On an Algorithm to Determine the Space Groups

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The discrete groups of motions of the euclidean space $\mathbb{R}^n$ with finite fundamental domain (space groups in n dimensions) contain n linearly independent translations. For $n = 3$, this was shown by SCHOENFLIESS [1] by geometric methods. BIEBERBACH [2, 3] proved the Fundamental Theorem in an arithmetic way for arbitray n. The proof was simpified by FROBENIUS [5].

It follows from the Fundamental Theorem that the translations in a given space group $\mathfrak{G}$ form a normal subgroup $\mathfrak{T}$ with finite quotient group, so that $\mathfrak{T}$ is a free abelian group in n generators. The translation subgroup $\mathfrak{T}$ is a uniquely determined as the largest abelian normal subgroup. Any subgroup containing $\mathfrak{T}$ is not abelian.

Two space groups are equivalent if they can be transformed into one another by an affinity. BIEBERBACH [3] shows two space groups are equivalent if and only if they are isomorphic.

In this article, we first prove the theorem that if a group $\overline{\mathfrak{G}}$ is constructed as the extension of a free abelian group $\overline{\mathfrak{T}}$ with finitely many generators $\overline{T}_1, \ldots, \overline{T}_n$ by a finite factor group, and if only the unit class $\overline{\mathfrak{T}}$ itself corresponds to the identity automorphism of $\overline{\mathfrak{T}}$, then $\overline{\mathfrak{G}}$ is isomorphic to a space group.

According to the above, determining the classes of equivalent space groups of $\mathbb{R}^n$ amounts to the problem posed by SPEISER [6] to find all types of non-isomorphic extensions of the free abelian group $\overline{\mathfrak{T}}$ in n generators with finite factor group $\overline{\mathfrak{F}}$, such that only the unit element in $\overline{\mathfrak{F}}$ corresponds to the identity automorphism of $\overline{\mathfrak{T}}$. BIEBERBACH [4] shows that this problem has only finitely many solutions.

The classification of space groups has so far been accomplished only for $n \leq 3$, and in a geometric manner.

In this article, an algebraic method to classify the space group is developed, which allows to computationally verify the results obtained geometrically, and which also shows a feasible way to obtain the classification for more than three dimensions.

At first, we realise that the automorphisms of $\overline{\mathfrak{T}}$ corresponding to elements of $\overline{\mathfrak{F}}$ can be represented as a group $\mathfrak{F}$ isomorphic to $\overline{\mathfrak{F}}$ of integer substitutions in n variables. Here, the group $\mathfrak{F}$ is uniquely determined by $\mathfrak{G}$ up to transformation with an integer matrix of determinant ± 1, that is, up to arithmetic equivalence.

We assume the knowledge of all classes of finite groups of integer substitutions under arithmetic equivalence. As BIEBERBACH [4] showed, there exists only finitely many such classes. In an older work [7], I provided practical methods to handle these classes. They are subject of further studies. For each class we assume a representative group $\mathfrak{F}$ to be chosen and solve the extension problem for this one.

To facilitate the computations, it is helpful to provide finitely many generators $A_1, \ldots, A_\nu$ for the group $\mathfrak{F}$ with finitely many defining relations:

$$R_j(A_1, \ldots, A_\nu) = E_n \quad (j = 1, \ldots, r),$$

where E_n is the $n \times n$-identity matrix.

Using the matrices in $\mathfrak{F}$ and the relations R_j, a matrix $\mathfrak{R}$ with rn rows and $n\nu$ columns is constructed. The product of the non-zero elementary divisors of $\mathfrak{R}$ is essentially identical to the number of space groups associated to $\mathfrak{F}$. A reduction can only happen if there exists integer substituions of determinant ± 1 (unimodular matrices) transforming $\mathfrak{F}$ into itself. All matrices of this form comprise a group $N_{\mathfrak{F}}$ which has finitely many generators $X_1, \ldots, X_\mu$ according to a theorem by SIEGEL [8]. By an additional computation we easily find which reduction of the above number is results from the X_i. The flow of the algorithm is illustrated by examples.

A systematic survey on the computations for $n = 3$ is intended as an addendum to this work. It is inevitable to concern oneself with the nomenclature of mineralogy. The number of 230 space groups of $\mathbb{R}^3$ given by SCHOENFLIESS [1] is confirmed.

