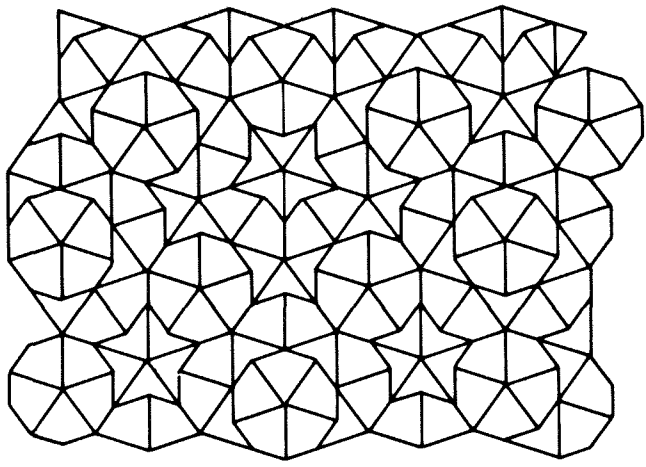
Symmetry Properties and Scaling Behaviour of Quasiperiodic Crystals



F.H.G.M. Wijnands

Symmetry Properties and Scaling Behaviour of Quasiperiodic Crystals

Symmetry Properties and Scaling Behaviour of Quasiperiodic Crystals

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de natuurwetenschappen,

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voor Esther

Contents

Chapter 1

Introduction

Quasiperiodic crystals include a wide variety of crystal structures, such as displacively modulated structures (de Wolff 1974, de Wolff *et al.* 1981, Janner and Janssen 1980a), composite structures (Janner and Janssen 1980b) and quasicrystals, which were discovered in 1984 (Shechtman *et al.* 1984). All these crystals have in common that the Fourier spectrum can be labeled with a finite number of indices, say n. The positions of the Bragg peaks of the diffraction pattern form a $\mathbf{Z}$-module of rank n, called the Fourier module. If the rank is greater than the physical dimension, say d, then the crystal is nonperiodic. Quasiperiodic structures can be described as an intersection of a higher-dimensional periodic structure with the physical space. The intersection of an n-dimensional periodic structure with a properly chosen d-dimensional subspace has a Fourier module of rank n. Conversely, a d-dimensional structure having a Fourier module of rank n can be described as the restriction of an n-dimensional periodic structure in the sense of Bohr (Bohr 1924; Janssen 1988).

These considerations can be used in the case of quasiperiodic tilings proposed as models for quasicrystals. Penrose introduced a nonperiodic tiling of the plane with two types of tiles (Penrose 1974, Penrose 1979). De Bruijn (1981) developed the grid method to show that the Penrose tiling can be described as a projected 5-dimensional periodic structure. This method was generalized to three dimensions by Kramer and Neri (1984). Using the fact that quasicrystal phases are special cases of quasiperiodic crystal phases, an embedding procedure has been given which had already been developed for incommensurately modulated crystal phases (Bak 1985, Janssen 1986). An-

other method is the cut-and-project method (Duneau and Katz 1985, Katz and Duneau 1986).
These n-dimensional structures have n-dimensional space group symmetry and in addition they often have the property of self similarity. This symmetry has consequences for physical properties such as phonon frequency spectra (Los and Janssen 1990) and electronic energy spectra (Kohmoto *et al.* 1983, Kohmoto and Banavar 1986). This self similarity also becomes apparent in the mathematical construction of quasicrystals in steps. A famous example is the Fibonacci chain. At each step the electronic energy spectrum can be determined in a tight-binding approximation. It turns out that the middle bands of the spectrum in one step appear in the spectrum of one of the succeeding steps in a rescaled version. The Fibonacci chain is characterized by a very special irrational number, the golden mean. The golden mean belongs to a family of quadratic irrationals for which generalized Fibonacci chains can be constructed.
In chapter 2 it is studied whether scaling properties, already determined for the Fibonacci chain by Kohmoto *et al.* (1983), are also valid for generalized Fibonacci chains. The numerically found values for the scaling properties are in agreement with the theoretical values found by linearizing a non-linear recursive mapping for the trace of a transfer matrix around certain orbits. Also the total bandwidth for each approximation is determined, indicating that the electronic states for the incommensurate limit seem to be neither extended nor localized.
Quasicrystals can be characterized by their local isomorphism class. Two quasicrystals are locally isomorphic if every finite part in one quasicrystal appears in the other quasicrystal. With use of the derived recursion formula which is valid for all quadratic irrationals in our family, it is proved in chapter 2 that generalized Fibonacci chains have the same energy spectrum if and only if they are locally isomorphic.

The special symmetry property studied in chapter 2 is a property in the physical space. For periodic crystals the symmetry is described by a space group. As noted above, quasiperiodic crystals can be embedded in a higher-dimensional Euclidean space with as minimal dimension the rank of the $\mathbf{Z}$-module of the Fourier spectrum. The higher-dimensional crystal can be constructed such that it is periodic. The symmetry group is a higher-

dimensional space group, called superspace group (de Wolff 1974, 1977; Janner and Janssen 1977). In order to discuss the classification of higher-dimensional space groups, we introduce some concepts.

An arithmetic (crystallographic, unimodular) point group is a representation $\Gamma(K)$ of a point group $K \subset O(n)$ on a basis of an invariant lattice. Therefore the representation entries are integers. Notice that for each $K \subset O(n)$ leaving an n-dimensional lattice invariant, there is such a $\Gamma(K)$. On the other hand, any finite subgroup of $Gl(n, \mathbf{Z})$ can be made to appear as a faithful representation of a point group $K \subset O(n)$.

Another basis for the same lattice gives an arithmetically equivalent point group. The two arithmetic point groups are said to belong to the same arithmetic crystal class. For given dimension, there is only a finite number of arithmetic crystal classes. For dimensions lower than five, all arithmetic crystal classes have been determined (Brown *et al.* 1978).

According to Ascher and Janner (1965), a space group G can be interpreted as a group extension of an n-dimensional lattice group, isomorphic to $\mathbf{Z}^n$, by a point group K, isomorphic to a finite subgroup of $Gl(n, \mathbf{Z})$. In this formalism, all non-isomorphic extensions of $\mathbf{Z}^n$ by K have only to be determined for one representative of each arithmetic equivalence class. The method to determine all non-isomorphic space groups for a given arithmetic point group, is described in the following section.

1.1 Space groups

Let the n-dimensional Euclidean group $IO(n)$ be defined, using the Wigner-Seitz notation, as:

$$IO(n) \equiv \{\{\alpha|\mathbf{t}\} \mid \alpha \in O(n),\ \mathbf{t} \in \mathbb{R}^n\} \tag{1.1}$$

where $\{\alpha|\mathbf{t}\}$ acts on $\mathbf{r} \in \mathbb{R}^n$ as:

$$\{\alpha|\mathbf{t}\}\mathbf{r} = \alpha\mathbf{r} + \mathbf{t}. \tag{1.2}$$

Let T denote the subgroup of $IO(n)$ consisting of all translations:

$$T \equiv \{\{\epsilon|\mathbf{t}\} \mid \mathbf{t} \in \mathbb{R}^n\},\ \epsilon = \mathbb{1}_n. \tag{1.3}$$

Definition 1.1.1 (Ascher and Janner 1965). An n-dimensional space group G is a subgroup of $IO(n)$ such that $G \cap T = A$, where:

(1) A is isomorphic to $\mathbf{Z}^n$ and
(2) A is generated by n linearly independent translations.

A space group G has two important properties:

$$A \trianglelefteq G \text{ and } G/A \simeq K\,, \tag{1.4}$$

where $O(n) \supset K = \{\alpha | \{\alpha|\mathbf{u}(\alpha)\} \in G\}$ is the point group of G. K is generated by the set $\{\alpha_1, \ldots, \alpha_s\}$, denoted as: $K =< \alpha_1, \ldots, \alpha_s >$. As a consequence of rel. (1.4), G can be decomposed into cosets w.r.t. its invariant subgroup A:

$$G = \bigcup_{\alpha \in K} \{\alpha|\mathbf{u}(\alpha)\} A \tag{1.5}$$

where $\{\alpha|\mathbf{u}(\alpha)\}$ is determined mod A. If we choose the lattice basis as the basis for $\mathbb{R}^n$, then the elements of A have integer components. This procedure comes down to the isomorphism given in Definition 1.1.1.

For given arithmetic point group, there are two equivalent ways to derive all non-isomorphic space groups. The first way uses the fact that (1.2) requires that for each $\alpha, \beta \in K$:

$$\{\alpha|\mathbf{u}(\alpha)\} A \{\beta|\mathbf{u}(\beta)\} A = \{\gamma|\mathbf{u}(\gamma)\} A \tag{1.6}$$

for some $\gamma \in K$. Hence we have to seek all solutions of the so called Frobenius congruences (Zassenhaus 1949):

$$\alpha\mathbf{u}(\beta) + \mathbf{u}(\alpha) - \mathbf{u}(\gamma) \equiv 0 \,(\text{mod } \mathbf{Z}^n),\ \forall \alpha, \beta \in K\ (\gamma = \alpha\beta). \tag{1.7}$$

Non-trivial solutions of these congruences are called non-primitive translations and the set $\mathbf{u}(K)$ defines a system of non-primitive translations. Brown (1969) followed this approach to determine non-isomorphic space groups. The second way is based upon a theorem by Ascher and Janner (1965) stating that each extension of a free abelian group A by a finite group K by a monomorphism $\Gamma : K \rightarrow Gl(n, \mathbf{Z})$ can be embedded as a space group in $IO(n)$ (a monomorphism $\Gamma : M \rightarrow N$ is an injective homomorphism of M into N). The properties (1.4) can be expressed as an exact sequence of group homomorphisms:

$$0 \;\rightarrow\; A \;\overset{\rho}{\rightarrow}\; G \;\overset{\sigma}{\rightarrow}\; K \;\rightarrow\; 1 \quad (\Gamma) \tag{1.8}$$

where 0 respectively 1 are the trivial subgroups of A and K. The sequence is exact since the image of each homomorphism is the kernel of the next homomorphism. Since $A \simeq \mathbf{Z}^n$, we can denote the free abelian group by $\mathbf{Z}^n$ instead of A.
Since $\Gamma(K)$ is a faithful representation of a finite group in $Gl(n, \mathbf{Z})$, it is an arithmetic point group, defined by K and the automorphism Γ in (1.8). The derivation of all non-isomorphic space groups G with arithmetic point group $\Gamma(K)$ can be achieved e.g. by the method developed by Janssen *et al.* (1969), also described by Fast and Janssen (1971). The main steps are briefly outlined below.

1.1.1 Non-equivalent extensions

First all non-equivalent extensions are derived. Each $g \in G$ can be written as: $g = r(\alpha)a$, $a \in \mathbf{Z}^n$, $\alpha \in K$ (here we identified $\mathbf{Z}^n$ with its isomorphic image $\rho\mathbf{Z}^n$, with ρ defined in (1.8)). Suppose K is presented as a set of words $\varphi_i(\alpha_1, \ldots, \alpha_s) = \epsilon$, $1 \leq i \leq r$, where ϵ is the identity of K and the $\varphi_i = \epsilon$ are called the defining relations. Then:

$$\varphi_i(r(\alpha_1), \ldots, r(\alpha_s)) = g_i \in \mathbf{Z}^n, \quad 1 \leq i \leq r. \tag{1.9}$$

These relations, together with the relations: $r(\alpha)ar(\alpha)^{-1} = \Gamma(\alpha)a$, $\forall \alpha \in K$, determine G completely. Now consider the integral group ring of K:

$$\left\{ \sum_{\alpha \in K} m_\alpha \times \alpha \mid m_\alpha \in \mathbf{Z}^n, \ \forall\, \alpha \in K \right\} \tag{1.10}$$

of which the elements act on $\mathbf{u} \in \mathbf{Z}^n$ as:

$$(\sum_\alpha m_\alpha \times \alpha)\mathbf{u} = \sum_\alpha m_\alpha \Gamma(\alpha)\mathbf{u}. \tag{1.11}$$

Suppose that another coset representative $r'(\alpha) = r(\alpha)\mathbf{u}(\alpha)$, $\mathbf{u}(\alpha) \in \mathbf{Z}^n$, is chosen. Then there exist elements $\pi_i(\alpha_j)$ of the integral group ring of K such that:

$$\varphi_i(r'(\alpha_1), \ldots, r'(\alpha_s)) = \sum_{j=1}^{s} \pi_i(\alpha_j) u(\alpha_j) + g_i \,, \quad 1 \leq i \leq r. \tag{1.12}$$

Now denote $n \times r$ by p and $n \times s$ by q and define a supervector Φ and a supermatrix Π as:

$$\Phi \equiv \begin{bmatrix} g_1 \\ \cdot \\ \cdot \\ g_r \end{bmatrix} \in \mathbf{Z}^p \,, \; \Pi \equiv \begin{bmatrix} \pi_1(\alpha_1) & . & . & . & \pi_1(\alpha_s) \\ & & \cdot & & \\ & & \cdot & & \\ & & \cdot & & \\ \pi_r(\alpha_1) & . & . & . & \pi_r(\alpha_s) \end{bmatrix} \in M_{p\times q}(\mathbf{Z}). \tag{1.13}$$

With use of a theorem by Hall (1938) it can be proved that Φ determines an extension if and only if $\Phi \in \Pi\,\mathbb{R}^q \cap \mathbf{Z}^p$; Φ and Φ' determine equivalent extensions if and only if $\Phi - \Phi' \in \Pi\mathbf{Z}^q$. The set of vectors Φ is an abelian group with the vector addition as group operation. Therefore all non-equivalent extensions are achieved once the abelian factor group

$$(\Pi\,\mathbb{R}^q \cap \mathbf{Z}^p)/\Pi\mathbf{Z}^q \tag{1.14}$$

is determined. First the supermatrix Π is diagonalized:

$$\Pi' = P\Pi Q = \begin{bmatrix} d_1 & 0 & . & & & 0 \\ 0 & d_2 & 0 & & & 0 \\ & & \cdot & & & \\ & & & & & \\ & & & & \cdot & \\ 0 & 0 & 0 & 0 & 0 & d_q \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, d_i \geq 0,\; 1 \leq i \leq q, \tag{1.15}$$

with $P \in Gl(p, \mathbf{Z})$, $Q \in Gl(q, \mathbf{Z})$. The factor group $(\Pi'\,\mathbb{R}^q \cap \mathbf{Z}^p)/\Pi'\mathbf{Z}^q$ is given by the set:

$$\{\Phi'\} = \left\{ \sum_{i=1}^{q} n_i \epsilon_i \mid 0 \leq n_i \leq max(0, d_i - 1) \right\} \tag{1.16}$$

where $\epsilon_i \in \mathbf{Z}^p$ is defined by: $(\epsilon_i)_j = \delta_{ij}$. Hence the non-equivalent extensions are given by:

$$\{\Phi\} = \left\{ P^{-1}\Phi' \right\} = \left\{ \sum_{i=1}^{q} n_i P^{-1} \epsilon_i \mid 0 \leq n_i \leq max(0, d_i - 1) \right\}. \tag{1.17}$$

Define a matrix $A \in M_{p\times q}(\mathbb{Z})$ by:

$$A_{ij} = \delta_{ij} \times \begin{cases} 1 & \text{if } d_i > 1 \\ 0 & \text{if } d_i \leq 1 \end{cases} . \tag{1.18}$$

Generators for the factor group (1.14) are formed by all columns $[P^{-1}A]_i$ for which d_i is greater than one. Each such column generates a group of order d_i. The d_i greater than one are called torsion numbers of the extension (1.14).

Since each extension of $\mathbb{Z}^n$ by a finite group K by a monomorphism $\Gamma : K \rightarrow Gl(n,\mathbb{Z})$ can be embedded as a space group $G \subset IO(n)$, its elements can be written as: $\{\alpha|\mathbf{u}(\alpha)\}$ for each $\alpha \in K$. Notice that each non-primitive translation $\mathbf{u}(\alpha)$ is known once the non-primitive translations $\mathbf{u}(\alpha_1), \ldots, \mathbf{u}(\alpha_s)$ for the point group generators are known by using the defining relations $\varphi_i(\alpha_1, \ldots, \alpha_s) = \epsilon$, $1 \leq i \leq r$. After defining a matrix $D \in M_{q\times p}(\mathbb{Q})$ by:

$$D_{ij} = \begin{cases} d_i^{-1}\delta_{ij} & \text{if } d_i > 0 \\ 0 & \text{if } d_i = 0 \end{cases} , \tag{1.19}$$

to each solution (1.17) corresponds a system of non-primitive translations $\mathbf{u}(K)$:

$$\mathbb{R}^q \ni \begin{Bmatrix} \mathbf{u}(\alpha_1) \\ \cdot \\ \cdot \\ \mathbf{u}(\alpha_s) \end{Bmatrix} \equiv U = QD\Phi' = \sum_{i=1}^{q} n_i Q D \epsilon_i . \tag{1.20}$$

Each non-equivalent extension can be expressed by a relation vector Φ in rel. (1.17) or by a system of non-primitive translations U in rel. (1.20). The vectors Φ and U are related: $\Phi = \Pi U$.

1.1.2 Non-isomorphic space groups

The isomorphism $A \simeq \mathbb{Z}^n$ is determined up to an automorphism χ of $\mathbb{Z}^n$. Due to this freedom, isomorphic space groups may be obtained from non-equivalent extensions with the same $\Gamma(K)$. Consider the following commu-

tative diagram with exact rows of group extensions:

$$\begin{array}{ccccccccc} & & & \overset{\rho_1}{} & & \overset{\sigma_1}{} & & & \\ 0 & \to & \mathbf{Z}^n & \to & G_1 & \to & K & \to & 1 \quad (\Gamma) \\ & & \chi \downarrow & & \psi \downarrow & & \omega \downarrow & & \\ & & & \overset{\rho_2}{} & & \overset{\sigma_2}{} & & & \\ 0 & \to & \mathbf{Z}^n & \to & G_2 & \to & K & \to & 1 \quad (\Gamma) \end{array} \tag{1.21}$$

The diagram (1.21) is a morphism of group extensions determined by the homomorphisms χ, ψ and ω. Notice that in the diagram (1.21), χ and ω are automorphisms and ψ is an isomorphism. We may assume that $\psi r_1(\alpha) = r_2(\omega\alpha)$, $\forall\ \alpha \in K$. From the relation: $r_1(\alpha)\rho_1 a[r_1(\alpha)]^{-1} = \rho_1\Gamma(\alpha)a$, it follows that $\rho_2\Gamma(\omega\alpha)\chi a = r_2(\omega\alpha)\rho_2\chi a[r_2(\omega\alpha)]^{-1} = \rho_2\chi\Gamma(\alpha)a$. The last equality is a consequence of the fact that (1.21) is a morphism of group extensions. Hence:

$$\Gamma(\omega\alpha) = \chi\Gamma(\alpha)\chi^{-1},\ \forall\alpha \in K, \tag{1.22}$$

and χ is an element of $N(\Gamma(K), Gl(n, \mathbf{Z}))$, abbreviated to $N(\Gamma(K))$. Here:

$$N(\Gamma(K)) = \left\{\mu \in Gl(n, \mathbf{Z}) \mid \mu\Gamma(\alpha)\mu^{-1} \in \Gamma(K),\ \forall\ \alpha \in K\right\} \tag{1.23}$$

is the normalizer of $\Gamma(K)$ in $Gl(n, \mathbf{Z})$. The two systems of non-primitive translations $\mathbf{u}_1(K)$ respectively $\mathbf{u}_2(K)$ of G_1 and G_2, are related by:

$$\mathbf{u}_2(\alpha) = \chi\mathbf{u}_1(\omega^{-1}\alpha)\ ,\ \forall\ \alpha \in K, \tag{1.24}$$

and are called equivalent. With help of the relation: $\mathbf{u}_1(\alpha\beta) \equiv \mathbf{u}_1(\alpha) + \alpha\mathbf{u}_1(\beta)\ (\mathrm{mod}\ \mathbf{Z}^n)$, $\forall\ \alpha, \beta \in K$, we can write:

$$\mathbf{u}_1(\omega^{-1}\alpha_i) \equiv \sum_{j=1}^{s} \Omega_{ij}\mathbf{u}_1(\alpha_j)\ \ (\mathrm{mod}\ \mathbf{Z}^n)\ ,\ 1 \leq i \leq s, \tag{1.25}$$

with Ω_{ij} in the integral group ring of K, defined in (1.10). After defining:

$$X \equiv \begin{bmatrix} \Omega_{11} & . & . & . & \Omega_{1s} \\ & . & & & . \\ & . & & & . \\ & . & & & . \\ \Omega_{s1} & . & . & . & \Omega_{ss} \end{bmatrix}, \tag{1.26}$$

we have the following relation:

$$U_2 \equiv XU_1 \pmod{\mathbf{Z}^q}. \tag{1.27}$$

In order to relate two equivalent systems of non-primitive translations, it suffices to determine X in rel. (1.26) for a set of generators $\{\chi_1, \ldots, \chi_m\}$ of $N(\Gamma(K))$.
Two space groups G_1 and G_2 which are conjugate by a translation $\mathbf{w}$ are clearly isomorphic and the non-primitive translations are related by: $\mathbf{u}_1(\alpha)$ is equivalent to $\mathbf{u}_2(\alpha) = \mathbf{u}_1(\alpha) + (\alpha - \mathbb{1}_n)\mathbf{w}$.

1.2 The role of the present work

In order to use the formalism described in the previous two subsections, one needs to know the defining relations (1.9) and a generating set for the normalizer defined in (1.23). In chapter 3, four different algorithmic procedures are described to construct a set of defining relations satisfied by a set of generators of a given arithmetic point group. Computer programs, written in FORTRAN77 and based upon these four methods, have been developed. The four methods are compared on the basis of results for several arithmetic point groups.
An algorithmic procedure to determine a set of generators for the normalizer of a given arithmetic point group is outlined in chapter 4. Also for this algorithmic procedure, a computer program has been written and results for some point groups are presented.

For the description of quasiperiodic crystals, the physical space should be treated as a distinguished subspace. Hence one can not use n-dimensional crystallography without taking the role of the physical space into account. Space groups describing quasiperiodic crystals are therefore called superspace groups instead of n-dimensional space groups. In chapter 5, the consequences of the existence of a distinguished subspace are discussed for point groups. The analysis is restricted to non-mixing point groups, i.e. point groups for which there is a subspace with the physical dimension, which is invariant under the action of the point group. A method is described to determine all non-equivalent choices for the physical space, such that the point group may be the symmetry group for a quasiperiodic structure. Also

the arithmetic equivalence of two arithmetic point groups is discussed. The analysis for quasiperiodic crystals gives rise to compatibility conditions for arithmetic point groups and leads to finer arithmetic equivalence classes.

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Chapter 2

Energy spectra and local isomorphism for one-dimensional quasiperiodic potentials

Energy spectra for one-dimensional tight-binding models, with two types of quasiperiodic potentials, are studied, for which the incommensurability is characterized by quadratic irrationals. One is the step potential model, for which the structure is a generalized Fibonacci chain. For special structures, scaling properties of the spectrum are found numerically, a critical index δ for the total bandwidth is determined. These scaling properties are in agreement with theoretical values found by linearizing a recursive mapping for the trace of transfer matrices. It is shown that generalized Fibonacci chains have the same energy spectrum if and only if they are locally isomorphic. The other potential is sinusoidal, for which the critical index δ is determined at the critical point.

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2.1 Introduction

There has been much interest (Hofstadter 1976, Andre and Aubry 1980, Kohmoto *et al.* 1983 and references therein, Thouless 1983, Ostlund *et al.* 1983, Ostlund and Pandit 1984, Wilkinson 1987) in a tight-binding model with the Schrödinger equation:

$$\Psi_{m+1} + \Psi_{m-1} + V(m\omega)\Psi_m = E\Psi_m \qquad (2.1)$$

$$V(t+1) = V(t).$$

This is the Schrödinger equation for an electron on a one-dimensional lattice with a periodic site potential. Here m labels the lattice site, E is the energy. The relation between the nature of the wavefunctions and the character of the energy spectrum has been studied for a number of models. If ω is rational, say $\omega = \frac{p}{q}$, p and q being relatively prime integers, the eigenspectrum consists of q bands and all eigenfunctions are extended. If ω is irrational, the question arises, what the nature is of the spectrum. The potential $V(m\omega) = \lambda \tan(2\pi[m\omega - \nu])$ gives localized states for "typical" irrational ω's, and the bands for $\omega = \frac{p}{q}$ have widths proportional to $e^{-\gamma q}$, as $q \to \infty$ (Grempel *et al.* 1982). An analytic weak potential $V(m\omega)$ gives extended states for almost every irrational ω (Bellissard *et al.* 1983). Rational $\omega = \frac{p}{q}$ give bandwidths proportional to q^{-1}, as $q \to \infty$ (Kohmoto *et al.* 1983).

Kohmoto *et al.* (1983) studied the case of a step potential:

$$V(t) = \begin{cases} V_0 & \text{for } -\omega < t \leq -\omega^3 \\ V_1 & \text{for } -\omega^3 < t \leq \omega^2 \end{cases}$$

where $\omega = \frac{\sqrt{5}-1}{2}$ is the inverse of the golden mean.

Because the bandwidths were proportional to $q^{-(1+\delta)}$, $\delta > 0$, the states were believed to be neither localized nor extended. This has been proved for certain values of $|V_0 - V_1|$ (Casdagli 1986, Delyon and Petritis 1986, Süto 1987). Kohmoto *et al.* (1983) analyzed the problem also by means of a mapping problem, making use of a recursion relation for the traces of transfer matrices.

The case $V(t) = \lambda \cos(2\pi t)$ has been studied extensively as well. With this choice of the potential, the model is self-dual, since the Fourier coefficients

of the wavefunctions Ψ_m obey the same equation, with different coefficients, as the Ψ_m. For $\omega = \frac{\sqrt{5}-1}{2}$, Kohmoto (1983) compared λ=1.98, 2.00 and 2.02. From the spectrum, the states turned out to be extended for λ=1.98, critical for λ=2.00 and localized for λ=2.02, in agreement with Andre and Aubry (1980) and Avron and Simon (1983).
Now $\omega = \frac{\sqrt{5}-1}{2}$ belongs to the family of positive solutions of the following quadratic equation:

$$\phi^2 + n\phi = 1 \tag{2.2}$$

with n a positive integer. Positive solutions are: $\phi = \frac{\sqrt{(n^2+4)}-n}{2}$. These ϕ can be rewritten as a continued-fraction expansion:

$$\phi = \cfrac{1}{n + \cfrac{1}{n + \cfrac{1}{n + \ldots}}} . \tag{2.3}$$

For $n = 1$, ϕ is the inverse of the golden mean.
The purpose of this paper is twofold. The first aim is to treat the localization problem for general n. For the step potential and for the potential $V(t) = \lambda \cos(2\pi t)$, the values n=1,2,3,4 are studied. For each n, energy spectra for systematic commensurate approximations are calculated. The description of the models is given in § 2.2. Numerical results for the total bandwidth and for scaling properties are presented in § 2.3. The derivation of recursion relations for the traces of transfer matrices, which will be useful in the following two sections, is contained in § 2.4. With help of the derived recursion relations, the numerical results on the scaling properties can be compared with theoretical values, as is outlined in § 2.5.
The second aim is to relate energy spectra of generalized Fibonacci chains (in particular, the step potential case) and the concept of local isomorphism (note that generalized Fibonacci chains can be considered as one-dimensional quasicrystals). Levine and Steinhardt (1986) argue that quasicrystals have the same diffraction pattern and the same free energy if and only if they belong to the same local isomorphism class. It will be studied whether generalized Fibonacci chains (not) belonging to the same local isomorphism class, have the same (a different) energy spectrum. In § 2.6, for a given arbitrary generalized Fibonacci chain, it will be studied which set of chains belongs to the same local isomorphism class and which set of chains has the same energy spectrum as the given one. Comparison of the two sets yields the answer on the relation between energy spectra and local isomorphism.

2.2 Transfer matrix formulation of the model

First, write the Schrödinger equation (2.1) in terms of transfer matrices as:

$$M(m\phi)\Theta_m \;=\; \Theta_{m+1} \;;\; M(t) \;=\; \begin{bmatrix} E-V(t) & -1 \\ 1 & 0 \end{bmatrix} \;;\; \Theta_m \;=\; \begin{bmatrix} \Psi_m \\ \Psi_{m-1} \end{bmatrix}. \tag{2.4}$$

Notice that the matrices $M(t)$ are periodic in t with period 1 and that the determinant of $M(t)$, denoted by $\det(M(t))$, is equal to one. Lattice sites m and $m+k$ can be related by repeating the procedure given in eq. (2.4):

$$M^{(k)}(m\phi)\Theta_m \;=\; \Theta_{m+k} \tag{2.5}$$

where $M^{(k)}(t)$ is defined recursively by:

$$M^{(k_1+k_2)}(t) \;=\; M^{(k_1)}(t+k_2\phi)M^{(k_2)}(t) \tag{2.6}$$

and $M^{(1)}(t) \equiv M(t)$. Rational approximations can be achieved by cutting off the continued-fraction expansion (2.3) after l steps:

$$\phi_l \;=\; \cfrac{1}{(n_1 + 1/(n_2 + \ldots + 1/n_l)\ldots)} \;,\; n_1 = \ldots = n_l = n. \tag{2.7}$$

Eq. (2.7) can be rewritten in the form: $\phi_l = \frac{q_{l-1}}{q_l}$, where q_l are generalized Fibonacci-numbers; q_l obey the recursion relations:

$$q_{l+1} \;=\; nq_l \;+\; q_{l-1}, \;\; q_0 \;=\; 1, \; q_1 \;=\; n. \tag{2.8}$$

Denote the trace of a matrix X by $Tr(X)$. For these rational values $\phi_l = \frac{q_{l-1}}{q_l}$, energies are allowed (forbidden) if $\left|Tr(M^{(q_l)}(t))\right|$ is less than (greater than) two.

In working out the models for the two types of potentials, the further approach is different, so they will be treated separately.

2.2.1 The step potential

The model can be described as follows. The site potential $V(m\phi)$ can take two values: V_0 and V_1. Consider a structure consisting of atoms of type A (then $V(m\phi) = V_1$) and of type B (then $V(m\phi) = V_0$) on sites m ($m =$

$0, 1, 2, ...$). For a generalized Fibonacci chain, the potential $V(m\phi)$ can be constructed as follows. We consider sequences of symbols A, B. Starting with sequence $S_0 = B$ at site $m = 0$ corresponding to V_0, $S_1 = AB^{n-1}$ at sites $m = 0, \ldots, (n-1)$ corresponding to $V_1, V_0, \ldots, V_0$, the juxtaposition rule is:

$$S_{k+1} = S_k^n S_{k-1} \quad (k \geq 1). \tag{2.9}$$

Note that the number of atoms after each step S_k is q_k, and the atoms are put on sites $m = 0, \ldots, (q_k - 1)$. A commensurate approximation is achieved by cutting off the construction after l steps and constructing a periodic structure with unit cell S_l at sites $m = 0, 1, 2, \ldots$; ϕ is replaced by ϕ_l. Energies are allowed if $\left|Tr(M^{(q_l)}(0))\right| \leq 2$ (for convenience, t is put equal to zero). $Tr(M^{(q_l)}(0))$ can be calculated by using a recursion relation for $M_k \equiv M^{(q_k)}(0)$ $(k \geq 0)$, after defining

$$M_B = \begin{bmatrix} E - V_0 & -1 \\ 1 & 0 \end{bmatrix} \quad , \quad M_A = \begin{bmatrix} E - V_1 & -1 \\ 1 & 0 \end{bmatrix} :$$

$$M_{k+1} = M_{k-1} M_k^n \quad ; M_0 = M_B, \; M_1 = M_B^{n-1} M_A \quad (k \geq 1). \tag{2.10}$$

Proof. M_0 corresponds to $S_0 = B \rightarrow M_0 = M_B$. M_1 corresponds to $S_1 = AB^{n-1} \rightarrow M_1 = M^{(q_1)}(0) = M^{(n)}(0) = M((n-1)\phi_l) \ldots M(0) = M_B^{n-1} M_A$. M_2 corresponds to $S_2 = S_1^n S_0 \rightarrow M_2 = M^{(q_2)}(0) = M^{(q_0 + nq_1)}(0)$ $= M^{(q_0)}(nq_1\phi_l) M^{(nq_1)}(0) = M_B (M_B^{n-1} M_A)^n = M_0 M_1^n$. Eq. (2.9) leads directly to eq. (2.10) because M_k corresponds to the reverse of S_k for each k. □

Note that eq. (2.10) also holds for the incommensurate limit (then the proof goes with ϕ instead of ϕ_l). Eq. (2.10) holds for general S_0, S_1, with M_0, M_1 corresponding to the reverse of S_0, S_1 respectively. Energies are allowed (forbidden) if $|Tr(M_l)|$ is less than (greater than) two.

