

ON THE STRUCTURE AND THE DETERMINATION OF n -DIMENSIONAL
PARTIALLY PERIODIC CRYSTALLOGRAPHIC GROUPS

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0. Introduction

Let \mathbb{E}^n be an n -dimensional Euclidean space. An n -dimensional crystallographic group can be defined as the group of rigid motions of \mathbb{E}^n fixing an n -dimensional "crystal structure". It is called a space group, a partially periodic crystallographic group, or a crystallographic point group if it contains just n , r with $0 < r < n$, or no linearly independent translations, respectively.

The structure of partially periodic crystallographic groups is somewhat different from the well-known structure of space groups. First of all, the linear constituent groups of partially periodic groups do not necessarily act faithfully on the translation subgroups. Therefore, Bieberbach's method of assigning an arithmetic crystal class i.e. a conjugate class (= \mathbb{Z} -class) of finite subgroups of $GL(n, \mathbb{Z})$ to each space group must be generalized, which implicitly has already been done by some authors, e.g. in [9].

Moreover, unlike the space groups, partially periodic groups can be isomorphic without being affinely equivalent. As in the case of space groups, from a crystallographic point of view, affine equivalence is the more natural equivalence relation. The question of which equivalence relation of partially periodic crystallographic groups can play the role that Bieberbach's arithmetic equivalence did in the case of space groups, apparently has not been studied systematically. The classifications occurring in the literature appear rather unnatural from this point of view. In fact, in some cases different class numbers have been given without explanation, e.g. in [3].

Using Maschke's theorem, it will be shown in this paper that every n -dimensional crystallographic group with exactly r linearly independent translations can be represented as an extension of \mathbb{Z}^r by a finite group $P < GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Z})$ and vice versa. Two finite subgroups of $GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Z})$ are called $\mathbb{Z} \times \mathbb{Q}$ -equivalent if they are conjugate in $GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q})$. This equivalence relation reduces to \mathbb{Z} -equivalence in the case of space groups ($r=n$) and to \mathbb{Q} -equivalence (= "geometric equivalence" ([8])) in the case of crystallographic point groups ($r=0$). The $\mathbb{Z} \times \mathbb{Q}$ -classes turn out to be an adequate generalization of Bieberbach's arithmetic crystal classes. They can be determined by an algorithm proposed in [6].

The first part of Zassenhaus' space group algorithm [18] can be applied to determine the, again finitely many, non-equivalent extensions of \mathbb{Z}^r by a finite group $P < GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Z})$. The affinely equivalent extensions can be identified by the second part of Zassenhaus' algorithm if the (finitely generated) \mathbb{Z} -normalizer used there is replaced by the factor group of the normalizer $N_{GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q})}(P)$ modulo the centralizer $C_1 \times_{GL(n-r, \mathbb{Q})}(P)$ which is again finitely generated.

By a modification of the developed algorithm crystallographic equivalence instead of affine equivalence can also be treated, and thus the enantiomorphic pairs of crystallographic groups can be determined.

A further modification which is not treated in this paper allows the determination of colour groups ([13]).

The algorithm was implemented on a computer, and all crystallographic groups of dimension $n \leq 3$ were calculated at the "Rechenzentrum der RWTH Aachen".

I have tried to use as little mathematical background as possible, so that the paper hopefully can be read also by crystallographers with some basic mathematical knowledge.

I like to thank Professor J. Neubüser for introducing me to the field of mathematical crystallography, for valuable advice during my investigations and for reading the different drafts of this paper and supplying helpful comments and criticism. Moreover, I owe special thanks to Dr. W. Plesken for fruitful discussions.

1. Definitions and Basic Properties of Crystallographic Groups

Throughout this paper let \mathbb{A}^n be a fixed *affine space*^{*}, i.e.

\mathbb{A}^n is a triple (A, V, \rightarrow)

where

A is a set (of *points*),

V is an n -dimensional vector space over the field of real numbers \mathbb{R} ,

and

$\rightarrow : A \times A \rightarrow V$ is a function assigning to each couple $(a, b) \in A \times A$ of points a vector $\overrightarrow{ab} \in V$

such that

- for each $a \in A$ and each $x \in V$ there is exactly one $b \in A$ such that $\overrightarrow{ab} = x$,
- $\overrightarrow{ab} + \overrightarrow{bc} = \overrightarrow{ac}$ for all $a, b, c \in A$.

An *affine mapping* is a bijective function $\alpha : A \rightarrow A$ such that

- $\overrightarrow{ab} = \overrightarrow{cd}$ implies $\overrightarrow{\alpha(a)\alpha(b)} = \overrightarrow{\alpha(c)\alpha(d)}$ for all $a, b, c, d \in A$,
- the function $\varphi_\alpha : V \rightarrow V$ defined by $\varphi_\alpha(\overrightarrow{ab}) = \overrightarrow{\alpha(a)\alpha(b)}$ for all $a, b \in A$ is a linear mapping of V , called the *linear constituent* of α .

If φ_α is the identity *id*, then α is called a *translation*. The translations form a normal subgroup T^n of the *affine group*, i.e. the group of all affine mappings.

^{*}) The reader who is not familiar with affine spaces may consult e.g. [11].

For all $o, \alpha \in A$ and all affine mappings α

$$\overrightarrow{o\alpha(a)} = \overrightarrow{o\alpha(o)} + \overrightarrow{\alpha(o)\alpha(a)} = \overrightarrow{o\alpha(o)} + \varphi_\alpha(\overrightarrow{o\alpha(o)}).$$

Thus choosing an *origin* $o \in A$, we can describe α by φ_α and a vector $t_\alpha := \overrightarrow{o\alpha(o)}$, which is called its *translation vector*. If α is a translation, its translation vector t_α is independent of the choice of the origin o , and thus there is a natural 1-1-correspondence between T^n and V . The translation corresponding to a vector $t \in V$ is denoted by τ_t .

The multiplication of affine mappings α and β is described by

$$(1) \quad t_{\beta \circ \alpha} + \varphi_{\beta \circ \alpha}(\overrightarrow{o\alpha}) = t_\beta + \varphi_\beta(t_\alpha) + \varphi_\beta \circ \varphi_\alpha(\overrightarrow{o\alpha}),$$

which shows that the function mapping α onto its linear constituent φ_α is a homomorphism.

Now let V be provided with a fixed positive definite scalar product $\Phi: V \times V \rightarrow \mathbb{R}$. This induces a metric $\overline{}: A \times A \rightarrow \mathbb{R}$ assigning to each couple $(a, b) \in A \times A$ of points their *distance*

$$\overline{ab} := |\overrightarrow{ab}| := \sqrt{\Phi(\overrightarrow{ab}, \overrightarrow{ab})}.$$

We call $\mathbb{E}^n := (\mathbb{A}^n, \Phi)$ an *Euclidean space*. Throughout this paper \mathbb{E}^n shall be fixed.

