action of P is given by

$$P' = \{X^{-1}gX \mid g \in P\}.$$

Since $L \neq L'$, we have that $X \notin GL_n(\mathbb{Z})$, but clearly $X \in GL_n(\mathbb{R})$.

Definition 57 Two space groups lie in the same *geometric class* if their point groups P and P' are conjugate by a real basis transformation, i.e. if $P' = \{X^{-1}gX \mid g \in P\}$ for some $X \in GL_n(\mathbb{R})$.

We will also say that two point groups $P, P' \leq GL_n(\mathbb{Z})$ lie in the same geometric class if they are conjugate by a matrix in $GL_n(\mathbb{R})$.

Point groups in the same geometric class are the actions of a matrix group on different lattices.

Historically, the geometric classes in dimension 3 were determined much earlier[24] than the space groups. They were obtained as the symmetry groups for the set of normal vectors of crystal faces which describe the morphological symmetry of macroscopic crystals.

Note: It is more familiar to speak of the geometric classes as the *types of point groups*. This emphasizes the point of view to regard a point group as the group of linear parts of a space group, written with respect to an *arbitrary basis* of $\mathbb{R}^n$ (not necessarily a lattice basis).

It is also common to state that *there are* 32 *point groups in* 3*-dimensional space*. This is just as imprecise as saying that *there are* 230 *space groups*, since there are in fact infinitely many point groups and space groups.

What is meant if we say that two space groups have *the same point group* is usually that their point groups are of the same type (i.e. lie in the same geometric class) and can thus be *made to coincide* by a basis transformation of $\mathbb{R}^n$.

Example: The space groups $\mathtt{P\bar{4}2m}$, $\mathtt{P\bar{4}m2}$, $\mathtt{I\bar{4}m2}$ and $\mathtt{I\bar{4}2m}$ all have the same point group type which is denoted both by $\mathtt{\bar{4}m2}$ and by $\mathtt{\bar{4}2m}$ in the ITA. However, from the symbols it is obvious that the information on the lattice type is dropped (by forgetting about `P` or `I`).

The numbers of geometric classes of space groups are given in Table 4.

dimension	1	2	3	4	5	6
geometric classes	2	10	32	227	955	7104

Table 4: Number of geometric classes in dimensions up to 6.

[24]The geometric classes were determined by Moritz Ludwig Frankenheim, 1801-1869, in 1826 and by Johann Friedrich Christian Hessel, 1796-1872, in 1830. The space group types were found independently by Arthur Schoenflies, 1853 - 1928 and Evgraf Stepanowitch Fedorov, 1853 - 1919, in 1890/1891.

Starting with the space group types, we get the classification into arithmetic classes if we keep the information about the point groups *and* lattices and forget about the SNoTs, and we get the classification into geometric classes if we also forget about the lattices, thus keeping only the point group information:

$$\text{space group types} \underset{\text{forget SNoT}}{\longrightarrow} \text{arithmetic classes} \underset{\text{forget lattice}}{\longrightarrow} \text{geometric classes}$$

Diagram of arithmetic classes

In Figure 3 the subgroup diagram of arithmetic classes in the hexagonal crystal family (this term will be explained below) in dimension 3 is displayed.

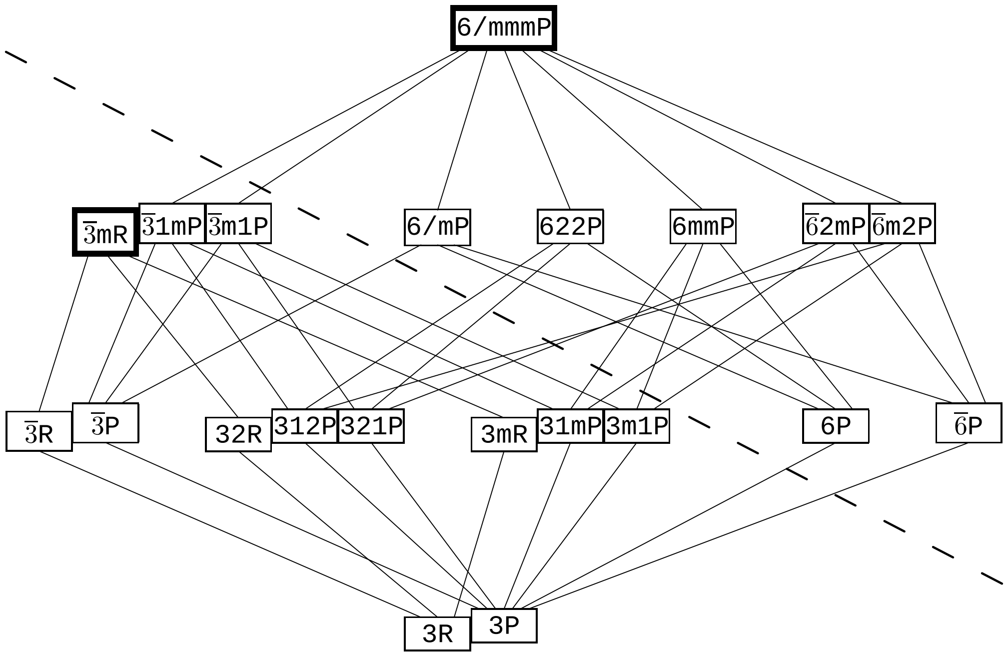


Figure 3: Arithmetic classes in the hexagonal crystal family.

This diagram illustrates the different possibilities of moving between arithmetic classes discussed so far:

- The boxes represent the arithmetic classes.
- The thick boxes represent the Bravais classes.
- If boxes are joined by a line, the lower group is a maximal[25] subgroup of the upper group.
- The Bravais flock of a Bravais class consists of those boxes which can be joined by a chain to the box of the Bravais class (note that in this diagram all groups have spaces of metric tensors of dimension 2).
- Boxes which are directly joined together horizontally lie in the same geometric class and are thus actions of the same group on different lattices.