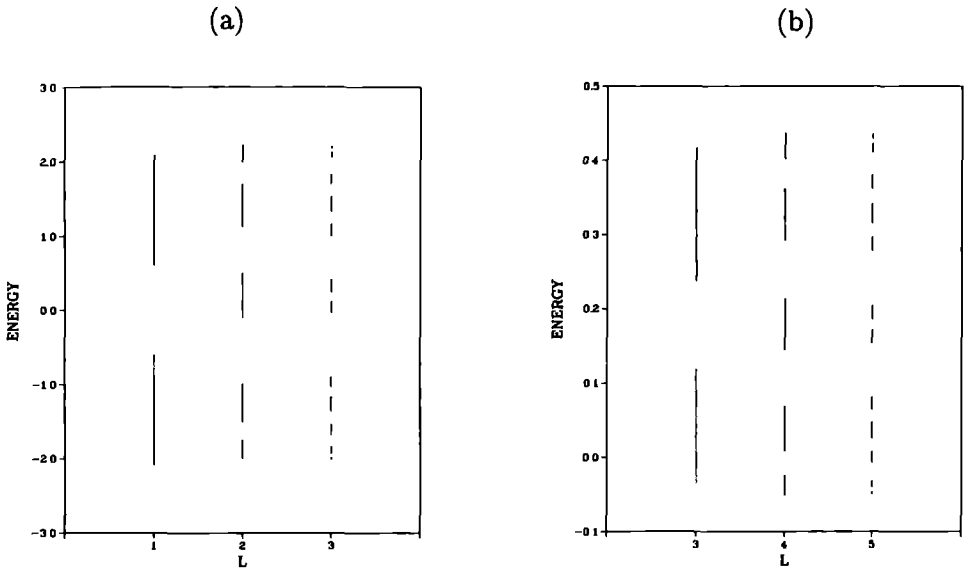

Figure 2.1. Allowed energies for the step potential, $n = 2$, $V_0 = -V_1 = 0.6$; (a) gives the bands for l=1,2,3, (b) gives the middle bands for l=3,4,5.

2.2.2 The sinusoidal potential

We now consider the potential $V(t) = \lambda \cos(2\pi t)$. For rational approximations $\phi_l = \frac{q_{l-1}}{q_l}$, $Tr(M^{(q_l)}(t))$ has to be calculated. Taking t equal to zero, $M^{(q_l)}(0)$ has the form:

$$M^{(q_l)}(0) = \prod_{m=1}^{q_l} \begin{bmatrix} E - \lambda \cos(2\pi[q_l - m]\phi_l) & -1 \\ 1 & 0 \end{bmatrix} \tag{2.11}$$

2.3 Spectra and scaling

For the step potential and for a fixed value of n, the energy spectra can be calculated for various commensurate approximations $\phi_l = \frac{q_{l-1}}{q_l}$ with help of eq. (2.10). In all calculations, $V_0 = -V_1 = 0.6$ in eq. (2.10).

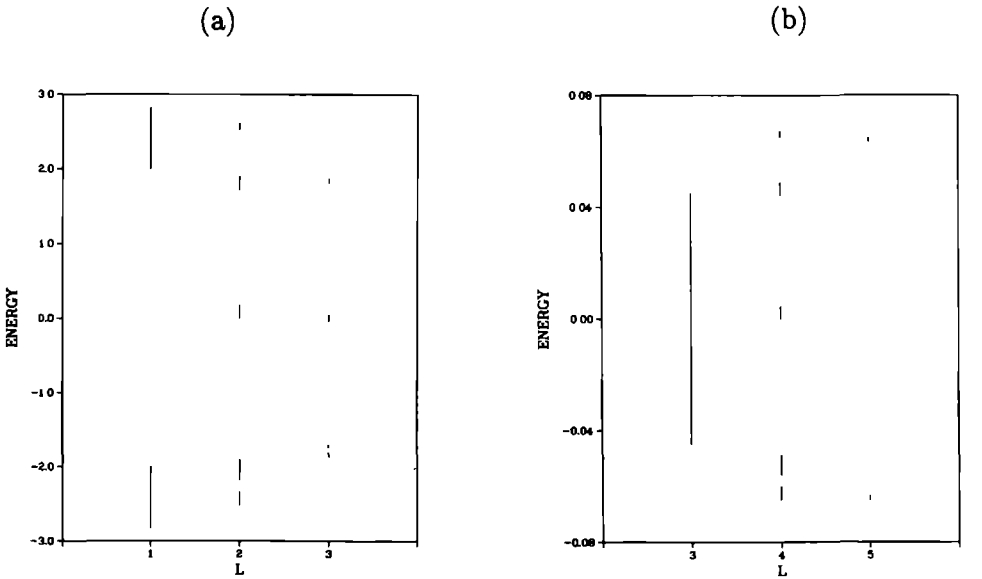

Figure 2.2. Allowed energies for the sinusoidal potential, n=2, λ=2.00; (a) shows the spectrum for l=1,2,3, (b) shows the middle bands for l=3,4,5. Notice that the middle band for l=3 consists of two bands that touch each other.

Figure 2.1(a) shows the energy bands for $n = 2$, $l = 1, 2, 3$, and in figure 2.1(b) the middle bands for $l = 3, 4, 5$ are plotted. Comparing 2.1(a) and 2.1(b), one sees that the spectrum for ϕ_l appears in the spectrum for ϕ_{l+2} in a rescaled version, given by the scaling parameter α. The greater the values of l, the more the scaling parameter α converges (for the middle bands and the middle gaps).

For $n = 1$ and $n = 3$, scaling is found by comparing ϕ_l and ϕ_{l+3} and for $n = 2$ and $n = 4$, ϕ_l and ϕ_{l+2} are compared. This is related to the fact that for n odd, every third generalized Fibonacci-number is even, and for n even, every second generalized Fibonacci-number is even.

Table 2.1 shows the values of the scaling parameter α for $n = 1, 2, 3, 4$; α has been calculated by comparing values of l up to $l = 21, 17, 13, 11$ for $n = 1, 2, 3, 4$ respectively.

For the sinusoidal potential, scaling is found at $\lambda = 2.00$ but scaling does not appear at $\lambda = 1.98$ and $\lambda = 2.02$. Figure 2.2 shows the spectrum for

	Step potential						*Sinusoidal potential*					
n	α			δ			α			δ		
1	5.618	$\pm$	0.008	0.354	$\pm$	0.005	14.0	$\pm$	0.1	1.00	$\pm$	0.01
2	8.77	$\pm$	0.05	0.349	$\pm$	0.002	39.7	$\pm$	0.2	1.00	$\pm$	0.01
3	80.3	$\pm$	0.5	0.340	$\pm$	0.003	1280	$\pm$	30	1.00	$\pm$	0.01
4	47.3	$\pm$	0.3	0.328	$\pm$	0.002	950	$\pm$	10	1.00	$\pm$	0.01

Table 2.1: Scaling parameter α and critical index δ for the step potential and the sinusoidal potential for $n = 1, 2, 3, 4$.

$l = 1, 2, 3$ (fig. 2.2(a)) and the middle bands for $l = 3, 4, 5$ (fig. 2.2(b)) for $n = 2$ and $\lambda = 2.00$, the self-dual point.
In Table 2.1 the values of the scaling parameter α of the middle bands and middle gaps for $n = 1, 2, 3, 4$ are given. For $n = 1, 2, 3, 4$ values of l up to $l = 21, 10, 7, 6$ were compared respectively.
Another quantity is the total bandwidth B_l as function of different approximations $\phi_l = \frac{q_{l-1}}{q_l}$ and fixed n. For the step potential, B_l is found numerically to go down as: $B_l = c[q_l]^{-\delta}$, as $q_l \to \infty$, in all cases $n = 1, 2, 3, 4$, each with its own value of c and δ. In the incommensurate limit, the wavefunctions seem to be critical: they are neither localized nor extended, according to Grempel *et al.* (1982) and Kohmoto *et al.* (1983). In Table 2.1, the values of δ, called the critical index of total bandwidth, are given for $n = 1, 2, 3, 4$.

For the sinusoidal potential, at $\lambda = 2.00$, B_l goes down as well as $B_l = c[q_l]^{-\delta}$, as $q_l \to \infty$, in all cases $n = 1, 2, 3, 4$. The values of δ are given in Table 2.1 for $n = 1, 2, 3, 4$. Surprisingly, δ is the same for each $n = 1, 2, 3, 4$. All cases $n = 1, 2, 3, 4$ give the same picture for $\lambda = 1.98$ and $\lambda = 2.02$: $\log B_l$ goes down faster than linearly to zero as function of l for $\lambda = 2.02$, $\log B_l$ goes down slower than linearly to its asymptotic value as function of l for λ=1.98, as $q_l \to \infty$.

2.4 Recursion relations

In order to treat the spectral problem for $n = 1$, Kohmoto *et al.* (1983) converted eq. (2.10) into a recursion relation for $x_k = Tr(M_k)$: $x_{k+1} = x_{k-1}x_k - x_{k-2}$, and constructed a 3-dimensional mapping operator T. If

$\mathbf{r}_k = (x_k, x_{k-1}, x_{k-2})$, then $\mathbf{r}_{k+1} = T\mathbf{r}_k = (x_{k-1}x_k - x_{k-2}, x_k, x_{k-1})$. Starting with $|x_0| \leq 2$ and $|x_1| \leq 2$, once $|x_k|$ and $|x_{k+1}|$ are greater than two, then an energy is forbidden for all approximations $l \geq k$. Gumbs and Ali (1988) derived similar recursion relations for $n = 2, 3$ and Holzer (1988) derived recursion relations for general n. The author derived similar recursion relations for general n independently. Since they will be of use in § 2.5 and § 2.6, a short proof will follow below. Taking eq. (2.10) as starting point, it holds that

$$M_{k+1} + [M_{k-2}]^{-1} = M_{k-1}[M_k]^n + [M_{k-1}]^n[M_k]^{-1}. \tag{2.12}$$

Using the relations:

$$Tr(AB) = Tr(BA) \text{ for every matrix } A,\ B; \tag{2.13a}$$

$$Tr(AB) + Tr(AB^{-1}) = Tr(A)Tr(B) \text{ and } Tr(A) = Tr(A^{-1}) \tag{2.13b}$$
$$\text{if } \det(A) = \det(B) = 1,$$

directly yields:

$$Tr(M_{k-1}[M_k]^m) = Tr(M_{k-1}[M_k]^{m-1})Tr(M_k) - Tr(M_{k-1}[M_k]^{m-2}) \tag{2.14a}$$

$$Tr([M_{k-1}]^m[M_k]^{-1}) = Tr([M_{k-1}]^{m-1}[M_k]^{-1})Tr(M_{k-1}) - Tr([M_{k-1}]^{m-2}[M_k]^{-1}). \tag{2.14b}$$

Defining $x(k) = Tr(M_k)$, $y(k,m) = Tr(M_{k-1}[M_k]^m)$, $z(k,m) = Tr([M_{k-1}]^m[M_k]^{-1})$, eq. (2.12) and (2.14(a,b)) can be rewritten as:

$$\begin{aligned} x(k+1) &= y(k,n-1)x(k) - y(k,n-2) \\ &+ z(k,n-1)x(k-1) - z(k,n-2) - x(k-2) \\ y(k,m) &= y(k,m-1)x(k) - y(k,m-2) \\ z(k,m) &= z(k,m-1)x(k-1) - z(k,m-2). \end{aligned}$$

Substituting $m = n$ in the last relation and using $z(k,n) = x(k-2)$ yields: $x(k-2) = z(k,n-1)x(k-1) - z(k,n-2)$, so that the resulting recursion relations become:

$$x(k+1) = y(k,n-1)x(k) - y(k,n-2) \tag{2.15a}$$

$$y(k,m) \;=\; y(k,m-1)x(k) \;-\; y(k,m-2) \qquad (2.15b)$$

with initial conditions: $x(1) = Tr(M_1)$, $x(0) = Tr(M_0)$, $y(0,n-1) = Tr(M_1[M_0]^{-1})$. With help of the relations $y(k,0) = x(k-1)$, $y(k,-1) = y(k-1,n-1)$, all $x(k)$ can be calculated.
Essentially, the recursion relations (2.15) are relations between variables of the form: $x(k_1)$ and $y(k_2,n-1)$, as becomes clear by calculating the recursion relations for $n = 1,2,3,4$:

$$\begin{aligned}
n=1: \quad x(k+1) &= x(k-1)x(k) - x(k-2) && (2.16)\\
n=2: \quad x(k+1) &= y(k,1)x(k) - x(k-1) \\
y(k,1) &= x(k-1)x(k) - y(k-1,1) && (2.17)\\
n=3: \quad x(k+1) &= y(k,2)x(k) - x(k-1)x(k) + y(k-1,2) \\
y(k,2) &= x(k-1)[x(k)]^2 - y(k-1,2)x(k) - x(k-1) && (2.18)\\
n=4: \quad x(k+1) &= x(k-1)[x(k)]^4 - y(k-1,3)[x(k)]^3 \\
&\quad -3x(k-1)[x(k)]^2 + x(k-1) + 2y(k-1,3)x(k) \\
y(k,3) &= x(k-1)[x(k)]^3 - y(k-1,3)[x(k)]^2 \\
&\quad -2x(k-1)x(k) + y(k-1,3). && (2.19)
\end{aligned}$$

We define $y(k) \equiv y(k,n-1)$ and $\mathbf{r}_k \equiv (x(k),x(k-1),y(k-1))$. Analogously to the $n=1$ case, a 3-dimensional mapping operator T can be defined with $\mathbf{r}_{k+1} = T\mathbf{r}_k = (x(k+1),x(k),y(k))$. The $x(k+1),y(k)$ are calculated according to eq. (2.15). There exists an invariant:

$$-4 + x(k)^2 + x(k-1)^2 + y(k-1)^2 - x(k)x(k-1)y(k-1) = (V_1 - V_0)^2 \qquad (2.20)$$

for each $k \geq 1$. The proof goes by induction to k. Therefore, for general n, the mapping is on a two-dimensional manifold.

2.5 Linearization around cycles

Following the analysis by Kohmoto and Oono (1984), one considers periodic orbits for the recursion relations (2.15). An orbit is a sequence of points $\mathbf{r}_0,\mathbf{r}_1,\ldots$ with $\mathbf{r}_k = (x(k),x(k-1),y(k-1))$, $\mathbf{r}_{k+1} = T\mathbf{r}_k = (x(k+1),x(k),y(k))$ as in § 2.4. All vectors $\mathbf{r}_k$ lie on the two-dimensional manifold (2.20). An orbit is periodic if there exists an $m \in \mathbf{N}$ such that

$\mathbf{r}_{k+m} = \mathbf{r}_k$, $\forall k \geq 0$. The orbit is then called an m-cycle. The nature of such m-cycles can be studied by linearization around m successive cycle points by determining the Jacobian of the mapping T^m. The values of the scaling parameter α in Table 2.1 turn out to be in agreement with the largest eigenvalue of the Jacobian of T^m for appropriate $m-$cycles.

$n = 1$. There is a six-cycle: $(0,0,a) \rightarrow (-a,0,0) \rightarrow (0,-a,0) \rightarrow (0,0,-a) \rightarrow (a,0,0) \rightarrow (0,a,0) \rightarrow (0,0,a)$ where $a^2 = (V_1 - V_0)^2 + 4$ because of eq. (2.20). Now because of eq. (2.16), the Jacobian of T at the point $\mathbf{r}_k = (x(k), x(k-1), x(k-2))$ can be written as:

$$\begin{bmatrix} x(k-1) & x(k) & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

Hence the three eigenvalues λ of the Jacobian of T^6 at the six-cycle are: $\lambda_1 = 1, \lambda_\pm = 8a^4 + 1 \pm \sqrt{64a^8 + 16a^4}$. The λ_i result from a comparison of each $k-$th and $(k+6)-$th approximation. The scaling parameter α for $n = 1$ in Table 2.1 was obtained by comparing each $k-$th and $(k+3)-$th approximation. Hence $\sqrt{\lambda_i}$ and α have to be compared. Now $\sqrt{\lambda_+} = 5.618$ for potential strength $V_0 = -V_1 = 0.6$ which is exactly the value for α in Table 2.1.

$n = 2$. There is a four-cycle: $(a,0,0) \rightarrow (0,a,0) \rightarrow (-a,0,0) \rightarrow (0,-a,0) \rightarrow (a,0,0)$. The Jacobian of T^4 at this four-cycle has eigenvalues: $\lambda_1 = 1, \lambda_\pm = 2a^4 - 4a^2 + 1 \pm \sqrt{4a^8 - 16a^6 + 20a^4 - 8a^2}$. Then $\sqrt{\lambda_+} = 8.766$, which equals the value of α.

$n = 3$. There is a six-cycle: $(0,0,a) \rightarrow (a,0,0) \rightarrow (0,a,0) \rightarrow (0,0,-a) \rightarrow (-a,0,0) \rightarrow (0,-a,0) \rightarrow (0,0,a)$. The Jacobian of T^6 at this six-cycle has $\lambda_1 = 1, \lambda_\pm = 8a^8 - 28a^6 + \frac{49}{2}a^4 + 1 \pm \sqrt{(8a^8 - 28a^6 + \frac{49}{2}a^4 + 1)^2 - 1}$ as eigenvalues. Hence $\sqrt{\lambda_+} = 80.31$, which is consistent with the value of α.

$n = 4$. There is a two-cycle: $(a,0,0) \rightarrow (0,a,0) \rightarrow (a,0,0)$. The Jacobian of T^2 at this two-cycle has eigenvalues: $\lambda_1 = 1, \lambda_\pm = \frac{3}{2}a^4 - 4a^2 + 1 \pm \sqrt{\frac{9}{4}a^8 - 12a^6 + 19a^4 - 8a^2}$. Then $\lambda_+ = 47.24$, the same as the value for α.

2.6 Spectra and local isomorphism

Up to now, energy spectra were discussed in relation to the nature of the electronic states. Another question is whether there is a relation between

energy spectra of generalized Fibonacci chains, and the concept of local isomorphism.

Definition. Two n-dimensional structures are locally isomorphic if and only if every sphere in one structure can be mapped on a sphere with the same radius and the same contents in the other structure by a translation and/or an orthogonal transformation.

For two generalized Fibonacci chains this means that two chains are locally isomorphic if and only if every finite sequence in one chain can be mapped on the same sequence in the other chain by a translation and/or an inversion. Consider an arbitrary generalized Fibonacci chain, as in § 2.2:

$$\begin{array}{lcll} S_0 & = & A^{a_1}B^{b_1}\ldots A^{a_m}B^{b_m} & (a_1,\ldots,\ b_m\ =\ 0,1,\ldots) \\ S_1 & = & A^{c_1}B^{d_1}\ldots A^{c_p}B^{d_p} & (c_1,\ldots,\ d_p\ =\ 0,1,\ldots) \\ S_{k+1} & = & S_k^n S_{k-1} & (k\ \geq\ 1). \end{array} \qquad (2.21)$$

The infinite chain is referred to as $S_\infty = \lim_{k\to\infty} S_k$. According to § 2.2, the energy spectrum for a commensurate approximation S_l consists of energies for which $|Tr(M_l)| \leq 2$, where M_l is determined by the procedure:

$$\begin{array}{lcl} M_0 & = & M_B^{b_m}M_A^{a_m}\ldots M_B^{b_1}M_A^{a_1}\ ; \quad M_1\ =\ M_B^{d_p}M_A^{c_p}\ldots M_B^{d_1}M_A^{c_1}; \\ M_{k+1} & = & M_{k-1}M_k^n. \end{array} \qquad (2.22)$$

In the following, for a given chain S_∞, the set of chains will be determined, which is locally isomorphic to S_∞, and the set which has the same energy spectrum as S_∞. Comparison of the two sets will provide the relation between energy spectrum and local isomorphism.

2.6.1 Locally isomorphic structures

In order to determine all T_∞ which are locally isomorphic to a given S_∞, two lemmas will be useful. First, some notation is introduced. With T_∞, a structure is meant which is constructed in the same way as S_∞ (see eq. (2.21)), but with $(T_0, T_1) \neq (S_0, S_1)$. For given S_k, S_k^r means the reverse of S_k (for example: if $S_k = A^aB^b$, then $S_k^r = B^bA^a$). For given S_k, let E be a product of A atoms and B atoms. Then ES_kE^{-1} is said to be a positive product if ES_kE^{-1} does not contain A^i or B^i with $i < 0$ (E^{-1}:

if, for example, $E = A^a B^b$, then $E^{-1} = B^{-b}A^{-a}$). Note that E is not necessarily a positive product.

Lemma 2.6.1. For given S_∞, let T_∞ be such that $T_0 = ES_0E^{-1}$, $T_1 = ES_1E^{-1}$ with the restriction on E, that T_0, T_1 be positive products. Then S_∞ and T_∞ are locally isomorphic and

$$T_k = ES_kE^{-1} \quad , \; k \geq 0. \tag{2.23}$$

Proof.

(i) Eq. (2.23) is evident for $k = 0, 1$.

(ii) Suppose eq. (2.23) holds for $k-1, k$. Then $T_{k+1} = T_k^n T_{k-1} = (ES_kE^{-1})^n ES_{k-1}E^{-1} = ES_k^n S_{k-1}E^{-1} = ES_{k+1}E^{-1}$. Since S_k and T_k differ by the same set of finite sequences at the edges for each k, the two infinite sequences are locally isomorphic. □

Lemma 2.6.2. For given S_∞, let T_∞ be such that $T_0 = S_0^r$, $T_1 = S_1^r$. Then S_∞ and T_∞ are locally isomorphic and:

$$\begin{array}{lll} (S_0S_1)^{-1}T_k^r(S_1S_0) = S_k & k \text{ even} \\ (S_1S_0)^{-1}T_k^r(S_0S_1) = S_k & k \text{ odd.} \end{array} \tag{2.24}$$

The rather lengthy proof is given in Appendix 2.1. Now all T_∞ can be determined, which are locally isomorphic to a given S_∞.

Theorem 2.6.3. For given S_∞, the structures T_∞ which are locally isomorphic to S_∞ are of one of the following forms:

$$\text{(a)} \qquad T_0 = ES_mE^{-1} \quad , \; T_1 = ES_{m+1}E^{-1} \quad , \; m \geq 0 \tag{2.25a}$$

$$\text{(b)} \qquad T_0 = ES_m^rE^{-1} \quad , \; T_1 = ES_{m+1}^rE^{-1} \quad , \; m \geq 0 \tag{2.25b}$$

$$\text{(c)} \qquad S_0 = ET_mE^{-1} \quad , \; S_1 = ET_{m+1}E^{-1} \quad , \; m > 0 \tag{2.25c}$$

$$\text{(d)} \qquad S_0 = ET_m^rE^{-1} \quad , \; S_1 = ET_{m+1}^rE^{-1} \quad , \; m > 0 \tag{2.25d}$$

with E an arbitrary product of A atoms and B atoms, such that T_0, T_1 are positive products.
For the proof, see Appendix 2.2.

2.6.2 Structures with the same energy spectrum

The next question is: for given S_∞, which T_∞ have the same energy spectrum as S_∞? The spectrum for S_∞ consists of energies, for which $|\lim_{k\to\infty} x(k)| \leq 2$ (see § 2.2); $x(k) = Tr(M_k)$ where M_k and S_k are related according to eq. (2.21), (2.22). The spectrum for T_∞ consists of energies for which $|\lim_{k\to\infty} x'(k)| \leq 2$; $x'(k) = Tr(M'_k)$, where M'_k and T_k are related according to eq. (2.21), (2.22). First, for given S_∞, the structures T_∞ of form (a)-(d) in Theorem 2.6.3, will be proved to have the same spectrum as S_∞. The following lemma will be useful.

Lemma 2.6.4. If $x'(0) = x(0)$, $x'(1) = x(1)$, $y'(0, n-1) = y(0, n-1)$, then S_∞ and T_∞ have the same energy spectrum.
Proof. According to the recursion relations (2.15), the starting conditions for $x(k)$ are $x(0)$, $x(1)$, $y(0, n-1)$; for $x'(k)$ they are $x'(0)$, $x'(1)$, $y'(0, n-1)$. If the starting conditions are the same, then $x'(k) = x(k)$ for each k and $\lim_{k\to\infty} x'(k) = \lim_{k\to\infty} x(k)$. Thus S_∞ and T_∞ have the same spectrum. □

Theorem 2.6.5. For given S_∞: S_∞ and the locally isomorphic structures T_∞ in eq. (2.25) of Theorem 2.6.3, have the same energy spectrum.
For the proof, see Appendix 2.3.

The final step is to prove that the T_∞ in eq. (2.25) of Theorem 2.6.3 are the only structures having the same energy spectrum as S_∞. Two lemmas will be useful.

Lemma 2.6.6. For arbitrary S_l and T_k (with corresponding $x(l) = Tr(M_l)$, $x'(k) = Tr(M'_k)$ respectively) the energy spectrum is the same if and only if $x(l) = x'(k)$.
Proof. The "if" part is trivial.
For the "only if" part: in order to get the same spectrum, S_l and T_k must contain the same number of atoms (since the number of bands equals the number of atoms), say s_l. Then $x(l)$ and $x'(k)$ are both polynomials in

E of order s_l. In order to have the same spectrum, $2s_l$ points $(E, x(l)(E))$, $(E, x'(k)(E))$ must be the same. Since a polynomial of order s_l is completely determined by s_l+1 points and since $s_l \geq 1$, the polynomials $x(l)$ and $x'(k)$ must be the same. □

In order to formulate the following lemma, we introduce some notation. Let s_k be the number of atoms contained in S_k; so s_0, s_1 is the number of atoms in S_0, S_1 respectively and $s_{k+1} = ns_k + s_{k-1}$; note that $s_k = q_k$, defined in eq. (2.8), if $s_0 = 1$, $s_1 = n$. Similarly, s'_k is the number of atoms contained in T_k. Let $aP(p)$ denote a polynomial of order p with highest-order coefficient a: $aP(p) = aE^p + O(< p)$.

Lemma 2.6.7. For S_∞ and T_∞ (with corresponding $x(k) = Tr(M_k)$, $x'(k) = Tr(M'_k)$ respectively) with $s_k = s'_k$ for each k, then it holds for each $k > 1$:

(*a*) if $x'(0) = x(0)$, $x'(1) = x(1)$, $y'(0, n-1) = y(0, n-1) - a_{-1}P(p_{-1})$, then:

$$\begin{aligned} x'(k) - x(k) &= a_{-1}q_{k-2}P(p_{-1} - s_0 - s_1 + s_k) \\ y'(k-1, n-1) - y(k-1, n-1) & \\ &= a_{-1}(q_{k-2} - q_{k-3})P(p_{-1} - s_0 - s_1 + s_k - s_{k-1}) \end{aligned} \tag{2.26a}$$

(*b*) if $y'(0, n-1) = y(0, n-1)$, $x'(1) = x(1)$, $x'(0) = x(0) - a_0P(p_0)$, then:

$$\begin{aligned} x'(k) - x(k) &= -a_0q_{k-2}P(p_0 - s_0 + s_k) \\ y'(k-1, n-1) - y(k-1, n-1) & \\ &= -a_0(q_{k-2} - q_{k-3})P(p_0 - s_0 + s_k - s_{k-1}) \end{aligned} \tag{2.26b}$$

(*c*) if $y'(0, n-1) = y(0, n-1), x'(0) = x(0), x'(1) = x(1) - a_1P(p_1)$, then:

$$\begin{aligned} x'(k) - x(k) &= -a_1q_{k-1}P(p_1 - s_1 + s_k) \\ y'(k-1, n-1) - y(k-1, n-1) & \\ &= -a_1(q_{k-1} - q_{k-2})P(p_1 - s_1 + s_k - s_{k-1}). \end{aligned} \tag{2.26c}$$

For the proof, see Appendix 2.4.

Now, for a given S_∞, the structures T_∞ can be determined, which have the same spectrum as S_∞. In order to have the same energy spectrum for S_∞ and T_∞, it must hold that $\lim_{k\to\infty} x(k) = \lim_{k\to\infty} x'(k)$ with $x(k)$, $x'(k)$ being polynomials of order s_k, s'_k respectively in E. Then there must be a $t \in \mathbf{Z}$, such that $\lim_{k\to\infty}[x'(k) - x(k+t)] = 0$. This means that $s'_k = s_{k+t}$ for $min(k, k+t) \geq 0$. Since $\lim_{k\to\infty} S_k = \lim_{k\to\infty} S_{k+t}$, we can start with S_0, S_1, T_0, T_1 such that $s_0 = s'_0, s_1 = s'_1$.
We now assume (assumption 1) that, if an $M \in \mathbf{N}$ can be found such that $x'(k) - x(k) = f(k)P(s_k - M)$ for each k, with $\lim_{k\to\infty} f(k) \neq 0$, then $\lim_{k\to\infty} x(k) \neq \lim_{k\to\infty} x'(k)$.
Consider, for given S_∞, a chain T_∞, with $s_k = s'_k$ for each k. Let $y'(0, n-1)$ $= y(0, n-1)$ - $a_{-1}P(p_{-1})$, $x'(0) = x(0)$ - $a_0P(p_0)$, $x'(1) = x(1)$ - $a_1P(p_1)$. Then, according to Lemma 2.6.7:

$$\begin{aligned} x'(k) - x(k) &= q_{k-2}[a_{-1}P(p_{-1} - s_0 - s_1 + s_k) \\ &\quad -a_0P(p_0 - s_0 + s_k)] - q_{k-1}a_1P(p_1 - s_1 + s_k) \end{aligned}$$

where only the highest-order terms count.
Then $x'(k) - x(k) = f(k)P(max[p_{-1} - s_0 - s_1, p_0 - s_0, p_1 - s_1] + s_k)$. Now the question is, whether $\lim_{k\to\infty} f(k) \neq 0$. First note that, if we are in case (a),(b) or (c) of Lemma 2.6.7, then $\lim_{k\to\infty} f(k) = \infty$. For combinations of these cases, choose S_0, S_1, T_0, T_1 such that S_{-2}, T_{-2}, S_{-1}, T_{-1} are positive products. Then the a_{-1} term does not provide the highest-order term: $p_{-1} - s_0 - s_1 < min(p_0 - s_0, p_1 - s_1)$. Then $\lim_{k\to\infty} f(k) = 0$ only if $p_0 - s_0 = p_1 - s_1$ and if $\lim_{k\to\infty}[q_{k-2}a_0 + q_{k-1}a_1] = 0 \to a_1 = -\phi a_0$. If V_0, V_1 are rational , then a_0, a_1 are rational, and $\lim_{k\to\infty} f(k) = \infty$.
For given C, D being products of M_A matrices and M_B matrices: if $Tr(C)$ $= Tr(D)$, then $D = ECE^{-1}$ or $D = EC^rE^{-1}$ with E being a product of M_A matrices and M_B matrices. Argument: write $D = PCQ$ (such P, Q can always be found). We now assume the following expression to hold (assumption 2): $Tr(D) = Tr(PCQ) = Tr(CQP) \neq Tr(C)$ if $P \neq Q^{-1}$ since $Tr(C)$ will then be a different polynomial in E than $Tr(D)$. Analogously, after noting that $Tr(C) = Tr(C^r)$ due to Theorem 2.6.5, $Tr(PC^rQ) \neq Tr(C)$ if $P \neq Q^{-1}$ (this is made plausible below Theorem 2.6.8).

Theorem 2.6.8. For rational V_0, V_1, for given S_∞: the T_∞ which have the same energy spectrum as S_∞ are exactly the T_∞ in eq. (2.25) of Theorem 2.6.3.

Proof. Suppose T_∞ has the same energy spectrum as S_∞. Then T_∞ must be of one of the following forms, due to assumption 1 and 2:

(a)	$T_0 = ES_mE^{-1}$	,	$T_1 = FS_{m+1}F^{-1}$	,	$m \geq 0$
(b)	$T_0 = ES_m^rE^{-1}$	,	$T_1 = FS_{m+1}^rF^{-1}$	,	$m \geq 0$
(c)	$S_0 = ET_mE^{-1}$	,	$S_1 = FT_{m+1}F^{-1}$	,	$m > 0$
(d)	$S_0 = ET_m^rE^{-1}$	,	$S_1 = FT_{m+1}^rF^{-1}$	,	$m > 0$.

The final step is to prove that $E = F$. The proof will be given for case (a); the proof for the other cases goes analogously. Define U_∞ by: $U_0 = S_m, U_1 = S_{m+1}, U_{k+1} = U_k^n U_{k-1}$. Then $U_\infty = S_\infty$. Thus T_∞ and U_∞ must be proved to have the same spectrum, where $T_0 = EU_0E^{-1}$, $T_1 = FU_1F^{-1}$. Let $x(k) = Tr(M_k)$ and $x'(k) = Tr(M_k')$ correspond to U_k and T_k respectively. Then $M_0' = M_E^{-1}M_0M_E$, $M_1' = M_F^{-1}M_1M_F$. Since then $x'(0) = x(0)$, $x'(1) = x(1)$, it must hold that $y'(0, n-1) = y(0, n-1)$ due to Lemma 2.6.7. Thus $Tr(M_1'(M_0')^{-1}) = Tr(M_1M_0^{-1}) \rightarrow Tr(M_F^{-1}M_1M_FM_E^{-1}M_0^{-1}M_E) = Tr(M_1M_0^{-1})$. The same argument as in assumption 2 yields: $M_E = M_F \rightarrow E = F$.
The statement that the T_∞ of form (a) have the same spectrum as S_∞ according to Theorem 2.6.5, completes the proof. □

It can be proved that Theorem 2.6.8 also holds ($\lim_{k\to\infty} f(k) \neq 0$) for V_0, V_1 not both rational, except for the following case (if existing !).

1) Let $s_k' = s_{k+t}$ for each k, for certain t (otherwise S_∞ and T_∞ will not have the same spectrum due to assumption 1);

2) Choose S_0, S_1, T_0, T_1 such that $t = 0$ and S_{-2}, T_{-2}, S_{-1}, T_{-1} are positive products;

3) Let $a_1 = -\phi a_0$ and $p_0 - s_0 = p_1 - s_1$;

4) For each k, S_k and T_k contain the same number of atoms of type A (thus also of type B, since $s_k = s_k'$): suppose $s_k = s_k'$; S_k, T_k contain A_k, A_k' atoms of type A respectively, $A_k \neq A_k'$. Then $x'(k)$ - $x(k) = (A_k' - A_k)(V_0 - V_1)P(s_k - 1)$;

5) For each k, S_k and T_k are of the form: $S_k = EA^{a_1}B^{b_1}\ldots A^{a_j}B^{b_j}E^{-1}$, $T_k = FA^{c_1}B^{d_1}\ldots A^{c_{j'}}B^{d_{j'}}F^{-1}$ with $j = j'$, where E, F are products

of A atoms and B atoms: suppose $A_k = A'_k$, $j \neq j'$. Then $x'(k)$ - $x(k)$ $= (j' - j)(V_0 - V_1)^2 P(s_k - 4)$.

