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

1991 J. Phys. A: Math. Gen. 24 5703

(http://iopscience.iop.org/0305-4470/24/24/008)

J. Phys. A: Math. Gen. **24** (1991) 5703–5720. Printed in the UK

An algorithm to find generators for the normalizer of an n-dimensional crystallographic point group in $\mathrm{Gl}(n, \mathbb{Z})$

Frank Wijnands

Institute for Theoretical Physics, University of Nijmegen, 6525 ED Nijmegen, The Netherlands

Received 30 April 1991, in final form 11 July 1991

Abstract. A new method for finding generators for the normalizer 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.

1. Introduction

As is well known, the normalizer $N(K)$

$$N(K) = \{m \in \mathrm{Gl}(n,\mathbb{Z}) | mkm^{-1} \in K \; \forall \; k \in K\} \tag{1}$$

of a finite group $K \subset \mathrm{Gl}(n,\mathbb{Z})$ (then K is called a finite unimodular group, crystallographic point group or arithmetic point group), is finitely generated (Siegel 1943). 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, Janssen *et al* 1969, Fast and Janssen 1971).

For n = 1,2,3 all finite subgroups of $\mathrm{Gl}(n,\mathbb{Z})$ and their normalizer have been well known for a long time. For n = 4, a complete list of finite subgroups of $\mathrm{Gl}(n,\mathbb{Z})$ and their normalizer was given by Brown *et al* (1973, 1978). For n = 5 all maximal finite subgroups of $\mathrm{Gl}(n,\mathbb{Z})$ have been determined by Ryskov (1972a, b) and Bülow (1973) and all maximal finite absolutely irreducible subgroups of $\mathrm{Gl}(n,\mathbb{Z})$ were computed up to $\mathbb{Z}$-equivalence by Plesken and Pohst for n = 5,7 (1977a) and for n = 6 (1977b). 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 section 2 the achievement of a set of generators is described due to the coset decomposition of the normalizer WRT the centralizer and due to the coset decomposition of a subgroup of the automorphism group of the point group WRT its inner automorphisms. Section 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 section 4. How one finds representatives of the cosets of the normalizer WRT the centralizer, is discussed in section 5. An algorithm based upon the methods described in sections 3,4,5 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 section 6. Results for some point groups for $n = 5$ and $n = 6$ are presented in section 7.

2. Organization of generators due to coset decomposition of the normalizer

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

$$C(K) = \{c \in \mathrm{Gl}(n,\mathbb{Z}) | ck = kc \;\forall\; k \in K\} \tag{2}$$

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

$$C(K) \trianglelefteq N(K). \tag{3}$$

It is possible to decompose $N(K)$ in cosets WRT $C(K)$:

$$N(K) = \bigcup_{i=1}^{p} n_i C(K) \tag{4}$$

where n_i corresponds to some automorphism $\varphi_i : K \to$ K, defined by:

$$\varphi_i(k) = n_i k n_i^{-1} \qquad \forall k \in K$$

$(n_1 \equiv I_n)$. Then

$$I(K) \trianglelefteq A(K) \subseteq \mathrm{Aut}(K) \tag{5}$$

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

$$C(K) = \langle c_1, ..., c_e \rangle \tag{6}$$

for a point group

$$K = \langle k_1, ..., k_s \rangle. \tag{7}$$

Due to relation (5), $A(K)$ can be decomposed in cosets WRT $I(K)$:

$$A(K) = \bigcup_{i=1}^{t} \varphi_i I(K) \tag{8}$$

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

$$I(K) = \langle \Theta_1, ..., \Theta_r \rangle \tag{9}$$

and coset representatives $\{\varphi_1, \ldots, \varphi_t\}$ according to equation (8). In the rest of this paper, n_i is a matrix corresponding to the automorphism φ_i.

3. How to find generators for a matrix group

As is pointed out in section 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 some $m \in \mathrm{G} \equiv \langle g_1, \ldots, g_f \rangle$ for a matrix group G. Say $m = g_1^2 g_4^{-1}$; now consider three different paths $m \to I_n$, such that at each step the number of terms in a word is decreased by one:

1. $m = g_1^2 g_4^{-1} \to g_1 g_4^{-1} \to g_4^{-1} \to I_n$
2. $m = g_1^2 g_4^{-1} \to g_1 g_4^{-1} \to g_1 \to I_n$
3. $m = g_1^2 g_4^{-1} \to g_1^2 \to g_1 \to I_n$.