[25] A group H is a *maximal subgroup* of G if there exists no subgroup of G that lies properly between G and H, i.e. if $H \leq K \leq G$ implies $K = H$ or $K = G$.

- Only for the sake of clearness some boxes are slightly lowered (the boxes with symbols ending on R) in order to emphasize that the action is on a *different* lattice.

In particular, we can read off that the 21 arithmetic classes fall into 12 geometric classes and 2 Bravais flocks, the Bravais flock of Bravais class 6/mmmP contains all arithmetic classes with symbols ending on P and contains the groups genuinely acting on a hexagonal lattice, the Bravais flock of Bravais class $\overline{3}$mR contains all classes with symbols ending on R and contains the groups acting on a rhombohedral lattice.

5.5 Lattice systems

The idea by which arithmetic classes are joined into geometric classes can analogously be applied to Bravais classes and Bravais flocks. If the full symmetry groups of two different lattices are conjugate by a basis transformation $X \in GL_n(\mathbb{R})$, the corresponding Bravais flocks may be joined into a larger class.

Definition 58 Two Bravais flocks are said to belong to the same *lattice system* if their Bravais classes belong to the same geometric class.

Analogously, we will say that two lattice types belong to the same lattice system if their full symmetry groups belong to the same geometric class.

On the one hand every lattice system contains a Bravais class, on the other hand all the Bravais classes in a lattice system lie in the same geometric class, hence there are as many lattice systems as there are geometric classes containing Bravais classes.

Definition 59 A geometric class is called a *holohedry* if at least one of the arithmetic classes contained in it is a Bravais class. A holohedry is thus a matrix group that is the full symmetry group of at least one of the lattices on which it acts.

Every holohedry belongs to precisely one lattice system and every lattice system contains precisely one holohedry.

Note: In the hexagonal crystal family displayed in Figure 3 every lattice system consists just of a single Bravais flock, since both holohedries contain only one Bravais class. This is not a typical situation, usually a holohedry contains more than one Bravais class the Bravais flocks of which are then joined into a lattice system.

In Table 5 the numbers of lattice systems which are the same as the numbers of holohedries are given for dimensions up to 6.

dimension	1	2	3	4	5	6
lattice systems	1	4	7	33	57	220

Table 5: Number of lattice systems in dimensions up to 6.

5.6 Crystal systems

For the geometric class of a point group P, the arithmetic classes contained in it determine on which lattices P acts. A further possibility to classify point groups therefore is given by joining those geometric classes which act on the same set of lattices.

Definition 60 Two geometric classes belong to the same *crystal system* if the arithmetic classes contained in them belong to the same set of Bravais flocks.

Example: In the hexagonal crystal family displayed in Figure 3, the dashed line separates the two crystal systems. The geometric classes below the dashed line act both on hexagonal and on rhombohedral lattices, this crystal system is called the *trigonal crystal system*. The geometric classes above the dashed line only act on hexagonal lattice and belong to the *hexagonal crystal system*.

A crystal system can contain at most one holohedry, and in the example above it does so. Indeed, all crystal systems in dimensions up to 4 contain a holohedry, but for higher dimensions this is no longer true.

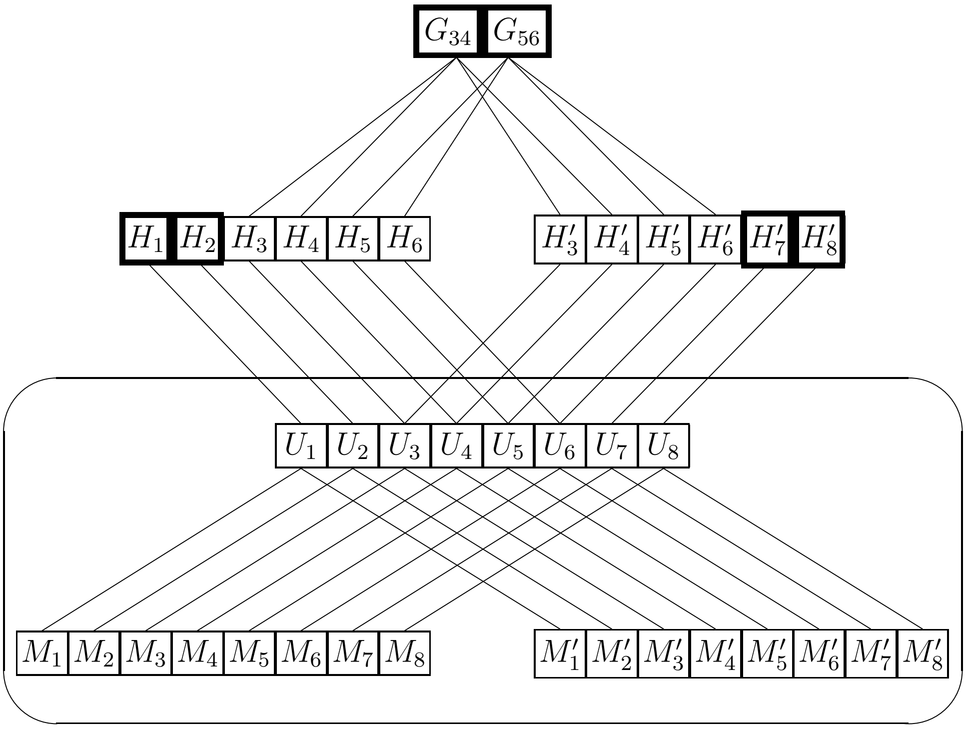


Figure 4: Crystal system without a holohedry in 5-dimensional space.

Figure 4 displays a part of the arithmetic classes in a crystal family in 5-dimensional space. There are six Bravais classes, indicated by the bold boxes, which represent six different lattices. But only the geometric classes in the oval frame act on all the six different lattices. The holohedries on the top level act on two of the lattices and the holohedries on the second level both act on four of the lattices. Thus, the geometric classes in the oval frame form a crystal system that does not contain a holohedry. The three holohedries form crystal systems on their own.