Comparing Theorem 2.6.3 and Theorem 2.6.8 leads to the conclusion that two generalized Fibonacci chains constructed by juxtaposition have the same energy spectrum if and only if they are locally isomorphic (except for the case mentioned below Theorem 2.6.8, for which it is not known). The proof of Theorem 2.6.3 shows that, if S_∞ and T_∞ are locally isomorphic, then there is an $m \in \mathbf{Z}$ such that the commensurate approximations T_k and S_{k+m} differ by a constant finite sequence at the edges for each k, or such that T_k and the reverse of S_{k+m} differ by a finite sequence for each k (constant for each even k, and constant for each odd k), for k large enough.

2.7 Conclusions

For the step potential, for which the system is critical in the incommensurate limit, and for the $\lambda = 2$ case of the sinusoidal potential, a scaling parameter α and a critical index for the total bandwidth δ is determined for n = 1,2,3,4 and the total bandwidth goes down as $c[q_l]^{-\delta}$, where q_l is the number of bands. For the step potential, recursion relations for general n have been derived to treat the spectral problem by means of a mapping problem. The numerically found values for α are in agreement with the eigenvalues of the linearization around certain cycles for this mapping problem.
Generalized Fibonacci chains are found to have the same energy spectrum if and only if they are locally isomorphic (except for one case, for which it is not known). It has been shown how two locally isomorphic chains are related.

Appendix 2.1. Proof of Lemma 2.6.2

Proof by induction. Define U_∞ by: $U_0 = S_0 = T_0^r$, $U_1 = S_1 = T_1^r$, $U_{k+1} = U_{k-1}U_k^n$ (the juxtaposition rule for U_k is different from the rule for S_k, T_k). Then:

(i) $(S_0S_1)^{-1}U_2(S_1S_0) = S_2$
(ii) $(S_1S_0)^{-1}U_3(S_0S_1) = S_3$
(iii) $(S_1S_0)^{-1}U_3U_2 = (S_0S_1)^{-1}U_2U_3$.

Proof by substituting $U_2 = S_0 S_1^n$, $U_3 = S_1[S_0 S_1^n]^n$. Induction step; for k even: suppose $(S_0S_1)^{-1}U_{k-2}(S_1S_0) = S_{k-2}$, $(S_1S_0)^{-1}U_{k-1}(S_0S_1) = S_{k-1}$, $(S_1S_0)^{-1}U_{k-1}U_{k-2} = (S_0S_1)^{-1}U_{k-2}U_{k-1}$. Then:

$$\text{(iv)}\quad (S_0S_1)^{-1}U_k(S_1S_0) = S_k$$
$$\text{(v)}\quad (S_0S_1)^{-1}U_kU_{k-1} = (S_1S_0)^{-1}U_{k-1}U_k.$$

Proof by substituting $U_k = U_{k-2}U_{k-1}^n$ and using the induction assumptions. Analogously one can prove, using the induction assumptions for odd k:

$$\text{(vi)}\quad (S_1S_0)^{-1}U_k(S_0S_1) = S_k$$
$$\text{(vii)}\quad (S_1S_0)^{-1}U_kU_{k-1} = (S_0S_1)^{-1}U_{k-1}U_k.$$

Relations (i)-(vii) lead to:

$$(S_0S_1)^{-1}U_k(S_1S_0) = S_k \quad \text{for } k \text{ even}$$
$$(S_1S_0)^{-1}U_k(S_0S_1) = S_k \quad \text{for } k \text{ odd}.$$

The final step in the proof is by noting that $U_k = T_k^r, k \geq 0$. This leads directly to:

$$(S_0S_1)^{-1}T_k^r(S_1S_0) = S_k \quad \text{for } k \text{ even}$$
$$(S_1S_0)^{-1}T_k^r(S_0S_1) = S_k \quad \text{for } k \text{ odd}. \quad \square$$

Appendix 2.2. Proof of Theorem 2.6.3

For given S_∞, define U_∞ by: $U_0 = S_m$, $U_1 = S_{m+1}$, $m \geq 0$, $U_{k+1} = U_k^n U_{k-1}$. Then $U_k = S_{k+m}$ for each k and $U_\infty = S_\infty$.

(a) Then T_∞, given by $T_0 = EU_0E^{-1} = ES_mE^{-1}$, $T_1 = EU_1E^{-1} = ES_{m+1}E^{-1}$, is locally isomorphic to S_∞ according to Lemma 2.6.1 and:

$$T_k = ES_{k+m}E^{-1}\ ,\ k \geq 0. \tag{A2.1}$$

The only restriction on E is that T_0, T_1 be positive products.

(b) Then T_∞, given by $T_0 = EU_0^rE^{-1} = ES_m^rE^{-1}$, $T_1 = EU_1^rE^{-1} = ES_{m+1}^rE^{-1}$, is locally isomorphic to S_∞ according to Lemma 2.6.1, 2.6.2 and:

$$\begin{aligned}(S_mS_{m+1})^{-1}E^rT_k^r(E^{-1})^r(S_{m+1}S_m) &= S_{k+m}, \quad k \text{ even}\\ (S_{m+1}S_m)^{-1}E^rT_k^r(E^{-1})^r(S_mS_{m+1}) &= S_{k+m}, \quad k \text{ odd}.\end{aligned} \tag{A2.2}$$

The restriction on E is that T_0, T_1 be positive products.

(c) For given S_∞: if positive products T_0, T_1 can be found, such that $S_0 = ET_mE^{-1}$, $S_1 = ET_{m+1}E^{-1}$ for certain E and $m > 0$, then S_∞ and T_∞ are locally isomorphic and:

$$S_k = ET_{k+m}E^{-1}\ ,\ k \geq 0,\ m > 0. \tag{A2.3}$$

(d) Analogously, for given S_∞: if positive products T_0, T_1 can be found, such that $S_0 = ET_m^rE^{-1}$, $S_1 = ET_{m+1}^rE^{-1}$ for certain E and $m > 0$, then S_∞ and T_∞ are locally isomorphic and:

$$\begin{array}{ll} (T_mT_{m+1})^{-1}E^rS_k^r(E^{-1})^r(T_{m+1}T_m) = T_{k+m}, & k \text{ even} \\ (T_{m+1}T_m)^{-1}E^rS_k^r(E^{-1})^r(T_mT_{m+1}) = T_{k+m}, & k \text{ odd.} \end{array} \tag{A2.4}$$

The next step is to prove that there are no other structures T_∞, which are locally isomorphic to a given S_∞.

(a) Without inversion.
With help of the relation $S_{k-1} = S_k^{-n}S_{k+1}$, S_l can also be defined for $l < 0$, if S_l is a positive product. Let p $\in \mathbf{Z}$ be such that S_l is a positive product for $l \geq p$, and S_{p-1} is not. Take an arbitrary T_∞ and write: $T_1 = DS_{t+1}C$, where $t+1$ is the largest integer for which S_{t+1} is included in T_1 (so C, D are positive products). If S_{p+1} is not included in T_1, then write $t = p$ (then C, D are not both positive products).
At first, sequences T_k and $ET_kE^{-1} (k \geq 0)$ will not be distinguished. Later on, this possibility of getting locally isomorphic chains (according to Lemma 2.6.1) will be taken into account.
Since we do not distinguish between T_k and CT_kC^{-1} $(k \geq 0)$ at this stage, write: $T_1 = CDS_{t+1}$. Then CD must be a product of sequences S_t and S_{t+1}: $T_1^2 = CDS_{t+1}CDS_{t+1}$ occurs in T_∞. Now S_∞ can be considered as built up out of S_t, S_{t+1}, occurring as powers $(S_{t+1})^n, (S_{t+1})^{n+1}, S_t$. Then $T_1 = (S_{t+1})^\gamma$ or $T_1 = (S_{t+1})^{i_1}S_t(S_{t+1})^{i_2}....(S_{t+1})^{i_{k-1}}S_t(S_{t+1})^{i_k}$. Since $t+1$ is the largest integer for which S_{t+1} is included in T_1, it holds that:

$$T_1 = (S_{t+1})^\gamma,\ 1 \leq \gamma \leq n \tag{A2.5}$$

or

$$T_1 = (S_{t+1})^{i_1}S_t(S_{t+1})^{i_2},\ i_1 \leq n-1,\ 1 \leq i_2 \leq n.$$

- $n = 1$.

$T_1 = S_{t+1}$ or $T_1 = S_t S_{t+1}$. Suppose $T_1 = S_t S_{t+1}$. Since we do not distinguish between T_k and $S_t^{-1} T_k S_t$ ($k \geq 0$) at this stage, we may write: $T_1 = S_t^{-1} S_t S_{t+1} S_t = S_{t+1} S_t = S_{t+2}$. Due to the fact that $t+1$ is the largest integer for which S_{t+1} is included in T_1, it holds that $T_1 = S_{t+1}$. The next step is to prove that $T_0 = S_t$. ${T_1}^2 T_0 {T_1}^2 = (S_{t+1})^2 T_0 (S_{t+1})^2$ occurs in T_∞. In order to be locally isomorphic to S_∞, it must hold that:

$$T_0 = S_t \quad \text{or} \quad T_0 = S_t (S_{t+1})^{i_1} \ldots (S_{t+1})^{i_k} S_t \; ; \quad i_1, \ldots, i_k = 1, 2.$$

In the latter case, $i_1 = i_k = 2$, because $T_0 T_1 T_0$ occurs in T_∞. Also $T_0 T_1^2 T_0$ occurs in T_∞, which means that $(S_{t+1})^2 S_t (S_{t+1})^2 S_t (S_{t+1})^2$ occurs; this sequence does not occur in S_∞. So $T_1 = S_{t+1}, T_0 = S_t$.

- $n > 1$.

Suppose $T_1 = (S_{t+1})^{i_1} S_t (S_{t+1})^{i_2}$ (see eq. (A2.5)). Now T_1^{n+1} occurs in T_∞. Since $n > 1$, $S_t (S_{t+1})^{(i_1+i_2)} S_t (S_{t+1})^{(i_1+i_2)} S_t$ occurs. This sequence only occurs in S_∞ when $i_1 + i_2 = n$. Write $T_1 = (S_{t+1})^{(n-i)} S_t (S_{t+1})^i$ ($i \geq 1$). Since we do not distinguish between T_k and $(S_{t+1})^i T_k (S_{t+1})^{-i}$ ($k \geq 0$) at this stage, write $T_1 = (S_{t+1})^n S_t = S_{t+2}$. Since $t+1$ was the largest integer for which S_{t+1} is included in T_1, T_1 must be $(S_{t+1})^\gamma, 1 \leq \gamma \leq n$. Now T_1^n occurs in T_∞. Since S_{t+1} occurs only as power $(S_{t+1})^n$ or $(S_{t+1})^{n+1}$ in S_∞, it must hold that $\gamma = 1$: $T_1 = S_{t+1}$.
The next step is to prove that $T_0 = S_t$. Now $T_1^{n+1} T_0 T_1^n = (S_{t+1})^{n+1} T_0 (S_{t+1})^n$ and $T_1^n T_0 T_1^{n+1} = (S_{t+1})^n T_0 (S_{t+1})^{n+1}$ occur in T_∞, which yields: $T_0 = S_t$ or $T_0 = S_t (S_{t+1})^{i_1} \ldots . (S_{t+1})^{i_k} S_t$; $i_1 = i_k = n; i_2, \ldots, i_{k-1} = n$ or $n+1$.
In the latter case, make use of the fact that $(T_1^n T_0)^n$ occurs in T_∞ and that, if $[(S_{t+1})^{n+1} S_t][(S_{t+1})^n S_t]^i [(S_{t+1})^{n+1} S_t]$ occurs in S_∞, then $i = n$ or $n-1$. This means, that T_0 must be of the kind:

$$T_0 = S_t [(S_{t+1})^n S_t]^{(n-i-j_0)} [(S_{t+1})^{n+1} S_t][(S_{t+1})^n S_t]^{j_1} \ldots$$

$$\ldots [(S_{t+1})^n S_t]^{j_s} [(S_{t+1})^{n+1} S_t][(S_{t+1})^n S_t]^i$$

with $i \geq 1, j_1, \ldots, j_s = n$ or $n-1$ and $j_0 = 1, 2$. Now $T_1^{n+1} T_0$ occurs in T_∞. In order to be locally isomorphic to S_∞, it must hold that $n - i - j_0 = n$ or $n - 1 \rightarrow i \leq 0$. Since $i \geq 1$, T_∞ and S_∞ cannot be locally isomorphic.

So $T_1 = S_{t+1}$, $T_0 = S_t$. Combining these results with Lemma 2.6.1 gives, as a conclusion, that the T_∞ which are locally isomorphic to S_∞, without taking inversion into account, are of form (A2.1) ($t \geq 0$) or of form (A2.3) ($t < 0$).

(b) With inversion.

Lemma 2.6.2 tells that, with $U_0 = S_0^r$, $U_1 = S_1^r$, $U_{k+1} = U_k^n U_{k-1}$, every finite sequence in S_∞ occurs in the reverse of U_∞ and vice versa. So the task is to search for T_∞ such that every sequence in T_∞ occurs in U_∞ and vice versa. Part (a) of the proof showed that, in order to get locally isomorphic chains T_∞ and U_∞ without taking inversion into account, it must hold that $T_0 = FU_tF^{-1}$, $T_1 = FU_{t+1}F^{-1}$, which means that the T_∞, which are locally isomorphic to S_∞, taking inversion into account, are of form (A2.2) or (A2.4). □

Appendix 2.3. Proof of Theorem 2.6.5

Suppose $T_0 = ES_tE^{-1}$, $T_1 = ES_{t+1}E^{-1}$, then we are in the cases (a) ($t \geq 0$) and (c) ($t < 0$) of Theorem 2.6.3. Say $U_0 = ES_0E^{-1}$, $U_1 = ES_1E^{-1}$, $U_{k+1} = U_k^n U_{k-1}$. Then $U_\infty = T_\infty$, since $\lim_{k\to\infty} ES_kE^{-1} = \lim_{k\to\infty} ES_{k+t}E^{-1}$. So we have to prove that U_∞ and S_∞ have the same spectrum.

Let E, S_k, U_k correspond to M_E, M_k, M_k' respectively according to eq. (2.21), (2.22). Then $M_0' = M_E^{-1}M_0M_E$, $M_1' = M_E^{-1}M_1M_E$. With use of the relation $Tr(CD) = Tr(DC)$ for arbitrary C, D, this directly yields: $x'(0) = x(0)$, $x'(1) = x(1)$, $y'(0, n-1) = y(0, n-1)$. Using Lemma 2.6.4, U_∞ and S_∞ have the same spectrum, thus T_∞ and S_∞ have the same spectrum.

Suppose $T_0 = ES_t^rE^{-1}$, $T_1 = ES_{t+1}^rE^{-1}$. Then we are in cases (b) ($t \geq 0$) and (d) ($t < 0$) of Theorem 2.6.3. Say $V_0 = E^{-1}T_0E = S_t^r$, $V_1 = E^{-1}T_1E = S_{t+1}^r$, $V_{k+1} = V_k^n V_{k-1}$. Then V_∞ and T_∞ have the same spectrum according to the proof above. So the next step is to prove that V_∞ and S_∞ have the same spectrum.

Say $U_0 = S_t$, $U_1 = S_{t+1}$, $U_{k+1} = U_k^n U_{k-1}$. Then $U_\infty = S_\infty$. We have to prove that U_∞ and V_∞ have the same spectrum (note that $V_0 = U_0^r$, $V_1 = U_1^r$).

Let M_k, M_k' correspond to U_k, V_k respectively. It must hold that: (1) $Tr(M_0^r) = Tr(M_0)$, (2) $Tr(M_1^r) = Tr(M_1)$, (3) $Tr(M_1^r(M_0^r)^{-1}) = Tr(M_1M_0^{-1})$. The relations (1), (2), (3) hold if $Tr(C) = Tr(C^r)$ for arbitrary $C = M_A^{a_1} \ldots M_B^{b_m}$

($a_1, \ldots, b_m \in \mathbf{Z}$). The proof goes by induction.
First, $Tr(C) = Tr(C^\tau)$ for $C = M_A^{a_1} M_B^{b_1}$, $C = M_A^{a_1} M_B^{b_1} M_A^{a_2}$, $C = M_B^{b_1} M_A^{a_1} M_B^{b_2}$ for all $a_1, a_2, b_1, b_2 \in \mathbf{Z}$, by using eq. (2.13).
The induction step: suppose $Tr(M_A^{a_1} \ldots M_A^{a_m}) = Tr(M_A^{a_m} \ldots M_A^{a_1})$. Then:

$$
\begin{aligned}
& Tr(M_A^{a_1} \ldots M_A^{a_m} M_B^{b_m}) \\
&= Tr(M_A^{a_1} \ldots M_B^{b_{m-1}}) Tr(M_A^{a_m} M_B^{b_m}) - Tr(M_A^{a_1} \ldots M_B^{(b_{m-1}-b_m)} M_A^{-a_m}) \\
&= Tr(M_B^{b_{m-1}} \ldots M_A^{a_1}) Tr(M_B^{b_m} M_A^{a_m}) - Tr(M_A^{-a_m} M_B^{(b_{m-1}-b_m)} \ldots M_A^{a_1}) \\
&= Tr(M_B^{b_m} M_A^{a_m} \ldots M_A^{a_1}),
\end{aligned}
$$

because of the induction assumption and with use of eq. (2.13). □

Appendix 2.4. Proof of Lemma 2.6.7

First, note that $x'(k)$ and $x(k)$ are polynomials with highest-order term E^{s_k}. The proof will be given for eq. (2.26(a)). The other two cases go analogously. The cases $n = 1$ and $n > 1$ are treated separately. Suppose $x'(0) = x(0), x'(1) = x(1), y'(0, n-1) = y(0, n-1) - a_{-1}P(p_{-1})$. The task will be to find the highest-order term of the difference polynomial $y'(k-1, n-1) - y(k-1, n-1)$ and $x'(k) - x(k)$. By "lower-order terms" will be meant terms which do not contribute to the highest-order term.

- *$n = 1$.*

For $n = 1$, $y(0, n-1) = x(-1)$, $y'(0, n-1) = x'(-1)$.

$$
\begin{aligned}
x'(2) &= x'(0)x'(1) - x'(-1) \\
&= x(0)x(1) - [x(-1) - a_{-1}P(p_{-1})] \\
&= x(2) + a_{-1}P(p_{-1}); \\
x'(3) &= x'(1)x'(2) - x'(0) \\
&= x(1)[x(2) + a_{-1}P(p_{-1})] - x(0) \\
&= x(3) + a_{-1}P(p_{-1} + s_1) \\
&= x(3) + a_{-1}P(p_{-1} - s_0 - s_1 + s_3); \\
x'(4) &= x'(2)x'(3) - x'(1) = \ldots \\
&= x(4) + a_{-1}P(p_{-1} - s_0 - s_1 + s_4).
\end{aligned}
$$

The induction step: suppose eq. (2.26(a)) holds for $k-1$, $k-2$, $k-3$. Then eq. (2.25(a)) also holds for k.
Proof by using $x'(k) = x'(k-2)x'(k-1) - x'(k-3)$ and substituting the terms on the right-hand side with help of the induction assumptions.

- $n > 1$

$$
\begin{aligned}
y'(1,n-1) &= y'(1,n-2)x'(1) - y'(1,n-3) \\
&= [y'(1,0)x'(1) - y'(1,-1)][x'(1)]^{n-2} + \text{lower-order terms} \\
&= [x'(0)x'(1) - y'(0,n-1)][x'(1)]^{n-2} + \text{lower-order terms} \\
&= y(1,n-1) + a_{-1}P(p_{-1} + (n-2)s_1); \\
x'(2) &= y'(1,n-1)x'(1) - y'(1,n-2) \\
&= x(2) + a_{-1}P(p_{-1} + (n-1)s_1) \\
&= x(2) + q_0 a_{-1}P(p_{-1} - s_0 - s_1 + s_2); \\
y'(2,n-1) &= y'(2,n-2)x'(2) - y'(2,n-3) \\
&= [x'(1)x'(2) - y'(1,n-1)][x'(2)]^{n-2} + \text{lower-order terms} \\
&= y(2,n-1) + a_{-1}P(p_{-1} + ns_1 + (n-2)s_2) \\
&\quad +(n-2)a_{-1}P(p_{-1} + ns_1 + (n-2)s_2) \\
&= y(2,n-1) + (q_1 - q_0)a_{-1}P(p_{-1} - s_0 - s_1 + s_3 - s_2); \\
x'(3) &= y'(2,n-1)x'(2) - y'(2,n-2) \\
&= x(3) + q_1 a_{-1}P(p_{-1} - s_0 - s_1 + s_3).
\end{aligned}
$$

The induction step: suppose eq. (2.26(a)) holds for $y(k-2,n-1)$, $x(k-2)$, $x(k-1)$. Then eq. (2.26(a)) also holds for $y(k-1,n-1)$, $x(k)$ by using the relations:

$$
\begin{aligned}
y'(k-1,n-1) &= y'(k-1,n-2)x'(k-1) - y'(k-1,n-3) \\
&= [x'(k-2)x'(k-1) - y'(k-2,n-1)][x'(k-1)]^{n-2} \\
&+ \text{lower-order terms}; \\
x'(k) &= y'(k-1,n-1)x'(k-1) - y'(k-1,n-2)
\end{aligned}
$$

and using the induction assumptions. □

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Chapter 3

Methods to determine generators and defining relations for an n-dimensional point group

Four methods to determine a generating set of matrices satisfying defining relations of an n-dimensional point group are described, given all point group elements or given a generating set, but without knowing defining relations. The first method makes use of the stepwise construction of the point group, adding a new generator at each step. Defining relations are achieved by making a coset decomposition at each step. Another approach is by use of the lower central series, yielding generators and relations according to a well known technique. If the point group is nonsolvable, there is a nontrivial subgroup which has itself as commutator group. The first method is then used to treat this subgroup. This approach is denoted as the second method. The third new method is a depth-first search method. At each step in the construction, a certain element is multiplied with a certain generator according to the depth-first search rule. In the fourth method, which is similar to the third method, the point group is constructed according to a breadth-first search rule. The first method gives better results than the other methods with respect to the number of defining relations and the computer time.

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3.1 Introduction

An interesting problem in group theory is the finite presentation of a finite group by means of a set of generators $\{g_1, \ldots, g_m\}$ and defining relations satisfied by these generators:

$$\varphi_i(g_1, \ldots, g_m) = \epsilon, \ 1 \leq i \leq r \tag{3.1}$$

where each $\varphi_i(g_1, \ldots, g_m)$ is a word in the letters $g_1, \ldots, g_m$ and their inverses $g_1^{-1}, \ldots, g_m^{-1}$ and ϵ is the unit element of the group.
In this paper, the finite group is an n-dimensional crystallographic point group (i.e. a finite subgroup of $Gl(n, \mathbf{Z})$) and the point group is supposed to be given either by all matrices contained in the point group, or by a generating set of matrices, without giving defining relations.
A number of methods has already been developed to treat related problems. One of them is the method of Todd and Coxeter (Todd and Coxeter 1936, also described by Coxeter and Moser (1957), pp. 12-18), for establishing the order of a finite group defined by some defining relations satisfied by a set of generators. Since this method assumes the defining relations to be known, the Todd-Coxeter method is not of much use for our problem. Algorithmic applications of these methods have been described e.g. by Leech (1963) and Mendelsohn (1965). For solvable groups, the problem is easy to solve. Nonsolvable crystallographic point groups occur in dimensions higher than three. For $n = 4$, a complete list of finite subgroups of $Gl(n, \mathbf{Z})$ has been given by Brown *et al.* (1973, 1978). The knowledge of defining relations satisfied by a generating set of a point group is of importance for the determination of space groups (Brown 1969, Janssen *et al.* 1969, Fast and Janssen 1971).
The paper is organized as follows. A set of generators and relations for solvable groups can be achieved by an already well known technique, using the lower central series. This technique is described in § 3.2. In the first new method, described in § 3.3, the point group is constructed by stepwise adding a generator to a subgroup already achieved, and then determining the larger subgroup. Once the latter subgroup has been decomposed into cosets w.r.t. the former subgroup, defining relations can be constructed. In the second method, by means of the lower central series, one ends up with a subgroup which has itself as commutator group. If the point group is solvable, then the second method coincides with the method, already described in § 3.2.

If the point group is nonsolvable, then the first method is used to treat this subgroup. For nonsolvable groups, the strategy of the second method is briefly outlined in § 3.3. The third new method is a depth-first search method. Each generator of the point group gets a certain priority. The point group is constructed in a number of steps. At each step, the elements obtained are multiplied by the generators with a certain priority, determined by the depth-first search rule. The fourth method, denoted as a breadth-first search method, is similar to the third method. Starting with the identity matrix, one determines stepwise the set achieved by multiplying all elements of the prior set with all generators, and by adding the extra elements to this prior set. At each step, defining relations are achieved. The third and fourth methods are outlined in § 3.4. All these methods yield a number of defining relations. Since, generally, most of them are redundant, a procedure has been developed to decrease this number. This procedure is treated in § 3.5. A computer program based upon these four methods has been developed. The algorithmic procedure of the program for the first two methods is pointed out in § 3.6. Examples and results for some point groups are given in § 3.7. The four methods are compared and evaluated in § 3.8.

3.2 Lower central series method

Consider a finite group $K \subset Gl(n, \mathbf{Z})$. Define $K^{(0)} \equiv K$. Let $i \geq 0$. The commutator group $K^{(i+1)}$ is defined inductively as the group, generated by the set:

$$\left\{ghg^{-1}h^{-1} \mid g,\ h \in K^{(i)}\right\}. \tag{3.2}$$

There is a $j \in \mathbf{N}$ such that $K^{(j+k)} = K^{(j)}$, $\forall\ k \in \mathbf{N}$. The series $K^{(0)} \supset \ldots \supset K^{(j)}$, called the lower central series, has length j then. The point group K is solvable if and only if $K^{(j)} = \{\mathbb{1}_n\}$, where $\mathbb{1}_n$ is the identity matrix, the unit element of K.
There are two important properties relating $K^{(i)}$ and its commutator group $K^{(i+1)}$ for each $0 \leq i < j$:

$$K^{(i+1)} \trianglelefteq K^{(i)}\ ;\ K^{(i)}/K^{(i+1)} \text{ is abelian.} \tag{3.3}$$

For the proof, see e.g. Hall (1959, p.138).
Since every finite abelian group is either a finite cyclic group or is isomorphic

to a direct product of finite cyclic groups (see e.g. Rotman 1965, pp. 58-62), eq. (3.3) can be rewritten as:

$$\exists\, p, m_1, \ldots, m_p \in \mathbf{N} \text{ such that } K^{(i)}/K^{(i+1)} \simeq C_{m_1} \times \ldots \times C_{m_p}. \quad (3.4)$$

For each i, generators and defining relations are achieved as follows.
The first task is to find all, say L, coset representatives of $K^{(i)}$ w.r.t. $K^{(i+1)}$. The first representative is $k_1 \equiv \mathbf{1}_n$. The second coset representative is a matrix $k_2 \in K^{(i)}$, $k_2 \notin K^{(i+1)}$. Then all matrices in the coset $k_2K^{(i)}$ are determined. If the number of cosets is greater than two, then a matrix $k_3 \in K^{(i)}$, $k_3 \notin K^{(i+1)}$, $k_3 \notin k_2K^{(i+1)}$ is sought and all matrices in the coset $k_3K^{(i)}$ are determined, etc.
The second task is to determine the value of $p, m_1, \ldots, m_p$ in rel. (3.4). To answer this question we need to know the orders of all elements of the factor group in rel. (3.4), i.e. the values x such that:

$$(k_z)^x \in K^{(i+1)}\,,\ (k_z)^y \notin K^{(i+1)},\ \forall\, y < x$$

for each non-trivial coset representative $k_z = k_2, \ldots, k_L$. When all these orders are known, the value of p and of the m_l can be determined. Suppose, for example, that $|K^{(i)}|/|K^{(i+i)}| = 12$. Then the problem is whether the direct product meant in rel. (3.4) is $C_{12}, C_6 \times C_2, C_3 \times C_2 \times C_2$ or $C_4 \times C_3$. For example, C_{12} has 4,2,2,2,1,1 elements of order 12,6,4,3,2,1 respectively, whereas $C_6 \times C_2$ has 6,2,3,1 elements of order 6,3,2,1 respectively.
Then there is, up to isomorphism, one and only one direct product with the same distribution of orders of its elements as the factor group. If two or more isomorphic direct products are possible, then we choose the direct product for which the number of cyclic groups is minimal.
The next step is to find matrices corresponding to the generator of each cyclic group, of which the orders $m_1, \ldots, m_p$ are known now. The generator g_k, $1 \le k \le p$, can be found inductively as follows:

$$g_k \in K^{(i)}\ ;\ (g_k)^{m_k} \in K^{(i+1)}\ ;\ (g_k)^{r_k} \notin (g_1)^{r_1} \ldots (g_{k-1})^{r_{k-1}} K^{(i+1)} \quad (3.5)$$

for $0 \le r_j < m_j$, $\forall j \le k$. When all generators, each of them corresponding to a cyclic group in the direct product of rel. (3.4), are determined, one can write each element $m \in K^{(i)}$ in the form:

$$m = (g_1)^{r_1} \ldots (g_p)^{r_p} \times h \quad (3.6)$$

where $r_l < m_l$, $1 \leq l \leq p$, and h is a matrix in $K^{(i+1)}$.
In this way the factor group $K^{(i)}/K^{(i+1)}$ yields some generators for each $i < j$ (notice that $K^{(j)} = \{\mathbb{1}_n\}$). If $i < j-1$, then once generators according to the factor group $K^{(i+1)}/K^{(i+2)}$ have been achieved, the matrices h in eq. (3.6) can be written in the form:

$$h = (h_1)^{q_1} \dots (h_s)^{q_s} \times k$$

where $h_1, \dots, h_s$ are generators according to the factor group $K^{(i+1)}/K^{(i+2)}$ and k is a matrix in $K^{(i+2)}$.
At the end, each element g of the point group K can be written in the form:

$$g = [(a_1)^{x_1} \dots (a_d)^{x_d}]_0 \left[(b_1)^{t_1} \dots (b_e)^{t_e}\right]_1 \dots\dots [(z_1)^{y_1} \dots (z_f)^{y_f}]_{j-1} \quad (3.7)$$

where the product enclosed by $[\ ]_i$ refers to a product of generators according to the factor group $K^{(i)}/K^{(i+1)}$.
Up to now, we have achieved a set of generators and have expressed each element of the point group as word in the generators. The last step is to determine a sufficient set of defining relations satisfied by the generators. These relations are established by the demand that the word problem has a solution for this point group K. The word problem for a finitely generated group can be formulated as follows.

Definition 3.2.1. Given a finitely presented group G, generated by a set $\{g_1, \dots, g_m\}$ satisfying defining relations $\varphi_i(g_1, \dots, g_m) = \epsilon, 1 \leq i \leq r$. Then the word problem has a solution if for an arbitrary word in the generators and their inverses $W(g_1, \dots, g_m)$, the question can be answered whether $W(g_1, \dots, g_m) = \epsilon$.

In our case, where the groups considered are finite, the word problem can be formulated in the following way.

Definition 3.2.2. Given a finitely presented group G, generated by a set $\{g_1, \dots, g_m\}$ satisfying defining relations $\varphi_i(g_1, \dots, g_m) = \epsilon$, $1 \leq i \leq r$. Suppose each group element is expressed as word $W_k(g_1, \dots, g_m)$, $1 \leq k \leq |K|$, in the generators and their inverses. Then the word problem has a solution if an arbitrary word $W(g_1, \dots, g_m)$ in the generators and their inverses corresponds to one and only one word $W_k(g_1, \dots, g_m)$.