An affine mapping α is called a *rigid motion* of \mathbb{E}^n if it preserves the distance of points, i.e.

$$\overline{ab} = \overline{\alpha(a)\alpha(b)} \text{ for all } a, b \in A.$$

The linear constituent φ_α of a rigid motion α is an *orthogonal mapping*, i.e. it preserves the scalar product

$$\Phi(x, y) = \Phi(\varphi_\alpha(x), \varphi_\alpha(y)) \text{ for all } x, y \in V.$$

The rigid motions of \mathbb{E}^n form a group B^n and the orthogonal mappings of V form the orthogonal group O^n .

An m -dimensional (point) *lattice* in \mathbb{E}^n is a set \overline{L} of points such that

the corresponding set of vectors

$$L := \{\overrightarrow{oa} \mid a \in \bar{L}\},$$

where o is any fixed element in \bar{L} , forms an m -dimensional *vector lattice*, i.e. L is the set

$$L = \{z_1 \cdot l_1 + \dots + z_m \cdot l_m \mid z_i \in \mathbb{Z}\}$$

of all integral linear combinations of m linearly independent vectors l_1, \dots, l_m in V .

A set (o, b_1, \dots, b_m) of $m+1$ points in \bar{L} is called a *coordinate system* of \bar{L} if the corresponding vectors $\overrightarrow{ob_1}, \dots, \overrightarrow{ob_m}$ form a *lattice basis* of L , i.e. L is generated by (the linearly independent vectors) $\overrightarrow{ob_1}, \dots, \overrightarrow{ob_m}$. Since by definition L is a finitely generated free abelian group, each subgroup M of L is again a vector lattice of dimension $s \leq m$ and the corresponding set of points

$$\bar{M}_o := \{a \in \bar{L} \mid \overrightarrow{oa} \in M\}$$

is an m -dimensional point lattice for every $o \in \bar{L}$. *)

The concept of a "periodical system" can be described in mathematical terms as follows. Let

$$f: A \rightarrow F$$

be a function assigning a property (e.g. a colour) $f(a)$ to each point $a \in A$. By $L(f)$ we denote the group of all vectors $t \in V$ whose corresponding translations τ_t leave f invariant, i.e.

$$L(f) := \{t \in V \mid f(\tau_t(a)) = f(a) \text{ for all } a \in A\}.$$

The group of all rigid motions fixing f

$$S(f) := \{\alpha \in B^n \mid f(\alpha(a)) = f(a) \text{ for all } a \in A\}$$

*) If $s = m$, \bar{L} or L is often called a centering of \bar{M}_o or M , respectively.

is called the *symmetry group* of f . If $L(f)$ is an r -dimensional vector lattice and $S(f)$ even fixes a function $f': A \rightarrow F'$ such that $L(f')$ is a lattice of dimension n , then f is called an (n,r) -*crystal structure*, and its symmetry group $S(f)$ is called a (*crystallographic*) (n,r) -*group* or, in brief, a *crystallographic group* of \mathbb{E}^n . We call it *space group*, *partially periodic group*, or *point group* if $n=r$, $0 < r < n$, or $r=0$, respectively. Since by definition every crystallographic group $S(f)$ fixes an (n,n) -crystal structure $f': A \rightarrow F'$ as well, $S(f)$ is a subgroup of the space group $S(f')$. On the other hand, we shall obtain as an immediate consequence of Proposition 1.3 that every subgroup U of a space group $S(f')$ is crystallographic, i.e. there exists an (n,r) -crystal structure $f: A \rightarrow F$ such that $U = S(f)$.

Let f be an (n,r) -crystal structure and $C := S(f)$ its symmetry group. The group

$$P(C) := \{\varphi_\alpha \mid \alpha \in C\}$$

is called the *linear constituent* of C .

The translations of C form a normal subgroup $T(C)$, called the *translation subgroup* of C . It is canonically isomorphic to the *translation lattice*

$$L(C) := \{t \in V \mid \tau_t \in T(C)\} = L(f)$$

of C .

From the multiplication rule (1) we obtain the conjugation formula

$$\alpha \circ \tau_t \circ \alpha^{-1} = \tau_{\varphi_\alpha(t)} \quad \text{for all } \alpha \in C, \tau_t \in T(C).$$

As $T(C)$ is normal in C , $\tau_{\varphi_\alpha(t)}$ must be an element of $T(C)$ and therefore

$$\varphi_\alpha(t) \in L(C) \quad \text{for all } t \in L(C), \varphi_\alpha \in P(C).$$

This means that the linear constituent $P(C)$ of C acts on the translation lattice $L(C)$ and thus $L(C)$ becomes a \mathbb{Z} -free $\mathbb{Z}P(C)$ -module, i.e. a $\mathbb{Z}P(C)$ -lattice.

Since the (n,r) -group C is a subgroup of a space group C' , its translation lattice $L(C)$ is a sublattice of $L(C')$ and its linear constituent $P(C)$ is a subgroup of $P(C')$. Therefore $P(C)$ acts on $L(C')$ and it must be finite as every subgroup of O^n acting on an n -dimensional vector lattice is finite (see also [8]).

We prepare our first proposition by a definition and a lemma.

1.1 Definition. A point $b \in A$ is called *a point in general position* with respect to a group of rigid motions C if $\alpha(b) = \beta(b)$ implies $\alpha = \beta$ for all $\alpha, \beta \in C$. \square

1.2 Lemma. Let C be a group of rigid motions fixing an n -dimensional point lattice \bar{L} . Then there exists a point in general position with respect to C not contained in \bar{L} .

Proof: A point $b \in A$ is in general position with respect to C if and only if $\gamma(b) = b$ implies $\gamma = id$ for each $\gamma \in C$. Fixing an origin $o \in A$ we can describe the equation $\gamma(b) = b$ by the system of linear equations $\overrightarrow{o\gamma(b)} = \overrightarrow{o b}$. For each $\gamma \neq id$ the set of solutions of this system of linear equations is empty or forms a residue class of a proper subspace of V . The union of all these residue classes and of the vector lattice L associated to \bar{L} is still properly contained in V since C is countable as an extension of its countable translation subgroup and its finite linear constituent. \square

1.3 Proposition. Let C be a group of rigid motions of \mathbb{E}^n acting on an n -dimensional point lattice. Then C is a crystallographic group.

Proof: Let \bar{L}' be an n -dimensional point lattice fixed by C and L' its associated vector lattice. The function $f': A \rightarrow \{-1, 0, 1\}$ defined by

$$f'(a) := \begin{cases} -1 & \text{if } a \in \bar{L}' \\ 0 & \text{if } a \notin \bar{L}' \end{cases}$$

is an (n,n) -crystal structure fixed by C . Let $b \in A$ be a point in general position with respect to the space group $S(f')$ such that $b \notin \bar{L}'$.