The numbers of lattice systems are given in Table 6.

dimension	1	2	3	4	5	6
crystal systems	1	4	7	33	59	251

Table 6: Number of crystal systems in dimensions up to 6.

Note that in dimension 6 there are already 31 crystal systems that do not contain a holohedry (251 crystal classes vs. 220 holohedries).

5.7 Crystal families

The coarsest classification level for space groups (and point groups) collects all arithmetic classes together which can be reached by moving inside Bravais flocks and inside geometric classes.

Definition 61 The *crystal family* of a space group G is the smallest set of arithmetic classes containing G which contains full Bravais flocks and full geometric classes.

If we graph all arithmetic classes of dimension n in the way shown in Figures 3 and 4, the crystal families are the connected components if we regard boxes joined by lines or directly joined horizontally as being linked.

Put in a different way, we can reach all point groups in a crystal family by an iteration of the following moves:

- move to a subgroup or supergroup with a space of metric tensors of the same dimension;
- move to a conjugate group by a basis transformation.

The numbers of crystal families are given in Table 7.

dimension	1	2	3	4	5	6
crystal families	1	4	6	23	32	91

Table 7: Number of crystal families in dimensions up to 6.

Note: Up to dimension 3 it seems exceptional that a crystal family splits into different crystal systems, since the only instance of this phenomenon is the splitting of the hexagonal crystal family into the trigonal and the hexagonal crystal systems. However, in higher dimensions it becomes rare that a crystal family consists of a single crystal system, hence this is actually the exceptional case and the splitting into several crystal systems is the rule.

Summary

We finish this section by collecting together the numbers of classes on the different classification levels for dimensions up to 6 in Table 8.

dimension	1	2	3	4	5	6
crystal families	1	4	6	23	32	91
lattice systems	1	4	7	33	57	220
crystal systems	1	4	7	33	59	251
lattice types	1	5	14	64	189	841
geometric classes	2	10	32	227	955	7104
arithmetic classes	2	13	73	710	6079	85311
space group types	2	17	230	4894	222079	28934974

Table 8: Number of classes on different classification levels in dimensions up to 6.

6 Site-symmetry groups

We have already discussed in Section 3.1 that the space $\mathbb{R}^n$ can be partitioned into congruent cells by translating the unit cell of a lattice basis by the vectors of the lattice. Note that we still assume that a space group is written with respect to a lattice basis of its translation lattice: If L is the translation lattice of a space group G and $(v_1, \ldots, v_n)$ is a lattice basis of L, then the unit cell C of L is given by

$$C := \{x_1 v_1 + \cdots + x_n v_n \mid 0 \leq x_i < 1 \text{ for } 1 \leq i \leq n\}.$$

This means that every cell contains precisely one lattice point, for the unit cell C this is the origin.

Important note: The terminology on unit cells is occasionally somewhat confusing. In Section 8.1.4. of ITA (p. 723) a unit cell is the parallelepiped spanned by a *crystallographic basis* of a lattice. In the case that such a basis is actually a lattice basis, it is called a *primitive basis* and the unit cell coincides with our notion here. However, if for a centred lattice a basis of the underlying primitive lattice is chosen as crystallographic basis, this unit cell contains more than one point of the centred lattice.

On the other hand, in Section 9.1.4. of ITA (p.743), the lattice bases are always primitive, but in addition *conventional bases* are defined which are (particularly nice) bases for the primitive lattices. These bases span what is called a *conventional cell*.

In order to avoid misunderstandings, we will always assume that the unit cell is the parallelepiped spanned by a lattice basis, and we will call a cell spanned by a conventional basis (which is not necessarily a lattice basis) a conventional cell (in line with Section 9.1.4. of ITA).

Since the translates of the unit cell by lattice vectors cover $\mathbb{R}^n$ without overlapping, an arbitrary point in $\mathbb{R}^n$ can be translated into the unit cell by a unique translation in the translation subgroup: Let $(v_1, \ldots, v_n)$ be the lattice basis and assume that with respect to this lattice basis a point $x \in \mathbb{R}^n$ has coordinate vector $\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$. Since the unit cell consists of the points with coordinate vectors having coordinates in the interval $[0, 1)$ (i.e. 1 is excluded), we have to subtract the *integer part* of each coordinate. The integer part of a real number x is denoted by $\lfloor x \rfloor$ and is defined as the largest integer $\leq x$. For example, $\lfloor 2.3 \rfloor = 2$ and $\lfloor -1.5 \rfloor = -2$.

The unique translation by which x is moved into the unit cell is thus given by

$$v = \lfloor x_1 \rfloor \cdot v_1 + \cdots + \lfloor x_n \rfloor \cdot v_n.$$

Example: For the rhombic lattice with lattice basis $\left(v_1 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, v_2 = \begin{pmatrix} -1 \\ 2 \end{pmatrix}\right)$, the coordinate vector of the point $x = \begin{pmatrix} 3.8 \\ 1.6 \end{pmatrix}$ is $\begin{pmatrix} 2.3 \\ -1.5 \end{pmatrix}$, since $x = 2.3 \cdot v_1 - 1.5 \cdot v_2$. The required translation is thus $v = \lfloor 2.3 \rfloor \cdot v_1 + \lfloor -1.5 \rfloor \cdot v_n = 2v_1 - 2v_2 = \begin{pmatrix} 4 \\ 0 \end{pmatrix}$. We have $x - v = \begin{pmatrix} -0.2 \\ 1.6 \end{pmatrix}$ which indeed lies in the unit cell because $x - v = 0.3 \cdot v_1 + 0.5 \cdot v_2$.

6.1 Crystallographic orbits

Since the elements of a space group provide symmetries of a crystal pattern, two points x and y which are mapped to each other by a space group element can be regarded as being *geometrically* *equivalent*. Starting from a point $x \in \mathbb{R}^n$, it is easy to obtain infinitely many points equivalent to x, we simply have to apply all space group elements to x. This idea gives rise to the notion of an *orbit* of a point under a space group G.