Theorem 3.2.3. Suppose for some $i < j$ that the commutator group $K^{(i+1)}$ of $K^{(i)}$ is generated by the set $\{h_1, \ldots, h_s\}$. Suppose that $K^{(i)}$ is generated by the set $\{h_1, \ldots, h_s, g_1, \ldots, g_p\}$ with $(g_k)^{m_k} \in K^{(i+1)}$, $(g_k)^{r_k} \notin K^{(i+1)}$, $\forall\, r_k < m_k$, $1 \leq k \leq p$.
Then each element of $K^{(i)}$ can be decided to belong to one and only one coset in the left coset decomposition of $K^{(i)}$ w.r.t. $K^{(i+1)}$, if the following defining relations satisfied by the generators $h_1, \ldots, h_s, g_1, \ldots, g_p$ are known:

$$\begin{array}{lcll} (g_k)^{m_k} & = & V_k(h_1, \ldots, h_s) & , \; 1 \leq k \leq p \\ g_k^{-1} g_l^{-1} g_k g_l & = & W_{kl}(h_1, \ldots, h_s) & , \; 1 \leq k, l \leq p \\ g_k^{-1} h_l g_k & = & X_{kl}(h_1, \ldots, h_s) & , \; 1 \leq k \leq p \,, \; 1 \leq l \leq s \end{array} \tag{3.8}$$

where $V_k(h_1, \ldots, h_s)$, $W_{kl}(h_1, \ldots, h_s)$, $X_{kl}(h_1, \ldots, h_s)$ are words in the generators and their inverses of the commutator group $K^{(i+1)}$.
Proof. Consider an arbitrary word $W(h_1, \ldots, h_s, g_1, \ldots, g_p)$ in $K^{(i)}$. With help of the relations (3.8), this word can be written in the form:

$$W(h_1, \ldots, h_s, g_1, \ldots, g_p) \;=\; (g_1)^{r_1} \ldots (g_p)^{r_p} W'(h_1, \ldots, h_s)$$

where $W'(h_1, \ldots, h_s)$ is a word in the generators of $K^{(i+1)}$. From the product $(g_1)^{r_1} \ldots (g_p)^{r_p}$ one can tell to which coset of $K^{(i)}$ w.r.t. $K^{(i+1)}$ the word W belongs, because all elements are expressed as words in the generators in precisely that manner (see rel. (3.7)). □

Using Theorem 3.2.3, a set of sufficient defining relations for the point group K can be constructed. For each $0 \leq i \leq j-1$, one calculates the matrices $g_k^{-1} g_l^{-1} g_k g_l$, $g_k^{-1} h_l g_k$ and $(g_k)^{m_k}$ and since each element of the point group K is expressed as word in the generators, the words V_k, W_{kl} and X_{kl} can be substituted in rel. (3.8).
Then consider an arbitrary word W in the generators. By successively using rel. (3.8), starting with $i = 0$, one can decide to which coset in the left coset decomposition of $K^{(i)}$ w.r.t. $K^{(i+1)}$ this word belongs. At the end, one has written the word W in the form (3.7), which is exactly the way in which each element of the point group was expressed. This means that the word problem has a solution according to Definition 3.2.2 and therefore we have found sufficient defining relations.

3.3 First and second method

In order to treat finite groups generally (solvable as well as nonsolvable), a different method has to be used to achieve sufficient defining relations satisfied by a generating set. The method described below is based upon the successive construction of a larger subgroup by adding a new generator and is called the first method. By carefully choosing defining relations satisfied by all coset representatives and the generators found at an earlier stage, one can solve the problem.

Suppose a point group K is given by a generating set of matrices, without knowing defining relations:

$$K = < g_1, \ldots, g_f > .$$

Consider the cyclic group $K_1 = < g_1 >$ with defining relation: $(g_1)^{m_1} = \epsilon$. Then K_1 is obviously completely determined by this defining relation. Next, consider the group:

$$K_2 = < g_1, g_2 > .$$

All elements of K_2 can be expressed as words in the generators g_1, g_2 (if K_2 is constructed, for example, by successive multiplication from the left with g_1 or g_2, then each new element can directly be expressed as word in the generators). K_2 can be decomposed into left cosets $c_i K_1$, $1 \leq i \leq L$, w.r.t. K_1, with $c_1 \equiv \epsilon$, $c_2 \equiv g_2$ and $L = \frac{|K_2|}{|K_1|}$ (throughout the paper, by a coset decomposition is meant a left coset decomposition). Now g_1, together with all coset representatives $c_2, \ldots, c_L$, are considered as generators for K_2. If $L > 2$, the representatives $c_3, \ldots, c_L$ are considered to be separate letters at the moment, although they are expressible as words in g_1, g_2. If $f \geq 3$, then $K_3 =< g_1, g_2, g_3 >$ is treated in exactly the same way, etc.
At the end, we have written each element g of the point group K in terms of g_1 and in terms of coset representatives in the form:

$$g = c(i_f)c(i_{f-1}) \ldots c(i_2)(g_1)^{r_1} \tag{3.9}$$

where $c(i_m)$ is some coset representative in the left coset decomposition of K_m w.r.t. K_{m-1} for each $2 \leq m \leq f$. Since all coset representatives are expressible as words in the generators, $c(i_m) = W(g_1, \ldots, g_m)$, $2 \leq m \leq f$,

each element g is expressed as word in the generators $g_1, \ldots, g_f$. Suppose that $|K_1| < |K|$, so $f \geq 2$ (otherwise K is cyclic and trivially defined). Consider the decomposition of K_m w.r.t. K_{m-1}, $2 \leq m \leq f$. If the number of cosets L is greater than two, then the coset representatives $c_3, \ldots, c_L$ are expressible as words in the elements $g_1, \ldots, g_m$ and their inverses. The defining relations can be achieved with use of the following theorem.

Theorem 3.3.1. Consider the point group K as being generated by $g_1, \ldots, g_f$. The word problem has a solution for K, if one knows the defining relations:

$$(g_k)^{m_k} = \epsilon \, , \; 1 \leq k \leq f \tag{3.10}$$

due to the order of the generators and the defining relations due to the left coset decomposition of K_m w.r.t. K_{m-1} for each $2 \leq m \leq f$ with coset representatives, say $c_2, \ldots, c_L$, all expressed as words $W_2(g_1, \ldots, g_m)$, ..., $W_L(g_1, \ldots, g_m)$:

$$g_k c_l = c_u V_{kl}(g_1, \ldots, g_{m-1}) \, , \; 1 \leq k \leq m \, , \; 2 \leq l \leq L \tag{3.11}$$

where the V_{kl} are words in $g_1, \ldots, g_{m-1}$ and their inverses.
Proof. Consider an arbitrary word $W(g_1, \ldots, g_f)$. It must be proved that one can decide the word W to be written as: $W(g_1, \ldots, g_f) = c(i_f)W'(g_1, \ldots, g_{f-1})$ for some coset representative $c(i_f)$ in the coset decomposition of K_f w.r.t. K_{f-1}. Suppose W does not contain the letter g_f, so $W = W(g_1, \ldots, g_{f-1})$. Then $c(i_f) = \epsilon$. Otherwise, the word W can be written as:

$$W(g_1, \ldots, g_f) = W''(g_1, \ldots, g_f) g_f W'(g_1, \ldots, g_{f-1})$$

so W' consists only of letters $g_1, \ldots, g_{f-1}$ or $g_1^{-1}, \ldots, g_{f-1}^{-1}$. Now $g_f = c_2$ in the decomposition. First, W'' is rewritten such that it contains only positive powers $(g_k)^{r_k}$, $\forall \; k \leq f$. Suppose $r_k < 0$, then replace $(g_k)^{r_k}$ by $(g_k)^{r_k + a m_k}$, with $a \in \mathbb{N}$ such that $r_k + a m_k \geq 0$ and $r_k + (a-1) m_k < 0$. This replacement is allowed because of the relations (3.10).
Then separate in W'' the first letter on the right-hand side, say g_k, $k \leq f$. Write: $W''(g_1, \ldots, g_f) = A(g_1, \ldots, g_f) g_k$. Then one of the defining relations (3.11) reads: $g_k c_2 = c_u V_{k2}(g_1, \ldots, g_{f-1})$ and the word W can be rewritten as:

$$W(g_1, \ldots, g_f) = A(g_1, \ldots, g_f) c_u V_{k2}(g_1, \ldots, g_{f-1}) W'(g_1, \ldots, g_{f-1}).$$

Notice that the number of letters in A is equal to the number of letters in W'' minus one. Then the same procedure can be applied to $A(g_1,\ldots,g_f)c_u$, etc. At the end, we have written the word W in the form:

$$W(g_1,\ldots,g_f) \;=\; c(i_f)Y(g_1,\ldots,g_{f-1}).$$

Then the whole process is repeated for the word $Y(g_1,\ldots,g_{f-1})$, ending up with Y being written in the form:

$$Y(g_1,\ldots,g_{f-1}) \;=\; c(i_{f-1})Z(g_1,\ldots,g_{f-2})$$

etc. Finally, we have written each word in the form (3.9), all coset representatives $c(i_m)$ being written as words $W_m(g_1,\ldots,g_m)$ for each $2 \leq m \leq f$. But this is exactly the way in which each element of the point group K is expressed in terms of the generators $g_1,\ldots,g_f$. Hence the word problem has a solution for K according to Definition 3.2.2 and the relations (3.10), (3.11) form a sufficient set of defining relations satisfied by the generators $g_1,\ldots,g_f$. Notice that the integers m_k in rel. (3.10) and the words V_{kl} in rel. (3.11) can be determined since one can calculate the explicit matrices and substitute the corresponding words V_{kl}, since each element of K_{m-1} is expressed in terms of $g_1,\ldots,g_{m-1}$ for all $2 \leq m \leq f$. □

One could also follow the method used in § 3.2, until a subgroup $K^{(j)} = K^{(j+1)}$ is reached and, if $K^{(j)} \neq \{\mathbf{1}_n\}$ (i.e. the point group is nonsolvable), then apply the first method to this subgroup. This method is denoted as the second method. The second method for solvable groups coincides with the method already described in § 3.2. For nonsolvable point groups, the approach is as follows.
Since the subgroup $K^{(j)}$ is given by all elements of $K^{(j)}$ without knowing a set of generators, the problem is how to choose the generators for this subgroup. If one takes as successive generators elements of maximal order, then there is the best change to have powers of the last generator added, as coset representatives. If the defining relations according to rel. (3.11) are determined, we expect more relations to be trivially eliminated if more coset representatives are powers of the last generator added.
If a point group is given by all point group elements, without giving a set of generators, then the argument mentioned above can also be applied in order to select the generators.

After determining the lower central series $K^{(0)} \supset \ldots \supset K^{(j)}$, each element $g \in K$ can be written as:

$$g = [(a_1)^{x_1} \ldots (a_d)^{x_d}]_0 \ldots\ldots [(z_1)^{y_1} \ldots (z_r)^{y_r}]_{j-1} \times h \qquad (3.12)$$

where h is a matrix in $K^{(j)}$. Once the first method has been applied to $K^{(j)}$, each h in rel. (3.12) can be expressed as a word in the generators of $K^{(j)}$. Defining relations satisfied by the generating set (the union of the generating sets achieved at each step of the lower central series, and the generating set of $K^{(j)}$) can be achieved with help of Theorem 3.2.3, 3.3.1. In Theorem 3.2.3, the generators h_l include the generators found for $K^{(j)}$.

3.4 Third and fourth method

The third method, to be described below, can be denoted as a depth-first search method (Aho *et al.* 1983 p. 216). Consider a point group $K = < g_1, \ldots, g_f >$. Each generator is given a priority: the i-th generator has i-th priority for all i, $1 \leq i \leq f$. The first element in the list is ϵ and at this point, this element has not been multiplied with any generator yet. Then the procedure is as follows.
Search for the last matrix in the list for which there is a generator with which this matrix has not yet been multiplied. If there are more such generators for a matrix, then choose the generator of maximal priority. If there is such a matrix, say m, expressed as $W(g_1, \ldots, g_f)$, and such a generator, say g_k, then there are two types of results r:
1. r is not in the list yet. Then the corresponding word is called unreferenced and is of the form: $g_k W = g_k W$. The new matrix is added to the list and the corresponding word $g_k W$ is stored;
2. r is already in the list. Then the corresponding word is called a reference and is of the form $g_k W = W'$, where W' is the word corresponding to the resulting matrix.
If all matrices in the list have been multiplied with all generators, then the procedure stops, otherwise the procedure is repeated. Then the defining relations can be constructed with use of the following theorem.

Theorem 3.4.1. A sufficient set of defining relations for the point group

$K = < g_1, \ldots, g_f >$ is formed by

$$(g_k)^{m_k} = \epsilon \,,\; 1 \leq k \leq f, \tag{3.13}$$

and all references

$$g_k W(g_1, \ldots, g_f) = W'(g_1, \ldots, g_f). \tag{3.14}$$

Proof. First it is proved that a sufficient set of defining relations is formed by the relations corresponding to all unreferenced multiplications and all references.
Suppose one knows the relations (3.13) and all referenced and unreferenced words. Consider an arbitrary word $W(g_1, \ldots, g_f)$. With help of rel. (3.13), all powers $(g_k)^{r_k}$ can be considered to be positive. Separate in W the letter on the right, say g_k: $W(g_1, \ldots, g_f) = W'(g_1, \ldots, g_f)g_k$. The matrix g_k is the result of the multiplication $g_k \times \epsilon$, where ϵ corresponds to the identity matrix. This multiplication can either be unreferenced (then the resulting matrix is expressed as g_k) or a reference (then the resulting matrix is expressed as some other word in the generators). In both cases the resulting expression is denoted as $X(g_1, \ldots, g_f)$. So $W = W'X$. Separate in W' the letter on the right, say g_i: $W'(g_1, \ldots, g_f) = W''(g_1, \ldots, g_f)g_i$. Then W can be written as: $W = W''g_iX$. The multiplication $g_i \times X$ yields a resulting expression $g_iX = Y$, which is known, since all referenced and all unreferenced words are known. So $W = W''Y$. The process is set forth by writing W'' as: $W'' = W'''g_p$. Again the resulting word $g_pY = Z$ is known, and $W = W'''Z$, etc. At the end, the word W is rewritten in the way in which one and only matrix was expressed. Hence the word problem has been solved according to Definition 3.2.2 and the supposed set of words forms a sufficient set of defining relations. Next, all unreferenced words can be trivially eliminated, since these words are of the form $g_kW = g_kW \Rightarrow \epsilon = \epsilon$.
□

The fourth method is related to the third method. It is a breadth-first search method (Aho *et al.* 1983 p. 242). Starting with the set $A_0 = \{g_1, \ldots, g_f\}$, the set A_{i+1} is defined inductively as:

$$A_{i+1} = A_i \cup \{g_k A_i |\; 1 \leq k \leq f\}.$$

We can proceed as in the third method. Two types of words can be distinguished:

1. words corresponding to a multiplication $g_k \times a$ yielding an element not yet in the list; these words are again called unreferenced;
2. words corresponding to a multiplication yielding an element, already in the list. Such a word is called a reference.

As for the third method, a sufficient set of defining relations is formed by the relations (3.13) and by all references (3.14).

3.5 Reduction of number of defining relations

In the previous sections, four methods have been described to determine a set of generators and a sufficient set of defining relations satisfied by these generators. In principle the problem is solved, but most of the defining relations probably are redundant.

Before turning to the reduction problem, notice that it is useful to order the generators such that the i-th generator does not have a smaller order than the $(i+1)$-th generator (except for the lower central series part of the second method, because then we are not free to choose the generators). For the first two generators in the first method, this follows from Theorem 3.3.1. The tests showed that for all methods (provided we are free to choose the generators), the generators have to be ordered as suggested, if we want to achieve the smallest number of defining relations. For the depth-first search method, an additional advantage is that the storage of the words is more efficient. One could store a word by placing all letters behind each other. It is more efficient to store the word as a product of powers of letters. If the generators are ordered as suggested, then this product has the minimum length.

The problem is to have a systematic procedure to decrease the number of relations. The procedure is the following.

First a standard minimization procedure is applied to each relation in order to minimize the number of its letters. The standard minimization consists of two components.

1. Let m_k be the order of the generator g_k. Suppose $(g_k)^{r_k}$ appears in an expression. If $|r_k - m_k| < |r_k|$, then replace $(g_k)^{r_k}$ by $(g_k)^{r_k - m_k}$. If $|r_k + m_k| < |r_k|$, then replace $(g_k)^{r_k}$ by $(g_k)^{r_k + m_k}$.

The only exception is the case that the defining relation is of the form: $(g_k)^{m_k} = \epsilon$, since the relation may not be used to eliminate itself.

2. If a defining relation contains a $(g_k)^{r_k}$ on the left and a $(g_k)^{t_k}$ on the right, then multiply the relation from the right with $(g_k)^{-t_k}$ and from the left with $(g_k)^{t_k}$.
If the standard minimization changes the word, then the procedure is applied again, etc., until the procedure does not alter the word.
Now search for the relation with the maximal number of letters. Suppose this number is N. Since each defining relation is of the form (3.1), one can insert another relation between two successive letters in the relation in question, and see if the resulting number of letters after the standard minimization procedure is applied, can be decreased. Consider such a relation to be inserted, with number of letters M. What are the possibilities for this insertion?
i. Insertion before the 1-th, ..., N-th letter of the relation in question: N possibilities;
ii. The relation inserted, can be permuted cyclically: M possibilities;
iii. The relation inserted, can be inverted: (combined with *ii*) M possibilities.
Hence $2MN$ combinations are possible.
Now use the following procedure: insert first all relations with number of letters equal to N into the relation in question, using all possibilities mentioned above, then insert all relations with number of letters smaller than the relation in question. (First, it seems practical to insert all relations for which the number of letters is less than or equal to, say, $2N$. It turned out for all point groups tested, that this option causes the same number of resulting relations as the other option and that it costs more computer time. Therefore this option is not incorporated in the algorithm. Second, the reason for first inserting all relations with the same number of letters as the relation in question is, that if two relations are equal up to inversion and/or cyclic permutation, then the relation in question is eliminated immediately). If there is no way to decrease the number of letters, then this defining relation is a permanent defining relation and is from now on only used to be inserted in other relations which are still to be examined. If for some combination the number of letters can be decreased, then the old (longer) word is replaced by the new (shorter) word, and again the relation with the maximal number of letters is sought.
Of course, one can use a modified method: once the number of letters of

a relation has been decreased, one replaces the old word by the new word and then tries to decrease the number of letters of the new word. So once a relation is started to be treated, this relation is eliminated or is decided to be permanent, before turning to another relation. It turned out for most point groups tested, that this procedure yields the same number of defining relations and costs the same computer time. For a few point groups, the alternative procedure costs less computer time, but gives a greater number of resulting defining relations. This modified method is not applied.
In the first and second method, defining relations were achieved in steps. The procedure described above can best be applied to the set of defining relations achieved at the last step. The defining relations achieved at previous steps are only used to be inserted.

3.6 Algorithm scheme

For all four methods, algorithms have been developed. If the point group is given by a set of generators, then these generators are supposed to be put in the right order. If the point group is given by all point group elements, then the generators are chosen to have maximal order. Denote the ordered or achieved set of generators as $\{g_1, \ldots, g_f\}$. The algorithm scheme for the various methods is as follows.

A. First method.

- 1. Determine all matrices contained in $K_1 = < g_1 >$ and put them in a list. The first defining relation is of the form: $(g_1)^{m_1} = \epsilon$.

- 2. Calculate the order m_2 of the second generator g_2. The second defining relation reads: $(g_2)^{m_2} = \epsilon$. Now the subgroup $K_2 =< g_1, g_2 >$ is determined as follows.
  First check for each power $(g_2)^{r_2}$, $r_2 < m_2$, whether the corresponding matrix belongs to the list. If not, then that power is chosen to be the next coset representative of K_2 w.r.t. K_1. All matrices in the coset $(g_2)^{r_2} K_1$ are calculated and are added to the list.

- 3. Then all other elements of K_2 are determined by successive multiplication from the left with g_1, g_2 (the breadth-first search procedure of § 3.4). Once a new element has been found, this element is a new

coset representative and all matrices in that coset are calculated. For each new element in the list, its expression in terms of the generators g_1 and g_2 is stored.

- 4. Now the defining relations can be formulated. Let L be the number of cosets of K_2 w.r.t. K_1. All matrices $g_1 c_l = c_u V_{1l}(g_1, g_2)$, $2 \leq l \leq L$, are calculated, and the words $X_l(g_1, g_2)$ respectively $Y_u(g_1, g_2)$ corresponding to c_l and c_u, are substituted to give the expression $g_1 X_l(g_1, g_2) = Y_u(g_1, g_2) V_{1l}(g_1, g_2)$.

- 5. The number of defining relations achieved in step A5 is reduced by the procedure of which the algorithmic steps were already outlined in § 3.5.

- 6. If $K_1 \subset K$, then turn to step A2 with g_2 replaced by g_3, etc.

B. Second method.

- 1. All matrices in the commutator group $K^{(1)}$ are calculated.

- 2. If $K^{(1)} \subset K^{(0)} \equiv K$, then coset representatives of $K^{(0)}$ w.r.t. $K^{(1)}$ are established as follows. Start with a matrix $k_2 \notin K^{(1)}$ and calculate all matrices in the coset $k_2 K^{(1)}$. If the number of cosets is greater than two, then search for a matrix $k_3 \notin K^{(1)}$, $k_3 \notin k_2 K^{(1)}$ and calculate all matrices in the coset $k_3 K^{(1)}$, etc.

- 3. Now we need to know the order of each element of the factor group $K^{(0)}/K^{(1)}$. Hence the smallest integer p_i must be found such that $(k_i)^{p_i} \in K^{(1)}$, $2 \leq i \leq L$ (L is the order of the factor group).

- 4. Find the, up to isomorphism unique, direct product of cyclic groups having the same order and with the same distribution of orders for its elements as the factor group.

- 5. The generators corresponding to each cyclic group in this direct product, can be found with help of rel. (3.23).

- 6. Each element of K can be expressed in terms of a product of powers of these generators times some matrix $h \in K^{(1)}$.

- 7. The steps B2-B6 are repeated with $K^{(i)}$ replaced by $K^{(i+1)}$ for each $0 \leq i \leq j-1$, with $K^{(j)} = K^{(j+1)}$. For step B6 this means that the matrices h are expressed in terms of powers of the new generators times some new matrix $h' \in K^{(i+1)}$.

- 8. If $K^{(j)} \neq \mathbf{1}_n$, then apply algorithm A to the point group $K^{(j)}$ with one modification. Since $K^{(j)}$ is given by its elements, successive generators are chosen such that they have maximal order. As in algorithm A, a set of defining relations satisfied by the generators of $K^{(j)}$ can be established and its number can be reduced with use of the algorithmic procedure of § 3.5.

- 9. Determine the defining relations (3.8) satisfied by the generators, found from the decomposition of $K^{(i)}$ w.r.t. $K^{(i+1)}$ for each $i = j-1$, $\ldots, 1$. Since all words corresponding to the words g_k, g_l, h_l in rel. (3.8) are known, these relations can be established. Notice that, if K is unsolvable, then the h_l should include also the achieved generators of $K^{(j)}$ found in step B8.

- 10. The number of defining relations is reduced for each $i = j-1, \ldots, 1$ with use of the procedure of § 3.5. For each such i: after turning to this value of i, the number is reduced only of the new defining relations. The defining relations already established when the reduction procedure for this i was started, together with the defining relations achieved in step B8, are permanent (and serve only to reduce the number of new relations).

Since the third and fourth method were described in the form of an algorithmic procedure in § 3.4 already, they are not treated again in this section.

3.7 Examples and Results

A computer program has been written in FORTRAN77, based upon the four methods described in § 3.3, 3.4 and the reduction procedure of § 3.5. The program ran on a SUN4-computer. The first point group is meant as an example for the first two methods. A subgroup of this point group serves as example for the third and the fourth method. The other point groups are discussed less extensively.

The first point group is a 3-dimensional full cubic point group $K \simeq O \times C_2$, which is solvable: $K = < g_1, g_2, g_3 >$

$$= < \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} > . \qquad (3.15)$$

- First method.

$K_1 = < g_1 >$. The defining relation reads: $\varphi_1 = g_1^4 = \epsilon$.
$K_2 =< g_1, g_2 >$. It turns out that $|K_2| = 24$. Since $g_2^3 = \epsilon$, the second defining relation reads: $\varphi_2 = g_2^3 = \epsilon$. The matrices contained in K_2 are expressed in terms of g_1, g_2 as follows:

$$\begin{array}{lllllll}
k_1 & = & \epsilon & & k_{13} & = & g_1 g_2 \\
k_2 & = & g_1 & & k_{14} & = & g_1 g_2 g_1 \\
k_3 & = & g_1^2 & & k_{15} & = & g_1 g_2 g_1^2 \\
k_4 & = & g_1^3 & & k_{16} & = & g_1 g_2 g_1^3 \\
k_5 & = & g_2 & & k_{17} & = & g_2 g_1 g_2 \\
k_6 & = & g_2 g_1 & & k_{18} & = & g_2 g_1 g_2 g_1 \\
k_7 & = & g_2 g_1^2 & & k_{19} & = & g_2 g_1 g_2 g_1^2 \\
k_8 & = & g_2 g_1^3 & & k_{20} & = & g_2 g_1 g_2 g_1^3 \\
k_9 & = & g_2^2 & & k_{21} & = & g_2^2 g_1 g_2 \\
k_{10} & = & g_2^2 g_1 & & k_{22} & = & g_2^2 g_1 g_2 g_1 \\
k_{11} & = & g_2^2 g_1^2 & & k_{23} & = & g_2^2 g_1 g_2 g_1^2 \\
k_{12} & = & g_2^2 g_1^3 & & k_{24} & = & g_2^2 g_1 g_2 g_1^3
\end{array}$$

with coset representatives:

$$\begin{array}{lllllllll}
c_1 & = & k_1 & = & \epsilon & c_4 & = & k_{13} & = & g_1 g_2 \\
c_2 & = & k_5 & = & g_2 & c_5 & = & k_{17} & = & g_2 g_1 g_2 \\
c_3 & = & k_9 & = & g_2^2 & c_6 & = & k_{21} & = & g_2^2 g_1 g_2
\end{array}$$

The defining relations $\varphi_i = \epsilon$ of the form (3.11) are:

i	$g_k c_l$	$=$	k_m	$\Rightarrow$	φ_i	$=$	ϵ
3	g_2c_2	$=$	k_9	$\Rightarrow$	ϵ	$=$	ϵ
4	g_2c_3	$=$	k_1	$\Rightarrow$	ϵ	$=$	ϵ
5	g_2c_4	$=$	k_{17}	$\Rightarrow$	ϵ	$=$	ϵ
6	g_2c_5	$=$	k_{21}	$\Rightarrow$	ϵ	$=$	ϵ
7	g_2c_6	$=$	k_{13}	$\Rightarrow$	ϵ	$=$	ϵ
8	g_1c_2	$=$	k_{13}	$\Rightarrow$	ϵ	$=$	ϵ
9	g_1c_3	$=$	k_8	$\Rightarrow$	$g_1g_2^{-1}g_1g_2^{-1}$	$=$	ϵ
10	g_1c_4	$=$	k_{22}	$\Rightarrow$	$g_1^2g_2g_1^{-1}g_2^{-1}g_1^{-1}g_2$	$=$	ϵ
11	g_1c_5	$=$	k_{19}	$\Rightarrow$	$g_1g_2g_1g_2g_1g_2^{-1}g_1^{-1}g_2^{-1}$	$=$	ϵ
12	g_1c_6	$=$	k_9	$\Rightarrow$	$g_1g_2^{-1}g_1g_2^{-1}$	$=$	ϵ

The relations in the column, headed by "$\varphi_i = \epsilon$", are achieved using the standard minimization procedure. Of all 10 relations (3.11), 6 relations are of the form: $\epsilon = \epsilon$, and are therefore eliminated. Hence the total number of defining relations to start with, is six. The defining relation with the maximal number of letters is $\varphi_5 = g_1g_2g_1g_2g_1g_2^{-1}g_1^{-1}g_2^{-1} = \epsilon$. Now consider the relation $\varphi_3 = g_1g_2^{-1}g_1g_2^{-1} = \epsilon$. When the inverse of φ_3 is placed before the first letter of φ_5, the result is:

$$\varphi_5 = \epsilon \rightarrow g_2g_1^{-1}g_2g_1^{-1} \times g_1g_2g_1g_2g_1g_2^{-1}g_1^{-1}g_2^{-1} \;=\; g_1^{-2}g_2^{-1}g_1g_2g_1g_2^{-1}$$

with use of the standard minimization procedure. Hence the number of letters has been decreased from 8 to 7 and φ_5 is written as:
$\varphi_5 = g_1^{-2}g_2^{-1}g_1g_2g_1g_2^{-1}$. The relation with the maximal number of letters is now φ_4. Consider the cyclic permutation $g_2^{-1}g_1g_2g_1g_2^{-1}g_1^{-2}$ of φ_5. Now put this word in front of φ_4. The result is:

$$\varphi_4 = \epsilon \rightarrow g_2^{-1}g_1g_2g_1g_2^{-1}g_1^{-2} \times g_1^2g_2g_1^{-1}g_2^{-1}g_1^{-1}g_2 \;=\; \epsilon.$$

Hence $\varphi_4 = \epsilon$ can be eliminated. The relation with the maximal number of letters is now $\varphi_5 = g_1^{-2}g_2^{-1}g_1g_2g_1g_2^{-1}$. Consider the inverse of φ_3: $g_2g_1^{-1}g_2g_1^{-1}$. Placing this word before φ_5 yields:

$$\varphi_5 = \epsilon \rightarrow g_2g_1^{-1}g_2g_1^{-1} \times g_1^{-2}g_2^{-1}g_1g_2g_1g_2^{-1} \;=\; g_2^{-1}g_1g_2^{-1}g_1.$$

After treating all defining relations as mentioned above, the remaining defining relations are:

$$\begin{aligned} \varphi_2 &= g_2^3 &&= \epsilon \\ \varphi_3 &= g_1 g_2^{-1} g_1 g_2^{-1} &&= \epsilon \end{aligned}$$

which are added to the relation $\varphi_1 = g_1^4 = \epsilon$, which was already permanent when K_2 was constructed.
$K_3 = < g_1, g_2, g_3 >$. The first additional defining relation reads: $\varphi_4 = g_3^2 = \epsilon$. Since $g_3^2 = \epsilon$, there is only one power of g_3 to serve as coset representative: $c_2 = g_3$. All matrices in the coset $c_2 K_2$ are determined and the corresponding words are stored. Multiplication from the left with g_1, g_2, g_3 yields no extra elements, as expected: $|K_3| = 48$, since $K_3 = K$.
One defining relation of the form (3.11), $g_3 c_2 = c_m V_{32}(g_1, g_2)$, is eliminated since $g_3^2 = \epsilon$. The other two relations read:

$$\begin{aligned} \varphi_5 &= g_1 g_3 g_1^{-1} g_3^{-1} &&= \epsilon \\ \varphi_6 &= g_2 g_3 g_2^{-1} g_3^{-1} &&= \epsilon \end{aligned}$$

None of the added relations can be eliminated.
The outcome of the calculation is, that K is generated by the set $\{g_1, g_2, g_3\}$ given in eq. (3.15), satisfying the defining relations:

$$\begin{aligned} \varphi_1 &= g_1^4 &&= \epsilon \\ \varphi_2 &= g_2^3 &&= \epsilon \\ \varphi_3 &= g_1 g_2^{-1} g_1 g_2^{-1} &&= \epsilon \\ \varphi_4 &= g_3^2 &&= \epsilon \\ \varphi_5 &= g_1 g_3 g_1^{-1} g_3^{-1} &&= \epsilon \\ \varphi_6 &= g_2 g_3 g_2^{-1} g_3^{-1} &&= \epsilon \end{aligned} \tag{3.16}$$

Hence of the 9 non-trivial defining relations, 3 relations can be eliminated.

- Second method.

All point group matrices are determined: $|K| = 48$. The commutator group $K^{(1)}$ has order 12. There are 4 left coset representatives to be determined. One of them is $\mathbb{1}_3$. The other three representatives are:

$$c_2 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, c_3 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, c_4 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \tag{3.17}$$

The distribution of orders of the factor group elements is determined. Since $c_2^2 \in K^{(1)}$, $c_3^2 \in K^{(1)}$, $c_4^2 \in K^{(1)}$, the factor group $K/K^{(1)}$ is isomorphic to $C_2 \times C_2$. The generators achieved are $d_1 = c_2$ and $d_2 = c_3$.
Each element of K is expressed as $(d_1)^{r_1}(d_2)^{r_2}h$, where h is a matrix in $K^{(1)}$. The procedure is repeated, until a subgroup is reached which has itself as commutator group. It turns out that $|K^{(2)}| = 4$, so the factor group $K^{(1)}/K^{(2)}$ can only be isomorphic to C_3. Hence we get one extra generator d_3. The commutator group $K^{(3)}$ turns out to consist of the identity matrix. The factor group $K^{(2)}/K^{(3)}$ is isomorphic to $C_2 \times C_2$. Therefore two extra generators, d_4 and d_5, are achieved. Since K is solvable, the first method does not have to be applied now. The defining relations (3.8) are constructed in the following sequence:

$$\begin{array}{llllllll}
i & \varphi_i & = & \epsilon & i & \varphi_i & = & \epsilon \\
1 & d_4^2 & = & \epsilon & 9 & d_1 d_2 d_1^{-1} d_2^{-1} & = & \epsilon \\
2 & d_5^2 & = & \epsilon & 10 & d_1^{-1} d_3 d_1 & = & d_3^{-1} d_4 \\
3 & d_4 d_5 d_4^{-1} d_5^{-1} & = & \epsilon & 11 & d_1^{-1} d_4 d_1 & = & d_5 \\
4 & d_3^3 & = & \epsilon & 12 & d_1^{-1} d_5 d_1 & = & d_4 \\
5 & d_3^{-1} d_4 d_3 & = & d_4 d_5 & 13 & d_2^{-1} d_3 d_2 & = & d_3 \\
6 & d_3^{-1} d_5 d_3 & = & d_4 & 14 & d_2^{-1} d_4 d_2 & = & d_4 \\
7 & d_1^2 & = & d_4 d_5 & 15 & d_2^{-1} d_5 d_2 & = & d_5 \\
8 & d_2^2 & = & \epsilon & & & &
\end{array} \tag{3.18}$$

satisfied by the generators d_1, d_2 (the matrices c_2 and c_3 of rel. (3.17)) and:

$$d_3 = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}, d_4 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, d_5 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \tag{3.19}$$

The 15 defining relations given in eq. (3.18) can not be decreased in number.

The second point group, meant as an example of the third and fourth method, is a cubic point group $K = < g_1, g_2 > \subset Gl(3, \mathbf{Z})$, with $K \simeq O$, and g_1, g_2 are defined in eq. (3.15).

- Third method.

$K =< g_1, g_2 >$. The generators g_1 respectively g_2 have first and second priority. Since $|K| = 24$, there are 23 multiplications yielding new elements.