The orbit $C(b) := \{\alpha(b) \mid \alpha \in C\}$ of b and \bar{L}' are disjoint, for $c \in C(b) \cap \bar{L}'$ would imply $b = \alpha(c) \in \alpha(\bar{L}') = \bar{L}'$ for a suitable $\alpha \in C$ which is a contradiction.

Therefore the function $f: A \rightarrow \{-1, 0, 1\}$ defined by

$$f(a) := \begin{cases} -1 & \text{if } a \in \bar{L}' \\ 1 & \text{if } a \in C(b) \\ 0 & \text{elsewhere} \end{cases}$$

is well defined. By the construction of f we obtain $C \leq S(f) \leq S(f')$ and thus $L(C) \leq L(f) \leq L(f') = L'$. Therefore f is an (n, r') -crystal structure with $r \leq r' \leq n$. It remains to show that C is the symmetry group $S(f)$ of f and therefore $L(f) = L'$ and $r = r'$. So let $\alpha \in S(f)$. From $f(\alpha(b)) = f(b) = 1$, i.e. $\alpha(b) \in C(b)$, it follows that $\alpha \in C$ for $C \leq S(f')$ and b is a point in general position with respect to $S(f')$. \square

1.4 Example. Let \bar{L}' be a "primitive cubic point lattice", i.e. the corresponding vector lattice $L' = \{\vec{o\alpha} \mid \alpha \in \bar{L}'\}$, o being a fixed point in \bar{L}' , is generated by mutually orthogonal vectors $l_1 = \vec{o\alpha_1}$, $l_2 = \vec{o\alpha_2}$, $l_3 = \vec{o\alpha_3}$ of the same length (forming an orthonormal basis of V). Then $f': A \rightarrow \{-1, 0, 1\}$ defined by

$$f'(a) := \begin{cases} -1 & \text{if } a \in \bar{L}' \\ 0 & \text{if } a \notin \bar{L}' \end{cases}$$

is an $(3, 3)$ -crystal structure because $L(f') = L'$.

It can easily be seen that for instance $b \in A$ with $\vec{ob} = l_1 + \sqrt{2} \cdot l_2 + \pi \cdot l_3$ is a point in general position with respect to $S(f')$. Let $\alpha \in B^3$ be the screw rotation about the 4-fold axis through o and α_1 with translation vector l_1 . Starting from b we arrive at

$$\begin{aligned} \alpha(b) & \text{ with } \vec{o\alpha(b)} = l_1 + l_1 - \pi \cdot l_2 + \sqrt{2} \cdot l_3, \\ \alpha^2(b) & \text{ with } \vec{o\alpha^2(b)} = 2 \cdot l_1 + l_1 - \sqrt{2} \cdot l_2 - \pi \cdot l_3, \quad \text{and} \\ \alpha^3(b) & \text{ with } \vec{o\alpha^3(b)} = 3 \cdot l_1 + l_1 + \pi \cdot l_2 - \sqrt{2} \cdot l_3, \end{aligned}$$

in turn.

Using the vector lattice L generated by $4 \cdot l_1$ and the point lattices

$$\bar{L}_i := \{a \in A \mid \overrightarrow{\alpha^i(b)} a \in L\}, \quad i = 0, 1, 2, 3,$$

we define $f: A \rightarrow \{-1, 0, 1\}$ by

$$f(a) := \begin{cases} -1 & \text{if } a \in \bar{L}_1' \\ 1 & \text{if } a \in \bar{L}_0 \cup \bar{L}_1 \cup \bar{L}_2 \cup \bar{L}_3 \\ 0 & \text{otherwise.} \end{cases}$$

Then f is an $(3,1)$ -crystal structure with $L(f) = L$ and $S(f)$ is generated by α . \square

2. Matrix Representations of Crystallographic Groups

For the description of the announced algorithm in Chapter 5 we introduce matrix representations of crystallographic groups for which we use normal letters instead of italic ones.

2.1 Proposition. a) Let C be a crystallographic (n,r) -group of \mathbb{E}^n . Then there exists a coordinate system $(o, \alpha_1, \dots, \alpha_n)$ of \mathbb{E}^n such that with respect to this coordinate system or the associated basis $(b_1 = \overrightarrow{o\alpha_1}, \dots, b_n = \overrightarrow{o\alpha_n})$ of V , respectively,

- the linear constituent $P(C)$ of C is (faithfully) represented by integral matrices of the form $p \in \text{GL}(r, \mathbb{Z}) \times \text{GL}(n-r, \mathbb{Z})$, i.e.

$$p = \begin{pmatrix} p' & 0 \\ 0 & p'' \end{pmatrix}, \quad p' \in \text{GL}(r, \mathbb{Z}), \quad p'' \in \text{GL}(n-r, \mathbb{Z}),$$

- the translation lattice $L(C)$ of C is represented by integral columns $t \in \mathbb{Z}^x$, i.e.

$$t = \begin{bmatrix} t_1 \\ \vdots \\ t_r \\ t_x \end{bmatrix}, \quad t_i \in \mathbb{Z},$$

- the elements of C are represented by

$$(v_p + t, p), \quad |P(C)| \cdot v_p \in \mathbb{Z}^x$$

their multiplication being defined by

$$(2) \quad (v_p + t, p) \cdot (v_q + s, q) = (v_p + t + p \cdot v_q + p \cdot s, p \cdot q)$$

(where $p = \begin{pmatrix} p' & 0 \\ 0 & p'' \end{pmatrix}$ acts on \mathbb{Z}^r and \mathbb{R}^r as p' does, e.g. $p \cdot v_q := p' \cdot v_q$)

The vector system $v: p \rightarrow v_p$ fulfills the characteristic congruence

$$v_{p \cdot q} \equiv v_p + p \cdot v_q \pmod{\mathbb{Z}^r}.$$

b) A set

$$(3) \quad \begin{cases} C = \{(v_p + t, p) \mid p \in P, t \in \mathbb{Z}^r\} \\ P \text{ a finite subgroup of } GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Z}) \\ |P| \cdot v_p \in \mathbb{Z}^r, v_{p \cdot q} \equiv v_p + p \cdot v_q \pmod{\mathbb{Z}^r} \text{ for all } p, q \in P \end{cases}$$

is a group with respect to the multiplication (2) representing an (n, r) -group.