Definition 62 Let G be a space group in n-dimensional space and let $x \in \mathbb{R}^n$ be a point. Then the (infinite) set

$$G(x) := \{\mathfrak{g}(x) \mid \mathfrak{g} \in G\}$$

is called the *orbit of x under G* or the *G-orbit of x*.

The G-orbit of x is the smallest subset of $\mathbb{R}^n$ that contains x and is closed under the action of G. It is also called a *crystallographic orbit*.

It is clear that the G-orbit of a point x is completely determined by its points in the unit cell, since on the one hand the orbit is invariant under the action of the translation subgroup T of G and on the other hand translating the unit cell by T entirely covers $\mathbb{R}^n$.

We also note that the above discussion has shown that for every element g in the point group P of G there is exactly one element $\mathfrak{g} \in G$ with linear part g such that $\mathfrak{g}(x)$ lies in the unit cell. In other words, every coset of T in G contains exactly one element $\mathfrak{g}$ such that $\mathfrak{g}(x)$ lies in the unit cell.

This means that the number of points of $G(x)$ which lie in the unit cell is at most the number of cosets of T in G, which is the same as the order $|P|$ of P.

We now have two obvious possibilities:

(1) The points in the orbit of x under G are all different. In this case there are indeed $|P|$ points of the orbit in the unit cell.

(2) Some points of the orbit coincide. In this case there are strictly less than $|P|$ points of the orbit in the unit cell. We will actually see that the number of points in the unit cell is a divisor of $|P|$.

If two points of the orbit of x under G coincide, this means that there are elements $\mathfrak{g} \neq \mathfrak{h} \in G$ such that $\mathfrak{g}(x) = \mathfrak{h}(x)$. But from this we see that $\mathfrak{h}^{-1} \cdot \mathfrak{g}(x) = x$, hence x is fixed by the nontrivial element $\mathfrak{h}^{-1} \cdot \mathfrak{g}$ of G.

Definition 63 The subgroup[26] $G_x := Stab_G(x) := \{\mathfrak{g} \in G \mid \mathfrak{g}(x) = x\}$ is called the *site-symmetry group* or the *stabilizer* of x in G.

Since translations fix no point in $\mathbb{R}^n$, site-symmetry groups can not contain translations. As a consequence, a site-symmetry group contains at most one element of a coset $T\mathfrak{g} = \{t\mathfrak{g} \mid t \in T\}$. This means that applying the homomorphism Π which forgets about the translation parts is an isomorphism from the site-symmetry group to a subgroup of the point group P of G.

Theorem 64 Let G_x be a site-symmetry group of G. Then the elements of G_x all have different linear parts and the homomorphism $\Pi : \{g \mid t\} \to g$ is an isomorphism from G_x to a subgroup of P.

In particular, the order of the site-symmetry group G_x is a divisor[27] of the order $|P|$ of the point group.

[26] The fact that the site-symmetry group is indeed a *subgroup* of G follows from the observation that $\mathfrak{g}(x) = x$ and $\mathfrak{h}(x) = x$ implies $\mathfrak{g} \cdot \mathfrak{h}(x) = \mathfrak{g}(x) = x$, i.e. G_x is closed under multiplication.

[27] The famous *Theorem of Lagrange* states that the order $|H|$ of a subgroup H of a finite group G divides $|G|$. This is an immediate consequence of the fact that the cosets of H in G all contain the same number of elements.

Remark: There is an alternative way to see that the linear parts of a site-symmetry group G_x form a subgroup of the point group of G. Since x is fixed by all elements of G_x, shifting the origin to x will necessarily result in augmented matrices with translation part 0. But shifting the origin is realized by conjugating with a translation and this does not change the linear parts of G_x.

In order to count the number of orbit points in the unit cell, we will now assume that x already lies in the unit cell. We already stated that from each coset $T\mathfrak{g}$ there is exactly one element $t\mathfrak{g}$ such that $y := t\mathfrak{g}(x)$ lies in the unit cell. We will denote this element by $\mathfrak{g}_u$.

If $y = x$, then $\mathfrak{g}_u \in G_x$ is an element in the site-symmetry group and we already know that there are $|G_x|$ elements for which this is the case. However, if y is different from x, then for every $\mathfrak{h} \in G_x$ we have $\mathfrak{g}_u \cdot \mathfrak{h}(x) = \mathfrak{g}_u(x) = y$. This means that multiplying $\mathfrak{g}_u$ (from the right) with all elements of G_x gives $|G_x|$ elements with different linear parts which map x to y. Thus, the point y is hit $|G_x|$ times.

We have thus seen that there are $|P|$ elements of G such that $\mathfrak{g}(x)$ lies in the unit cell and that every point of the orbit lying in the unit cell is hit $|G_x|$ times. This means that the number of different orbit points in the unit cell is $|P|/|G_x|$.

Lemma 65 Let $x \in \mathbb{R}^n$ be a point with site-symmetry group G_x of order $|G_x|$. Then every point in the orbit $G(x)$ of x is obtained via $|G_x|$ different elements of G.

In particular, the number of points of the G-orbit of x which lie in the unit cell is $|P|/|G_x|$.

If we are dealing with centred lattices, then the conventional cell of the lattice (which is the unit cell of the primitive lattice) contains $k > 1$ translates of the unit cell of the centred lattice. This means that the conventional cell contains k points of the centred lattice.

In this case, the number of points of the G-orbit of x which lie in the *conventional cell* of the centred lattice is $k \cdot |P|/|G_x|$.

6.2 Points in general and in special position

The general idea behind applying group theory to crystallography is the concept, that objects are classified via their symmetry properties. One example for this concept is to regard two crystal patterns as equivalent if their symmetry groups are space groups of the same type.