Introduce the norm of a matrix in a straightforward way:

$$N(m) = \sum_{i,j=1}^{n} (m_{ij})^2. \tag{10}$$

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 $\{g_1, \ldots, g_f\}$ if there exists a path

$$m \equiv m(0) \to m(1) \to \cdots \to m(L) \equiv I_n (L \in \mathbb{N})$$

such that

$$\forall 0 \leqslant i < L \, \exists \, 1 \leqslant j \leqslant f \qquad q \in \{-1, 1\}$$

either

$$N(g_j^q m(i)) < N(m(i)) \Rightarrow m(i+1) = g_j^q m(i)$$

or

$$N(m(i) g_j^q) < N(m(i)) \Rightarrow m(i+1) = m(i) g_j^q \tag{11}$$

or

$$i = L - 1 \text{ and } m(i) = g_j^q.$$

The criterion (11) ensures, that by a finite number of steps ($\leqslant N(m)$) a matrix m is decided to be in a generating set or not. Of course, in principle more paths $m \to I_n$, satisfying condition (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 $\{k_1, \ldots, k_s\}$ of K (see relation (7)) forms the input. Now $C(K)$ can be defined in a way equivalent to definition (2) as follows:

$$C(K) = \{c \in M_{n \times n}(\mathbb{Z}) | c k_j = k_j c, 1 \leqslant j \leqslant s\} \cap \mathrm{Gl}(n, \mathbb{Z}). \tag{12}$$

According to definition (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 $m_{ij}, 1 \leqslant i, j \leqslant n$, 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:

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

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

$$F : C_R(K) \to \mathbb{R}^N \qquad F(m) = (x_1, \ldots, x_N) \tag{13}$$

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:

$$M' = \{x \in \mathbb{Z}^N \| x_j | \leqslant D, j \in \{1, \ldots, N\}\}$$

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

$$M'' = \{F^{-1}(x) | x \in M'\}$$

according to relation (13), and M consists of all matrices m in the set M'' satisfying the following two conditions:

1. $m_{rs} \in \mathbb{Z}$ 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 (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 (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 (11).

As pointed out before, there can (and in general will) exist more paths $m \to I_n$. Suppose for example:

1. $$m \to mc_3^{-1} \to c_2^{-1}mc_3^{-1} \to c_2^{-1}mc_3^{-1}c_2^{-1} = I_n$$
2. $$m \to mc_4^{-1} \to c_1^{-1}mc_4^{-1} = I_n$$

are two possible paths. Then

$$m = c_2^2c_3 = c_1c_4 \Rightarrow c_4 = c_1^{-1}c_2^2c_3$$

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 WRT the decision whether a matrix m can be expressed as a word in some generating set. If no path $m \to I_n$ has been found, the process is carried out for m^{-1} instead of m with the same criterion (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 (11), but of which the inverses satisfy criterion (11), is denoted by $J = \{j_1, \ldots, j_a\}$ for some $a \in \mathbb{N}$.

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:

$$T = \left\{ a \in M_{n\times n}(\mathbb{R}) | a k_j = k_j a, 1 \leqslant j \leqslant s \wedge \nexists j \in \left\{1, \ldots, e\right\}, \right.$$
$$\left. q \in \left\{-1, 1\right\} [N(c_j^q a) < N(a) \text{ or } N(a c_j^q) < N(a)] \right\}. \tag{14}$$

So T consists of all matrices $a \in M_{n\times n}(\mathbb{R})$ commuting with each $k \in K$, of which the norm can not be decreased by left- or right-multiplication with any generator c_j or its inverse.

All $j_k \in J$ are added to the c_i of definition (14). This is permitted, since J consists of all matrices for which the criterion (11) is satisfied after inversion.