Proof: a) Let C be a subgroup of the space group C' . Then its linear constituent $P(C)$ acts on the translation lattices $L(C)$ and $L(C')$. Therefore $P(C)$ also acts on the vector space $RL(C)$ consisting of the real linear combinations of the vectors of $L(C)$. Since $P(C)$ is an orthogonal group, the orthogonal complement $RL(C)^\perp$ of $RL(C)$ is mapped onto itself and the elements $\varphi \in P(C)$ commute with the orthogonal projection $\pi: V \rightarrow RL(C)^\perp$, i.e. $\pi(\varphi(x)) = \varphi(\pi(x))$ for all $x \in V$. Therefore $P(C)$ acts also on $L^* := \pi(L(C'))$, which is an $(n-r)$ -dimensional lattice in $RL(C)^\perp$ as we shall show now.

The lattice $L(C')$ is a direct sum of the r -dimensional lattice $L := RL(C) \cap L(C')$ and an $(n-r)$ -dimensional lattice L' , say ([10, p. 100]). Let (b'_{r+1}, \dots, b'_n) be a basis of L' . Then $b_i := \pi(b'_i) = b'_i + l_i$ for suitable $l_i \in L$, $i = r+1, \dots, n$, and thus b_{r+1}, \dots, b_n are linearly independent and form a lattice basis of $\pi(L') = L^*$.

With respect to a basis (b_1, \dots, b_n) of V where (b_1, \dots, b_r) and (b_{r+1}, \dots, b_n) are lattice bases of $L(C)$ and L^* , respectively, $P(C)$ and $L(C)$ are represented as stated in the proposition.

For the representation of C we have to choose a suitable origin o . For each $\psi \in P(C)$ let $\alpha_\psi \in C$ with linear constituent $\varphi_{\alpha_\psi} = \psi$, i.e. $\{\alpha_\psi \mid \psi \in P(C)\}$ is a set of representatives of the cosets of $T(C)$ in C . Then $C = \{\tau_t \alpha_\psi \mid t \in L(C), \psi \in P(C)\}$. Let o' be any origin and (o', a'_1, \dots, a'_n) the coordinate system with $\overrightarrow{o' a'_i} = b_i$. With respect to this coordinate system the translation vector $v'_\psi := \overrightarrow{t'_{\alpha_\psi} o'} = \overrightarrow{o' \alpha_\psi(o')}$ of α_ψ is represented by a vector $v'_\psi \in \mathbb{R}^n$, p being the representation of ψ with respect to the basis (b_1, \dots, b_n) . Thus C is represented by elements $(v_p + t, p)$, their multiplication rule (2) following immediately from the corresponding multiplication rule (1). The characteristic congruence is obvious. It remains to show that there is an origin o such that $v_\psi := \overrightarrow{o \alpha_\psi(o)} \in |P(C)| \cdot L(C)$. We show that the point o defined by

$$\overrightarrow{o' o} = |P(C)|^{-1} \cdot \sum_{\chi \in P(C)} v'_\chi$$

is suitable.

Summing up the characteristic congruence

$$v'_{\psi \circ \chi} \equiv v'_\psi + \psi(v'_\chi) \pmod{L(C)} \text{ for all } \psi, \chi \in P(C)$$

we obtain

$$\sum_{\chi \in P(C)} v'_{\psi \circ \chi} \equiv |P(C)| \cdot v'_\psi + \psi\left(\sum_{\chi \in P(C)} v'_\chi\right) \pmod{L(C)},$$

i.e. $|P(C)| \cdot v'_\psi + (\psi - id) \cdot \sum v'_\chi \in L(C)$, and thus

$$\begin{aligned} |P(C)| \cdot v_\psi &= |P(C)| \cdot \overrightarrow{o \alpha_\psi(o)} \\ &= |P(C)| \cdot (\overrightarrow{o o'} + \overrightarrow{o' \alpha_\psi(o')} + \overrightarrow{\alpha_\psi(o') \alpha_\psi(o)}) \\ &= |P(C)| \cdot (\overrightarrow{o o'} + v'_\psi + \psi(\overrightarrow{o' o})) \\ &= |P(C)| \cdot v'_\psi + (\psi - id) \cdot \sum v'_\chi \in L(C). \end{aligned}$$

b) Because of the characteristic congruence, C forms a group with respect to the multiplication (2). The finite group P fixes the positive definite scalar product $\phi_o : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ defined by

$$\Phi_o(x,y) := x^t \left(\sum_{p \in P} p^t \cdot p \right) \cdot y \quad (x^t \text{ being the transpose matrix of } x)$$

There exists a basis (b_1, \dots, b_n) of V such that Φ_o is the representation of the given scalar product Φ of \mathbb{E}^n ([17, p. 153]), i.e. if $x, y \in \mathbb{R}^n$ are the representations of $x, y \in V$ with respect to this basis, then

$$\Phi(x,y) = \Phi_o(x,y).$$

Therefore, the group P represented by P with respect to (b_1, \dots, b_n) is orthogonal. As P acts on \mathbb{Z}^n , P acts on $L' := \{z_1 \cdot b_1 + \dots + z_n \cdot b_n \mid z_i \in \mathbb{Z}\}$. Since $v_p \in |P|^{-1} \cdot \mathbb{Z}^x$ for all $p \in P$, C acts on the n -dimensional vector lattice $|P|^{-1} \cdot \mathbb{Z}^n$.

Let o be any origin and C the group of rigid motions of \mathbb{E}^n represented by C with respect to the coordinate system (o, a_1, \dots, a_n) with $\vec{o a_1} = b_1, \dots, \vec{o a_n} = b_n$. Then C acts on the point lattice corresponding to $|P|^{-1} \cdot L'$ and therefore C is a crystallographic group by Proposition 1.3. Since its translation lattice $L(C)$ is generated by b_1, \dots, b_n , C is an (n,r) -group. \square

2.2 Example. The symmetry group of the $(3,1)$ -crystal structure f of Example 1.4 can be represented by the matrix group

$$\left\langle \left([1/4], \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \right) \right\rangle = \left\{ \left([1/4] + t, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \right), \right. \\ \left. \left([1/2] + t, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right), \left([3/4] + t, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \right), (t, e) \mid t \in \mathbb{Z} \right\}.$$

From now on, when speaking of a crystallographic group, we mean - if not otherwise stated - a group of the form (3). Its *linear constituent* P is denoted by $P(C)$, its *translation lattice* \mathbb{Z}^x by $L(C)$, and the corresponding *translation subgroup* by $T(C)$.

3. Equivalence of Crystallographic Groups

We shall show in this chapter that affine equivalence of crystallographic groups can be expressed by an equivalence relation of the associated linear constituents, called $\mathbb{Z} \times \mathbb{Q}$ -equivalence, and a relation of the associated vector systems.