We are now ready for a further application of this principle. When we analyze crystals, one of the crucial questions is to determine the actual positions of the atoms. It turns out that often the atoms occupy positions that have a nontrivial site-symmetry group. This suggests to classify the points in $\mathbb{R}^n$ into equivalence classes according to their site-symmetry groups.

Definition 66 A point $x \in \mathbb{R}^n$ is called a point in *general position* for the space group G if its site-symmetry group contains only the identity element of G, i.e. if $G_x = \{id\}$.

Otherwise, x is called a point in *special position*.

The distinction into general and special positions is of course very coarse. But we already noted that two points in the same orbit under the space group are geometrically equivalent. However, such points do not have the *same* site-symmetry group, but they have *conjugate* site-symmetry groups.

Definition 67 Two subgroups H_1 and H_2 of a group G are said to be *conjugate in G* if there is an element $g \in G$ such that

$$H_2 = \{g^{-1}hg \mid h \in H_1\}.$$

If two subgroups are conjugate by an element g one briefly writes $H_2 = g^{-1}H_1 g$.

Note: The importance of the notion of conjugation lies in the fact that conjugation is an *isomorphism* from H_1 to H_2. It is easy to see that conjugation respects the multiplication, since $g^{-1}(hk)g = (g^{-1}hg)(g^{-1}kg)$. Moreover, if $g^{-1}hg = 1$, then $h = gg^{-1} = 1$, hence only the identity is mapped to the identity, and hence conjugation is an isomorphism.

The crucial observation for points in one orbit is that if $\mathfrak{h} \in G_x$ and if $\mathfrak{g} \in G$ is an element mapping x to y, i.e. $\mathfrak{g}(x) = y$ and $x = \mathfrak{g}^{-1}(y)$, then

$$\mathfrak{g}\mathfrak{h}\mathfrak{g}^{-1}(y) = \mathfrak{g}\mathfrak{h}(x) = \mathfrak{g}(x) = y,$$

i.e. $\mathfrak{g}\mathfrak{h}\mathfrak{g}^{-1}$ lies in G_y.

Lemma 68 Let x and y be points in the same orbit of a space group G, i.e. there exists $\mathfrak{g} \in G$ such that $\mathfrak{g}(x) = y$. Then for the site-symmetry groups one has $G_y = \mathfrak{g} \cdot G_x \cdot \mathfrak{g}^{-1}$, i.e. the site-symmetry groups are conjugate by the element mapping y to x.

Example: Let G be the space group of type p4gm generated by the augmented matrices

$$\mathfrak{g} = \left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right)$$

and the translations of the standard lattice.

Let $x = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$ be a point in the unit cell. One easily checks that the site-symmetry group G_x (of point group type 2) is generated by

$$\mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & 1 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right).$$

The point x is mapped to the point $y = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$ (also lying in the unit cell) by $\mathfrak{g}$. Hence the site-symmetry group G_y of y is generated by

$$\mathfrak{g}\mathfrak{h}\mathfrak{g}^{-1} = \left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \left(\begin{array}{cc|c} -1 & 0 & 1 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) = \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right)$$

One immediately sees that the last matrix indeed fixes the point y.

Exercise 8.

Let G be the space group of type p4gm generated as above by the matrices

$$\mathfrak{g} = \left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right)$$

and the translations of the standard lattice. Let $x = \begin{pmatrix} 0.2 \\ 0.7 \end{pmatrix}$ be a point in the unit cell.

(i) Determine the site-symmetry group G_x of x in G and show that it has point group type $\mathtt{m}$.

(ii) Find the points in the unit cell that lie in the orbit of x under G. (Hint: Since the point group P of G has order 8 and $|G_x| = 2$, you should find 4 points.)

(iii) Find elements of G mapping x to each of the other three orbit points in the unit cell and determine the site-symmetry groups of these points.

6.3 Affine and Euclidean normalizers of space groups

Since we want to declare points in one orbit under the space group G to be equivalent, we certainly have to collect all those points in one class which have site-symmetry groups that are conjugate in G. However, even if the site-symmetry groups of two points are not conjugate, they still may play equivalent roles. This is due to the fact that G can be seen as the subgroup of a much larger group, e.g. of the Euclidean group $\mathcal{E}_n$ or the full affine group $\mathcal{A}_n$. It may happen that two subgroups of G are not conjugate by an element of G, but by an element of such a larger group.

What we have to consider here is the *normalizer* of a group in a larger group. We actually already saw an instance where a normalizer plays an important role, namely in the context of constructing space groups with given translation lattice and point group. There the action of the *integral normalizer* of the point group on the SNoTs had to be taken into account.

Definition 69 Let G be a group and let H be a subgroup of G. Then the *normalizer* of H in G is the subgroup $N_G(H)$ of elements of G that fix H under conjugation, i.e.

$$N_G(H) = \{g \in G \mid g^{-1}Hg = H\}.$$

Since $h^{-1}Hh = H$ for all $h \in H$, it is clear that $H \leq N_G(H) \leq G$. Moreover, H is a normal subgroup of G if and only if $N_G(H) = G$.

There are two main issues why the normalizer N of H in G is interesting:

(1) The different conjugate subgroups of H in G (i.e. the orbit of H under the conjugation action of G) are in one-to-one correspondence with the cosets of N in G.

(2) Since the normalizer fixes H, conjugating by a normalizer element result in an automorphism of H. Such an automorphism permutes the subgroups of H and two subgroups of H which are not conjugate in H may lie in the same orbit under the normalizer.

In particular the second issue is important for space groups. We have seen that the augmented matrices of a space group change under shifts of the origin and basis transformations, i.e. under affine transformations. This can be realized as conjugation by elements of the affine group $\mathcal{A}_n$. The orbit of a space group under this conjugation action is the set of space groups that belong to the same space group type.

The normalizer of a space group G in the affine group now consists precisely of those coordinate transformations of $\mathbb{R}^n$ that leave G unchanged as a whole. This means that the elements of G are relabelled without changing their geometric properties.