Analogously to relation (13), the set $T \subseteq M_{n\times n}(\mathbb{R})$, defined in definition (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 definition (10) and the fact that all dependent coefficients depend linearly on the N free parameters). Since all matrices $m \in C(K)$ for which $|x_i| \leqslant D$ ($F(m) = \boldsymbol{x} \in \mathbb{Z}^N$ according to relation (13)) have already been evaluated, it holds for these m that $m \notin T$ and the corresponding $\boldsymbol{x} \notin T'$. The completeness of the set $\{c_1, \ldots, c_e\}$ is proved if

$$T \cap \mathrm{Gl}(n, \mathbb{Z}) = \{\emptyset\}. \tag{15}$$

Before the proof is outlined, first some useful properties will be described. Let $\lambda \in \mathbb{R}\backslash_{\{0\}}$. Then

$$\boldsymbol{x} \in T' \Leftrightarrow \lambda \boldsymbol{x} \in T' \tag{16}$$

because of the fact, that T' is defined by homogeneous polynomials of second degree in the N free parameters. Let $\det(\boldsymbol{x})$ denote $\det(g)$, where g corresponds to $\boldsymbol{x}$ in accordance with relation (13). Then

$$\det(\lambda \boldsymbol{x}) = \lambda^n \det(\boldsymbol{x}) \qquad (\lambda \in \mathbb{R}) \tag{17}$$

because the determinant is a homogeneous polynomial of degree n in the N free parameters. For this reason it is also true that:

$$\frac{\partial}{\partial x_j} \det(\boldsymbol{x} = \lambda \boldsymbol{x}_0) = \lambda^{n-1} \frac{\partial}{\partial x_j} \det(\boldsymbol{x} = \boldsymbol{x}_0) \tag{18}$$

for some $\boldsymbol{x}_0 \in \mathbb{R}^N, \lambda \in \mathbb{R}, j \in \{1, \ldots, N\}$. These three properties are useful for the argument of the proof, which is outlined below.

Consider a hypercube in $\mathbb{R}^N$, centred in $(0, \ldots, 0)$ with edge length $2E$ ($E \in \mathbb{N}$). The surface of this cube is divided into hypersquares S_i of edge length 1. Every S_i produces a tube T_i enclosed by

$$\{\lambda \boldsymbol{P} | \lambda \geqslant 0, \boldsymbol{P} \text{ on the boundary of } S_i\}.$$

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 an upper bound on $|x_j|, 1 \leqslant j \leqslant N$, for $\boldsymbol{x} = (x_1, \ldots, x_N)$ with $\det(\boldsymbol{x}) = \pm 1$, $\boldsymbol{x} \in T_i$, is determined if the condition is satisfied 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 this condition is satisfied. If $S_i \cap T' = \{\emptyset\}$, then $T_i \cap T' = \{\emptyset\}$ due to relation (16), and the next tube is to be examined. If $S_i \cap T' \neq \{\emptyset\}$, it must be determined whether

$$\{\boldsymbol{x} \in T_i | \det(\boldsymbol{x}) = \pm 1\} \cap \mathbb{Z}^N = \{\emptyset\}.$$

First calculate $\det(\boldsymbol{x}_M)$, where $\boldsymbol{x}_M$ is the point in the centre of S_i. If $\det(\boldsymbol{x}_M) > 0$, then one has to calculate a lower bound (referred to as LB) for $\det(\boldsymbol{x})$ for $\boldsymbol{x} \in S_i$. If $\det(\boldsymbol{x}_M) < 0$, 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 $\boldsymbol{x} \in T_i$. For example, suppose

$$N = 4 \qquad \det(x_1, x_2, x_3, x_4) = x_1^2 x_2^2 - x_3^2 x_4^2.$$

Suppose

$$S_i = \left\{(3, 2 + \beta, 1 + \gamma, \delta) \in \mathbb{R}^4 | \, 0 \leqslant \beta, \gamma, \delta < 1\right\}.$$

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

Method 2. For any $1 \leqslant j \leqslant N$, $\partial \det(\boldsymbol{x}) / \partial x_j$ 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

$$(36, -4, -8) \text{for} \left(\frac{\partial}{\partial x_2} \det(\boldsymbol{x}), \frac{\partial}{\partial x_3} \det(\boldsymbol{x}), \frac{\partial}{\partial x_4} \det(\boldsymbol{x}) \right)$$

respectively. Now a bound on the determinant is achieved as follows.