3.1 Definition. Let C and C^* be crystallographic groups of the form (3).

- a) C and C^* are called *affinely equivalent* if they are conjugate in the *affine group*

$$A(n, \mathbb{R}) := \{(t, x) \mid t \in \mathbb{R}^n, x \in GL(n, \mathbb{R})\}$$

where $GL(n, \mathbb{R})$ is the group of all regular $n \times n$ -matrices and $(t, x) \in A(n, \mathbb{R})$ acts on \mathbb{R}^n by means of

$$(t, x) \cdot s := t + x \cdot s \quad \text{for } s \in \mathbb{R}^n,$$

i.e. C and C^* are affinely equivalent if there exists a mapping $(t, x) \in A(n, \mathbb{R})$ such that $C = (t, x) \cdot C^* \cdot (t, x)^{-1}$. (Here we have identified $(t, p) \in C$ with $(\begin{bmatrix} t \\ 0 \end{bmatrix}, p) \in A(n, \mathbb{R})$.)

- b) C and C^* are called *crystallographically equivalent* if they are conjugate under the *proper affine group*

$$A(n, \mathbb{R})^+ := \{(t, x) \mid t \in \mathbb{R}^n, x \in GL(n, \mathbb{R}), \det x > 0\}.$$

- c) C and C^* are called *translationally equivalent* if they are conjugate under the *group of translations*

$$T(n, \mathbb{R}) := \{(t, e) \mid t \in \mathbb{R}^n\} \quad (e \text{ being the identity matrix}).$$

- d) C and C^* are said to be *enantiomorphic* if they are affinely but not crystallographically equivalent. \square

We shall not deal in detail with crystallographic equivalence, although it can be treated in quite an analogous way as affine equivalence. The interested reader is referred to [12], [13].

Of course conjugation by elements of a group induces an equivalence relation and therefore translational, affine, and crystallographic equivalence define a decomposition of the crystallographic groups into classes of equivalent ones.

We have introduced the above equivalence relations only for the matrix representations of crystallographic groups, the analogues for groups of rigid motions of \mathbb{E}^n being obvious.

Affine classes of crystallographic groups and of their representations are obviously in 1-1-correspondence. However, this is not true for single groups because different choices of coordinate systems of \mathbb{E}^n may yield different representations.

3.2 Theorem. Let $C = \{(v_p + t, p) \mid p \in P, t \in \mathbb{Z}^r\}$ and $C^* := \{(v_{p^*}^* + t^*, p^*) \mid p^* \in P^*, t^* \in \mathbb{Z}^r\}$ be (n, r) -groups. Then C and C^* are

a) translationally equivalent, if and only if $P = P^*$ and for a suitable $u \in \mathbb{Q}^r$

$$(4) \quad v_p \equiv v_p^* + (e-p)u \pmod{\mathbb{Z}^r} \text{ for all } p \in P,$$

b) affinely (crystallographically) equivalent, if and only if there exist $x \in GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q})$ (with $\det x > 0$) and $u \in \mathbb{Q}^r$ such that

$$(5) \quad \begin{aligned} x P^* x^{-1} &= P \quad \text{and} \\ v_p &\equiv x \cdot v_{x^{-1}p x}^* + (e-p)u \pmod{\mathbb{Z}^r} \text{ for all } p \in P. \end{aligned}$$

(Notice in particular that for $P^* = P$ the condition $x P^* x^{-1} = P$ means that x lies in the normalizer $N_{GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q})}(P)$.)

Proof:

a) follows from b) by specialization.

b) By definition, C and C^* are affinely equivalent if and only if there exists a matrix

$$\tilde{x} = \begin{pmatrix} x' & x_{12} \\ x_{21} & x'' \end{pmatrix} \in GL(n, \mathbb{R}) \text{ and a vector } \tilde{u} = \begin{bmatrix} u \\ u'' \end{bmatrix} \in \mathbb{R}^n$$

such that $(\tilde{u}, \tilde{x}) \cdot C^* \cdot (\tilde{u}, \tilde{x})^{-1} = C$. Since translations are transformed onto translations, it follows that $(\tilde{u}, \tilde{x}) \cdot T(C^*) \cdot (\tilde{u}, \tilde{x})^{-1} = T(C)$ and therefore $\tilde{x} \cdot \mathbb{Z}^r = \mathbb{Z}^r$, that is to say $x_{21} = 0$ and $x' \in GL(r, \mathbb{Z})$, and thus $x'' \in GL(n-r, \mathbb{R})$. Using the fact that $P, P^* \leq GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Z})$, it can be seen by direct

computations that

$$\left(\begin{bmatrix} u \\ u'' \end{bmatrix}, \begin{pmatrix} x' & x_{12} \\ 0 & x'' \end{pmatrix} \right) \cdot C^* \cdot \left(\begin{bmatrix} u \\ u'' \end{bmatrix}, \begin{pmatrix} x' & x_{12} \\ 0 & x'' \end{pmatrix} \right)^{-1} = C$$

implies that even

$$\left(\begin{bmatrix} u \\ 0 \end{bmatrix}, \underbrace{\begin{pmatrix} x' & 0 \\ 0 & x'' \end{pmatrix}}_x \right) \cdot C^* \cdot \left(\begin{bmatrix} u \\ 0 \end{bmatrix}, \underbrace{\begin{pmatrix} x' & 0 \\ 0 & x'' \end{pmatrix}}_x \right)^{-1} = C$$

and thus

$$\begin{aligned} & \{(v_p + t, p) \mid p \in P, t \in \mathbb{Z}^r\} = \\ & = (u, x) \cdot \{(v_{p^*}^* + t^*, p^*) \mid p^* \in P^*, t^* \in \mathbb{Z}^r\} \cdot (-x^{-1}u, x^{-1}) = \\ & = \{(u + x \cdot v_{p^*}^* + \underbrace{x \cdot t^*}_t - \underbrace{x p^* x^{-1}}_p \cdot u, \underbrace{x p^* x^{-1}}_p) \mid p^* \in P^*, t^* \in \mathbb{Z}^r\} = \\ & = \{(x \cdot v_{x^{-1}p x}^* + (e - p) \cdot u + t, p) \mid p \in x P^* x^{-1}, t \in x \cdot \mathbb{Z}^r\} \end{aligned}$$

Now the stated formulas (5) follow immediately. Moreover, we can assume without loss of generality that x'' and u are rational instead of real because they are solutions of the systems of rational linear equations

$$x'' \cdot p^* = p'' \cdot x'' \text{ for } p^* = \begin{pmatrix} p^{*'} & 0 \\ 0 & p^{*''} \end{pmatrix} \in P^* \text{ and suitable } p = \begin{pmatrix} p' & 0 \\ 0 & p'' \end{pmatrix} \in P$$

and

$$(e - p) \cdot u = v_p - x \cdot v_{x^{-1}p x}^* + t_p \text{ for } p \in P \text{ and suitable } t_p \in \mathbb{Z}^r,$$

respectively. Since $\mathbb{Q}^{(n-r) \times (n-r)}$ is a dense subset of $\mathbb{R}^{(n-r) \times (n-r)}$ and the determinant is a continuous function, there exists a solution $x'' \in GL(n-r, \mathbb{Q})$ if there is one in $GL(n-r, \mathbb{R})$ (see [10, p.200]).