The 24 elements of K are expressed as:

$$
\begin{array}{lcllcl}
k_1 & = & \epsilon & k_{13} & = & g_2g_1g_2g_1^2g_2g_1^3 \\
k_2 & = & g_1 & k_{14} & = & g_1g_2g_1g_2g_1^2g_2g_1^3 \\
k_3 & = & g_1^2 & k_{15} & = & g_1^2g_2g_1g_2g_1^2g_2g_1^3 \\
k_4 & = & g_1^3 & k_{16} & = & g_1^3g_2g_1g_2g_1^2g_2g_1^3 \\
k_5 & = & g_2g_1^3 & k_{17} & = & g_2g_1g_2g_1g_2g_1^2g_2g_1^3 \\
k_6 & = & g_1g_2g_1^3 & k_{18} & = & g_1g_2g_1g_2g_1g_2g_1^2g_2g_1^3 \\
k_7 & = & g_1^2g_2g_1^3 & k_{19} & = & g_1^2g_2g_1g_2g_1g_2g_1^2g_2g_1^3 \\
k_8 & = & g_1^3g_2g_1^3 & k_{20} & = & g_1^3g_2g_1g_2g_1g_2g_1^2g_2g_1^3 \\
k_9 & = & g_2g_1^2g_2g_1^3 & k_{21} & = & g_2^2g_1g_2g_1g_2g_1^2g_2g_1^3 \\
k_{10} & = & g_1g_2g_1^2g_2g_1^3 & k_{22} & = & g_1g_2^2g_1g_2g_1g_2g_1^2g_2g_1^3 \\
k_{11} & = & g_1^2g_2g_1^2g_2g_1^3 & k_{23} & = & g_1^2g_2^2g_1g_2g_1g_2g_1^2g_2g_1^3 \\
k_{12} & = & g_1^3g_2g_1^2g_2g_1^3 & k_{24} & = & g_1^3g_2^2g_1g_2g_1g_2g_1^2g_2g_1^3
\end{array}
$$

The defining relations of which the number has to be reduced are formed by the first two relations, expressing the orders of the generators: $\varphi_1 = g_1^4 = \epsilon$, $\varphi_2 = g_2^3 = \epsilon$, and the referenced words:

$$
\begin{array}{lllcll}
i & g_k k_l & = & k_m & \Rightarrow & \varphi_i & = \epsilon \\
3 & g_1k_4 & = & k_1 & \Rightarrow & \epsilon & = \epsilon \\
4 & g_1k_8 & = & k_5 & \Rightarrow & \epsilon & = \epsilon \\
5 & g_2k_8 & = & k_1 & \Rightarrow & g_2g_1^{-1}g_2g_1^{-1} & = \epsilon \\
6 & g_1k_{12} & = & k_9 & \Rightarrow & \epsilon & = \epsilon \\
7 & g_2k_{12} & = & k_8 & \Rightarrow & g_2g_1^{-1}g_2g_1^{-1} & = \epsilon \\
8 & g_2k_{11} & = & k_2 & \Rightarrow & (g_2g_1^2)^3 & = \epsilon \\
9 & g_1k_{16} & = & k_{13} & \Rightarrow & \epsilon & = \epsilon \\
10 & g_2k_{16} & = & k_{11} & \Rightarrow & g_2g_1^{-1}g_2g_1^{-1} & = \epsilon \\
11 & g_2k_{15} & = & k_3 & \Rightarrow & (g_2g_1^2g_2g_1)^2 & = \epsilon \\
12 & g_1k_{20} & = & k_{17} & \Rightarrow & \epsilon & = \epsilon
\end{array}
$$

etc. Of all 27 defining relations, 7 relations can be rewritten in the form $\epsilon = \epsilon$ with help of the standard minimization procedure, so the number of defining relations to be reduced, is 20.
With use of the reduction procedure (for an extensive application, see the

first example) the number of defining relations can be reduced to three:

$$\begin{array}{lllll} \varphi_1 & = & g_1^4 & = & \epsilon \\ \varphi_2 & = & g_2^3 & = & \epsilon \\ \varphi_3 & = & g_2 g_1^{-1} g_2 g_1^{-1} & = & \epsilon \end{array} \tag{3.20}$$

- Fourth method.

First the two generators are put in a list. There are 21 multiplications yielding a matrix which was not yet in the list. The 24 elements are expressed in terms of g_1, g_2 as:

$$\begin{array}{llllll} k_1 & = & \epsilon & k_9 & = & g_1^2 g_2 \\ k_2 & = & g_1 & k_{10} & = & g_1 g_2 g_1 \\ k_3 & = & g_2 & k_{11} & = & g_1 g_2^2 \\ k_4 & = & g_1^2 & k_{12} & = & g_2 g_1^2 \\ k_5 & = & g_1 g_2 & k_{13} & = & g_2 g_1 g_2 \\ k_6 & = & g_2 g_1 & k_{14} & = & g_2^2 g_1 \\ k_7 & = & g_2^2 & k_{15} & = & g_1^2 g_2 g_1 \\ k_8 & = & g_1^3 & k_{16} & = & g_1^2 g_2^2 \end{array} \qquad \begin{array}{llll} k_{17} & = & g_1 g_2 g_1^2 \\ k_{18} & = & g_1 g_2 g_1 g_2 \\ k_{19} & = & g_2 g_1 g_2 g_1 \\ k_{20} & = & g_2 g_1 g_2^2 \\ k_{21} & = & g_2^2 g_1^2 \\ k_{22} & = & g_2^2 g_1 g_2 \\ k_{23} & = & g_1^2 g_2 g_1^2 \\ k_{24} & = & g_1^2 g_2 g_1 g_2 \end{array}$$

Again the first two defining relations express the orders of g_1, g_2. The other defining relations are achieved by means of the references:

$$\begin{array}{llllll} i & g_k k_l & = & k_m & \Rightarrow & \varphi_i & = \epsilon \\ 3 & g_2 k_7 & = & k_1 & \Rightarrow & \epsilon & = \epsilon \\ 4 & g_1 k_8 & = & k_1 & \Rightarrow & \epsilon & = \epsilon \\ 5 & g_1 k_9 & = & k_{14} & \Rightarrow & g_1^{-1} g_2 g_1^{-1} g_2 & = \epsilon \\ 6 & g_1 k_{14} & = & k_3 & \Rightarrow & g_1 g_2^{-1} g_1 g_2^{-1} & = \epsilon \\ 7 & g_2 k_8 & = & k_{11} & \Rightarrow & g_2 g_1^{-1} g_2 g_1^{-1} & = \epsilon \\ 8 & g_2 k_9 & = & k_{10} & \Rightarrow & g_2 g_1^2 g_2 g_1^{-1} g_2^{-1} g_1^{-1} & = \epsilon \\ 9 & g_2 k_{14} & = & k_2 & \Rightarrow & \epsilon & = \epsilon \\ 10 & g_1 k_{15} & = & k_{21} & \Rightarrow & g_1^{-1} g_2 g_1^{-1} g_2 & = \epsilon \\ 11 & g_1 k_{16} & = & k_{22} & \Rightarrow & g_1^{-1} g_2 g_1^{-1} g_2 & = \epsilon \\ 12 & g_1 k_{19} & = & k_{13} & \Rightarrow & g_1 g_2 g_1 g_2 g_1 g_2^{-1} g_1^{-1} g_2^{-1} & = \epsilon \end{array}$$

etc. Of all 27 defining relations, 5 relations can be eliminated immediately with use of the standard minimization procedure. Hence the number of

defining relations to be reduced is 22. There are 3 resulting defining relations

$$\begin{array}{lcll} \varphi_1 & = & g_1^4 & = \epsilon \\ \varphi_2 & = & g_2^3 & = \epsilon \\ \varphi_3 & = & g_1 g_2^{-1} g_1 g_2^{-1} & = \epsilon \end{array} \tag{3.21}$$

The third point group has order 120:

$$K = < \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} > . \tag{3.22}$$

For the first method, the resulting defining relations are:

$$\begin{array}{lcll} \varphi_1 & = & g_1^6 & = \epsilon \\ \varphi_2 & = & g_2^2 & = \epsilon \\ \varphi_3 & = & (g_1 g_2)^6 & = \epsilon \\ \varphi_4 & = & g_2 g_1^{-2} g_2 g_1 g_2 g_1^{-1} g_2^{-1} g_1^{-1} g_2^{-1} g_1 & = \epsilon \end{array} \tag{3.23}$$

The point group K is isomorphic to S_5, the permutation group of 5 elements. For example, consider the following integral representation L of S_5:

$$L = < \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} > . \tag{3.24}$$

The first method applied to L yields exactly the defining relations (3.23).

The fourth point group to be considered, is a 4-dimensional face-centred hypercubic point group, of order 1152:

$$K = < \begin{bmatrix} -1 & 0 & 0 & 1 \\ 0 & 0 & -1 & 1 \\ -1 & -1 & -1 & 1 \\ -1 & -1 & -1 & 2 \end{bmatrix}, \begin{bmatrix} -1 & -1 & -1 & 2 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & -1 & 0 & 1 \end{bmatrix}, \tag{3.25}$$

$$\left[\begin{matrix} 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & -1 \\ 1 & 1 & 1 & -2 \end{matrix}\right], \left[\begin{matrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & -1 \end{matrix}\right], \left[\begin{matrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{matrix}\right] > .$$

According to the first method, K is generated by 5 generators satisfying the following 21 defining relations $\varphi_i = \epsilon$:

$$\begin{aligned}
\varphi_1 &= g_1^{12} & \varphi_{12} &= g_2 g_1 g_3^{-1} g_1^{-1} g_2^{-1} g_1 g_3 g_1^{-1} \\
\varphi_2 &= g_2^4 & \varphi_{13} &= g_4^2 \\
\varphi_3 &= g_2^2 g_1{}^{-6} & \varphi_{14} &= g_1 g_4 g_1^2 g_2 g_3 g_1^{-1} g_3^{-1} g_4^{-1} \\
\varphi_4 &= g_2^2 g_1 g_2^{-2} g_1^{-1} & \varphi_{15} &= g_2 g_4 g_2 g_4^{-1} \\
\varphi_5 &= g_1^{-2} g_2 g_1 g_2 g_1 g_2 & \varphi_{16} &= g_3 g_4 g_3 g_4^{-1} \\
\varphi_6 &= g_3^3 & \varphi_{17} &= g_5^2 \\
\varphi_7 &= g_1 g_3 g_1 g_3^{-1} g_2^2 g_1^{-1} g_3 g_1^{-1} g_3^{-1} & \varphi_{18} &= g_1 g_5 g_1 g_2^{-1} g_3^{-1} g_1^{-1} g_5^{-1} \\
\varphi_8 &= (g_1 g_3)^3 & \varphi_{19} &= g_2 g_5 g_1 g_3 g_1^{-1} g_3^{-1} g_5^{-1} \\
\varphi_9 &= g_1^2 g_3^{-1} g_1^{-2} g_3 & \varphi_{20} &= g_3 g_5 g_1 g_2 g_5^{-1} \\
\varphi_{10} &= g_2 g_3^{-1} g_2^{-1} g_3 & \varphi_{21} &= g_4 g_5 g_4^{-1} g_5^{-1} \\
\varphi_{11} &= g_1^{-1} g_2 g_1^2 g_2 g_1^{-1} g_2^{-1}
\end{aligned} \tag{3.26}$$

Brown *et al.* (1978) presented this point group by 28 defining relations satisfied by 7 generators.

The fifth point group is a 6-dimensional representation of the icosahedral group I, of order 60, which is isomorphic to the alternating group A_5:

$$K = < \left[\begin{matrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{matrix}\right], \left[\begin{matrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{matrix}\right] > . \tag{3.27}$$

The following defining relations are the result of the first method:

$$\begin{aligned}
\varphi_1 &= g_1^5 &&= \epsilon \\
\varphi_2 &= g_2^3 &&= \epsilon \\
\varphi_3 &= g_1 g_2 g_1 g_2 &&= \epsilon
\end{aligned} \tag{3.28}$$

(a)

no	*method 1*				*method 2*			
	f	*Rs*	*Rr*	*time*	*f*	*Rs*	*Rr*	*time*
1	3	9	6	0.2	5	15	15	1.7
2	2	6	3	0 2	4	10	10	0.7
3	2	14	4	1.4	3	16	8	168.7
4	2	26	21	14.4	9	39	39	5756.5
5	2	11	3	0.9	2	13	5	216.9
6	2	279	12	1309.0	4	47	22	75854.4

(b)

no	*method 3*				*method 4*			
	f	*Rs*	*Rr*	*time*	*f*	*Rs*	*Rr*	*time*
1	3	82	6	4.7	3	89	6	2.2
2	2	20	3	0.4	2	22	3	0.3
3	2	84	4	67.5	2	78	4	8.4
4	2	4494	?	>300000	2	4614	154	39542.6
5	2	50	3	4.4	2	53	3	1.2
6	2	1603	?	> 300000	2	1848	8	6673.2

Table 3 1 Results for 6 point groups for the coset method (method 1) and the lower central series method (method 2) (a) and the depth-first search method (method 3) and the breadth-first search method (method 4) (b) The numbers in column "*no*" refer to the number of the point group as treated in this section. The number of generators is denoted by *f* The number of relations to be reduced is denoted by *Rs* The resulting number of relations is denoted by *Rr* The column "*time*" denotes the running time in CPU-seconds

The sixth and last point group to be considered, is of order 1920:

$$K = < \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} > . \qquad (3.29)$$

The first method gives the following resulting defining relations:

$$
\begin{array}{rcll}
\varphi_1 & = & g_1^6 & = \epsilon \\
\varphi_2 & = & g_2^5 & = \epsilon \\
\varphi_3 & = & g_2^{-1}g_1^{-2}g_2g_1g_2g_1g_2^{-1}g_1^{-2}g_2g_1g_2g_1 & = \epsilon \\
\varphi_4 & = & g_2g_1g_2^2g_1^{-2}g_2^{-1}g_1^2g_2^2g_1^3 & = \epsilon \\
\varphi_5 & = & g_2g_1^2g_2^2g_1g_2g_1g_2g_1^2g_2^2g_1g_2g_1 & = \epsilon \\
\varphi_6 & = & g_1g_2g_1g_2g_1g_2g_1^2g_2g_1^3g_2^{-1}g_1^{-1}g_2^{-1}g_1^{-1}g_2^{-2} & = \epsilon \\
\varphi_7 & = & g_2g_1g_2g_1^{-1}g_2^{-1}g_1g_2g_1g_2g_1g_2^2g_1g_2g_1^2 & = \epsilon \\
\varphi_8 & = & g_1^2g_2^{-1}g_1^{-1}g_2g_1g_2^{-1}g_1^{-1}g_2g_1g_2^{-2}g_1^2g_2^{-2} & = \epsilon \\
\varphi_9 & = & g_2^2g_1^2g_2^{-1}g_1^{-1}g_2g_1^2g_2g_1^2g_2^2g_1^{-2}g_2^{-1}g_1^{-1} & = \epsilon \\
\varphi_{10} & = & g_2g_1^{-1}g_2g_1^{-1} & = \epsilon
\end{array}
\tag{3.30}
$$

In order to compare the four different methods, the results for the 6 point groups mentioned above, are tabulated in Table 3.1. Notice that for the third method in Table 3.1, the running time for two point groups exceeded 300000 CPU-seconds and the program was stopped.

3.8 Concluding remarks

The results in § 3.7 show, that the first method gives better results than the three other methods: running times are much shorter, and, generally, the number of resulting defining relations is equal or smaller. The reason that the running times for the third and fourth method are longer than for the first method is the much larger number of defining relations to be reduced. Table 3.1 also shows that the running times for the third method are longer than for the fourth method, also for point groups for which the number of defining relations to start with, is smaller in the third method than in the fourth method. The reason is that the words and the relations contain many more letters in the third method than in the fourth method, which is a consequence of the search method (the way in which all point group elements are expressed for the third and the fourth method in the second example in § 3.7, confirms this argument). The running times for the second method are longer than for the first method, because the determination of a commutator group requires much time. These results also reflect the well known fact that the number of generators, achieved with the lower central series method (i.e. the second method), in general does not yield the minimal

number of generators. The first method gives a reasonably small number of defining relations, satisfied by a set of generators, in a reasonably small running time, even for large order point groups.

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Chapter 4

An algorithm to find generators for the normalizer of an n-dimensional crystallographic point group in Gl(n,Z)

A new method for finding generators for the normalizer in $Gl(n, \mathbf{Z})$ of an n-dimensional crystallographic (arithmetic) point group is described. First a set of generators for the centralizer is determined, whereafter the completeness of the found set is checked. After evaluating all inner automorphisms, representatives of the outer automorphisms, if existent, are determined. A complete generating set for the normalizer of some point groups for n = 5,6 is determined with use of an algorithm, based upon this method.

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4.1 Introduction

As is well known, the normalizer $N(K)$ in $Gl(n, \mathbf{Z})$ of a finite group $K \subset Gl(n, \mathbf{Z})$:

$$N(K) = \left\{ m \in Gl(n, \mathbf{Z}) \mid mkm^{-1} \in K, \ \forall\, k \in K \right\} \tag{4.1}$$

is finitely generated (Siegel 1943). Such a group K is called a finite unimodular group, crystallographic point group or arithmetic point group.
The problem is to have a procedure to find a complete set of generators for the normalizer, given a generating set for the point group. The normalizer of a point group is of importance for the determination of space groups (Brown 1969, Ascher and Janner 1965, Janssen *et al.* 1969, Fast and Janssen 1971). For n = 1,2,3 all finite subgroups of $Gl(n, \mathbf{Z})$ and their normalizer are well known already a long time. For $n = 4$, a complete list of finite subgroups of $Gl(n, \mathbf{Z})$ and their normalizer was given by Brown *et al.* (1973, 1978). For $n = 5$, all maximal finite subgroups of $Gl(n, \mathbf{Z})$ have been determined by Ryskov (1972a,b) and Bülow (1973) and all maximal finite absolutely irreducible subgroups of $Gl(n, \mathbf{Z})$ were computed up to $\mathbf{Z}$-equivalence by Plesken and Pohst for n = 5,7 (1977a), $n = 6$ (1977b), $n = 8$ (1980a) and for $n = 9$ (1980b).
Brown *et al.* (1973) described methods to find a generating set for the normalizer, making use of the specific structure of the point group (like isomorphism class). The method described in this paper, is intended to determine a generating set for the normalizer without knowledge about the structure of the point group. It is suitable for any point group for arbitrary n, with its generators as input.
The paper is organized as follows. In § 4.2 the achievement of a set of generators is described due to the coset decomposition of the normalizer w.r.t. the centralizer and due to the coset decomposition of a subgroup of the automorphism group of the point group w.r.t. its inner automorphisms. § 4.3 contains a new method to find a generating set for a matrix group, which will be applied to the case of a matrix group being the centralizer of a point group. The procedure to check whether the found set was complete, is outlined in § 4.4. How one finds representatives of the cosets of the normalizer w.r.t. the centralizer, is discussed in § 4.5. An algorithm based upon the methods described in § 4.3, 4.4, 4.5 has been developed in order to determine

a generating set for the normalizer of a point group. A scheme of the different steps in the algorithm follows in § 4.6. Results for some point groups for $n = 5$ and $n = 6$ are presented in § 4.7.

4.2 Organization of generators due to coset decomposition of the normalizer

Consider an arithmetic point group $K \subset Gl(n, \mathbf{Z})$. The centralizer $C(K)$ in $Gl(n, \mathbf{Z})$:

$$C(K) = \{c \in Gl(n, \mathbf{Z}) \mid ck = kc, \ \forall\, k \in K\} \tag{4.2}$$

is an invariant subgroup of $N(K)$:

$$C(K) \trianglelefteq N(K). \tag{4.3}$$

It is possible to decompose $N(K)$ in cosets w.r.t. $C(K)$:

$$N(K) = \bigcup_{i=1}^{d} n_i C(K) \tag{4.4}$$

where n_i corresponds to some automorphism $\varphi_i : K \rightarrow K$, defined by: $\varphi_i(k) = n_i k n_i^{-1}$, $\forall\, k \in K$ ($n_1 \equiv \mathbf{1}_n$). Then

$$I(K) \trianglelefteq A(K) \subseteq Aut(K) \tag{4.5}$$

where $A(K) \equiv \{\varphi_1, \ldots, \varphi_d\}$ (the order of $A(K)$, $|A(K)|$, is equal to d) and $I(K)$ is the group of inner automorphisms of K: $I(K) = \{\Theta_i\}$, where $\Theta_i : K \rightarrow K$ is defined by : $\Theta_i(k) = a_i k a_i^{-1}$, $\forall\, k \in K$ for some $a_i \in K$. Since $|K|$ is finite, the number of automorphisms of K, $|Aut(K)|$, is finite ($|Aut(K)| \leq |K|!$), so p also is finite. Suppose one has found e generators for $C(K)$:

$$C(K) = < c_1, ..., c_e > \tag{4.6}$$

for a point group

$$K = < k_1, ..., k_s > . \tag{4.7}$$

Due to rel. (4.5), $A(K)$ can be decomposed in cosets w.r.t. $I(K)$:

$$A(K) = \bigcup_{i=1}^{t} \varphi_i I(K), \tag{4.8}$$

where φ_i is some representative for the i-th coset and $\varphi_1 \equiv id$. Then one has to find generators for $I(K)$:

$$I(K) = < \Theta_1, ..., \Theta_r > \tag{4.9}$$

and coset representatives $\{\varphi_1, \ldots, \varphi_t\}$ according to eq. (4.8). In the rest of this paper, n_i is a matrix corresponding to the automorphism φ_i.

4.3 How to find generators for a matrix group

As is pointed out in § 4.2, the first step is to determine a set of generators for the centralizer $C(K)$. With the method described below, a set of generators for any matrix group can be determined. This group can be defined in several ways. One can give all group elements, or the group can be determined by some defining relations. In the following, the matrix group is considered to be the centralizer of a point group, but the method is suitable for any matrix group.

Suppose one has a generating set of a matrix group. The problem is to find a procedure, according to which an arbitrary element can be expressed in terms of the generators by a finite number of steps. The central idea in the procedure is the following.

Consider an $m \in G$ for an n-dimensional matrix group $G \equiv < g_1, \ldots, g_f >$. Say $m = g_1^2 g_4^{-1}$. Now consider three different paths $m \rightarrow \mathbb{1}_n$, such that at each step the number of terms in a word is decreased by one:

$$\begin{aligned}
1. \quad m &= g_1^2 g_4^{-1} \rightarrow g_1 g_4^{-1} \rightarrow g_4^{-1} \rightarrow \mathbb{1}_n \\
2. \quad m &= g_1^2 g_4^{-1} \rightarrow g_1 g_4^{-1} \rightarrow g_1 \rightarrow \mathbb{1}_n \\
3. \quad m &= g_1^2 g_4^{-1} \rightarrow g_1^2 \rightarrow g_1 \rightarrow \mathbb{1}_n.
\end{aligned}$$

Introduce the norm $N(m)$ of a matrix m in a straightforward way:

$$N(m) = \sum_{i,j=1}^{n} (m_{ij})^2. \tag{4.10}$$

Then $\sqrt{N(m)}$ is a matrix norm (Lancaster 1969). Now a matrix m is decided to be expressible as a word in the generating set $\{g_1, ..., g_f\}$ if there exists a path

$$m \equiv m(0) \rightarrow m(1) \rightarrow \ ..... \ \rightarrow m(L) \equiv \mathbb{1}_n \ (\ L \in \mathbf{N})$$

such that there exist $j,\ q,\ 1 \leq j \leq f,\ q \in \{-1, 1\}$ for which

$$\begin{aligned} &\text{either} \quad N(g_j^q m(i)) < N(m(i)) \Rightarrow m(i+1) = g_j^q m(i) \\ &\text{or} \quad\ N(m(i) g_j^q) < N(m(i)) \Rightarrow m(i+1) = m(i) g_j^q \\ &\text{or} \quad\ i = L - 1 \text{ and } m(i) = g_j^q, \end{aligned} \tag{4.11}$$

for all $0 \leq i < L$. The criterion (4.11) ensures, that by a finite number of steps ($\leq N(m)$) a matrix m is decided to be in a generating set or not. Of course, in principle more paths $m \rightarrow \mathbb{1}_n$, satisfying condition (4.11), are allowed. This makes it possible to achieve generator relations, as will become clear in the description below. The method works as follows.
The generating set $\{k_1, ..., k_s\}$ of K (see rel. (4.7)) forms the input. Now $C(K)$ can be defined in a way equivalent to def. (4.2) as follows:

$$C(K) = \{c \in M_{n\times n}(\mathbb{Z}) \mid ck_j = k_j c\ ,\ 1 \leq j \leq s\ \} \cap Gl(n, \mathbb{Z}). \tag{4.12}$$

According to def. (4.12), a matrix $m \in C(K)$ is determined by the $s \times n^2$ linear equations for its n^2 coefficients, by the requirement that the coefficients $m_{ij},\ 1 \leq i, j \leq n$, are integers and by the requirement for the determinant of m (referred to as $\det(m)$) to be ± 1.
First, these $s \times n^2$ linear equations are to be solved, resulting in N independent parameters, the $n^2 - N$ other coefficients being 0 or depending linearly on these N independent parameters. Now define the following set of matrices:

$$C_R(K) = \{c \in M_{n\times n}(\mathbb{R}) \mid ck_j = k_j c\ ,\ 1 \leq j \leq s\}.$$

Then each $m \in C_R(K)$ can be mapped upon an N-dimensional vector by the bijection F:

$$F : C_R(K) \rightarrow \mathbb{R}^N\ ;\ F(m) = (x_1, \ldots, x_N) \tag{4.13}$$

where F assigns to each $m \in C_R(K)$ the values of its N independent coefficients. Now a set of matrices M is constructed, by considering the set:

$$M' = \left\{\mathbf{x} \in \mathbb{Z}^N \mid\mid x_j \mid \leq D\ ,\ j \in \{1, \ldots, N\}\right\}$$

for some $D \in \mathbf{N}$. Then the set M' corresponds to a set

$$M'' = \left\{ F^{-1}(\mathbf{x}) \mid \mathbf{x} \in M' \right\}$$

according to rel. (4.13), and M consists of all matrices m in the set M'' satisfying the following two conditions:
1. $m_{rs} \in \mathbf{Z}$ for m_{rs} dependent coefficients;
2. $\det(m) = \pm 1$.
The resulting set of matrices M is put in order with increasing norm.
The selection of the generators out of the set M is performed as follows. The first generator c_1 is the first matrix in the set M (with lowest norm). Now consider the second matrix, say $m \in M$. The criterion (4.11) can be applied with $f = 1$ in order to decide if $m \in < c_1 >$. If $m \notin < c_1 >$, then m becomes the second generator: $c_2 = m$, and the third element is treated according to criterion (4.11) with $f = 2$; if $m \in < c_1 >$, then the third member is treated with $f = 1$, etc. In this way the whole set M is examined, ending up with a set of generators and all other members being written as words in this generating set according to criterion (4.11).

As pointed out before, there can (and in general will) exist more paths $m \rightarrow \mathbb{1}_n$. Suppose for example:

$$\begin{aligned} 1. \quad & m \rightarrow mc_3^{-1} \rightarrow c_2^{-1} mc_3^{-1} \rightarrow c_2^{-1} mc_3^{-1} c_2^{-1} = \mathbb{1}_n \\ 2. \quad & m \rightarrow mc_4^{-1} \rightarrow c_1^{-1} mc_4^{-1} = \mathbb{1}_n \end{aligned}$$

are two possible paths. Then $m = c_2^2 c_3 = c_1 c_4$ so that $c_4 = c_1^{-1} c_2^2 c_3$ is a generator relation. In principle a dependent generating set $\{c_1 \ldots, c_e\}$ will be found, and with help of the generator relations as in the example above, the number of independent generators can be decreased.
In order to minimize the number of generators, one extra degree of freedom is allowed w.r.t. the decision whether a matrix m can be expressed as a word in some generating set. If no path $m \rightarrow \mathbb{1}_n$ has been found, the process is carried out for m^{-1} instead of m with the same criterion (4.11). Of course, this inversion is not allowed inside a path, since then the number of steps would not be ensured to be finite. The set of matrices which do not satisfy criterion (4.11), but of which the inverses satisfy criterion (4.11), is denoted by $J = \{j_1, \ldots, j_a\}$ for some $a \in \mathbf{N}$.

4.4 Check of completeness of generating set for $C(K)$

Now all matrices in the set M have been shown to be expressible as words in the set $\{c_1, \ldots, c_e\}$ but it still has to be proved that $< c_1, \ldots, c_e > = C(K)$. Consider the set:

$$T = \{a \in M_{n\times n}(\mathbb{R}) |\ ak_j = k_j a,\ 1 \leq j \leq s \text{ and there is no } j \in \{1, \ldots, e\},\ q \in \{-1, 1\} \text{ such that } N(c_j^q a) < N(a) \text{ or } N(ac_j^q) < N(a)\}. \tag{4.14}$$

So T consists of all matrices $a \in M_{n\times n}(\mathbb{R})$ commuting with each $k \in K$, of which the norm cannot be decreased by left- or rightmultiplication with any generator c_j or its inverse.
All $j_k \in J$ are added to the c_i of def. (4.14). This is permitted, since J consists of all matrices for which the criterion (4.11) is satisfied after inversion.
Analogously to rel. (4.13), the set $T \subseteq M_{n\times n}(\mathbb{R})$, defined in def. (4.14), corresponds to a set $T' \subseteq \mathbb{R}^N$. The set T' is defined by inequalities for a number of homogeneous polynomials of second degree in the N free parameters (because of def. (4.10) and the fact that all dependent coefficients depend linearly on the N free parameters). Since all matrices $m \in C(K)$ for which $|x_i| \leq D$ ($F(m) = \mathbf{x} \in \mathbb{Z}^N$ according to rel. (4.13)) have already been evaluated, it holds for these m that $m \notin T$ and the corresponding $\mathbf{x} \notin T'$. The completeness of the set $\{c_1, \ldots, c_e\}$ is proved if an upper bound can be determined on:

$$|x_j|,\ 1 \leq j \leq N, \text{ for } \mathbf{x} = (x_1, \ldots, x_N) \in T,\ \det(m(\mathbf{x})) = \pm 1. \tag{4.15}$$

Before the procedure to check rel. (4.15) is outlined, first some useful properties will be described. Let $\lambda \in \mathbb{R}\setminus_{\{0\}}$. Then

$$\mathbf{x} \in T' \Leftrightarrow \lambda\mathbf{x} \in T' \tag{4.16}$$

because of the fact that T' is defined by homogeneous polynomials of second degree in the N free parameters. Let $m(\mathbf{x})$ be the matrix corresponding to $\mathbf{x}$ and $\mathbf{x}(m)$ be the vector corresponding to the matrix m in accordance with rel. (4.13). Then $m(\lambda\mathbf{x}) = \lambda m(\mathbf{x})$ for all $\lambda \in \mathbb{R}$ and $\det(m(\mathbf{x}))$ is a homogeneous polynomial of degree n in the N free parameters. Then:

$$\det(m(\lambda\mathbf{x})) = \lambda^n \det(m(\mathbf{x})) \quad (\lambda \in \mathbb{R},\ \mathbf{x} \in \mathbb{R}^N) \tag{4.17}$$

$$\frac{\partial}{\partial x_j} \det(m(\lambda \mathbf{x})) \;=\; \lambda^{n-1} \frac{\partial}{\partial x_j} \det(m(\mathbf{x})) \tag{4.18}$$

for all $\mathbf{x}_0 \in \mathbb{R}^N$, $\lambda \in \mathbb{R}$, $j \in \{1, \ldots, N\}$. The three properties (4.16), (4.17), (4.18) are useful for the procedure to check rel. (4.15), which is outlined below.

Consider a hypercube in $\mathbb{R}^N$, centred in $(0, \ldots, 0)$ with edge length $2E$, with $E \in \mathbb{N}$. The surface of this cube is divided into hypersquares S_i of edge length equal to one. Every S_i produces a tube T_i enclosed by

$$\{\lambda \mathbf{P} |\; \lambda \geq 0\,,\; \mathbf{P} \text{ on the boundary of } S_i\}\,.$$

Then $\uplus\, T_i = \mathbb{R}^N$. In the following, the analysis is performed per square S_i (i.e. per tube T_i).
The idea is that we try to determine an upper bound on the absolute values of the independent parameters x_j, $1 \leq j \leq N$, on the determinant $= \pm 1$ surface inside the tube T_i, provided that $S_i \cap T' \neq \{\emptyset\}$. Note that, since S_i, and therefore also T_i, are defined by inequalities for second degree homogeneous polynomials in the N free parameters, there is an exact answer to the question whether or not $S_i \cap T' \neq \{\emptyset\}$.
If $S_i \cap T' = \{\emptyset\}$, then $T_i \cap T' = \{\emptyset\}$ due to rel. (4.16), and the next tube can be examined. If $S_i \cap T' \neq \{\emptyset\}$, then an upper bound must be determined on

$$|x_j|,\; 1 \leq j \leq N,\; \text{for } \mathbf{x} \;=\; (x_1, \ldots, x_N) \;\in\; T_i,\; \det(m(\mathbf{x})) \;=\; \pm\, 1.$$

First calculate $\det(m(\mathbf{x}_M))$, where $\mathbf{x}_M$ is the point in the centre of S_i. If $\det(m(\mathbf{x}_M)) > 0$, then one has to calculate a lower bound (referred to as LB) for $\det(m(\mathbf{x}))$ for $\mathbf{x} \in S_i$. If $\det(m(\mathbf{x}_M)) < 0$, then an upper bound, denoted by UB, must be calculated. In the following, with the bound B is meant LB or UB. Two methods are used to calculate such a bound.
Method 1. As already pointed out before, the determinant is a homogeneous polynomial of degree n. In order to find a bound, choose the most negative (LB) or positive (UB) value of the determinant term by term for $\mathbf{x} \in T_i$. For example, suppose $N = 4$ and:

$$\det(m(x_1, x_2, x_3, x_4)) \;=\; x_1^2 x_2^2 \;-\; x_3^2 x_4^2.$$

Consider:

$$S_i \;=\; \Big\{(3, 2+\beta, 1+\gamma, \delta) \;\in\; \mathbb{R}^4 \mid 0 \;\leq\; \beta, \gamma, \delta \;<\; 1\Big\}.$$

Since $\det(m(\mathbf{x}_M)) > 0$, a lower bound has to be determined: $LB = 9 \times 4 - 4 \times 1 = 32$.