First $\det(\boldsymbol{y})$ is calculated, where $\boldsymbol{y} \in S_i$ has property $y_j = \min(x_j), 1 \leqslant j \leqslant N$, so $\boldsymbol{y}$ 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

$$LB = \det(y) + \sum_{j \neq k}^{N} \min\left(0, \left[\frac{\partial}{\partial x_j} \det(x)\right]_{x \in S_i}\right) \equiv \det(y) + \delta_-$$
$$UB = \det(y) + \sum_{j \neq k}^{N} \max\left(0, \left[\frac{\partial}{\partial x_j} \det(x)\right]_{x \in S_i}\right) \equiv \det(y) + \delta_+ \tag{19}$$

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 $|x_j|, 1 \leqslant j \leqslant N$, for $\det(x) = \pm 1$ and $x \in T_i$, note that:

$$|x_j| \leqslant E \qquad 1 \leqslant j \leqslant N \qquad \text{for } x \in S_i .$$

Therefore

$$|x_j| \leqslant \frac{E}{\sqrt[n]{|B|}} \qquad 1 \leqslant j \leqslant N \qquad \text{for} \det(x) = \pm 1 \tag{20}$$

where B is the bound, UB or LB. Now the two cases $E/\sqrt[n]{|B|} < D + 1$ and $E/\sqrt[n]{|B|} \geqslant D + 1$ have to be distinguished. In section 3 all $m \in C(K)$ were examined, for which the corresponding $|x_j| \leqslant D (1 \leqslant j \leqslant N)$. So if $E/\sqrt[n]{|B|} < D + 1$, then all matrices $m \in C(K)$ with corresponding $x \in T_i$, have already been examined in section 3. If $E/\sqrt[n]{|B|} \geqslant D + 1$, then consider the set:

$$\left\{ x \in T_i \cap \mathbb{Z}^N | \exists\, t \in \{1, \ldots, N\}[|x_t| \geqslant D] \wedge |x_q| \leqslant \frac{E}{\sqrt[n]{|B|}}, 1 \leqslant q \leqslant N \right\}. \tag{21}$$

For all x in this set it is checked whether or not the following four conditions are fulfilled:

1. if $x \in T'$ and
2. $\det(x) = \pm 1$ and
3. $m_{rs} \in \mathbb{Z}$ for m_{rs} dependent coefficients of $m = F^{-1}(x)$ and
4. $m^{-1} \notin < c_1, \ldots, c_e >$ according to criterion (11), then add m to the set of generators.

If $LB \leqslant 0$ (or, if an upper bound is to be determined, $UB \geqslant 0$), then it is possible that $|x_k| \to \infty$ for some $x \in T'$ for which $\det(x) = \pm 1$. In that case use a refinement strategy, which consists of the following. Let

$$S_i \to 2S_i = \{2x | x \in S_i\}.$$

Since $2S_i$ has edge length 2, it can be divided into $2^{(N-1)}$ squares of edge length 1: $S_{i,m}^{(2)}$, with $1 \leqslant m \leqslant 2^{(N-1)}$, the upper index (2) denoting the level of refinement.

Every square $S^{(2)}_{i,m}$ corresponds to a tube $T^{(2)}_{i,m}$, 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 $T^{(2)}_{i,m} \cap T' \neq \{\emptyset\}$. If so, $\det(\boldsymbol{x}_M)$ is calculated, where $\boldsymbol{x}_M$ is the point in the centre of $S^{(2)}_{i,m}$. Then a lower bound (if $\det(\boldsymbol{x}_M) > 0$) or an upper bound (if $\det(\boldsymbol{x}_M) < 0$) 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 equation (18) with $\lambda = 2$, as bound B may be taken:

$$B = \det(\boldsymbol{y}) + 2^{(p-1)(n-1)}\delta \tag{22}$$

with $p = 2$ denoting the level of refinement, δ corresponding to the sum term in equation (20) for S_i (refinement level 1), $\boldsymbol{y} \in S^{(2)}_{i,m}$ has again property $y_j = \min(x_j), 1 \leqslant j \leqslant N$. The reason for using this strategy is the following. Suppose the determinant surface in $\mathbb{R}^N$ is relatively flat. Then, after refining:

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

according to equation (17), whereas

$$\delta(\det) \rightarrow 2^{n-1}\delta(\det)$$

according to the analysis described above.