The converse is true by the above computation. The same proof holds for crystallographic instead of affine equivalence if x is required to have a positive determinant. \square

3.3 Corollary and Definition. Let C and C^* be affinely equivalent (n,r) -groups with linear constituents $P, P^* < GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Z})$. Then P and P^* are conjugate in $GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q})$, i.e.

$$xP^*x^{-1} = P \text{ for a suitable } x \in GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q}).$$

Such matrix groups P and P^* are called $\mathbb{Z} \times \mathbb{Q}$ -equivalent. \square

For $r=0$ the $\mathbb{Z} \times \mathbb{Q}$ -equivalence reduces to geometrical and for $r=n$ to arithmetical equivalence (see e.g. [14]). It is the natural generalization of these concepts, while the analogously defined $\mathbb{Q} \times \mathbb{Q}$ -equivalence, which is often used in the literature (e.g. in [3]), does not embrace the concept of arithmetical equivalence.

4. The Structure of Crystallographic Groups.

We show in this chapter that each (n,r) -group is a subdirect product of an r -dimensional space group and an $(n-r)$ -dimensional finite unimodular group, and that at the same time it is an extension of its translation lattice \mathbb{Z}^r by a subdirect product of finite subgroups of $GL(r, \mathbb{Z})$ and $GL(n-r, \mathbb{Z})$, respectively. Moreover, each such extension represents an (n,r) -group. Therefore it is possible to construct the partially periodic groups ($r < n$) either as subdirect products of space groups and finite unimodular groups or as extensions. The first method was used by several authors (e.g. [9]), but it seems to become rather uncomfortable for $r \geq 2$ since then the equivalence problem is probably hard to solve. We prefer the construction by solving the extension problem and propose an algorithm for it in the next chapter, which is a natural generalization of Zassenhaus' space group algorithm.

4.1 Theorem. Let $C = \{(v_p + t, p) \mid p \in P, t \in \mathbb{Z}^r\}$ be an (n,r) -group.

- a) The functions mapping $(v_p + t, p) \in C$ with $p = \begin{pmatrix} p' & 0 \\ 0 & p'' \end{pmatrix} \in P$ onto $(v_p + t, p')$ and onto p'' are homomorphisms onto an (r,r) -group C' and a group $P'' < GL(n-r, \mathbb{Z})$, respectively. The intersection of the kernels of these homomorphisms is the identity $\{(0, e)\}$, i.e. C is a subdirect product

of the space group C' and the finite unimodular group P'' .

- b) The functions mapping $p = \begin{pmatrix} p' & 0 \\ 0 & p'' \end{pmatrix} \in P$ onto p' and p'' , respectively, are homomorphisms, the intersection of their kernels being the identity $\{e\}$, i.e. P is a subdirect product of finite unimodular groups $P' < GL(r, \mathbb{Z})$ and $P'' < GL(n-r, \mathbb{Z})$. Thus C is an extension of $L(C) = \mathbb{Z}^r$ by the subdirect product $P = P(C)$.

Let P' and P'' be finite subgroups of $GL(r, \mathbb{Z})$ and $GL(n-r, \mathbb{Z})$, respectively, and let C' be a space group of \mathbb{R}^r with linear constituent P' .

- a*) Every subdirect product C of C' and P'' is canonically isomorphic to an (n, r) -group.
 b*) Every extension of \mathbb{Z}^r by a subdirect product P of P' and P'' is isomorphic to an (n, r) -group.

Proof: a) and b) are trivial consequences of 2.1 b).

- a*) Let $\pi' : C \rightarrow C'$ and $\pi'' : C \rightarrow P''$ be epimorphisms with $\ker \pi' \cap \ker \pi'' = 1$. We define the action of an element c of C on $\mathbb{R}^n = \mathbb{R}^r \oplus \mathbb{R}^{n-r}$ by

$$c \cdot x := \pi'(c) \cdot x' + \pi''(c) \cdot x'' \text{ for } x = x' + x'', x' \in \mathbb{R}^r, x'' \in \mathbb{R}^{n-r}.$$

Then C acts on \mathbb{R}^n as an (n, r) -group by 2.1 b).

- b*) Because of Proposition 2.1 b) we have only to show that any extension of \mathbb{Z}^r by P can be described by a vector system $v : P \rightarrow |P|^{-1} \cdot \mathbb{Z}^r$. An elementary proof of this fact can be found in [18]. Moreover, it follows immediately from cohomology theory (see e.g. [1]), \square

We do not need this structure theorem for the determination of all (n, r) -groups with the announced Algorithm 5.1 because we shall only deal with vector systems and can directly apply Proposition 2.1 b).

4.2 Example. The $(3, 1)$ -group of Example 2.2 is a subdirect product of the $(1, 1)$ -group $C' = \langle (1/4, e) \rangle$ (Hermann-Maughin-symbol:1) and the unimodular

group $P'' = \left\langle \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right\rangle$ (Hermann-Maughin-symbol:4). \square

5. An Algorithm for the Determination of the Affine Classes of Crystallographic Groups.

Theorem 3.2 and Proposition 2.1 b enable us to formulate an algorithm for the determination of representatives for the affine classes of (n,r) -groups.

5.1 Algorithm.

- 1) Calculate a representative set P of the finite subgroups P of $GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Z})$ with respect to $\mathbb{Z} \times \mathbb{Q}$ -equivalence.

For each group $P \in P$

- 2) determine a set V of vector systems $v: P \rightarrow |P|^{-1} \cdot \mathbb{Z}^r$ which describes a representative set of the (n,r) -groups with linear constituent P with respect to translational equivalence;
- 3) identify those vector systems $v \in V$ which define affinely equivalent (n,r) -groups.

We describe the three steps more precisely.

- ad 1) By a theorem of Jordan and Minkowski there are only finitely many \mathbb{Z} -classes of finite subgroups of $GL(m, \mathbb{Z})$ for each fixed natural number m ([10, p.559]). Representative sets for these classes are well-known for $m \leq 4$ ([5]). From the finite number of those representatives $P' < GL(r, \mathbb{Z})$ and $P'' < GL(n-r, \mathbb{Z})$ only finitely many subdirect products

$$P < P' \times P'' = \left\{ \begin{pmatrix} p' & 0 \\ 0 & p'' \end{pmatrix} \mid p' \in P', p'' \in P'' \right\} \text{ can be derived and in [6] an algorithm}$$

is given for the calculation of representatives of the " $\mathbb{Z} \times \mathbb{Z}$ -classes" of these subdirect products. By an obvious modification of this algorithm also $\mathbb{Z} \times \mathbb{Q}$ -equivalence can be treated.

- ad 2) The (finite) set of vector systems V can be determined by the first part of Zassenhaus' algorithm as follows.