Definition 70 Let G be a space group and let $N_{\mathcal{A}} := N_{\mathcal{A}_n}(G)$ be the normalizer of G in the affine group. Then $N_{\mathcal{A}}$ is called the *affine normalizer* of G.

Since not all elements of the affine group are isometries, the affine normalizer may alter the metric tensor of the translation lattice of a space group. This is due to the fact that a point group not only fixes the metric tensor of the translation lattice of its space group, but, as we have seen in Section 3.1, it fixes metric tensors from a whole space of metric tensors. Under a coordinate transformation with an element from the affine normalizer this space of metric tensors is fixed as a whole but the single metric tensors may not be fixed.

Example: We have already seen that the point group of the space group of type `p2mm` fixes all metric tensors of the form $\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$ with $a, b \in \mathbb{R}$. The affine normalizer contains an element with linear part $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and transforming with this element changes the metric tensor from $\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$ to $\begin{pmatrix} b & 0 \\ 0 & a \end{pmatrix}$. This means that the roles of the short and the long basis vector in the rectangular lattice are interchanged.

Note: If the linear parts of the affine normalizer form a *finite* group N (which is not necessarily the case), there is a little trick by which the affine normalizer of a space group G can be turned into a group of isometries for a suitable lattice: We apply all elements $n_1, \ldots, n_{|N|}$ of N to the metric tensor F, this gives a set of $|N|$ (not necessarily different) metric tensors $n_i^{tr} F n_i$ and we now form the sum

$$F_0 := n_1^{tr} F n_1 + \cdots + n_{|N|}^{tr} F n_{|N|} = \sum_{i=1}^{|N|} n_i^{tr} F n_i$$

of these metric tensors. Then F_0 is fixed by all elements of N, since transforming by an element of N only permutes the tensors in the sum.

It is clear that F_0 is also fixed by the point group P of G, since P is a subgroup of N, hence we can regard G as a space group with translation lattice with metric tensor F_0. Then the affine normalizer is indeed a group of isometries.

In the above example, the metric tensor F_0 would be the sum

$$\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} + \begin{pmatrix} b & 0 \\ 0 & a \end{pmatrix} = \begin{pmatrix} a+b & 0 \\ 0 & a+b \end{pmatrix}$$

which is the metric tensor of a square lattice. But on a square lattice the matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is indeed an isometry.

If we insist that the metric tensor is preserved by the normalizer, we have to restrict to affine mappings which are isometries, i.e. to coordinate transformations in the Euclidean group.

Definition 71 Let G be a space group and let $N_{\mathcal{E}} := N_{\mathcal{E}_n}(G)$ be the normalizer of G in the Euclidean group. Then $N_{\mathcal{E}}$ is called the *Euclidean normalizer* of G.

The Euclidean normalizer can not be derived from the augmented matrices of a space group alone, one also explicitly needs the metric tensor of the translation lattice. Depending on the parameters of the metric tensor, the Euclidean normalizer may then be different, e.g. for $a = b$ in the rectangular lattice (which is thus a square lattice) it is larger than for $a \neq b$.

In other words, the Euclidean normalizer is not a property of the space-group type, but may differ for space groups of the same type.

Determining affine and Euclidean normalizers

Since the affine and the Euclidean normalizers are both subgroups of the affine group $\mathcal{A}_n$, we may apply the homomorphism Π to a normalizer N. The image $\Pi(N)$ is the group P_N of linear parts and the kernel is the group T_N of translations in N.

We first consider the translation subgroup T_N. Since translations are isometries, the translation subgroups of $N_{\mathcal{A}}(G)$ and of $N_{\mathcal{E}}(G)$ are actually the same.

We still assume that the space group G is written with respect to a lattice basis of its translation lattice. Working out the transformation of a space group element $\{g \mid t\}$ by a translation v gives

$$\left(\begin{array}{c|c} 1 & -v \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} 1 & v \\ \hline 0 & 1 \end{array}\right) = \left(\begin{array}{c|c} g & g \cdot v - v + t \\ \hline 0 & 1 \end{array}\right).$$

This shows that the translation vector v has to conform to $g \cdot v - v \in \mathbb{Z}^n$ for all g in the point group P of G.

Lemma 72 The translation subgroup of both the affine and the Euclidean normalizer of a space group G contains the translations by vectors v for which

$$g \cdot v - v \in \mathbb{Z}^n \text{ for all } g \text{ in the point group } P \text{ of } G.$$

In order to find the translation subgroup of the affine normalizer one therefore has to solve a system of linear congruences for the generators of the point group.

Examples:

(1) The point group of a space group of type `p2mm` is generated by

$$g = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \ h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For $v = \begin{pmatrix} x \\ y \end{pmatrix}$ we have $g \cdot v - v = \begin{pmatrix} -2x \\ 0 \end{pmatrix}$ and $h \cdot v - v = \begin{pmatrix} 0 \\ -2y \end{pmatrix}$, thus $x \in \frac{1}{2}\mathbb{Z}$ and $y \in \frac{1}{2}\mathbb{Z}$.

The translation subgroup of the space group is thus a subgroup of index[28] 4 in the translation subgroup of the affine normalizer.

(2) The point group of a space group of type `c2mm` is generated by

$$g = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ h = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

For $v = \begin{pmatrix} x \\ y \end{pmatrix}$ we have $g \cdot v - v = \begin{pmatrix} y - x \\ x - y \end{pmatrix}$ and $h \cdot v - v = \begin{pmatrix} -y - x \\ -x - y \end{pmatrix}$. This shows that either $x, y \in \mathbb{Z}$ or $x, y \in \frac{1}{2} + \mathbb{Z}$.

The translation subgroup of the space group is thus a subgroup of index 2 in the translation subgroup of the affine normalizer.

[28] The *index* of a subgroup H in G is the number of cosets of H in G.

(3) The point group of a space group of type `p1m1` is generated by $g = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$.