Of course, also at this second refinement level, there can be tubes $T^{(2)}_{i,m}$ with $LB \leqslant 0$ or $UB \geqslant 0$. Up to some maximum, as many refinements as necessary are allowed in order to achieve an exact analysis for each tube

$$T^{(p)}_{i,m_2,\ldots,m_p} \qquad (1 \leqslant m_j \leqslant 2^{(N-1)}\ \forall\ 1 \leqslant j \leqslant p)$$

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 there are no tubes for which $LB \leqslant 0$ (if $\det(\boldsymbol{x}_M) > 0$) or $UB \geqslant 0$ (if $\det(\boldsymbol{x}_M) < 0$) for $p = p_{\max}$. Then the found generator set is proved to be complete.

Suppose there are such tubes. Then consider the set :

$$\left\{\boldsymbol{x} \in T^{(p_{\max})}_{i,m_2,\ldots,m_{p_{\max}}} \cap \mathbb{Z}^N \mid \exists\ t \in \{1,\ldots,N\}\ [|x_t| \geqslant D] \wedge |x_q| \leqslant E \times 2^{(p_{\max}-1)}, 1 \leqslant q \leqslant N\right\} \tag{23}$$

For each $\boldsymbol{x}$ in this set it is checked whether the four conditions below relation (21) are satisfied, and if so, then the corresponding $m \in C(K)$ is added to the generator set.

Hence it has been proved that:

$$m \in C(K), |x_j| \leqslant E \times 2^{(p_{\max}-1)}\ \forall\ j \in \{1,\ldots,N\} \Rightarrow m \in < c_1,\ldots,c_{e+u} > \tag{24}$$

where $\boldsymbol{x} = F(m)$ according to relation (13), and u denotes the number of eventually 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.

5. Finding representatives for the cosets of $N(K)$ WRT $C(K)$

In section 2 it was already pointed out, how $N(K)$ can be decomposed in cosets WRT $C(K)$ (equation (4)). The resulting representatives $\{n_1, \dots, n_p\}$ correspond to the set automorphisms $\{\varphi_1, \dots, \varphi_p\}$. This set is the group $A(K)$ from relation (5). The ith automorphism φ_i is completely determined once

$$\varphi_i(k_j) = x k_j x^{-1} \qquad x \in n_i C(K) \tag{25}$$

is known for all point group generators $k_1, \dots, k_s$. The first consideration is how to construct all possible automorphisms of the kind of relation (25). A necessary (but, as will be shown, not sufficient) condition for such an automorphism, say φ_i, is that

$$\det(k_j - \lambda I_n) = 0 \Leftrightarrow \det(\varphi_i(k_j) - \lambda I_n) = 0 \qquad 1 \leqslant j \leqslant s \tag{26}$$

i.e. each generator k_j must satisfy the same characteristic equation and, as a consequence, 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, $\det(k - \lambda I_n) = 0$, has to be calculated for each $k \in K$. For $n \leqslant 6$, use can be made of the following lemma.

Lemma 1. If $n \leqslant 6$, 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: $k^m = I_n, k^j \neq I_n$ 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 the lemma described above, 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

$$\{g(j,1), \dots, g(j,a_j)\} \qquad 1 \leqslant j \leqslant s. \tag{27}$$

Then the number of homomorphisms of the kind of equation (25) to be considered, is

$$\prod_{j=1}^{s} a_j .$$

Now consider a homomorphism:

$$k_j \to \varphi(k_j) = g(j, m_j) \qquad 1 \leqslant m_j \leqslant a_j \ \forall\, 1 \leqslant j \leqslant s. \tag{28}$$

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

$$< (g(1, m_1), \ldots, g(s, m_s) >= K \tag{29}$$

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

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

$$K \supseteq H = \left\langle \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \right\rangle$$

but $|K| = 8$ whereas $|H| = 4$.