Let $E = \{p_1, \dots, p_k\}$ be a set of matrices generating the group P and

$$r_1 = r_1(p_1, \dots, p_k) = e, \dots, r_m = r_m(p_1, \dots, p_k) = e$$

a system of defining relations of P . If we know v_{p_1}, \dots, v_{p_k} , we can determine v_p (up to \mathbb{Z}^r) for each matrix $p \in P$ by expressing p as a word in the generators p_1, \dots, p_k and then recursively applying the characteristic congruence in (3) to this word. It can be shown ([18]) that v_{p_1}, \dots, v_{p_k} define a vector system v if and only if for the vectors v_{r_1}, \dots, v_{r_m} derived in this way, the congruences

$$v_{r_i} \equiv 0 \pmod{\mathbb{Z}^r} \text{ for } i = 1, \dots, m$$

hold. This system of $r \cdot m$ simultaneous congruences can be combined to

$$R \cdot V \equiv 0 \pmod{\mathbb{Z}^{r \cdot m}}$$

$$\text{where } V := \begin{bmatrix} v_{p_1} \\ \vdots \\ v_{p_k} \end{bmatrix} \in \mathbb{R}^{r \cdot k} \text{ and}$$

$R = (a_{ij}), a_{ij} \in \mathbb{Z}^{r \times r}$ for $i = 1, \dots, m$ and $j = 1, \dots, k$ is defined by

$$v_{r_i} = \sum_{j=1}^k a_{ij} \cdot v_{p_j} \text{ for } i = 1, \dots, m.$$

The matrix $R \in \mathbb{Z}^{r \cdot m \times r \cdot k}$ can be transformed to diagonal form

$$Z \cdot R \cdot S = \begin{pmatrix} d_1 & & & & \\ & \ddots & & & \\ & & d_s & & \\ & & & \ddots & \\ & & & & 0 \\ & & & & \vdots \\ & & & & & 0 \end{pmatrix}, \quad Z \in GL(r \cdot m, \mathbb{Z}), \quad S \in GL(r \cdot k, \mathbb{Z})$$

by means of row operations (multiplying R by Z from the left) and column operations (multiplying R by S from the right).

Now it can be shown that

$$V := \left\{ V := S \cdot \begin{bmatrix} e_1/d_1 \\ \vdots \\ e_s/d_s \\ 0 \\ \vdots \\ 0 \end{bmatrix} \mid 0 < e_i < d_i, e_i \in \mathbb{Z} \text{ for } i = 1, \dots, s \right\}$$

is a set of vectors $V = \begin{bmatrix} v_{p_1} \\ \vdots \\ v_{p_k} \end{bmatrix}$ defining a representative

set of the classes of translationally equivalent (n,r) -groups with linear constituent P ([18], [4]).

- ad 3) By a modification of the second part of Zassenhaus' algorithm the vector systems of affinely equivalent groups are identified. By Theorem 3.2 on the characterization of affine equivalence, we have to determine the orbits of V with respect to the operation of the normalizer $N_{\mathbb{Z} \times \mathbb{Q}}(P) := N_{GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q})}(P)$, where an element $x \in N_{\mathbb{Z} \times \mathbb{Q}}(P)$ acts on the set of vector systems by means of

$$v_p \rightarrow v_p^x := x \cdot v_p \cdot x^{-1}_{px}$$

thus inducing a permutation on V .

The centralizer $C_{1 \times \mathbb{Q}}(P) := C_{1 \times GL(n-r, \mathbb{Q})}(P)$ acts trivially on the vector systems because

$$x \cdot v_p \cdot x^{-1}_{px} = e \cdot v_p = v_p \quad \text{for } x = \begin{pmatrix} e & 0 \\ 0 & x'' \end{pmatrix} \in C_{1 \times \mathbb{Q}}(P).$$

Therefore we have only to determine the orbits with respect to the factor group $N_{\mathbb{Z} \times \mathbb{Q}}(P)/C_{1 \times \mathbb{Q}}(P)$ which is finitely generated by a theorem of Siegel [16].

Since $v^{x \cdot y} = (v^x)^y$ for $x, y \in N_{\mathbb{Z} \times \mathbb{Q}}(P)$, it is sufficient to determine the orbits induced by the action of a finite set $\{x_1, \dots, x_t\}$ which together with $C_{1 \times \mathbb{Q}}(P)$ generates the normalizer $N_{\mathbb{Z} \times \mathbb{Q}}(P)$. The set $\{x_1, \dots, x_t\}$ can be found as the union of a generating set of $C_{\mathbb{Z} \times 1}(P) := C_{GL(r, \mathbb{Z}) \times 1}(P)$, which is known for $r \leq 4$, with a set of representatives of the cosets of $C_{\mathbb{Z} \times \mathbb{Q}}(P)$ in $N_{\mathbb{Z} \times \mathbb{Q}}(P)$. This can be determined by checking of which automorphisms of P are induced by matrices in $GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q})$ (see also [7], [15]).

The orbits under an element $x = \begin{pmatrix} x' & 0 \\ 0 & x'' \end{pmatrix} \in N_{\mathbb{Z} \times \mathbb{Q}}(P)$ are calculated in analogy to [18] and [4] as follows:

Let $x^{-1}p_i x = w_i$ be a representation of $x^{-1}p_i x$ as a word w_i in the generators p_1, \dots, p_k of P . By recursively applying the characteristic congruence to v_{w_i} we can express $v_{x^{-1}p_i x}$ as

$$v_{x^{-1}p_i x} = \sum_{j=1}^k b_{ij} \cdot v_{p_j}, \quad b_{ij} \in \mathbb{Z}^{r \times r} \text{ for } i=1, \dots, k.$$

If we define $B = (x' \cdot b_{ij}) \in \mathbb{Z}^{r \cdot k \times r \cdot k}$, we get

$$V^x := \begin{bmatrix} v_{p_1}^x \\ \vdots \\ v_{p_k}^x \end{bmatrix} = B \cdot \begin{bmatrix} v_{p_1} \\ \vdots \\ v_{p_k} \end{bmatrix} = B \cdot S \cdot \begin{bmatrix} e_1/d_1 \\ \vdots \\ e_s/d_s \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

$$\text{The vectors } V^x \text{ and } V^* = \begin{bmatrix} v_{p_1}^* \\ \vdots \\ v_{p_k}^* \end{bmatrix} = S \cdot \begin{bmatrix} e_1^*/d_1 \\ \vdots \\ e_s^*/d_s \\ 0 \\ \vdots \\ 0 \end{bmatrix} \in V \text{ define}$$

translationally equivalent groups if and only if

$$V^x - V^* = S \cdot \begin{bmatrix} z_1 \\ \vdots \\ z_s \\ * \\ \vdots \\ * \end{bmatrix} \quad \text{for } z_i \in \mathbb{Z} \text{ and rational numbers } *$$