For $v = \begin{pmatrix} x \\ y \end{pmatrix}$ we have $g \cdot v - v = \begin{pmatrix} -2x \\ 0 \end{pmatrix}$, thus $x \in \frac{1}{2}\mathbb{Z}$ and y is arbitrary.

Remarks:

(1) If the affine normalizer of a space group G has a larger translation subgroup than G, this reveals an *inherent ambiguity* in the choice of the origin.

In Example (1), the origin of the space group `p2mm` is usually chosen in a point where two reflection lines intersect, thus in a twofold rotation point. But the unit cell of the translation lattice also contains rotation points in $\begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$, thus each of these points could equally well be chosen as origin. Under the affine normalizer, these rotation points all lie in the orbit of the origin.

(2) Examples (1) and (2) show that the affine normalizer depends on the arithmetic class of a space group, not only on the type of its point group.

(3) Example (3) shows that the affine normalizer may contain translations of arbitrarily small length. This means that the translation subgroup of the affine (or Euclidean) normalizer is not necessarily a lattice, hence the affine normalizer does not need to be a space group itself.

We now look at the group P_N of linear parts of the affine and of the Euclidean normalizer.

For the Euclidean normalizer, the group P_N has to fix the metric tensor of the translation lattice L of G. Therefore P_N is a subgroup of the full symmetry group B of the lattice L and thus P_N can be found in the normalizer of the point group of G in B.

Lemma 73 Let G be a space group with point group P and translation lattice L. Let F be the metric tensor of the lattice basis of L and let $B = \{g \in GL_n(\mathbb{Z}) \mid g^{tr}Fg = F\}$ be the full symmetry group of L.

Then the group P_N of linear parts of the Euclidean normalizer $N_{\mathcal{E}}$ is a subgroup of the normalizer of P in B, i.e. $P_N \leq N_B(P)$.

Note: Since the action of the linear parts may not be compatible with the SNoT of G, not every element of $N_B(P)$ may give rise to an element of the Euclidean normalizer of G.

Example: Let G be the space group of type $\mathtt{P4_1}$ generated by the screw rotation

$$\left(\begin{array}{ccc|c} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{4} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \text{ and the translations of the lattice } L \text{ with metric tensor } \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

Then the full symmetry group B of L normalizes the point group of G, but of the elements

$$g = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ h = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \text{ and } gh = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

of B only gh gives rise to an element in the Euclidean normalizer of G.

Obtaining the group P_N of linear parts of the affine normalizer is in general more difficult than for the Euclidean normalizer. First of all, this group may be infinite in which case it can not be found as a subgroup of the symmetry group of some lattice. But even in the case that P_N is finite it is not a priori clear in which Bravais class it is contained, since it may fix an arbitrary metric tensor in the space of metric tensors for the point group P.

However, for the space groups in low dimensions the group P_N can always be found by checking which of the abstract automorphisms of P are given by conjugation by an integral matrix.

Finally, once the translation subgroup T_N and the group P_N of linear parts of the affine or Euclidean normalizer have been determined, one still has to compute a system of nonprimitive translations, since in general the normalizer is not a semidirect product of T_N and P_N.

This can be done along the same lines as determining the translation subgroup T_N of the normalizer by writing out the conjugation and solving a system of linear congruences.

6.4 Wyckoff positions and Wyckoff sets

In classifying point positions by their site-symmetry groups we have already noted that we will certainly regard points in the same orbit under the space group as equivalent. Since points in one orbit have conjugate site-symmetry groups, we thus have to collect points with conjugate site-symmetry groups into the same class.

Note however, that it is possible that two points x and y which do not lie in one orbit under G actually have the same site-symmetry group, e.g. if both points lie on the same rotation axis.

The equivalence classes obtained by defining points with conjugate site-symmetry groups as equivalent are called *Wyckoff positions*.

Definition 74 Two points x and y belong to the same *Wyckoff position* if their site-symmetry groups G_x and G_y are conjugate subgroups of G.

In particular, the Wyckoff position containing a point x also contains the full orbit $G(x)$ of x under G.

Due to the action of the affine normalizer $N_{\mathcal{A}}$ of G, some of the Wyckoff positions may still have the same geometric properties. This is the case if the site-symmetry groups G_x and G_y of two points x and y are conjugate in $N_{\mathcal{A}}$ but not in G. Joining also these points into the same equivalence class results in a coarser classification with larger classes which are called *Wyckoff sets*.

Definition 75 Two points x and y belong to the same *Wyckoff set*[29] if their site-symmetry groups G_x and G_y are conjugate subgroups of the affine normalizer $N_{\mathcal{A}}$ of G.

In particular, the Wyckoff set containing a point x also contains the full orbit $N_{\mathcal{A}}(x)$ of x under the affine normalizer of G.

Example: Let G be the space group of type `p2mm` generated by the augmented matrices

$$\left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right)$$

[29]The Wyckoff sets are given in Section 14.2, Table 14.2.3.1 (2-dimensional space) and Table 14.2.3.2 (3-dimensional space) on pages 850-870 of the ITA.

and the translations of the standard lattice. One sees that G has four Wyckoff positions with site-symmetry group of type m, these are represented by the points

$$(e)^{30} \begin{pmatrix} x \\ 0 \end{pmatrix}, \quad (f) \begin{pmatrix} x \\ \frac{1}{2} \end{pmatrix}, \quad (g) \begin{pmatrix} 0 \\ y \end{pmatrix}, \quad (h) \begin{pmatrix} \frac{1}{2} \\ y \end{pmatrix}.$$

Note that we assume that x and y are generic and not special values. In this case this means that $x, y \notin \{0, \frac{1}{2}\}$, since otherwise the site-symmetry group would be larger.

One checks that the site-symmetry groups for the four Wyckoff positions are generated by:

$$(e) \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad (f) \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right), \quad (g) \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad (h) \left(\begin{array}{cc|c} -1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right)$$

which are indeed not conjugate in G.