Method 2. For any $1 \leq j \leq N$, $\frac{\partial}{\partial x_j}\det(m(\mathbf{x}))$ is a homogeneous polynomial of degree $n-1$. Now the extremal partial derivative of the determinant is calculated term by term, $\forall\, j \in \{1,\ldots,N\}\setminus_{\{k\}}$, when x_k is fixed. For the example mentioned above, lower bounds on the partial derivatives are

$$(36,-4,-8) \quad \text{for} \quad (\frac{\partial}{\partial x_2}\det(m(\mathbf{x})),\ \frac{\partial}{\partial x_3}\det(m(\mathbf{x})),\ \frac{\partial}{\partial x_4}\det(m(\mathbf{x}))\ )$$

respectively. Now a bound on the determinant is achieved as follows. First $\det(m(\mathbf{y}))$ is calculated, where $\mathbf{y}$ has property $y_j = min(x_j)$, $1 \leq j \leq N$, $\mathbf{x} = (x_1,\ldots,x_N) \in S_i$. So $\mathbf{y}$ is on the edge of S_i. Next, when a lower (upper) bound is sought, and a partial derivative can only be positive (negative), then that partial derivative does not give a contribution. So

$$LB = \det(m(\mathbf{y})) + \sum_{j\neq k}^{N} min(0,\ [\frac{\partial}{\partial x_j}\det(m(\mathbf{x}))]_{\mathbf{x}\in S_i}\ ) \equiv \det(m(\mathbf{y})) + \delta_- \tag{4.19}$$

$$UB = \det(m(\mathbf{y})) + \sum_{j\neq k}^{N} max(0,\ [\frac{\partial}{\partial x_j}\det(m(\mathbf{x}))]_{\mathbf{x}\in S_i}\ ) \equiv \det(m(\mathbf{y})) + \delta_+$$

For the example mentioned above, LB = 36-0-4-8 = 24. The values for the bounds determined with these two methods, are compared and the highest (LB case) or lowest (UB case) value for the bound is taken. Suppose $LB > 0$ ($UB < 0$). In order to determine an upper bound on the $|x_j|$, $1 \leq j \leq N$, for $\det(m(\mathbf{x})) = \pm 1$ and $\mathbf{x} \in T_i$, note that:

$$|x_j| \leq E\ ,\ 1 \leq j \leq N\ ,\ \text{for}\ \mathbf{x} \in S_i.$$

Therefore

$$|x_j| \leq \frac{E}{\sqrt[n]{|B|}}\ ,\ 1 \leq j \leq N\ ,\ \text{for}\ \det(m(\mathbf{x})) = \pm 1 \tag{4.20}$$

where B is the bound, UB or LB. Now the two cases $\frac{E}{\sqrt[n]{|B|}} < D+1$ and $\frac{E}{\sqrt[n]{|B|}} \geq D+1$ have to be distinguished. In § 4.3 all $m \in C(K)$ were examined,

for which the corresponding $|x_j| \leq D$, $1 \leq j \leq N$. So if $\frac{E}{\sqrt[n]{|B|}} < D+1$, then all matrices $m \in C(K)$ with corresponding $\mathbf{x} \in T_i$, have already been examined in § 4.3. If $\frac{E}{\sqrt[n]{|B|}} \geq D+1$, then consider the set:

$$\left\{ \mathbf{x} \in T_i \cap \mathbf{Z}^N \mid \text{there is a } t \in \{1,\ldots,N\} \text{ such that } |x_t| \geq D \right. \\ \left. \text{and } |x_q| \leq \frac{E}{\sqrt[n]{|B|}},\ 1 \leq q \leq N \right\}. \tag{4.21}$$

For all $\mathbf{x}$ in this set it is checked, whether or not the following four conditions are fulfilled:
1. if $\mathbf{x} \in T'$ and
2. $\det(m(\mathbf{x})) = \pm 1$ and
3. $m(\mathbf{x})_{rs} \in \mathbf{Z}$ for $m(\mathbf{x})_{rs}$ dependent coefficients of $m(\mathbf{x})$ and
4. $m(\mathbf{x})^{-1} \notin < c_1, \ldots, c_e >$ according to criterion (4.11),

then add $m(\mathbf{x})$ to the set of generators.
If $LB \leq 0$ (or, if an upper bound is to be determined, $UB \geq 0$), then it is possible that $|x_k| \rightarrow \infty$ for some $\mathbf{x} \in T'$ for which $\det(m(\mathbf{x})) = \pm 1$. In that case we use a refinement strategy, which consists of the following. Consider, instead of S_i, $2S_i \equiv \{2\mathbf{x} \mid \mathbf{x} \in S_i\}$. Since $2S_i$ has edge length 2, it can be divided into $2^{(N-1)}$ squares of edge length 1: $S^{(2)}_{i,v}$, with $1 \leq v \leq 2^{(N-1)}$, the upper index (2) denoting the level of refinement. Every square $S^{(2)}_{i,v}$ corresponds to a tube $T^{(2)}_{i,v}$, and in fact nothing else has been done but subdividing the tube T_i. For each new tube the analysis is restarted in a slightly different way than for the first refinement level. First it is checked whether $T^{(2)}_{i,v} \cap T' \neq \{\emptyset\}$. If so, then $\det(m(\mathbf{x}_M))$ is calculated, where $\mathbf{x}_M$ is the point in the centre of $S^{(2)}_{i,v}$. Then a lower bound (if $\det(m(\mathbf{x}_M)) > 0$) or an upper bound (if $\det(m(\mathbf{x}_M)) < 0$) on the determinant is determined. Method 1 is used for that purpose in exactly the same way as before. Method 2 works differently if the level of refinement is not 1. Use is being made of the fact that a refinement has taken place. Using eq. (4.18) with $\lambda = 2$, as bound B may be taken:

$$B = \det(m(\mathbf{y})) + 2^{(p-1)(n-1)}\,\delta_{\pm} \tag{4.22}$$

with $p = 2$ denoting the level of refinement, δ corresponding to the sum term in eq. (4.19) for S_i (refinement level 1), $\mathbf{y}$ has again property $y_j =$

$min(x_j)$, $1 \leq j \leq N$, $\mathbf{x} = (x_1, \ldots, x_N) \in S^{(2)}_{i,v}$. The reason for using this strategy is the following. Suppose the determinant surface in $\mathbb{R}^N$ is relatively flat. Then after refining:

$$\det(m(\mathbf{y})) \rightarrow \approx \det(m(2\mathbf{y})) = 2^n \det(m(\mathbf{y}))$$

according to eq. (4.17), whereas $\delta(\det) \rightarrow 2^{n-1}\delta(\det)$ according to the analysis described above. It follows from eq. (4.22) that we then have a better chance to determine a bound B.
Of course, also at this second refinement level there can be tubes $T^{(2)}_{i,v}$ with $LB \leq 0$ or $UB \geq 0$. Up to some maximum, as many refinements as necessary are allowed in order to achieve an exact analysis for each tube

$$T^{(p)}_{i,v_2,\ldots,v_p} \quad (1 \leq v_j \leq 2^{(N-1)}, \ \forall\, 1 \leq j \leq p)$$

where p denotes the refinement level. At each refinement level $p \neq 1$, the same analysis as for $p = 2$, is used. The outcome of the analysis described above is as follows.
Suppose we put a maximum p_{max} on the number of refinements and there are no tubes $T^{(p_{max})}_{i,v_2,\ldots,v_{p_{max}}}$, with centre $\mathbf{x}_M$, for which $LB \leq 0$ (if $\det(m(\mathbf{x}_M)) > 0$) or $UB \geq 0$ (if $\det(m(\mathbf{x}_M)) < 0$). Then the found generator set is proved to be complete. Suppose there are such tubes. Then consider the set:

$$\Big\{\mathbf{x} \in T^{(p_{max})}_{i,v_2,\ldots,v_{p_{max}}} \cap \mathbf{Z}^N \mid \text{there is a } t \in \{1,\ldots,N\} \text{ such that } |x_t| \geq D \text{ and } |x_q| \leq E \times 2^{(p_{max}-1)},\ 1 \leq q \leq N\Big\}. \tag{4.23}$$

For each $\mathbf{x}$ in this set it is checked whether the four conditions below rel. (4.21) are satisfied, and if so, then the corresponding $m(\mathbf{x}) \in C(K)$ is added to the generator set. Hence it has been proved that:

$$m(\mathbf{x}) \in C(K)\ ,\ |x_j(m)| \leq E \times 2^{(p_{max}-1)},\ \forall\, j \in \{1,\ldots,N\}$$
$$\Rightarrow\ m(\mathbf{x}) \in < c_1, \ldots, c_{e+u} > \tag{4.24}$$

where u denotes the number of possibly added generators due to the analysis described above (for all point groups tested, the author never encountered the situation $u \neq 0$). In other words, the generator set has not been proved to be complete, but each matrix in the subgroup of $C(K)$ generated by all $m \in C(K)$ with coefficients up to some maximal absolute value, has been proved to be expressible as word in the found generating set.

4.5 Finding representatives for the cosets of $N(K)$ w.r.t. $C(K)$

In § 4.2 it was already pointed out, how $N(K)$ can be decomposed in cosets w.r.t. $C(K)$ (eq. (4.4)). The resulting representatives $\{n_1, \ldots, n_d\}$ correspond to the set automorphisms $\{\varphi_1, \ldots, \varphi_d\}$. This set is the group $A(K)$ from rel. (4.5). The i-th automorphism φ_i is completely determined once

$$\varphi_i(k_j) \;=\; m k_j m^{-1} \;,\; m \;\in\; n_i C(K) \tag{4.25}$$

is known for all point group generators $k_1, \ldots, k_s$. The first consideration is how to construct all possible automorphisms of the kind of rel. (4.25). A necessary (but, as will be shown, not sufficient) condition for such an automorphism, say φ_i, is that

$$\det(k_j \;-\; \lambda \mathbb{1}_n) \;=\; 0 \;\Leftrightarrow\; \det(\varphi_i(k_j) \;-\; \lambda \mathbb{1}_n) \;=\; 0 \;,\; 1 \;\leq\; j \;\leq\; s \tag{4.26}$$

i.e. each generator k_j must satisfy the same characteristic equation and, as a consequence, must have the same eigenvalues, as $\varphi_i(k_j)$. Therefore all point group elements have to be determined, which have the same eigenvalues as the generators. Now the characteristic equation, $\det(k - \lambda \mathbb{1}_n) = 0$, has to be calculated for each $k \in K$. For $n \leq 6$, use can be made of the following lemma.

Lemma 4.5.1. If $n \leq 6$, then the eigenvalues of a point group element k are completely determined by:
1. $\det(k)$, the determinant of the matrix k;
2. $\mathrm{tr}(k)$, the trace of the matrix k;
3. the order m of k: $k^m = \mathbb{1}_n$, $k^j \neq \mathbb{1}_n$ if $j < m$;
4. if $n = 6$ and $m = 4$ or 6, then it must be checked whether $\lambda = 1$ is an eigenvalue of k.

Proof. For given n, all possible orders m for a point group element k can be determined (see e.g. Hiller 1985). For example, for $n = 6$, the possible orders are 1,2,3,4,5,6,7,8,9,10,12,14,15,18,20,24 and 30. For given dimension n and order m, it is easy to classify all possibilities for the set of eigenvalues. □

Of course, one could determine the characteristic equation and not use Lemma 5.4.1, but in order to get information about the point group (like the order of all point group elements), the lemma is useful. Let the point

group elements having the same eigenvalues as k_j, be denoted as

$$\{g(j,1),\ldots,g(j,r_j)\},\ 1 \leq j \leq s. \tag{4.27}$$

Then the number of homomorphisms of the kind of eq. (4.25) to be considered, is $\prod_{j=1}^{s} r_j$. Now consider a homomorphism:

$$k_j \rightarrow \varphi(k_j) = g(j,m_j),\ 1 \leq m_j \leq r_j,\ \forall\ 1 \leq j \leq s. \tag{4.28}$$

In order to be an automorphism, it must hold that:

$$< (g(1,m_1),\ldots,g(s,m_s) > = K \tag{4.29}$$

which is not always the case. As an example, consider:

$$K = < \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} >$$

$$K \supseteq H = < \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} >$$

but $|K| = 8$ whereas $|H| = 4$. Excluding these homomorphisms, which are not automorphisms, representatives for the automorphisms have to be determined. According to rel. (4.8), however, it is convenient to search first for all inner automorphisms. The set of inner automorphisms is the set $\{\Theta_i\}$:

$$\Theta_i(k_j) = a_i k_j a_i^{-1}\ ,\ a_i \in K$$

for each generator k_j. Since all point group elements are known, all inner automorphisms can be determined exactly. They form a group, $I(K)$, and $|I(K)| \equiv r$. From now on, once a representative n_i is found (see rel. (4.4)), at the same time r representatives are found, according to rel. (4.8).
For each automorphism φ_i, a corresponding representative n_i is to be determined. As was the case for the centralizer matrices, n_i satisfies $s \times n^2$ linear equations for its coefficients. In order to find a matrix $n_i \in Gl(n,\mathbf{Z})$, the same procedure as in § 4.3 is used. Say there are P independent coefficients, $x_1,\ldots,x_P$, determining the coset $n_i C(K)$. Then all matrices for which

$$|x_j| \leq F\ ,\ \forall\ 1 \leq j \leq P, \tag{4.30}$$

are considered, for some $F \in \mathbf{N}$. Now suppose no representative can be found. Let again $m(x_1, \ldots, x_P) \in n_i C(K)$ be the matrix uniquely corresponding to $\mathbf{x}$. The determinant, which is a homogeneous polynomial of degree n in the P free parameters, can always be written as:

$$\det(m(x_1, \ldots, x_P)) = \frac{a}{b}(s_1 f_1 + \ldots + s_q f_q) \tag{4.31}$$

with a and b relatively prime, the f_j are the polynomial terms $x_1^{a_{1j}} \ldots x_P^{a_{Pj}}$ and $s_j \in \mathbf{Z}$, $1 \leq j \leq q$. When the factorization of the determinant in the form (4.31) gives $a \neq \pm 1$, then there cannot exist an $n_i \in Gl(n, \mathbf{Z})$ satisfying the linear equations defining n_i, since then there are no integer solutions for x_j, $1 \leq j \leq P$, such that $\det(m(x_1, \ldots, x_P)) = \pm 1$ in eq. (4.31). Once this is proved, it is proved for r representatives, since the automorphism in question can be combined with all inner automorphisms, giving r automorphisms of which it is proved that they cannot be of the form given by rel. (4.25).
If the determinant in the form (4.31) gives $a = \pm 1$, then it has not been proved, that there exists no representative for the automorphism considered (for example, by increasing the value of F in rel. (4.30), a representative perhaps might have been found). This means that it has not been proved that all coset representatives in $N(K)$ w.r.t. $C(K)$ have been found, and therefore the completeness of the generator set of $N(K)$ has not been proved. It must be noted, however, that for all point groups tested, once representatives could not be found, their non-existence could be proved with help of the factorization (4.31) of the determinant. Hence the coset decomposition of $N(K)$ w.r.t. $C(K)$ has been exactly tested for all point groups considered (also see § 4.7).

4.6 Algorithm scheme

An algorithm has been developed which is based upon the methods described in § 4.3, 4.4, 4.5. A generating set of a point group forms the input, the output is formed by a generating set of (a subgroup of) the normalizer. The algorithm scheme consists of the following steps.

A. Find a generating set for (a subgroup of) the centralizer C(K).

1. Determine independent parameters for $C(K)$ and the linear equations

determining the other, dependent coefficients (eq. (4.12)).

2. Construct a finite subset M of $C(K)$ by varying the absolute values of the independent parameters between zero and some constant D and by adding the corresponding matrix to M if its determinant is equal to ± 1 and if all dependent coefficients have integer values.

3. Put the elements of M in order with increasing norm.

4. The elements of M, starting with the element having lowest norm, are treated as follows.

- The first element of M becomes the first generator c_1;
- If an element can be expressed as a word in the already found generators, $c_1, \ldots, c_f$ for some $f \in \mathbb{N}$, according to criterion (4.11), then the next element is treated using the same set of generators;
- If an element cannot be expressed, the criterion (4.11) is applied to the inverse of this element (reason: more freedom in expressing a matrix as a word in a set of generators). If the inverse of the element is expressible as a word in the generators, then this element has to be stored in a list (although the element can be expressed as a word in the generators, it has to be used in the completeness check; see discussion at the end of § 4.3 and eq. (4.14)). Otherwise this element must be added to the set of generators.

5. Treating all elements of the set M as in step 4, M can be divided into generators, and elements expressible as words in these generators.

B. Completeness check.

6. The next step is to check, whether the found set is complete. Suppose, N is the number of independent parameters determining the centralizer. Then $\mathbb{R}^N$ is divided into tubes T_i, defined in § 4.4.

7. For each tube T_i it is checked, whether T_i contains vectors, for which the norm of the corresponding matrix (according to rel. (4.13)) cannot be decreased (this can be checked, since it requests solving a finite number of second degree inequalities);
a. If so, calculate an upper bound on the maximal absolute values of the

coefficients for vectors for which the corresponding matrix has determinant equal to ± 1 in this tube (see two methods described in § 4.4). If such an upper bound exists, then check for all vectors $\mathbf{x} \in \mathbf{Z}^N$, $\mathbf{x} \in T_i$ with maximal absolute values for their coefficients lower than the upper bound, whether the corresponding matrix is in $C(K)$, whether its norm cannot be decreased and whether its inverse cannot be expressed as a word in the generators according to criterion (4.11). If these three conditions are all satisfied, then this matrix has to be added to the set of generators;
b. If not, then turn to the next tube.

8. If all tubes T_i satisfy 8b or satisfy 8a such that an upper bound can be determined, then a complete generating set for the centralizer has been determined.

C. Find coset representatives.

9. The next step is to determine coset representatives for the cosets of the normalizer w.r.t. the centralizer. First, all point group elements with the same invariants as the generators are determined.

10. Each combination defines a homomorphism. For each homomorphism it is checked whether the images of the generators generate the whole point group. If so, this homomorphism is an automorphism.

11. All inner automorphisms are determined (the group of inner automorphisms, $I(K)$, is a subgroup of the group described in step 10, the group $A(K)$ (see § 4.2). So once all inner automorphisms are known, the number of coset representatives to be determined, is decreased considerably).

12. For each element of $A(K)$ a representative matrix is to be determined following the same procedure as in step 1,2 (so this matrix is determined by, say P, independent parameters, and the absolute values of these P parameters are varied between zero and some constant F).

13. Once one matrix has (not) been found, at the same time $|I(K)|$ matrices have (not) been found, according to step 11.

14. If a representative cannot be found, then try to prove, with help of the expression of the determinant in terms of the P independent parameters, that the determinant cannot be equal to ± 1, when the parameters have in-

teger values. If for at least one representative this proof cannot be given, then the algorithm cannot guarantee completeness of the determined generating set for the normalizer.

15. The generating set for (a subgroup of) the normalizer is formed by:

- the generating set for (a subgroup of) the centralizer (step 4),
- the point group elements for which the corresponding automorphisms generate the group of inner automorphisms (one can also simply take the point group generators, but if $|I(K)| < |K|$, then there are also point group elements in $C(K)$; see step 11),
- the coset representatives according to steps 12, 13.

4.7 Results

A computer program, following the algorithm scheme described in § 4.6, has been written in FORTRAN77 and ran on a SUN4 computer. The program is to be integrated in a software package for the determination of n-dimensional space groups.
Results for some point groups for $n = 5$ and $n = 6$ are given, together with a brief discussion about the completeness of the found set. The analysis for the first point group is meant as an example of how the algorithm works, and is therefore described more extensively.
Consider a point group K, mentioned by Janssen (1990), denoted by $7mm \subset Gl(6, \mathbf{Z})$, which is in the isomorphism class D_7 ($|K| = 14$. K consists of matrices of order 7,2,1 with determinant 1, -1, 1 respectively):

$$K =< k_1, k_2 >=< \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} > . \tag{4.32}$$

1. First, the equations relating the coefficients m_{ij} of $m \in C(K)$ (see def. (4.12)) are determined, resulting in three free parameters, x_1, x_2, x_3. Of the 33 remaining coefficients, 6 of them are zero and 27 coefficients depend

on x_1, x_2, x_3 linearly.

2. Then a set of matrices $\{m\} \equiv M$ is constructed by considering all $m \in C(K)$ for which $|x_j(m)| \leq 8$, $j = 1, 2, 3$. The result is a set of 143 matrices with highest norm 3206.

3. For this set M, for each norm (starting with the lowest norm), all elements with that particular norm are evaluated as follows. There are two matrices with norm 6: $g_1 = \mathbb{1}_6$ and $g_2 = -\mathbb{1}_6$ (notice that $\pm \mathbb{1}_n$ occur in every centralizer). The first generator, c_1, is g_2:

$$c_1 = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}. \tag{4.33}$$

The second norm occurring in M is 18. There are 6 matrices with this norm:

$$\left\{ \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ -1 & 1 & 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & -1 & 1 & 1 \\ 0 & 0 & -1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \end{bmatrix}, \right.$$

$$\begin{bmatrix} 0 & -1 & 1 & 0 & -1 & 1 \\ 0 & -1 & 0 & 1 & -1 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & -1 & 1 & 0 & -1 & 0 \\ 1 & -1 & 0 & 1 & -1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 & 1 \\ 1 & -1 & 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 & -1 & 1 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}, \tag{4.34}$$

$$\left. \begin{bmatrix} 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 1 & -1 & -1 \\ 0 & 0 & 1 & 1 & 0 & -1 \\ -1 & 0 & 1 & 1 & 0 & 0 \\ -1 & -1 & 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & -1 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 & 1 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 1 & -1 & 0 & 1 & 0 \\ -1 & 1 & 0 & -1 & 1 & 0 \end{bmatrix} \right\}$$

denoted by $\{g_i\}$, $i = 3, \ldots, 8$ respectively. Now g_3, $g_3^{-1} \notin < c_1 >$ according to criterion (4.11), so $c_2 = g_3$; g_4, $g_4^{-1} \notin < c_1, c_2 >$, so $c_3 = g_4$;
$g_5 \notin < c_1, c_2, c_3 >$, but $g_5^{-1} = c_2^{-1} c_3^{-1}$, so according to the notation adopted at the end of § 4.3, $j_1 = g_5$; $g_6 = c_1 c_2$, $g_7 = c_1 c_3$; $g_8 \notin < c_1, c_2, c_3 >$, but $g_8^{-1} = c_2^{-1} c_3^{-1} c_1$, so $j_2 = g_8$.
All other matrices in the set M turn out to be expressible as words in terms of c_1, c_2, c_3 according to criterion (4.11), except for two matrices with norm 106, denoted by j_3, j_4, which can be expressed in terms of c_1, c_2, c_3 only after inversion.

4. The next step is to prove that the set $\{c_1, c_2, c_3\}$ is complete. First the set T of def. (4.14) is determined by multiplying an arbitrary $a \in C(K)$ with all $g \in \{c_1, c_2, c_3, j_1, j_2, j_3, j_4\}$ and their inverses. This procedure results in eight constraints. The 143 matrices already evaluated, are certainly not in T. Now rel. (4.15) has to be proved. The determinant is a sixth degree polynomial in three parameters (so $N = 3$). Then a cube in $\mathbb{R}^3$ is constructed with edge length 6 (so $E = 3$). The analysis is done per tube T_i corresponding to a square S_i, where S_i is of the form:

$$S_i = \{(\pm 3,\ y_2 + \beta,\ y_3 + \gamma) |\ 0 \leq \beta, \gamma < 1\}\ ,\ y_2, y_3 \in \{-3, -2, -1, 0, 1, 2\}$$

or permutations. The maximal number of refinements allowed is put equal to 6 (so $p_{max} = 7$). This means that, if the analysis cannot prove completeness, it can prove that all matrices $m \in C(K)$, for which $|x_j(m)| \leq 3 \times 2^6 = 192$ are expressible as words in the set $\{c_1, \ldots, c_{3+u}\}$, where u denotes the number of possibly extra generators (see rel. (4.24)). It turns out, that the analysis for this point group is exact:

$$C(K) = < c_1, c_2, c_3 > \tag{4.35}$$

$$= \left\langle -\mathbb{1}_6, \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ -1 & 1 & 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & -1 & 1 & 1 \\ 0 & 0 & -1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \end{bmatrix} \right\rangle .$$

5. Now representatives for the coset decomposition of $N(K)$ w.r.t. $C(K)$ are to be determined. As $|K| = 14$, the number of inner automorphisms

$|I(K)| \leq 14$. It turns out that $|I(K)| = 14$, and the group of corresponding point group elements $I'(K)$, $I'(K) \simeq I(K)$, is equal to K itself. Hence $I'(K) =< k_1, k_2 >$. With use of Lemma 4.5.1, there are six respectively seven point group elements having the same eigenvalues as k_1 and k_2 (see rel. (4.32)). Therefore 42 homomorphisms of the kind of rel. (4.25) are possible, all of which are automorphisms, since they all satisfy condition (4.29). According to rel. (4.8), there are three representatives n_1, n_2, n_3 to be determined. Now n_1 is the representative corresponding to the coset $n_1 C(K) = C(K)$, so $n_1 \equiv \mathbf{1}_6$. The two remaining representatives are:

$$n_2 = \begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & -1 & 0 \\ -1 & -1 & 1 & 1 & -1 & 0 \\ 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & -1 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & -1 \end{bmatrix}, \quad n_3 = \begin{bmatrix} -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1 & 0 & -1 \\ -1 & 1 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 1 & 0 & 1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \end{bmatrix}. \tag{4.36}$$

This completes the analysis for this point group. The found generating set for the normalizer has been proved to be complete:

$$N(K) = < c_1, c_2, c_3, k_1, k_2, n_2, n_3 > . \tag{4.37}$$

The running time for this point group was 73.9 CPU-seconds.

As a second example, consider the point group:

$$K =< k_1, k_2 >= \left\langle \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \right\rangle. \tag{4.38}$$

Its generators have orders 6 and 2 respectively, both have determinant 1. $|K| = 120$ and possible orders for point group elements are 6,5,4,3,2,2,1, each number corresponding to a particular set of eigenvalues (note that K contains elements of order 2 with trace = -3 and trace = 1 for example; see Lemma 4.5.1). There are two independent coefficients, x_1, x_2, determining each $m \in C(K)$. A set M is constructed by considering

$$\left\{ \mathbf{x} \in \mathbf{Z}^3 \mid |x_j| \leq 3 \, , \, 1 \leq j \leq 2 \right\}.$$

It turns out that $C(K) =< -\mathbb{1}_5 >$. The algorithm can prove completeness of the found generating set. Now 20 respectively 15 point group elements have the same eigenvalues as the generators k_1 and k_2. This means that there are 300 homomorphisms of the kind (4.25). It turns out, that 60 homomorphisms do not satisfy condition (4.29), and are therefore no automorphisms. There are 120 inner automorphisms, and the corresponding group of point group elements is K itself. Due to the coset decomposition of $A(K)$ w.r.t. $I(K)$, there are (300-60)/120 = 2 representatives to be determined (the first representative is trivial: $n_1 \equiv \mathbb{1}_5$). The other representative, n_2, cannot exist in $Gl(5, \mathbf{Z})$, since $\det(n_2) = 0$, due to rel. (4.25). The result is:

$$N(K) \ = < -\mathbb{1}_5, k_1, k_2 > . \tag{4.39}$$

The running time for this point group was 4.4 CPU-seconds.

The third example to be considered, is the point group:

$$K =< k_1, k_2 >= \left\langle \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} , \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \right\rangle . \tag{4.40}$$

Its generators have orders 6 and 5 respectively, both have determinant 1. $|K| = 1920$ and possible orders for point group elements are 12,8,6,6,5,4,4,4,3, 2,2,1, each number corresponding to a particular set of eigenvalues. There is one independent coefficient, from which directly follows, that

$$C(K) \ = < -\mathbb{1}_5 > . \tag{4.41}$$

Now 320 respectively 384 point group elements have the same eigenvalues as the generators k_1 and k_2. This means that there are 122844 homomorphisms of the kind (4.25). It turns out that 69084 homomorphisms do not satisfy condition (4.29), and are therefore no automorphisms. There are 1920 inner automorphisms, and the corresponding group of point group elements is K itself. Due to the coset decomposition of $A(K)$ w.r.t. $I(K)$, there are (122844-69084)/1920 = 28 representatives to be determined (the first representative is trivial: $n_1 \equiv \mathbb{1}_5$). The 27 other representatives must have

determinant $\neq \pm 1$ due to the relations (4.25) determined by the defining automorphism (and have therefore been proved to be non-existent). The result is:

$$N(K) = < -\mathbb{1}_5, k_1, k_2 > . \tag{4.42}$$

The running time for this point group was 179.5 CPU-minutes.

The fourth case is meant as an example of a point group for which completeness of a generating set for its centralizer cannot be proved by our method. Only the centralizer part is treated here. This point group and its normalizer have already been treated by Brown *et al.* (1973). The point group is in isomorphism class D_6:

$$K =< k_1, k_2 >= \left\langle \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \right\rangle . \tag{4.43}$$

$C(K)$ has four independent coefficients, x_1, x_2, x_3, x_4. The algorithm finds five generators, c_1, c_2, c_3, c_4, c_5, with $c_5 = c_1 c_2$. Then

$$C(K) \supseteq \left\langle -\mathbb{1}_5, \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & -2 & 1 & 0 \\ 2 & 1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & -1 & -2 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \right\rangle$$

$$= < c_1, c_2, c_3, c_4 > . \tag{4.44}$$

Comparison with the results by Brown *et al.* (1973) shows that the set $\{c_1, c_2, c_3, c_4\}$ generates $C(K)$, but this cannot be proved by the check procedure of § 4.4. This can be seen as follows. The determinant of each $m \in C(K)$ in terms of the independent coefficients x_1, x_2, x_3, x_4 is:

$$\det(m(x_1, x_2, x_3, x_4)) = x_1^2 x_4^2 + 9x_2^2 x_3^2 + 6x_1 x_2 x_3 x_4. \tag{4.45}$$

Take for example a hypersurface S_i such that $(E, 0, 0, 0) \in S_i$. Now

$$\det(m(E, 0, 0, 0)) = 0 \ ; \ (E, 0, 0, 0) \in T' \tag{4.46}$$

using rel. (4.45) and the explicit form of the second degree inequalities defining T' . Then also:

$$\det(m(2^{(p-1)}E,0,0,0)) \;=\; 0\;;\; (2^{(p-1)}E,0,0,0) \;\in\; T' \;\; (p \;\in\; \mathbf{N}) \quad (4.47)$$

according to eq. (4.17) and eq. (4.16). This means that every T_i containing $(E,0,0,0)$ does not have an upper bound on the coefficients x_1, x_2, x_3, x_4 on the $\det m((\mathbf{x})) = \pm 1$ surface. According to rel. (4.47) however, for each refinement level $p \in \mathbf{N}$, tubes

$$T^{(p)}_{i,v_2,\ldots,v_p} \;\ni\; (E,0,0,0) \;\;,\; T^{(p)}_{i,v_2,\ldots,v_p} \;\cap\; T' \;\neq\; \{\emptyset\}$$

will exist, having no upper bound on the coefficients x_1, x_2, x_3, x_4 on the $\det(m(\mathbf{x})) = \pm 1$ surface. Therefore the completeness of the found set, given by rel. (4.44), can only be proved for the subgroup of $C(K)$ defined in rel. (4.24).

As a last remark, there are also point groups, for which completeness of the found generating set cannot be proved by the procedure described in § 4.4, although inspection of the determinant shows, that the centralizer must be finite. The maximum absolute value on the coefficients of $C(K)$ can then lead to a proof of completeness.

4.8 Concluding remarks

The algorithm described in this paper, for the determination of a generating set for the normalizer $N(K)$ in $Gl(n,\mathbf{Z})$ of an arithmetic point group K turns out to be powerful (in practice). Although completeness of the found set for the centralizer $C(K)$ can be proved only *a posteriori*, it turns out that for a number of point groups the proof exists. The accuracy of the analysis can be increased significantly, by using less rough determinant-bound determining methods (see § 4.4). The method to construct generators corresponding to the coset decomposition of $N(K)$ w.r.t. $C(K)$ turns out to be exact for all examples mentioned (even for all point groups tested).

As a last remark about the computer program, consider the bounds given a value by the user in a computer session. The values of the bounds related to the centralizer (the bounds D below rel. (4.13), E below eq. (4.18) and p_{max} above rel. (4.23)) should be chosen in accordance with the number of independent parameters determining the centralizer. The bigger this number

gets, the smaller these values should be chosen, in order to get reasonable running times. The value of the bound related to the coset decomposition of the normalizer w.r.t. the centralizer (the bound F in rel. (4.30)) should be chosen in accordance with the order of the point group.