Excluding these homomorphisms, which are not automorphisms, representatives for the automorphisms have to be determined. According to relation (8), however, it is convenient to search first for all inner automorphisms. The set of inner automorphisms is the set $\{\Theta_i\}$:

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

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 relation (4)), at the same time r representatives are found, according to relation (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 $n_i \in \mathrm{Gl}(n, \mathbb{Z})$, the same procedure as in section 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

$$|x_j| \leqslant F \qquad \forall 1 \leqslant j \leqslant P \tag{30}$$

are considered, for some $F \in \mathbb{N}$. Now suppose no representative can be found.

The determinant, which is a homogeneous polynomial of degree n in the P free parameters, can always be written as:

$$\det(x_1, \ldots, x_P) = \frac{a}{b}(s_1 f_1 + \ldots + s_m f_m) \tag{31}$$

with a and b relatively prime, the f_j are the polynomial terms $x_1^{a_{1j}} \ldots x_P^{a_{Pj}}$ and $s_j \in \mathbb{Z}, 1 \leqslant j \leqslant P$. When the factorization of the determinant in the form (31) gives $a \neq \pm 1$, then there cannot exist an $n_i \in \mathrm{Gl}(n, \mathbb{Z})$ satisfying the linear equations defining n_i, since then there are no integer solutions for $x_j, 1 \leqslant j \leqslant P$, such that $\det(x_1, \ldots, x_P) = \pm 1$ in equation (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 relation (25).

If the determinant in the form (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 relation (30), a representative perhaps might have been found). This means that it has not been proved that all coset representatives in $N(K)$ WRT $C(K)$ 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 (31) of the determinant. Hence the coset decomposition of $N(K)$ WRT $C(K)$ has been exactly tested for all point groups considered (also see section 7).

6. Algorithm scheme

An algorithm has been developed which is based upon the methods described in sections 3, 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 (equation (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 n^2 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 (11), then the next element is treated using the same set of generators;
   - if an element cannot be expressed, the criterion (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 section 3 and equation (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 section 4.

7. For each tube T_i it is checked, whether T_i contains points, for which the norm of the corresponding matrix (according to relation (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 points with det $= \pm 1$ in this tube (see two methods described in section 4). If such an upper bound exists, then check for all points $\boldsymbol{x} \in \mathbb{Z}^N, \boldsymbol{x} \in T_i$ 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 (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 7b or satisfy 7a 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 WRT 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 section 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 steps 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 integer 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 $|I(K)| < |K|$, there are also point group elements in $C(K)$; see step 11);
- the coset representatives according to steps 12, 13.

7. Results

A computer program, following the algorithm scheme described in section 6, has been written in FORTRAN77 and run 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, mentioned by Janssen (1990), denoted by 7mm $\subset \mathrm{Gl}(6,\mathbb{Z})$, which is in the isomorphism class D_7 ($|K| = 14$. K consists of matrices of order 7,2,1 with determinants 1, −1, 1 respectively) :

$$K = \left\langle \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \right\rangle. \tag{32}$$

1. First, the equations relating the coefficients $m_{ij} \in C(K)$ (see definition (12)) are determined, resulting in three free parameters, x_1, x_2, x_3. Of the 33 remaining coefficients, six 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 $|x_j| \leqslant 8, j = 1,2,3$. 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. One is trivial (I_6), the other is $-I_6$ (and occurs in every centralizer), which becomes the first generator:

$$c_1 = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}. \tag{33}$$

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

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

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

$$\left.\begin{bmatrix} 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 1 & -1 & -1 \\ 0 & 0 & 1 & 1 & 0 & -1 \\ -1 & 0 & 1 & 1 & 0 & 0 \\ -1 & -1 & 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & -1 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 & 1 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 1 & -1 & 0 & 1 & 0 \\ -1 & 1 & 0 & -1 & 1 & 0 \end{bmatrix}\right\} \qquad (34)$$