([4])^{*}, i.e.

$$B \cdot S \cdot \begin{bmatrix} e_1/d_1 \\ \vdots \\ e_s/d_s \\ 0 \\ \vdots \\ 0 \end{bmatrix} - S \cdot \begin{bmatrix} e_1^*/d_1 \\ \vdots \\ e_s^*/d_s \\ 0 \\ \vdots \\ 0 \end{bmatrix} = S \cdot \begin{bmatrix} z_1 \\ \vdots \\ z_s \\ * \\ \vdots \\ * \end{bmatrix}$$

or

$$S^{-1} \cdot B \cdot S \cdot \begin{bmatrix} e_1/d_1 \\ \vdots \\ e_s/d_s \\ 0 \\ \vdots \\ 0 \end{bmatrix} - \begin{bmatrix} e_1^*/d_1 \\ \vdots \\ e_s^*/d_s \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} z_1 \\ \vdots \\ z_s \\ * \\ \vdots \\ * \end{bmatrix}$$

This can be checked for every pair $V, V^* \in V$.

^{*}) This characterization of translational equivalence yields a method for determining the affine class of an (n,r) -group C by comparison with a list of the (n,r) -groups obtained from the generalized Zassenhaus algorithm.

- 1) Find the $\mathbb{Z} \times \mathbb{Q}$ -class of $P(C)$ and transform C into C^* by conjugation with a matrix $x \in GL(r, \mathbb{Z}) \times GL(n-r, \mathbb{Q})$ such that $P(C^*) = x \cdot P(C) \cdot x^{-1}$ appears in the list.
- 2) Find the translation class of C^* by comparing its vector system with those of the (n,r) -groups in the list whose linear constituent is $P(C^*)$. This can be achieved using the above condition.

5.2 Example. The linear constituent $P = \langle p \rangle = \left\langle \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \right\rangle$ of the examples 2.2 and 4.2 has a defining relation

$$r_1 = r_1(p) = p^4$$

and thus

$$\begin{aligned} v_{r_1} &= v_{p^4} \\ &= v_p + p \cdot v_{p^3} \\ &= v_p + p \cdot (v_p + p \cdot v_{p^2}) \\ &= v_p + p \cdot (v_p + p \cdot (v_p + p \cdot v_p)) \\ &= (e + p + p^2 + p^3) \cdot v_p \\ &= (1 + 1 + 1 + 1) \cdot v_p \\ &= 4 \cdot v_p \end{aligned}$$

Therefore $R = \langle 4 \rangle$ and R has already diagonal form and thus $S = Z = \langle 1 \rangle$. We get

$$\nu := \{[0], [1/4], [2/4], [3/4]\}$$

and there are four classes of translationally equivalent $(3,1)$ -groups with linear constituent P .

As $C_{\mathbb{Z} \times 1}(P) = \left\langle \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\rangle$ and the only automorphism $p \rightarrow p^3$ of P

is induced by the matrix $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$,

we have $N_{\mathbb{Z} \times \mathbb{Q}}(P) = \left\langle C_{1 \times \mathbb{Q}}(P), \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\rangle$.

Since $x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \in C_{\mathbb{Z} \times 1}$, we get

$$v_{x^{-1}p \ x} = v_p, \quad \text{i.e. } b_{11} = (1)$$

and therefore $B = (-1) \cdot (1) = (-1) = S^{-1} \cdot B \cdot S$.

As

$$S^{-1} \cdot B \cdot S \cdot [0] - [0] = [0],$$

$$S^{-1} \cdot B \cdot S \cdot [1/4] - [3/4] = [-1],$$

$$S^{-1} \cdot B \cdot S \cdot [1/2] - [1/2] = [-1],$$

$$S^{-1} \cdot B \cdot S \cdot [3/4] - [1/4] = [-1],$$

the orbits of V under x are $\{[0]\}$, $\{[1/4], [3/4]\}$, and $\{[1/2]\}$.

For $x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ we get

$$v_{x^{-1}p \ x} = v_{p^3} = v_p + p \cdot (v_p + p \cdot v_p)$$

$$= v_p + 1 \cdot (v_p + 1 \cdot v_p)$$

$$= 3 \cdot v_p, \quad \text{i.e. } b_{11} = (3),$$

and therefore $B = (1) \cdot (3) = (3) = S^{-1} \cdot B \cdot S$.

As

$$S^{-1} \cdot B \cdot S \cdot [0] - [0] = [0],$$

$$S^{-1} \cdot B \cdot S \cdot [1/4] - [3/4] = [0],$$

$$S^{-1} \cdot B \cdot S \cdot [1/2] - [1/2] = [1],$$

$$S^{-1} \cdot B \cdot S \cdot [3/4] - [1/4] = [2],$$

the orbits of V under x are again $\{[0]\}$, $\{[1/4], [3/4]\}$, and $\{[1/2]\}$ and there are three classes of affinely equivalent $(3,1)$ -groups with linear constituent P . \square

6. Closing Remarks

As crystallographic groups are extensions of their translation subgroups by their linear constituents, they can also be described by means of cohomology theory (see e.g. [1], [2]).

The method for the construction of the crystallographic groups proposed in this paper can be generalized to determine crystallographic colour groups (see e.g. [8]) which we define as follows:

6.1 Definition: Let $f: A \rightarrow F$ be an (n,r) -crystal structure and Π a group of permutations of "the colours" F . The group

$$F_{\Pi}(f) := \{(\pi, \alpha) \mid \pi \in \Pi, \alpha \in B^n, f(\alpha(a)) = \pi(f(a)) \text{ for all } a \in A\}$$

is called the *colour group* of f with respect to Π . It is called *crystallographic* if F is finite and if its *geometrical constituent*

$$C(F_{\Pi}(f)) := \{\alpha \in B^n \mid (\Pi, \alpha) \in F_{\Pi}(f) \text{ for a suitable } \pi \in \Pi\}$$

is a crystallographic group. \square

A crystallographic colour group $G = F_{\Pi}(f)$ is an extension of the *translation lattice*

$$L(G) := L(f)$$

by the *linear colour constituent*

$$P F(G) := \{(\pi, \varphi_{\alpha}) \mid (\pi, \alpha) \in G \text{ for a suitable } \alpha \in B^n\}$$

which itself is a subdirect product of the *colour constituent*

$$S(G) := \{\pi \in \Pi \mid (\pi, \alpha) \in G \text{ for a suitable } \alpha \in B^n\}$$

and the linear constituent $P(C(G))$ of the geometrical constituent $C(G)$ of G .

Defining equivalence of crystallographic colour groups in a natural way, we can construct the colour groups by the methods used for the determination of crystallographic groups. (The interested reader is referred to [13].)

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