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Chapter 5

Arithmetic equivalence of point groups for quasiperiodic structures

Necessary and sufficient conditions are formulated for an n-dimensional arithmetic point group such that it may be the symmetry group of a d-dimensional quasiperiodic but not periodic, i.e. incommensurate, structure with Fourier module of rank n. Only point groups leaving invariant a d-dimensional subspace (the physical space) are considered. For an arithmetic point group describing an incommensurate structure, all equivalent choices for the internal space are related by the normalizer in $Gl(n, \mathbf{Z})$ of the point group. Also the conditions on arithmetic equivalence of two point groups allowing an incommensurate structure are discussed. These conditions yield a further partition of the arithmetic crystal classes.

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5.1 Introduction

A well known problem in crystallography is the determination of non-isomorphic n-dimensional space groups. According to Ascher and Janner (1965), a space group G can be interpreted as a group extension of $\mathbf{Z}^n$ by a finite subgroup $\Gamma(K) \subset Gl(n, \mathbf{Z})$, a faithful representation of a point group $K \subset O(n)$. In this formalism, all non-isomorphic extensions of $\mathbf{Z}^n$ can be obtained by taking one representative $\Gamma(K)$ of each arithmetic equivalence class, which consists of conjugate subgroups of $Gl(n, \mathbf{Z})$. Notice that group extensions for arithmetically non-equivalent point groups are not isomorphic. For each representative arithmetic point group $\Gamma(K)$ all non-equivalent extensions can be determined. For this construction the knowledge of the presentation of the point group in terms of a set of defining relations satisfied by its generators is needed. Algorithms have been developed to construct a set of defining relations satisfied by the generators of an n-dimensional arithmetic point group (Wijnands and Thiers 1992).
Among the non-equivalent extensions, some might give isomorphic space groups. Two isomorphic extensions obtained from the same arithmetic point group are related by an element of the n-dimensional normalizer of $\Gamma(K)$ in $Gl(n, \mathbf{Z})$ (Ascher and Janner 1965; Janssen *et al.* 1969; Fast and Janssen 1971). An algorithm has been developed to determine a generating set for the normalizer in $Gl(n, \mathbf{Z})$ of an n-dimensional arithmetic point group (Wijnands 1991).
For $n = 3$, all non-isomorphic space groups have been tabulated (International Tables for X-ray Crystallography 1969). For $n = 4$, all arithmetic equivalence classes, their normalizers and space groups are known (Brown *et al.* 1978). All maximal finite subgroups of $Gl(5, \mathbf{Z})$ have been determined by Ryskov (1972a,b) and Bülow (1973). For $n = 6,7,8,9$ all maximal irreducible subgroups of $Gl(n, \mathbf{Z})$ have been determined (Plesken and Pohst 1977, 1980).
Crystallography for dimensions higher than three is important for the description of incommensurate modulated structures (de Wolff 1974; de Wolff *et al.* 1981, Janner and Janssen 1980a), composite incommensurate structures (Janner and Janssen 1980b) and quasicrystals (Bak 1985, Janssen 1986). All these structures are quasiperiodic. A quasiperiodic structure in the physical space (called external space, position space or parallel space) can be obtained by intersecting this space with a lattice periodic structure in

a higher-dimensional embedding space. Because of the distinguished physical subspace, the groups describing the symmetry of quasiperiodic structures are n-dimensional space groups, satisfying appropriate additional requirements. They are called superspace groups.
In this paper, for a given n-dimensional crystallographic point group, we present a method to determine all different distinguished subspaces which can play the role of the physical space. This comes down to determining all different sums of real irreducible representations carried by the orthogonal complement of the physical space (called internal space or perpendicular space) such that the point group allows an incommensurate structure. For each such choice, the formalism is given how to find all equivalent choices for the internal space. These ideas are based upon two papers. Janssen (1992) has given necessary conditions to be satisfied by a crystallographic point group (these conditions being proved to be sufficient in the case of a cyclic point group) in order to allow an incommensurate structure. The case of a cyclic point group has also been described by Baake *et al.* (1991). The second paper gives conditions satisfied by two arithmetic point groups to be arithmetically equivalent (Janssen 1991).
In § 5.2 the conditions satisfied by a crystallographic point group in order to allow an incommensurate structure, are formulated. In § 5.3 the problem of arithmetic equivalence of two arithmetic point groups describing quasiperiodic structures is discussed. The more severe conditions and the problem of arithmetic equivalence for modulated structures (a quasiperiodic structure of which in the diffraction pattern main and satellite reflections can be distinguished) are discussed in § 5.4. Examples and results are presented in § 5.5. Examples and results are presented in § 5.5.

5.2 Conditions on incommensurate structures

Let K be an abstract finite point group generated by a set $\{k_1, \ldots, k_s\}$, denoted as $K = < k_1, \ldots, k_s >$. Suppose there exists an integral faithful n-dimensional representation $\Gamma(K) =< \Gamma(k_1), \ldots, \Gamma(k_s) > \subset Gl(n, \mathbf{Z})$ of K. Then $\Gamma(K)$ is called an arithmetic point group. Note that on an appropriate basis, there exists a faithful representation of K acting on the space $\mathbb{R}^n$ as a group of orthogonal transformations. Therefore we may also consider K as a subgroup of $O(n)$.

In this section we formulate necessary and sufficient conditions to be satisfied by a given arithmetic point group $\Gamma(K)$ such that it may be the symmetry group of an incommensurate structure. Denote the physical dimension by d. A point group $\Gamma(K)$ is called non-mixing, if there is a d-dimensional subspace of $\mathbb{R}^n$ such that $\Gamma(K)$ leaves this subspace invariant. If no such subspace can be found, then the point group is mixing. In this paper only non-mixing point groups are considered, since intensity spots for a d-dimensional diffraction pattern have never been observed to be related by a mixing point group (Janssen 1992). We assume the character table of K and the irreducible representation matrices $\Gamma^i(k_j)$, for $\Gamma^i(K)$ in the decomposition of $\Gamma(K)$, to be known (throughout the paper, irreducible representations, irreps, are considered as complex representations, $\mathbb{C}$-irreps, unless stated otherwise). In order to check whether $\Gamma(K)$ is non-mixing, $\Gamma(K)$ has to be decomposed into real irreducible representations, $\mathbb{R}$-irreps. The reduction goes as follows. Consider the decomposition of $\Gamma(K)$ into $\mathbb{C}$-irreps:

$$\Gamma(K) \;=\; C^{-1}\left[\bigoplus_i m_i\Gamma^i(K)\right]C\;,\;\; C \;\in\; Gl(n,\mathbb{C}) \tag{5.1}$$

where m_i is the multiplicity of $\mathbb{C}$-irrep $\Gamma^i(K)$ in the decomposition. Each $\mathbb{C}$-irrep $\Gamma^j(K)$ is of one of three types:

- type 1: $\Gamma^j(K)$ is $\mathbb{C}$-equivalent to an $\mathbb{R}$-irrep. We assume that the irrep is given as a real irrep then;
- type 2: $\Gamma^j(K)$ is not $\mathbb{C}$-equivalent to an $\mathbb{R}$-irrep, but it is $\mathbb{C}$-equivalent to its complex conjugate $\Gamma^{j*}(K)$;
- type 3: $\Gamma^j(K)$ is not $\mathbb{C}$-equivalent to its complex conjugate $\Gamma^{j*}(K)$.

In the two latter cases, the corresponding $\mathbb{R}$-irrep can be constructed using:

$$\Gamma^j_r \;=\; B^{-1}\begin{bmatrix}\Gamma^j & 0\\ 0 & \Gamma^{j*}\end{bmatrix}B,\; B \;=\; \begin{bmatrix}\mathbb{1}_{d_j} & i\mathbb{1}_{d_j}\\ \mathbb{1}_{d_j} & -i\mathbb{1}_{d_j}\end{bmatrix}, \tag{5.2}$$

where $\mathbb{1}_{d_j}$ is the identity matrix of dimension d_j, the dimension of $\Gamma^j(K)$. It is easy to prove that Γ^j_r is irreducible over $\mathbb{R}$. The Frobenius-Schur criterion (Frobenius and Schur 1906; e.g. see Jansen and Boon 1967) can be used to determine the type of a $\mathbb{C}$-irrep $\Gamma^j(K)$.

Theorem 5.2.1. (Frobenius and Schur 1906). Let $\Gamma^j(G)$ be a $\mathbb{C}$-irrep of a finite group G of order $|G|$. Denote the character of $\Gamma^j(g)$ by $\chi(g)$, $\forall\, g \in G$. Then

$$\frac{1}{|G|}\sum_{g\in G}\chi(g^2) = \begin{cases} 1 & \text{if } \Gamma^j \text{ is potentially real (type 1)} \\ -1 & \text{if } \Gamma^j \text{ is pseudo}-\text{real (type 2)} \\ 0 & \text{if } \Gamma^j \text{ is essentially complex (type 3).} \end{cases} \tag{5.3}$$

Next, consider all choices for the d-dimensional external space, denoted by V_E, and its orthogonal complement V_I (recall that the point group is non-mixing):

$$\Gamma(K) = S^{-1}\Gamma_r(K)S = S^{-1}\left[\bigoplus_i m_{i,E}\Gamma_r^{i,E}(K) \oplus \bigoplus_j m_{j,I}\Gamma_r^{j,I}(K)\right]S, \tag{5.4}$$

where $S \in Gl(n,\mathbb{R})$ and $m_{i,E}$ ($m_{j,I}$) denotes the multiplicity of the $\mathbb{R}$-irrep $\Gamma_r^{i,E}$ ($\Gamma_r^{j,I}$) carried by the external (internal) space. For each such choice, one can check whether the point group allows an incommensurate structure as follows. Two or more $\mathbb{R}$-irreps are called partners if each $\mathbb{Z}$-irrep carrying one of these $\mathbb{R}$-irreps, also carries the other(s).

Condition 5.2.2. A non-mixing point group of the form (5.4) allows an incommensurate structure with Fourier module of rank n if and only if:

- 5.2.2.1. the external space carries a faithful (i.e. injective) representation,
  and at least one of the following two conditions is satisfied by each $\mathbb{R}$-irrep $\Gamma_r^{j,I}$ carried by V_I:

- 5.2.2.2a. V_E carries an $\mathbb{R}$-irrep, $\mathbb{R}$-equivalent to $\Gamma_r^{j,I}$;

- 5.2.2.2b. V_E carries a partner of $\Gamma_r^{j,I}$.

Proof. The "if" part: The case of cyclic groups has been proved by Janssen (1992). The arguments for the general case are analogous:

-Condition 5.2.2.2a is based upon the following argument. Consider the representation $\Gamma(K) = \Gamma^i(K) \oplus \Gamma^i(K)$ on a basis $\{\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_{2d_i}\}$, where $\hat{\mathbf{e}}_j$ is defined by: $(\hat{\mathbf{e}}_j)_i = \delta_{ij}$ and d_i is the dimension of $\Gamma^i(K)$. Suppose the internal space V_I has basis $\{\hat{\mathbf{e}}_{d_i+1}, \ldots, \hat{\mathbf{e}}_{2d_i}\}$. Then V_I carries $\Gamma^i(K)$. Consider as basis for another V_I': $\{\alpha\hat{\mathbf{e}}_1 + \beta\hat{\mathbf{e}}_{d_i+1}, \ldots, \alpha\hat{\mathbf{e}}_{d_i} + \beta\hat{\mathbf{e}}_{2d_i}\}$, then $\Gamma^i(K)$ is also carried by V_I'. By suitably choosing α and β, one may achieve that the lattice $\mathbb{Z}^n$ does not have a d-dimensional sublattice in common with the external space. Then the structure described in the external space is incommensurate.
Notice that the freedom in choosing α and β is totally covered in the freedom to choose the coefficients in the transformation matrix S in eq. (5.4). The matrix S is determined by linear equations satisfied by its n^2 coefficients.
-If Condition 5.2.2.2b is satisfied, then there is no basis in the external space V_E such that the matrices are integer valued. Hence there is no d-dimensional lattice in V_E, whereas the n-dimensional space contains a lattice (since the n-dimensional point group is arithmetic).
The "only if" part: One can bring $\Gamma(K)$ into the form $\Gamma^1(K) \oplus \Gamma^2(K)$ by a matrix $Q \in Gl(n, \mathbb{Q})$, where $\Gamma^1(K)$ contains all $\mathbb{R}$-irreps of $\Gamma(K)$ which are either $\mathbb{R}$-equivalent to an $\mathbb{R}$-irrep carried by V_E or to a partner of an $\mathbb{R}$-irrep carried by V_E. Both $\Gamma^1(K)$ and $\Gamma^2(K)$ can be chosen to be integer representations (if $\Gamma^i(K)$, $i = 1, 2$, carries an $\mathbb{R}$-irrep, then it also carries its partners; therefore Q can be chosen to be in $Gl(n, \mathbb{Q})$). The reciprocal space carries the adjoint representation $\Gamma^*(K) = \Gamma^{1*}(K) \oplus \Gamma^{2*}(K)$. This means that the basis vectors in the space carrying $\Gamma^{2*}(K)$ are projected on the origin in V_E. Therefore, if this space is not empty, then the rank of the module is smaller than n. □

Below we give some remarks on Condition 5.2.2.
First, the problem of constructing an integral representation for a given $\mathbb{R}$-irrep is not trivial. If we restrict ourselves to cyclic point groups, then this construction assumes the knowledge of the invariants of the generating matrix (Janssen 1992). In order to check Condition 5.2.2.2b, the easier problem has to be solved whether or not there is an integer representation possible in the external and the internal space. The solution is the knowledge that all one-, two- and three-dimensional arithmetic point groups for $d \leq 3$ do not need partners (since their real representations are all $\mathbb{R}$-equivalent to

integral representations). We restrict ourselves to $d \leq 3$.
Consider an n-dimensional arithmetic point group which is not isomorphic to a 1,2,3-dimensional arithmetic point group. If this point group satisfies Condition 5.2.2.1, then it also satisfies Condition 5.2.2.2b. Otherwise there should be a faithful two- or three-dimensional $\mathbb{R}$-irrep in V_E needing no partner in V_I. This contradicts the fact that the point group is non-crystallographic in V_E.
Second, the construction of a Fourier module of rank $\leq n$ follows from the reducing matrix. Let $\Gamma(K) \subset Gl(n, \mathbf{Z})$ act in the reciprocal space and let d be the physical dimension. There is a reducing matrix U such that $U\Gamma(K)U^{-1} = \Gamma_r(K)$. Suppose for convenience that $\Gamma_r(K)$ acts on basis $\{\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_n\}$ with V_E having as basis $\{\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_d\}$. Then the n columns of U, projected on V_E respectively V_I, form a $\mathbf{Z}$-module of rank $\leq n$ (consisting of the first d and the last $n-d$ components of the n columns of U) transforming according to the integral representation $\Gamma(K)$ under the action of the representation carried by V_E and V_I (Kramer 1987). Only if Condition 5.2.2 is satisfied, the rank is equal to n. In that case there exists an n-dimensional lattice periodic structure having the constructed Fourier module (Bohr 1924, Janssen 1988).

5.3 Arithmetic equivalence of point groups

Two n-dimensional arithmetic point groups $\Gamma(K)$ and $\Gamma'(K)$ are called arithmetically equivalent if there is an intertwining matrix $m \in Gl(n, \mathbf{Z})$ such that:

$$m\Gamma(K)m^{-1} = \Gamma'(K). \tag{5.5}$$

Then m induces an isomorphism:

$$\varphi : \Gamma(K) \rightarrow \Gamma'(K) : \varphi(\Gamma(k)) = m\Gamma'(k)m^{-1}. \tag{5.6}$$

To check whether such a matrix m can be found we can use a method which is very similar to a method used to determine the normalizer for an arithmetic point group (Wijnands 1991). The algorithmic procedure is the following.
1. First, all point group elements $\Gamma'(k) \in \Gamma'(K)$ are determined which have the same invariants as the point group generators $\Gamma(k_1), \ldots, \Gamma(k_s)$ of $\Gamma(K)$.
2. Since the isomorphism φ in eq. (5.6) has the property that the invariants of $\Gamma(k_i)$ and of $\varphi(\Gamma(k_i))$ have to be the same, we can restrict ourselves to

all combinations of images determined in step 1. For each combination we proceed as follows.
3. The task is to find a matrix $m \in Gl(n, \mathbf{Z})$ satisfying:

$$m\Gamma(k_i)m^{-1} = \Gamma'(k_i) \quad , \; 1 \leq i \leq s.$$

The matrix m is determined by $s \times n^2$ linear equations. Of all coefficients, some are independent; all other coefficients depend linearly on them. Now the independent coefficients are varied between two bounds. For each set of values of the coefficients, it is checked whether the resulting matrix is unimodular. If so, then we have found an intertwining matrix, and the two point groups are arithmetically equivalent. The procedure is stopped then. If not, then we turn to the next set of values.
4. If no matrix has been found, there are two possibilities.
- There does not exist an $m \in Gl(n, \mathbf{Z})$. By deriving the expression of the determinant of m, denoted by $\det(m)$, in terms of its independent coefficients, it can possibly be proved from the factorization of this expression, that integer values of the independent coefficients can never yield a value $det(m) = \pm 1$. In that case it has been proved that there does not exist such an $m \in Gl(n, \mathbf{Z})$.
- There does exist a matrix m of the desired form, but the required set of values for the coefficients exceeds the bounds we had put on the coefficients.
Only if a matrix m has been found or if non-existence of $m \in Gl(n, \mathbf{Z})$ has been proved with help of the determinant expression, the analysis is exact.
5. We turn to the next combination in step 3.

If quasiperiodic structures are considered, the problem is how to incorporate the role of the physical space as distinguished subspace in the problem of arithmetic equivalence of arithmetic point groups.

Condition 5.3.1. Two point groups $\Gamma(K)$ respectively $\Gamma'(K)$ with given choice for the internal space V_I and V_I', are arithmetically equivalent if and only if they are arithmetically equivalent as n-dimensional arithmetic point groups by a matrix m (eq. (5.5)) which maps V_I of $\Gamma(K)$ on V_I' of $\Gamma'(K)$.

This condition is again based on the fact that V_E (and V_I) is a distinguished subspace. Condition 5.3.1 can be checked as follows. As described in § 5.2,

the two point groups can be decomposed into $\mathbb{R}$-irreps:

$$S^{-1}\Gamma(K)S \;=\; \Gamma_r(K),\; T^{-1}\Gamma'(K)T \;=\; \Gamma'_r(K),\; S,T \in Gl(n,\mathbb{R}) \qquad (5.7)$$

where S,T have the property that $\Gamma_r(k) \;=\; \Gamma'_r(k),\; \forall\, k \;\in\; K$. Suppose an intertwining matrix m satisfying eq. (5.5) has been found. Then:

$$(T^{-1}mS)\Gamma_r(K)(S^{-1}m^{-1}T) \;=\; \Gamma_r(K), \qquad (5.8)$$

or, after defining $U \equiv T^{-1}mS$:

$$U\Gamma_r(K)U^{-1} \;=\; \Gamma_r(K). \qquad (5.9)$$

Of course, the coordinates of a vector $\mathbf{x} \in V_I$ depend on the choice of the basis, or equivalently, on the form of the representation. For fixed V_I, let $V_I(\Gamma(K))$ denote the set of coordinates of the internal space V_I on the basis on which the representation has the form $\Gamma(K)$. Analogously, $V'_I(\Gamma'(K))$ denotes the set of coordinates of another internal space V'_I on a basis, on which the representation has the form $\Gamma'(K)$. Then $V_I(\Gamma(K)) \;=\; SV_I(\Gamma_r(K))$. Given a fixed basis on which the representation has the form $\Gamma_r(K)$, the basis on which the representation takes the form $\Gamma(K)$ is determined up to a basis transformation due to the freedom in the reducing matrix S in eq. (5.7).
If the isomorphism (5.5) is regarded as a basis transformation, then $V_I(\Gamma(K))$ $= SV_I(\Gamma_r(K))$ is mapped by m on $V'_I(\Gamma'(K)) = mSV_I(\Gamma_r(K))$ using eqs. (5.7), (5.8).
If $\Gamma'(K) = \Gamma(K)$, then the matrix m is in the normalizer of $\Gamma(K)$ in $Gl(n,\mathbf{Z})$, defined by:

$$N(\Gamma(K)) \;=\left\{m \in Gl(n,\mathbf{Z}) \;\mid m\Gamma(k)m^{-1} \;\in\; \Gamma(K),\; \forall\, k \in K\right\}. \qquad (5.10)$$

Throughout this paper, with the normalizer is meant the normalizer in $Gl(n,\mathbf{Z})$. Following the analysis about the arithmetic equivalence of two arithmetic point groups, an arithmetic point group $\Gamma(K)$ with internal space V_I is arithmetically equivalent to $\Gamma(K)$ with internal space V'_I if and only if Condition 5.3.1 is satisfied. If Condition 5.3.1 is satisfied, then V_I and V'_I are called equivalent choices for the internal space (in fact, equivalent choices for the internal space refer to a permutation of the conjugacy classes due to

an automorphism).
With respect to the partition in arithmetic conjugacy classes, Condition 5.3.1 gives rise to a further partition: each arithmetic conjugacy class representative gives a number of arithmetically non-equivalent point groups in the sense of Condition 5.3.1. Now the normalizer can be decomposed into cosets w.r.t. the centralizer in $Gl(n, \mathbf{Z})$, defined by:

$$C(\Gamma(K)) = \left\{ m \in Gl(n, \mathbf{Z}) \mid m\Gamma(k)m^{-1} = \Gamma(k), \forall k \in K \right\}. \quad (5.11)$$

Denote this decomposition by:

$$N(\Gamma(K)) = \bigcup_{i=1}^{p} m_i C(\Gamma(K)). \quad (5.12)$$

Each coset $m_i C(\Gamma(K))$ corresponds to an automorphism φ_i: $\varphi_i(\Gamma(k)) = m_i\Gamma(k)m_i^{-1}$, $\forall k \in K$. A further decomposition can be made. The set of automorphisms $\{\varphi_1, \ldots, \varphi_p\}$ forms a group $A(K)$. A subgroup of $A(K)$ is formed by all inner automorphisms $\varphi_1, \ldots, \varphi_q$ defined by: $\varphi_i(\Gamma(k)) = m_i\Gamma(k)m_i^{-1}$, $\forall k \in K$, $m_i \in \Gamma(K)$. This further decomposition can be written as:

$$N(\Gamma(K)) = \bigcup_{i=1}^{p/q} m_i\Gamma(K)C(\Gamma(K)). \quad (5.13)$$

Now the representation of $\Gamma(K)$ carried by the internal space V_I is the same as the representation of $m\Gamma(K)m^{-1}$ on mV_I for each $m \in N(\Gamma(K))$. If $m \in C(\Gamma(K))$ or if $m \in \Gamma(K)$, then mV_I can be replaced by V_I (up to the freedom to vary V_I by the freedom in the matrix S in eq. (5.7)). For $m \in C(\Gamma(K))$ this is obvious from definition (5.11). For $m \in \Gamma(K)$ we can use the fact that on the reduced basis the matrix $S^{-1}mS$ has the same block form as any other $\Gamma_r(k) \in \Gamma_r(K)$. Hence the internal space is left unchanged (up to the changes due to the freedom of the reducing matrix S). Therefore, if we want to determine all non-equivalent choices for the internal space, only the p/q coset representatives of the normalizer w.r.t. the subgroup $\Gamma(K)C(\Gamma(K))$ have to be considered.

5.4 Modulated structures

If a modulated structure of dimension d is defined as a quasiperiodic structure for which main and satellite reflections can be distinguished in the

diffraction pattern, then there has to be a standard basis on which the point group matrices are of the form:

$$\Gamma(K) = \begin{bmatrix} \Gamma^E(K) & 0 \\ \Gamma^M(K) & \Gamma^I(K) \end{bmatrix} \subset Gl(n, \mathbf{Z}) \tag{5.14}$$

in direct space and of the form:

$$\Gamma^*(K) = \begin{bmatrix} \Gamma^{E^*}(K) & \Gamma^{M^*}(K) \\ 0 & \Gamma^{I^*}(K) \end{bmatrix} \subset Gl(n, \mathbf{Z}) \tag{5.15}$$

in reciprocal space. The representations $\Gamma(K)$ and $\Gamma^*(K)$ are related (Janssen and Janner 1987):

$$\Gamma(k) = \left[\Gamma^*(k^{-1})\right]^T, \ \forall k \in K, \tag{5.16}$$

where T means transposed. Hence the point groups $\Gamma^E(K)$ respectively $\Gamma^I(K)$ are crystallographic point groups in a d- and $(n-d)$-dimensional space.

Condition 5.4.1. An arithmetic point group $\Gamma(K)$ allows a modulated structure with Fourier module of rank n if and only if:

- 5.4.1.1. there is an $S \in Gl(n, \mathbf{Z})$ such that $S\Gamma(K)S^{-1}$ is of the form (5.14) in direct space or (5.15) in reciprocal space;
- 5.4.1.2. $\Gamma^E(K)$ is a faithful d-dimensional representation of K;
- 5.4.1.3. for each $\mathbb{R}$-irrep carried by the internal space there is an $\mathbb{R}$-equivalent $\mathbb{R}$-irrep carried by the external space.

Notice that it follows from Condition 5.4.1.1 that no $\mathbb{R}$-irrep carried by V_E should need any partner in V_I. Hence only arithmetic point groups which are crystallographic in a d-dimensional space have to be considered.
If we restrict ourselves to physical dimensions $d \leq 3$, then all $\mathbb{R}$-irreps are $\mathbb{R}$-equivalent to $\mathbf{Z}$-irreps. We assume these $\mathbf{Z}$-irreps to be known. So we have $\Gamma_r^{i,E}(K)$, $\Gamma_r^{j,I}(K) \subset Gl(n, \mathbf{Z})$ in eq. (5.4).
Consider an arithmetic point group $\Gamma(K)$. For each possible choice for the sum of $\mathbf{Z}$-irreps to be carried by V_I, the analysis is as follows. The first

problem is to find a matrix $S \in Gl(n, \mathbf{Z})$ bringing the point group on a standard basis (Condition 5.4.1.1). The matrices $\Gamma(k_i)$, $\Gamma^E(k_i)$, $\Gamma^I(k_i)$ for each point group generator k_i are known for d, $n-d \leq 4$. Furthermore the $\Gamma^M(k_i) \in M_{n-d,d}(\mathbf{Z})$ satisfy the following additional conditions. The Fourier spectrum corresponding to the basic structure has basis $\{\mathbf{a}_1{}^*, \ldots, \mathbf{a}_d{}^*\}$ and the modulation can be described in terms of modulation vectors $\mathbf{q}_1, \ldots, \mathbf{q}_{n-d}$. The set $\{\mathbf{a}_1{}^*, \ldots, \mathbf{a}_d{}^*, \mathbf{q}_1, \ldots, \mathbf{q}_{n-d}\}$ forms a d-dimensional $\mathbf{Z}$-module of rank n. The vectors $\mathbf{q}_j$ can be expressed in terms of the basic structure as:

$$\mathbf{q}_j = \sum_{i=1}^{d} \sigma_{ji} \mathbf{a}_i{}^* \ , \ 1 \leq j \leq n-d. \tag{5.17}$$

For actual systems, the coefficients $\sigma(p,T)_{ji}$ depend on pressure and temperature. Furthermore, since the modulation vectors $\mathbf{q}_j$ can be chosen inside the basic unit cell, the coefficients of σ satisfy:

$$0 \leq \sigma_{ji} < 1, \ 1 \leq j \leq n-d, \ 1 \leq i \leq d. \tag{5.18}$$

Then $\Gamma^M(k)$ satisfies the relation (Janner and Janssen 1979):

$$M_{n-d,d}(\mathbf{Z}) \ni \Gamma^M(k) = \sigma\Gamma^E(k) - \Gamma^I(k)\sigma, \quad \forall\, k \in K, \tag{5.19}$$

and the matrix σ can be written as:

$$\sigma = \sigma^i + \sigma^r \ ; \ \sigma^i \in M_{n-d,d}(\mathbb{R}) \ , \ \sigma^r \in M_{n-d,d}(\mathbb{Q}), \tag{5.20}$$

where σ^i and σ^r satisfy:

$$\sigma^i\Gamma^E(k) - \Gamma^I(k)\sigma^i = 0, \ \sigma^r\Gamma^E(k) - \Gamma^I(k)\sigma^r = \Gamma^M(k), \ \forall k \in K. \tag{5.21}$$

These relations limit the possibilities of the entries of the block Γ^M. If for each possible choice of $\Gamma^M(K)$ in rel. (5.19) no S can be found, and it can be proved that there does not exist such an S (with the technique of which the algorithmic steps have been described in § 5.3), then Condition 5.4.1.1 is proved to be violated, and $\Gamma(K)$ cannot describe a modulated structure.

Condition 5.4.2. Consider two n-dimensional arithmetic point groups $\Gamma(K)$ respectively $\Gamma'(K)$ with internal (external) space V_I (V_E) and V_I' (V_E'), both V_I and V_I' having dimension $n-d$. Denote the internal (external) space

$V_{I,st}$ ($V_{E,st}$) on which a point group on standard form acts, by its basis $\{\hat{\mathbf{e}}_{d+1}, \ldots, \hat{\mathbf{e}}_n\}$ ($\{\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_d\}$). Then $\Gamma(K)$ and $\Gamma'(K)$ are arithmetically equivalent as describing modulated structures if and only if:

- 5.4.2.1. There are matrices S, $T \in Gl(n, \mathbf{Z})$ such that $\Gamma_b(K) = S\Gamma(K)S^{-1}$ and $\Gamma'_b(K) = T\Gamma'(K)T^{-1}$ have the same block form (5.14) or (5.15);

- 5.4.2.2. In direct space: if $\mathbf{x} \in V_I$, then $S\mathbf{x} \in V_{I,st}$; if $\mathbf{x} \in V'_I$, then $T\mathbf{x} \in V_{I,st}$. In reciprocal space: if $\mathbf{x} \in V_E$, then $S\mathbf{x} \in V_{E,st}$; if $\mathbf{x} \in V'_E$, then $T\mathbf{x} \in V_{E,st}$;

- 5.4.2.3. There is an intertwining matrix m of the same block form as $\Gamma_b(K)$ and $\Gamma'_b(K)$ satisfying $m\Gamma_b(K)m^{-1} = \Gamma'_b(K)$.

Comparison with Condition 5.2.2 shows that the conditions on arithmetic equivalence are stronger. The reason is the following. Since the Fourier spectrum consists of main and satellite reflections, main reflections have to be mapped on main reflections by a point group element (Janner and Janssen 1979). Therefore S and T should be such that $\Gamma^E(K)$ respectively $\Gamma^I(K)$ are $\mathbf{Z}$-equivalent to $\Gamma^{E'}(K)$ and $\Gamma^{I'}(K)$. From now on, $\Gamma(K)$ and $\Gamma'(K)$ are assumed to be already on standard form. For the case that $\Gamma'(K) = \Gamma(K)$, this means that the normalizer of a point group $\Gamma(K)$ which is already on standard form, must have the same block form as $\Gamma(K)$.
The method to determine the normalizer of an arbitrary arithmetic n-dimensional point group can easily be applied to a modulated structure with the point group on a standard basis. For an n-dimensional point group, each normalizer element m is determined by linear equations satisfied by its n^2 coefficients. For a modulated structure, m has to satisfy the additional condition that $m_{ij} = 0$ for $1 \leq i \leq d$, $d+1 \leq j \leq n$ in direct space and $m_{ij} = 0$ for $1 \leq j \leq d$, $d+1 \leq i \leq n$ in reciprocal space. The procedure to determine a generating set for (a subset of) the normalizer and the procedure to check whether the set generates the whole normalizer are then completely the same (Wijnands 1991). Notice that for the general case of a quasiperiodic structure there is no such restriction on the normalizer.

5.5 Examples and Results

The first example is a point group isomorphic to $D_2 = < k_1,\ k_2 >$,

$$\Gamma(D_2) = < \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} > . \tag{5.22}$$

The representation $\Gamma(D_2)) \sim 2B_1 \oplus 2B_3$, where B_1 and B_3 are irreps of Klein's group, is already in reduced form: $\Gamma_r(D_2) = \Gamma(D_2)$. The matrix S in eq. (5.4) has the form:

$$S = \begin{bmatrix} \alpha & \gamma & 0 & 0 \\ \beta & \delta & 0 & 0 \\ 0 & 0 & \mu & \nu \\ 0 & 0 & \lambda & \eta \end{bmatrix} \in Gl(4,\mathbb{R}). \tag{5.23}$$

Since D_2 is abelian, there is only one inner automorphism. The only outer automorphism candidate is: $\varphi(\Gamma(k_1)) = \Gamma(k_2)$, $\varphi(\Gamma(k_2)) = \Gamma(k_1)$. A coset representative is:

$$m = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}. \tag{5.24}$$

The coset representative m in eq. (5.24) corresponds to the following automorphism:

$$\Gamma_r = \begin{bmatrix} B_1 & 0 & 0 & 0 \\ 0 & B_1 & 0 & 0 \\ 0 & 0 & B_3 & 0 \\ 0 & 0 & 0 & B_3 \end{bmatrix} \rightarrow m\Gamma_r m^{-1} = \begin{bmatrix} B_3 & 0 & 0 & 0 \\ 0 & B_3 & 0 & 0 \\ 0 & 0 & B_1 & 0 \\ 0 & 0 & 0 & B_1 \end{bmatrix} \tag{5.25}$$

Suppose the external space is three-dimensional. Then V_I can carry either B_1 or B_3. Suppose V_I carries B_1. Take $\{\hat{\mathbf{e}}_1\}$ as basis for $V_I(\Gamma_r)$. Then $V_I(\Gamma) = SV_I(\Gamma_r)$ is transformed by the matrix m to $mSV_I(m\Gamma_r m^{-1}) =$

$mSV_I(\Gamma_\tau) = mV_I(\Gamma)$:

$$V_I(\Gamma) \text{ with basis } \left\{ \begin{bmatrix} \alpha \\ \beta \\ 0 \\ 0 \end{bmatrix} \right\} \rightarrow mV_I(\Gamma) \text{ with basis } \left\{ \begin{bmatrix} 0 \\ 0 \\ \beta \\ \alpha \end{bmatrix} \right\}. \quad (5.26)$$

With use of rel. (5.25) we see that $mV_I(m\Gamma(D_2)m^{-1})$ and $V_I(\Gamma(D_2))$ carry the same sum of $\mathbb{R}$-irreps. Notice that $m\Gamma(D_2)m^{-1}$ and $\Gamma(D_2)$ are the same arithmetic point group. They are ordered differently due to the automorphism induced by m.
It follows from rel. (5.26) and from the fact that there is only one coset representative to be considered, that there are two choices for the internal space carrying B_1, and they are equivalent. The analysis for V_I carrying B_3 is completely analogous, yielding two equivalent choices for V_I, with the same basis vectors as in rel. (5.26).
In the case of a point group $\Gamma(C_2)$, generated by the first matrix in eq. (5.22), the two choices for the internal space given in rel. (5.26) are non-equivalent, since then there is no normalizer element relating them.