The affine normalizer of G contains on the one hand translations by $\begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$ (as computed before), which shows that the Wyckoff positions (e) and (f) lie in the same Wyckoff set just as (g) and (h) do. On the other hand the affine normalizer also contains the basis transformation interchanging the two coordinates, therefore also Wyckoff positions (e) and (g) lie in the same Wyckoff set. This shows that actually all four Wyckoff positions belong to the same Wyckoff set.

Geometrically, the positions in this Wyckoff set can be described as those points that lie on reflection lines but are not rotation points.

In the ITA, the Wyckoff positions are included in the description of the space groups. The convention is to label the Wyckoff positions by alphabetically by letters, starting with a for the largest site-symmetry group and ending with the last letter (depending on the number of Wyckoff positions) for the general position with trivial site-symmetry group. Also a symbol for the site-symmetry group is given that provides information about the type of the group and about its orientation with respect to the lattice. Moreover, for a Wyckoff position with site-symmetry group of order $|G_x|$, there are $|P|/|G_x|$ points of the orbit given such that the full orbit is obtained from these points by translations from the translation lattice. The given points do not necessarily lie in a unit cell of the translation lattice, but can be translated into the unit cell by lattice vectors and thus yield $|P|/|G_x|$ different orbit points in the unit cell.

> Note that the multiplicities given for the Wyckoff positions refer to a *conventional cell*, not to a *unit cell* (in our terminology). Thus, for a centred lattice the multiplicity for the general position is $k \cdot |P|$ where k is the ratio of the volumes of the conventional cell and the unit cell.

Exercise 9.
Let G be the space group of type p2gg generated by the augmented matrices

$$\left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right).$$

[30] We use the ITA notation for the Wyckoff positions, which is explained below.

Show that there are two Wyckoff positions of type 2 and that these Wyckoff positions belong to a single Wyckoff set. (Hint: It is enough to determine the translation part of the affine normalizer of G.)

Determining Wyckoff positions

We have seen that forgetting about the translation part shows that site-symmetry groups are isomorphic to subgroups of the point group P.

We can thus obtain all Wyckoff positions by running over representatives of the conjugacy classes of subgroups of P and checking whether the elements of a subgroup (with suitable translation parts) have a fixed point.

The crucial observation is that an element $\{g \mid t_g + t\}$ in the coset $T\{g \mid t_g\}$ fixes a point x if

$$\left(\begin{array}{c|c} g & t_g + t \\ \hline 0 & 1 \end{array}\right) \begin{pmatrix} x \\ \hline 1 \end{pmatrix} = \begin{pmatrix} gx + t_g + t \\ \hline 1 \end{pmatrix} = \begin{pmatrix} x \\ \hline 1 \end{pmatrix},$$

$$\text{thus if} \quad (g - id)x + t_g \equiv 0 \bmod \mathbb{Z}^n.$$

Lemma 76 Let G be a space group with point group P. Let H be a subgroup of P generated by $g_1, \ldots, g_r$ and let $\{g_1 \mid t_1\}, \ldots, \{g_r \mid t_r\}$ be elements in G with the linear parts of the generators.

If x is a solution of the system of congruences

$$(g_i - id)x + t_i \equiv 0 \bmod \mathbb{Z}^n \text{ for } 1 \le i \le r$$

then the site-symmetry group of x contains a subgroup isomorphic with H.

It may happen that the site-symmetry group of a fixed point x of H is strictly larger than H. Therefore it is useful to process the subgroups of P from large to small and check whether a Wyckoff position obtained is actually new.

Example: The point group P of the space group `p3m1` is generated by

$$g = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad h = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

The subgroup lattice of the point group P of type 3m is shown in Figure 5. The three reflections subgroups of order 2 are conjugate subgroups.

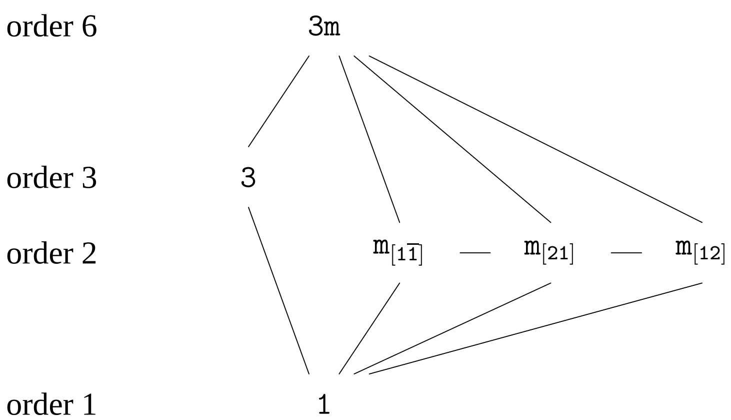


Figure 5: Subgroup lattice of the point group of type 3m.

For the reflection h we have $h - id = \begin{pmatrix} -1 & -1 \\ -1 & -1 \end{pmatrix}$ and we get

$$\begin{pmatrix} -1 & -1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x-y \\ -x-y \end{pmatrix} \equiv \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \text{ hence } -x-y \in \mathbb{Z}, \text{ i.e. } y = -x.$$

This gives the Wyckoff position $(x, \overline{x})$ with site-symmetry group of type m.

For the threefold rotation g we have $g - id = \begin{pmatrix} -1 & -1 \\ 1 & -2 \end{pmatrix}$ and we get

$$\begin{pmatrix} -1 & -1 \\ 1 & -2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x-y \\ x-2y \end{pmatrix} \equiv \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \text{ hence } 3x \in \mathbb{Z} \text{ and } -x-y \in \mathbb{Z}.$$

This gives the three Wyckoff positions $(0,0)$, $(\frac{1}{3}, \frac{2}{3})$ and $(\frac{2}{3}, \frac{1}{3})$, which are all also fixed by h. Thus these Wyckoff positions all have a site-symmetry group of type 3m and there is no Wyckoff position with site-symmetry group of type 3.

Some useful literature

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