denoted by $\{g_i\}, i = 3, \ldots, 8$, respectively. Now $g_3, g_3^{-1} \notin < c_1 >$ according to criterion (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 $j_1 = g_5$ (see section 3). $g_6 = c_1 c_2$, $g_7 = c_1 c_3$. $g_8 \notin < c_1, c_2, c_3 >$, 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 (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 definition (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 relation (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:

$$S_i = \{(\pm 3, y_2 + \beta, y_3 + \gamma) \in \mathbb{R}^3 \mid 0 \leqslant \beta,\ \gamma < 1\}$$

or permutations. The maximal number of refinements allowed is put equal to 7 (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 $|x_j| \leqslant 3 \times 2^6 = 192$ are expressible as words in the set $\{c_1, \ldots, c_{3+u}\}$, where u denotes the number of eventually extra generators (see relation (24)). It turns out that the analysis for this point group is exact:

$$C(K) = < c_1, c_2, c_3 >$$
$$= \left\langle -I_6, \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ -1 & 1 & 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 & 1 & -1 \\ -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & -1 & 1 & 1 \\ 0 & 0 & -1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \end{bmatrix} \right\rangle. \qquad (35)$$

5. Now representatives for the coset decomposition of $N(K)$ WRT $C(K)$ are to be determined. As $|K| = 14$, the number of inner automorphisms $|I(K)| \leqslant 14$. 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. So $I'(K) = < k_1, k_2 >$. With use of lemma 1, there are six respectively seven point group elements having the same eigenvalues as k_1 and k_2 (see relation (33)). Therefore 42 homomorphisms of the kind of relation (25) are possible, all of which are automorphisms, since they all satisfy condition (29). According to relation (8), there are three representatives n_1, n_2, n_3 to be determined. Now n_1 is the representative corresponding with the coset $n_1 C(K) = C(K)$, so $n_1 \equiv I_6$. The two remaining representatives are:

$$n_2 = \begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & -1 & 0 \\ -1 & -1 & 1 & 1 & -1 & 0 \\ 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & -1 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & -1 \end{bmatrix} \qquad n_3 = \begin{bmatrix} -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1 & 0 & -1 \\ -1 & 1 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 1 & 0 & 1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \end{bmatrix} . \tag{36}$$

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

$$N(K) = < c_1, c_2, c_3, k_1, k_2, n_2, n_3 > . \tag{37}$$

The running time for this point group was 73.9 seconds.

As a second example, consider the point group:

$$K = \left\langle \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \right\rangle . \tag{38}$$

Its generators have orders 6 and 2, 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 1 for example (see lemma 1)). There are two independent coefficients, x_1, x_2, determining each $m \in C(K)$. A set M is constructed by considering

$$\left\{ \boldsymbol{x} \in \mathbb{Z}^3 \| x_j | \leqslant 3, 1 \leqslant j \leqslant 2 \right\} .$$

It turns out that $C(K) = < -I_5 >$.

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 (25). It turns out that 60 homomorphisms do not satisfy condition (29), and are therefore not automorphisms. There are 120 inner automorphisms, and the corresponding group of point group elements is K itself. Due to the coset decomposition of $A(K)$ WRT $I(K)$, there are $(300 - 60)/120 = 2$ representatives to be determined (the first representative is trivial: $n_1 \equiv I_5$). The other representative, n_2, cannot exist in $\mathrm{Gl}(5, \mathbb{Z})$, since $\det(n_2) = 0$, due to relation (25).

The result is:

$$N(K) = < -I_5, k_1, k_2 > \tag{39}$$

The running time for this point group was 4.4 seconds.