The second example is a representation of the icosahedral group I: $\Gamma(I)$

$$=<\Gamma(k_1),\Gamma(k_2)>=<\begin{bmatrix} 1&0&0&0&0&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\\0&1&0&0&0&0 \end{bmatrix}, \begin{bmatrix} 0&0&0&0&0&1\\1&0&0&0&0&0\\0&0&0&0&1&0\\0&0&-1&0&0&0\\0&0&0&-1&0&0\\0&1&0&0&0&0 \end{bmatrix}>. \quad (5.27)$$

The character table of I is as follows:

I	ϵ	k_1	${k_1}^2$	k_2	k_1k_2
Γ^1	1	1	1	1	1
Γ^2	3	$-\tau$	$1+\tau$	0	-1
Γ^3	3	$1+\tau$	$-\tau$	0	-1
Γ^4	4	-1	-1	1	0
Γ^5	5	0	0	-1	1

(5.28)

On the $\mathbb{R}$-reduced basis we have: $\Gamma_r(I) = \Gamma^3 \oplus \Gamma^2$, with:

$$\Gamma^3(I) = < \frac{1}{2}\begin{bmatrix} 1 & \tau & -1-\tau \\ \tau & 1+\tau & 1 \\ 1+\tau & -1 & \tau \end{bmatrix}, \frac{1}{2}\begin{bmatrix} -1 & -\tau & -1-\tau \\ \tau & 1+\tau & -1 \\ 1+\tau & -1 & -\tau \end{bmatrix} > \tag{5.29}$$

$$\Gamma^2(I) = < \frac{1}{2}\begin{bmatrix} -\tau & 1+\tau & -1 \\ 1+\tau & 1 & \tau \\ 1 & -\tau & -1-\tau \end{bmatrix}, \frac{1}{2}\begin{bmatrix} -\tau & 1+\tau & 1 \\ -1-\tau & -1 & \tau \\ 1 & -\tau & 1+\tau \end{bmatrix} > \tag{5.30}$$

where $\tau = (\sqrt{5}-1)/2$ is the golden mean. In order to have a non-mixing point group, the external space has to be of dimension three. Since I is non-crystallographic in a three-dimensional space, the representation carried by V_E needs a partner in V_I. Indeed Γ^2 and Γ^3 are partners. The most general form for a matrix S satisfying $S^{-1}\Gamma(I)S = \Gamma_r(I)$ is:

$$S = \begin{bmatrix} -\tau\alpha & -\alpha & 0 & \beta & (1+\tau)\beta & 0 \\ \tau\alpha & -\alpha & 0 & \beta & -(1+\tau)\beta & 0 \\ 0 & -\tau\alpha & -\alpha & -(1+\tau)\beta & 0 & -\beta \\ -\alpha & 0 & -\tau\alpha & 0 & -\beta & (1+\tau)\beta \\ -\alpha & 0 & \tau\alpha & 0 & -\beta & -(1+\tau)\beta \\ 0 & -\tau\alpha & \alpha & -(1+\tau)\beta & 0 & \beta \end{bmatrix} \tag{5.31}$$

with $\mathbb{R} \ni \alpha, \beta$ such that $\det(S) \neq 0$. There are 24 respectively 20 point group elements with the same invariants as k_1 and k_2. Hence there are 480 automorphism candidates of the form (5.5). Since the inner automorphism group of I has order 60, there are 480/60=8 coset representatives to be determined. Of six of them the determinant expression shows that integer matrix coefficients can never yield a determinant equal to ± 1. The remaining two representatives are the unit matrix and the matrix:

$$m = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}. \tag{5.32}$$

On the $\mathbb{R}$-reduced basis the matrix $U = S^{-1}mS$ defines the following automorphism:

$$U\Gamma_r U^{-1} = \begin{bmatrix} 0 & U_1 \\ U_2 & 0 \end{bmatrix} \begin{bmatrix} \Gamma^3 & 0 \\ 0 & \Gamma^2 \end{bmatrix} \begin{bmatrix} 0 & U_1 \\ U_2 & 0 \end{bmatrix}^{-1} \sim \begin{bmatrix} \Gamma^2 & 0 \\ 0 & \Gamma^3 \end{bmatrix}.$$

Suppose V_I carries Γ^2. Then $V_I(\Gamma_r)$ has basis $\{\hat{\mathbf{e}}_4, \hat{\mathbf{e}}_5, \hat{\mathbf{e}}_6\}$ and $UV_I(\Gamma_r)$ has basis $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$. Hence there are two equivalent choices for the internal space carrying Γ^2. The case that V_I carries Γ^3 is completely analogous and yields the same equivalent choices for V_I. On the basis on which the point group is integral, the most general form for the basis of the internal space is given either by the first three or by the last three columns of S in eq. (5.31).

The third example is the point group denoted by $7mm =< \Gamma(k_1), \Gamma(k_2) > \subset Gl(6, \mathbf{Z})$, which is in the isomorphism class D_7 (Janssen 1990):

$$7mm = < \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} > . \quad (5.33)$$

The character table of D_7 is given below:

D_7	ϵ	k_1	${k_1}^2$	${k_1}^3$	k_2
Γ^1	1	1	1	1	1
Γ^2	1	1	1	1	-1
Γ^3	2	$2cos(\frac{2\pi}{7})$	$2cos(\frac{4\pi}{7})$	$2cos(\frac{6\pi}{7})$	0
Γ^4	2	$2cos(\frac{4\pi}{7})$	$2cos(\frac{8\pi}{7})$	$2cos(\frac{12\pi}{7})$	0
Γ^5	2	$2cos(\frac{6\pi}{7})$	$2cos(\frac{12\pi}{7})$	$2cos(\frac{18\pi}{7})$	0

(5.34)

It turns out that $\Gamma \sim \Gamma_r = \Gamma^3 \oplus \Gamma^4 \oplus \Gamma^5$, all being $\mathbb{C}$-equivalent to $\mathbb{R}$-irreps. The generators $\Gamma^{j+2}(k_1)$ and $\Gamma^{j+2}(k_2)$, $1 \leq j \leq 3$, can be chosen to be:

$$\begin{bmatrix} cos(\frac{2\pi j}{7}) - 3sin(\frac{2\pi j}{7}) & 4sin(\frac{2\pi j}{7}) \\ -5/2sin(\frac{2\pi j}{7}) & cos(\frac{2\pi j}{7}) + 3sin(\frac{2\pi j}{7}) \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ \frac{3}{2} & -1 \end{bmatrix}. \quad (5.35)$$

The normalizer of $7mm$ has been determined (Wijnands 1991). There are six respectively seven point group elements having the same invariants as the point group generators k_1 and k_2. Therefore there are 42 candidates for automorphisms. Since the inner automorphism group of D_7 has order 14, there are three outer automorphisms to be determined. One coset representative is $\mathbb{1}_6$, the two others are:

$$n_2 = \begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & -1 & 0 \\ -1 & -1 & 1 & 1 & -1 & 0 \\ 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & -1 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & -1 \end{bmatrix}, n_3 = \begin{bmatrix} -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1 & 0 & -1 \\ -1 & 1 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 1 & 0 & 1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \end{bmatrix}. \tag{5.36}$$

In order to have a non-mixing point group, the external space has to be two-dimensional (since we restrict ourselves to physical dimensions lower than four). Consider a subspace $\mathbb{R}^6 \supset V_m = V_E(\Gamma_r)$ with basis $\{\hat{\mathbf{e}}_{2m-1}, \hat{\mathbf{e}}_{2m}\}$, $1 \leq m \leq 3$. Then coset representative n_2 transforms V_1 to V_3, V_2 to V_1 and V_3 to V_2. Representative n_3 transforms V_1 to V_2, V_2 to V_3 and V_3 to V_1. Hence all choices for the internal space: $V_I = V_a \cup V_b$, $1 \leq a < b \leq 3$, are equivalent.

The fourth example is the point group $\Gamma(O \times C_2) = m\bar{3}m \oplus m\bar{3}m$, $K = O \times C_2$, for the incommensurate phase of wustite, $Fe_{1-x}O$, described by Yamamoto (1982). In the incommensurate phase, wustite has a three-dimensional cubic fundamental cell with a three-dimensional modulation with arithmetic point group $\Gamma(K) =< \Gamma(k_1), \Gamma(k_2), \Gamma(k_3) >$

$$= < \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}, -\mathbb{1}_6 > . \tag{5.37}$$

There is only one choice for the basis of the internal space $V_I(\Gamma)$: $\{\alpha\hat{\mathbf{e}}_1 + \beta\hat{\mathbf{e}}_4, \alpha\hat{\mathbf{e}}_2 + \beta\hat{\mathbf{e}}_5, \alpha\hat{\mathbf{e}}_3 + \beta\hat{\mathbf{e}}_6\}$. In the incommensurate phase of wustite, main and satellite reflections can be distinguished. Suppose we have two point groups, one with internal space $V_I(\Gamma)$ having as basis $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$, the other with

another internal space $V_I'(\Gamma)$ having as basis $\{\hat{\mathbf{e}}_4, \hat{\mathbf{e}}_5, \hat{\mathbf{e}}_6\}$. First the two point groups have to be transformed to a standard form. On standard form, the two point groups are identical, and therefore the two choices for the internal space are equivalent.

Using the notation of Janner *et al.* (1983), wustite has symmetry group $Pm\bar{3}m(\alpha,0,0)$, meaning that $\Gamma^E(K)$ and $\Gamma^I(K)$ are full cubic point groups without centering and one of the modulation basis vectors can be chosen to be $\mathbf{q}_1 = (\alpha,0,0)$ in coordinates w.r.t. the conventional unit cell. According to Table 1 in the paper of Janner *et al.* (1983), there are ten arithmetically non-equivalent (when considered as describing modulated structures) point groups with full cubic symmetry in the external and internal space. The question is: which of these point groups are arithmetically equivalent when considered as describing quasiperiodic structures? Since in all ten cases $\Gamma^E(K)$ and $\Gamma^I(K)$ are $\mathbb{R}$-equivalent, there is only one choice for the internal space, and the question comes down to finding all arithmetically equivalent point groups (regarded as n-dimensional point groups). First the form of $\Gamma^M(k_i)$ for the point group generators k_i in rel. (5.37) has to be determined for the ten point groups under consideration.
Suppose $\Gamma^E(K) = \Gamma^I(K) = Pm\bar{3}m$. Starting with an arbitrary matrix σ, we have, with use of rel. (5.20):

$$\sigma = \begin{bmatrix} \alpha & \beta & \beta \\ \beta & \alpha & \beta \\ \beta & \beta & \alpha \end{bmatrix} \in M_{3\times3}(\mathbb{R}),\ 0 \le \alpha < 1,\ \beta = 0 \text{ or } \beta = \frac{1}{2}. \qquad (5.38)$$

Hence the two possible arithmetic point groups are $Pm\bar{3}m(\alpha,0,0)$, with:

$$\sigma^z = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix},\ \sigma^r = 0 \Rightarrow \Gamma^M(k) = 0,\ \forall k \in K \qquad (5.39)$$

and $Pm\bar{3}m(\alpha, \frac{1}{2}, \frac{1}{2})$, with the same σ^z but:

$$\sigma^r = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix} \Rightarrow \Gamma^M(k_1) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & -1 & 0 \\ 0 & -1 & 0 \end{bmatrix}, \qquad (5.40$$

and $\Gamma^M(k_2) = \Gamma^M(k_3) = 0$ for the generators k_1, k_2, k_3 of rel. (5.37). These two point groups are arithmetically non-equivalent when regarded as describing modulated structures. The same analysis shows that the eight other arithmetic point groups have $\Gamma^M(k) = 0$, $\forall k \in K$. First we try to find an intertwining matrix m for two point groups $\Gamma(K)$ and $\Gamma'(K)$, each having $\Gamma^M(K) = 0$:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} \Gamma^E(K) & 0 \\ 0 & \Gamma^I(K) \end{bmatrix} = \begin{bmatrix} \Gamma^{E'}(K) & 0 \\ 0 & \Gamma^{I'}(K) \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix}.$$

Suppose $\Gamma^I(K)$ is not $\mathbf{Z}$-equivalent to $\Gamma^{I'}(K)$. Then $D = 0$ because of Schur's Lemma. Hence $B, C = \pm\mathbb{1}_3$ otherwise $\det(m) = 0$. Consequently, Schur's Lemma tells that $\Gamma^I(K) \sim \Gamma^{E'}(K)$ and $\Gamma^E(K) \sim \Gamma^{I'}(K)$.
Suppose $\Gamma^I(K)$ is $\mathbf{Z}$-equivalent to $\Gamma^{I'}(K)$. Then $D = \pm\mathbb{1}_3$. We have either
1) $\Gamma^E(K) \sim \Gamma^{E'}(K)$, so $A = \pm\mathbb{1}_3$, or
2) $\Gamma^E(K) \not\sim \Gamma^{E'}(K)$, so $A = 0$. Then $B, C = \pm\mathbb{1}_3$ otherwise $\det(m) = 0$. Consequently $\Gamma^I(K) \sim \Gamma^{E'}(K)$ and $\Gamma^E(K) \sim \Gamma^{I'}(K)$ but then also $\Gamma^E(K) \sim \Gamma^{E'}(K)$ which is contradicting the assumption that $\Gamma^E(K) \not\sim \Gamma^{E'}(K)$.
Therefore $\mathbf{Z}$-equivalence for the nine point groups with $\Gamma^M(K) = 0$ comes down to interchanging $\Gamma^E(K)$ and $\Gamma^I(K)$, e.g. by the following intertwining matrix:

$$m = \begin{bmatrix} 0 & \mathbb{1}_3 \\ \mathbb{1}_3 & 0 \end{bmatrix} : \begin{array}{lcl} Pm\bar{3}m(\alpha,\alpha,\alpha) & \sim & Fm\bar{3}m(\alpha,0,0); \\ Im\bar{3}m(\alpha,0,0) & \sim & Pm\bar{3}m(0,\alpha,\alpha); \\ Im\bar{3}m(\alpha,\alpha,\alpha) & \sim & Fm\bar{3}m(0,\alpha,\alpha). \end{array} \tag{5.41}$$

The only other possible equivalence is between $\Gamma(K) = Pm\bar{3}m(\alpha, \frac{1}{2}, \frac{1}{2})$ and one of the other nine point groups. It turns out that $\Gamma(K)$ is $\mathbf{Z}$-equivalent to $\Gamma'(K) = Im\bar{3}m(\alpha,\alpha,\alpha)$:

$$m\Gamma(K)m^{-1} = \Gamma'(K),\ m = \begin{bmatrix} 1 & 1 & 1 & 0 & -1 & -1 \\ 1 & 1 & 1 & -1 & 0 & -1 \\ 1 & 1 & 1 & -1 & -1 & 0 \\ 0 & 1 & 1 & 1 & -1 & -1 \\ 1 & 0 & 1 & -1 & 1 & -1 \\ 1 & 1 & 0 & -1 & -1 & 1 \end{bmatrix}. \tag{5.42}$$

Hence there are six arithmetic equivalence classes splitting into ten arithmetic equivalence classes when the point groups are considered to describe

modulated structures.

The fifth example is also an illustration that two arithmetically equivalent point groups describing quasiperiodic structures can be arithmetically non-equivalent when the point groups are to describe modulated structures. Consider the following two realizations of C_2:

$$\Gamma(C_2) = < \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & -1 \end{bmatrix} > , \; \Gamma'(C_2) = < \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} > . \quad (5.43)$$

Then $\Gamma(C_2)$, $\Gamma'(C_2) \sim A \oplus 2B$. The basisvectors of the internal space $V_I(\Gamma)$ respectively $V_I'(\Gamma')$ are $(\alpha, 0, \beta)^T$ and $(\gamma, -\gamma, \delta)^T$. Hence if $\Gamma(C_2)$ and $\Gamma'(C_2)$ are arithmetically equivalent as n-dimensional point groups, they are also arithmetically equivalent as point groups describing a quasiperiodic structure. There is an intertwining matrix:

$$m = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & -1 \\ 1 & 0 & 0 \end{bmatrix} , \; m\Gamma(C_2)m^{-1} = \Gamma'(C_2) \quad (5.44)$$

and the point groups describing quasiperiodic structures are arithmetically equivalent.

Next, the problem of equivalence is studied for modulated structures. Suppose that main and satellite reflections can be distinguished. The problem is worked out in direct space. The first problem is to determine all possible choices for the block form (5.14) with $\Gamma^E(C_2) = A \oplus B$ and $\Gamma^I(C_2) = B$. For $\Gamma^I(C_2)$ there is only one possible representation: $\Gamma^I(C_2) =< -1 >$. For $\Gamma^E(C_2)$ there are two $\mathbf{Z}$-inequivalent representations:

$$\Gamma^E(C_2) = < \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} > \text{ or } \Gamma^{\mathrm{E}}(\mathrm{C}_2) = < \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} > . \quad (5.45)$$

It follows from rel. (5.18), (5.19) that the only possibilities for the block form (5.14) are:

$$pm(\alpha, 0) = < \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} >, \; pm(\alpha, \frac{1}{2}) = < \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 1 & 0 & -1 \end{bmatrix} >,$$

$$\text{and } cm(\alpha,0) = < \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} >, \tag{5.46}$$

all with standard basisvector $(0,0,1)^T$. Considered as 3-dimensional arithmetic point groups, the first of these three point groups is arithmetically non-equivalent to the latter point groups, which are arithmetically equivalent. Hence there are at most two non-equivalent choices of the internal space for our point groups $\Gamma(C_2)$ and $\Gamma'(C_2)$ (recall that $\Gamma(C_2)$ and $\Gamma'(C_2)$ are arithmetically equivalent 3-dimensional arithmetic point groups).
Now $\Gamma(C_2)$ with V_I having basisvector $(0,0,1)^T$ describing a modulated structure, is arithmetically equivalent to $pm(\alpha, \frac{1}{2})$: with

$$S = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \text{ it holds that } S\Gamma(C_2)S^{-1} = < \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 1 & 0 & -1 \end{bmatrix} >, \tag{5.47}$$

and S maps the basisvector $(0,0,1)^T$ on $(0,0,1)^T$, the standard basisvector of the internal space for $pm(\alpha, \frac{1}{2})$. Then $\Gamma'(C_2)$ with basis $(1,-1,0)^T$ for $V_I'(\Gamma')$ is also arithmetically equivalent to $pm(\alpha, \frac{1}{2})$, since $\Gamma(C_2)$ and $\Gamma'(C_2)$ are arithmetically equivalent as 3-dimensional arithmetic point groups, and also $mV_I(\Gamma) = V_I'(\Gamma')$, as follows from rel. (5.44).
In the same way it can be proved that $V_I(\Gamma)$ with basisvector $(1,0,0)^T$ and $V_I'(\Gamma')$ with basisvector $(0,0,1)^T$ are equivalent choices for the internal space, using rel. (5.44). With use of (5.46) we see that both point groups are of type $cm(\alpha,0)$.
On the other hand, $V_I(\Gamma)$ with basisvector $(0,0,1)^T$ and $V_I'(\Gamma')$ with basisvector $(0,0,1)^T$ are non-equivalent choices for the internal space since $mV_I(\Gamma)$ has a non-zero component in the external space $V_E'(\Gamma')$. For the same reason $V_I(\Gamma)$ with basisvector $(1,0,0)^T$ and $V_I'(\Gamma')$ with basisvector $(1,-1,0)^T$ are non-equivalent choices for the internal space.
Hence for both point groups $\Gamma(C_2)$ and $\Gamma'(C_2)$ there are two arithmetic equivalence class representatives. As representatives one can take $\Gamma(C_2)$ and $\Gamma'(C_2)$, both with $(0,0,1)^T$ as basis vector for the internal space. Then $\Gamma(C_2) = pm(\alpha, \frac{1}{2})$ and $\Gamma'(C_2) = cm(\alpha,0)$.

5.6 Concluding remarks

A procedure has been described to verify whether a given arithmetic point group allows an incommensurate structure. If so, then for a given sum of real irreducible representations to be carried by the internal space, the most general form for this internal space is determined. Equivalent choices for the internal space can be given in the most general form by using the action of the normalizer of the point group. Two point groups, arithmetically equivalent as n-dimensional point groups, can be arithmetically non-equivalent when considered as describing quasiperiodic structures. This gives a further partition of the arithmetic crystal classes.

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Dutch summary

Samenvatting

Dit proefschrift behandelt ruimtegroepsymmetrie-eigenschappen van quasiperiodieke kristallen en de relatie tussen een schalingssymmetrie-eigenschap en het gedrag van elektronen voor een bepaald type 1-dimensionale quasiperiodieke kristallen.
Quasiperiodieke kristallen kunnen worden beschreven als doorsnijding van een hoger-dimensionale struktuur met de fysische ruimte. De hoger-dimensionale struktuur kan als periodiek gekozen worden. In de hoger-dimensionale ruimte is er dan een eenheidscel en een rooster aan te geven. Het quasiperiodieke kristal kan periodiek zijn of niet periodiek.

Voor fysische eigenschappen is kennis van de symmetrie zeer belangrijk. Voor periodieke kristallen kan deze symmetrie beschreven worden met behulp van een ruimtegroep. Deze bevat alle Euclidische transformaties die het kristal invariant laten. Ruimtegroep-elementen zijn combinaties van operaties die een punt, de oorprong, invariant laten (i.e. een element van de puntgroep van het kristal) en translaties. In drie dimensies zijn er 219 niet-equivalente ruimtegroepen, d.w.z. ruimtegroepen die niet door een affiene transformatie in elkaar over te voeren zijn (11 paren zijn equivalent, ze zijn echter niet geconjugeerd door een orientatie-behoudende affiene transformatie; zulke paren noemt men enantiomorf). Als twee ruimtegroepen equivalent zijn, dan zijn ze ook isomorf. Volgens een stelling van Bieberbach geldt ook het omgekeerde: isomorfe ruimtegroepen zijn altijd geconjugeerd door een affiene transformatie.

Hoewel quasiperiodieke kristallen niet periodiek hoeven te zijn, bezitten zij wel een perfecte orde. Quasikristallen, die pas in 1984 ontdekt werden, bezitten bovendien vaak een schalingssymmetrie-eigenschap genaamd zelfsimilariteit. Als men een deel van het kristal schaalt met een welbepaalde factor, dan vallen de atoomposities in de nieuwe struktuur samen met atoomposities in het niet-geschaalde kristal. Deze schalingseigenschap wordt ook

teruggevonden in de konstruktie van een quasikristal in stappen. Een bekend voorbeeld is de Fibonacci-keten, die is opgebouwd uit korte en lange intervallen (of, in een equivalente beschrijving, uit atomen van twee typen). Achtereenvolgende periodieke benaderingen van de Fibonacci-keten kunnen als volgt verkregen worden. Startend met een lang interval, wordt bij iedere stap in de konstruktie een lang interval vervangen door een lang gevolgd door een kort interval, en een kort interval wordt vervangen door een lang interval. De na elke stap verkregen eindige sequentie vormt dan de eenheidscel van het oneindige kristal. Na oneindig veel stappen verkrijgt men de Fibonacci-keten. Voor elke stap in de konstruktie van de Fibonacci-keten, kan men het energiespectrum voor de elektronen berekenen met behulp van een transfer-matrix methode (merk op dat elke benadering bij konstruktie periodiek is) met een zekere site-potentiaal. Wanneer de berekening gedaan wordt in een tight-binding benadering, blijkt dat een deel van het spectrum voor een bepaalde benadering, in verkleinde vorm verschijnt bij een volgende benadering. Wanneer men zich beperkt tot de middelste banden van ieder spectrum, kan, door de juiste benaderingen met elkaar te vergelijken, een uniforme schalingsfactor gevonden worden.

In hoofdstuk 2 van dit proefschrift wordt dit schalingsgedrag onderzocht voor de familie van gegeneraliseerde Fibonacci-ketens, waartoe de Fibonacci-keten behoort, ieder met een eigen substitutieregel en met als site-potentiaal een stap-potentiaal of een sinusvormige potentiaal. Voor 4 typen wordt numeriek een schalingsparameter van het middelste deel van het energiespectrum bepaald. Tevens wordt voor de stap-potentiaal een voor de hele familie geldende niet-lineaire recursieve afbeelding gekonstrueerd. De numeriek gevonden schalingswaarden zijn in overeenstemming met de waarden verkregen door linearisatie van deze afbeelding rond bepaalde cykels.
Ook de totale bandbreedte voor iedere benadering wordt numeriek bepaald voor de 4 typen en voor beide potentialen. Op grond van het gedrag van de totale bandbreedte als funktie van het aantal banden schijnt het spectrum singulier continue te zijn, hetgeen erop wijst dat de elektrongolffunkties in de limiet (i.e. voor het quasikristal) noch gelocaliseerd noch uitgebreid zijn. Hoewel quasikristallen niet periodiek zijn, bezitten zij wel de interessante lokale eigenschap dat ieder eindig deel van het kristal op een orthogonale transformatie na, voorkomt elders in het kristal. Op deze manier kan men ook quasikristallen met elkaar vergelijken. Indien elk eindig deel van het ene

kristal, eventueel na een Euclidische transformatie, in het andere quasikristal voorkomt, noemt men deze kristallen lokaal isomorf.

In hoofdstuk 2 wordt voor ieder type, afhankelijk van de beginvoorwaarden, bestudeerd welke gegeneraliseerde Fibonacci-ketens lokaal isomorf zijn. Gegeneraliseerde Fibonacci-ketens blijken hetzelfde energiespectrum te hebben dan en slechts dan als ze lokaal isomorf zijn.

De klassificatie van niet-isomorfe ruimtegroepen in dimensies hoger dan vier is nog niet bekend, terwijl voor sommige quasiperiodieke strukturen een 6-dimensionale beschrijving nodig is. Een deel van die klassificatie is wel reeds mogelijk.
In gegeven dimensie bestaan slechts eindig veel arithmetische kristalklassen (een arithmetische puntgroep is een eindige groep matrices met gehele coefficienten, aangezien een rooster invariant dient te worden gelaten. Arithmetisch equivalente puntgroepen beschrijven dezelfde puntgroep op een andere roosterbasis. Een arithmetische kristalklasse bestaat uit alle arithmetisch equivalente puntgroepen). Voor een representant van elke kristalklasse kunnen alle niet-isomorfe ruimtegroepen gekonstrueerd worden met het formalisme van groepsuitbreidingen, door de ruimtegroep op te vatten als uitbreiding van de translatie-normaalondergroep met de puntgroep. Deze konstruktie verloopt in twee fasen.
Eerst worden alle niet-equivalente uitbreidingen afgeleid. Daarvoor is het belangrijk dat de presentatie van de puntgroep in termen van generatoren en definierende relaties, i.e., woorden in de generatoren die de puntgroepstruktuur geheel vastleggen, bekend is. Voor een willekeurige puntgroep in een willekeurige dimensie was dit probleem nog niet opgelost.

In hoofdstuk 3 van dit proefschrift worden vier algorithmische methodes gepresenteerd om, gegeven een verzameling generatoren van een arithmetische puntgroep, een verzameling definierende relaties te bepalen. Als criterium om te bepalen of een set woorden een set definierende relaties vormt, wordt genomen dat het woordprobleem kan worden opgelost. Van de vier besproken methodes blijkt één methode het meest efficient te zijn. In deze methode wordt de puntgroep in stappen geanalyseerd. Startend met de ondergroep, gegenereerd door de eerste generator, wordt de volgende ondergroep gegenereerd door de groep uit de vorige stap samen met de volgende generator. Daarna wordt een cosetdecompositie t.o.v. de ondergroep uit

de vorige stap uitgevoerd, en nieuwe definierende relaties worden gekonstrueerd.
De tweede stap in de konstruktie is het herkennen welke ruimtegroepen door een andere keuze van de roosterbasis in elkaar zijn over te voeren. Hiervoor is de normalizator van de arithmetische puntgroep van belang. Een ruimtegroep is isomorf met een andere ruimtegroep met dezelfde arithmetische puntgroep, als de ene groep door conjugatie met een normalizator-element in de andere (modulo het rooster en modulo een oorsprongverschuiving) overgaat. In dimensies hoger dan vier is, mede vanwege het gebrek aan klassificatie van arithmetische kristalklassen, niet de normalizator van elke klasserepresentant bekend.

In hoofdstuk 4 wordt een algorithmische methode beschreven om, gegeven een set generatoren van een arithmetische puntgroep in een willekeurige dimensie, een set generatoren van (een ondergroep van) de normalizator te vinden.
Eerst wordt gepoogd een set generatoren van de centralizator te konstrueren. Daartoe wordt uit een eindige subset van de centralizator een set generatoren gedestilleerd door te eisen dat alle matrices in deze subset volgens een welgedefinieerd criterium in termen van deze generatoren uit te drukken zijn. Vervolgens wordt onderzocht of de gevonden set niet slechts een eindige ondergroep van de centralizator genereert. Het succes van deze procedure hangt van de puntgroep af. Voor sommige puntgroepen kan volledigheid bewezen worden, voor andere kan volledigheid slechts aannemelijk worden gemaakt.
De laatste stap is het bepalen van cosetrepresentanten van de normalizator t.o.v. de centralizator. Elke coset correspondeert met een ander automorfisme van de puntgroep. De set automorfismen wordt onderverdeeld in inwendige en uitwendige automorfismen. De bepaling van een volledige set cosetrepresentanten blijkt voor alle onderzochte puntgroepen exact te zijn.

De ruimtegroepen voor quasiperiodieke kristallen zijn niet gewone hoger-dimensionale ruimtegroepen doch zogenaamde superruimtegroepen. De fysische ruimte is een in de hoger-dimensionale ruimte onderscheidbare ruimte. Rekening hiermee houdend, komt men tot een fijnere equivalentierelatie. Twee puntgroepen die arithmetisch equivalent zijn als hoger-dimensionale puntgroep, d.w.z. zonder een fysische ruimte te onderscheiden, kunnen in-

equivalent zijn wanneer er wel zo'n ruimte is.

In hoofdstuk 5 wordt bestudeerd aan welke eisen een arithmetische puntgroep moet voldoen om een quasiperiodieke maar niet periodieke struktuur te beschrijven. De analyse beperkt zich tot puntgroepen die, gegeven een bepaalde dimensie van de fysische ruimte, niet mengend zijn, d.w.z. puntgroepen die de fysische ruimte niet mengen met de additionele ruimte, die loodrecht op de fysische ruimte staat. Dan is er een deelruimte met de fysische dimensie die een geheel aantal, over de reele getallen irreducibele, representaties draagt. De eis voor niet periodieke quasiperiodiciteit is dat elke representatie, gedragen door de additionele ruimte, ofwel een partner in de fysische ruimte heeft (omdat de representatie zelf over de reele getallen niet equivalent is met een gehele representatie), ofwel een equivalente representatie in de fysische ruimte heeft (door een geschikte draaiing van het assenstelsel kan dan een niet periodieke quasiperiodieke struktuur toegestaan zijn). Tevens dient de fysische ruimte een trouwe representatie van de arithmetische puntgroep te dragen.
Twee puntgroepen die voldoen aan deze eis, ieder met een keuze voor de fysische ruimte, zijn dan en slechts dan arithmetisch equivalent wanneer zij arithmetisch equivalent zijn als hoger-dimensionale puntgroep via een transformatiematrix die de fysische ruimte van de ene puntgroep overvoert in de fysische ruimte van de andere puntgroep. Op deze manier kan men ook bepalen welke keuzen van de fysische ruimte voor een gegeven puntgroep inequivalent zijn. Inequivalente keuzen corresponderen met inequivalente arithmetische kristalklassen.
Voor het speciale geval van een gemoduleerde kristalfase, waarbij in het diffractiepatroon hoofd- en satellietreflecties kunnen worden onderscheiden, is de voorwaarde voor equivalentie van twee puntgroepen strenger. Een puntgroepelement dient hoofdreflecties af te beelden op hoofdreflecties. Dit leidt tot een fijnere equivalentierelatie dan voor algemene quasiperiodieke kristallen. Ook is er dan een extra eis voor de gedaante van de normalizatorelementen.

Op basis van de hierboven beschreven groepentheoretische algorithmische methodes (hoofdstuk 3,4,5) zijn computerprogramma's, geschreven in Fortran77, ontwikkeld waarmee voor verschillende arithmetische puntgroepen resultaten berekend werden.

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