The third example to be considered is the point group:

$$K = \left\langle \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \right\rangle . \tag{40}$$

Its generators have orders 6 and 5, 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 it directly follows that

$$C(K) = < -I_5 > . \tag{41}$$

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 (25). It turns out that 69084 homomorphisms do not satisfy condition (29), and are therefore not automorphisms. There are 1920 inner automorphisms, and the corresponding group of point group elements is K itself. Due to the coset decomposition of $A(K)$ WRT $I(K)$, there are $(122844 - 69084)/1920 = 28$ representatives to be determined (the first representative is trivial: $n_1 \equiv I_5$). The 27 other representatives must have determinant $\neq \pm 1$ due to the relations (25) determined by the defining automorphism (and have therefore been proved to be non-existent). The result is:

$$N(K) = < -I_5, k_1, k_2 > . \tag{42}$$

The running time for this point group was 179.5 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 :

$$K = \left\langle \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \right\rangle . \tag{43}$$

$C(K)$ 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

$$C(K) \supseteq \left\langle -I_5, \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & -2 & 1 & 0 \\ 2 & 1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & -1 & -2 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \right\rangle . \tag{44}$$

Comparison with the results by Brown *et al* (1973) yields that the set $\{c_1, c_2, c_3, c_4\}$ generates $C(K)$, but this cannot be proved by the check procedure of section 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:

$$\det(x_1, x_2, x_3, x_4) = x_1^2 x_4^2 + 9x_2^2 x_3^2 + 6x_1 x_2 x_3 x_4. \tag{45}$$

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

$$\det(E, 0, 0, 0) = 0 \qquad (E, 0, 0, 0) \in T' \tag{46}$$

using relation (45) and the explicit form of the second degree inequalities defining T'. Then also

$$\det(2^{(p-1)}E, 0, 0, 0) = 0 \qquad (2^{(p-1)}E, 0, 0, 0) \in T'(p \in \mathbb{N}) \tag{47}$$

according to equations (17) and (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 $\det(\boldsymbol{x}) = \pm 1$ surface. According to relation (47), however, for each refinement level $p \in \mathbb{N}$, tubes

$$T^{(p)}_{i, m_2, \ldots, m_p} \ni (E, 0, 0, 0) \qquad T^{(p)}_{i, m_2, \ldots, m_p} \cap T' \neq \{\emptyset\}$$

will exist, having no upper bound on the coefficients x_1, x_2, x_3, x_4 on the $\det(\boldsymbol{x}) = \pm 1$ surface. Therefore the completeness of the found set, given by relation (44), can only be proved for the subgroup of $C(K)$ defined in relation (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 section 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.

8. Concluding remarks

The algorithm described in this paper, for the determination of a generating set for the normalizer $N(K)$ 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 section 4). The method to construct generators corresponding to the coset decomposition of $N(K)$ WRT $C(K)$ 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 an interactive computer session. The values of the bounds related to the centralizer (the bounds D below relation (13), E below equation (18) and $p_{\max}$ above relation (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 WRT the centralizer (the bound F in relation (30)), should be chosen in accordance with the order of the point group.

Acknowledgment

I would like to thank Dr T Janssen for suggesting the problem and for very useful and interesting discussions.

References

Brown H 1969 *Math. Comput.* **23** 499

Brown H, Bülow R, Neubüser J, Wondratschek H and Zassenhaus H 1978 *The Crystallographic Groups of Four-dimensional Space* (New York: Wiley)

Brown H, Neubüser J and Zassenhaus H 1973 *Math. Comput.* **27** 167

Bülow R 1973 Über Dadegruppen in $Gl(n, \mathbb{Z})$ *Dissertation* Aachen

Fast G and Janssen T 1971 *J. Comput. Phys.* **7** 1

Hiller H 1985 *Acta Cryst.* A **41** 541

Janssen T 1990 *Quasicrystals* (Springer Series in Solid-State Sciences **93**) ed T Fujiwara and T Ogawa (Berlin: Springer)

Janssen T, Janner A and Ascher E 1969 *Physica* **42** 41

Lancaster P 1969 *Theory of Matrices* (New York: Academic)

Plesken W and Pohst M 1977a *Math. Comput.* **31** 536

—— 1977b *Math. Comput.* **31** 552

Ryskov S 1972a *Dokl. Akad. Nauk SSSR* **204** 561 (Engl. transl. 1972 *Soviet Math. Dokl.* **13** 720)

—— 1972b *Trudy Mat. Inst. Steklov.* **128** 183 (Engl. transl. 1972 *Proc. Steklov. Inst. Math.* **128** 217)

Siegel C 1943 *Ann. Math.* **44** 674