§ 1

Let $\overline{\mathfrak{T}}$ be the free abelian group with n generators $\overline{T}_1, \ldots, \overline{T}_n$, $\overline{\mathfrak{G}}$ a group containing $\overline{\mathfrak{T}}$ as a normal subgroup with factor group $\overline{\mathfrak{F}}$. The elements $\overline{A}$ in $\overline{\mathfrak{F}}$ are the residue classes of $\overline{\mathfrak{G}}$ over $\overline{\mathfrak{T}}$:

$$\overline{A} = \overline{\mathfrak{T}} \overline{S}_{\overline{A}},$$

where the elements $\overline{S}_{\overline{A}}$ form a system of representatives of $\overline{\mathfrak{G}}$ over $\overline{\mathfrak{T}}$. By defining

$$\overline{A} \mapsto \left(\overline{T} \mapsto \overline{S}_{\overline{A}} \cdot \overline{T} \cdot \overline{S}_{\overline{A}}^{-1}\right) \quad (\overline{T} \in \overline{\mathfrak{T}}),$$

a unique automorphism of $\overline{\mathfrak{T}}$ is assigned to $\overline{A}$, such that the product of two residue classes over $\overline{\mathfrak{T}}$ is assigned the product of the respective automorphisms of $\overline{\mathfrak{T}}$. Here, the unit class $\overline{\mathfrak{T}}$ is assigned the identity automorphism. If we write

$$\overline{S}_{\overline{A}} \cdot \overline{T}_k \cdot \overline{S}_{\overline{A}}^{-1} = \overline{T}_1^{\alpha_{1k}(\overline{A})} \cdots \overline{T}_n^{\alpha_{nk}(\overline{A})},$$

we find the associated automorphism to be uniquely determined by the $n \times n$-matrix $A = (\alpha_{ik}(\overline{A}))$. One checks that the product of two automorphisms corresponds to the product of the respective matrices. All matrices A comprise a group $\mathfrak{F}$ of unimodular matrices homomorphic to $\overline{\mathfrak{F}}$.

Theorem 1 *If the group $\mathfrak{F}$ is finite and isomorphic to $\overline{\mathfrak{F}}$, then $\overline{\mathfrak{G}}$ is isomorphic to a space group in dimension n.*

PROOF: By assumption there is an isomorphism

$$\overline{A} \mapsto A$$

between $\overline{\mathfrak{F}}$ and $\mathfrak{F}$. We construct an isomorphism between $\mathfrak{T}$ and the group $\overline{\mathfrak{T}}$ of integer translations in $\mathbb{R}^n$ by defining

$$T = (E_n, \mathrm{t}) \mapsto \overline{T}_1^{t_1} \cdots \overline{T}_n^{t_n} = \overline{T},$$

where

$$\mathrm{t} = \begin{pmatrix} t_1 \\ \vdots \\ t_n \end{pmatrix} \qquad \text{and} \qquad t_1, \ldots, t_n \text{ are integers.}$$

Then

$$\overline{T}^{\overline{S}_{\overline{A}}} = \overline{S}_{\overline{A}} \cdot \overline{T} \cdot \overline{S}_{\overline{A}}^{-1} = \prod_{k=1}^{n} (\overline{S}_{\overline{A}} \cdot \overline{T}_k \cdot \overline{S}_{\overline{A}}^{-1})^{t_k} = \prod_{i=1}^{n} \overline{T}_i^{\sum_{k=1}^{n} \alpha_{ik}(A) t_k} = \overline{(E_n, A\mathrm{t})},$$

$$\overline{\mathfrak{T}}\overline{S}_{\overline{A}} \cdot \overline{\mathfrak{T}}\overline{S}_{\overline{B}} = \overline{\mathfrak{T}}\overline{S}_{\overline{AB}},$$

$$\overline{S}_{\overline{A}} \cdot \overline{S}_{\overline{B}} = \overline{T}_{A,B}\overline{S}_{\overline{AB}} \quad \text{with } T_{A,B} \in \mathfrak{T}.$$

From the law of associativity $\overline{S}_{\overline{A}}(\overline{S}_{\overline{B}}\overline{S}_{\overline{C}}) = (\overline{S}_{\overline{A}}\overline{S}_{\overline{B}})\overline{S}_{\overline{C}}$ the *associativity relations* for the factor system consisting of the elements $\overline{T}_{A,B}$:

$$\overline{T}_{B,C}^{\overline{S}_{\overline{A}}} \overline{T}_{A,BC} = \overline{T}_{A,B} \overline{T}_{AB,C}.$$

If we set $T_{A,B} = (E_n, \mathfrak{t}_{A,B})$, then it follows that

$$\mathfrak{t}_{A,BC} + A\mathfrak{t}_{B,C} = \mathfrak{t}_{A,B} + \mathfrak{t}_{AB,C}.$$

Averaging over $\mathfrak{F}$ yields

$$\mathfrak{m}_A + A\mathfrak{m}_B = \mathfrak{t}_{A,B} + \mathfrak{m}_{AB}, \tag{1}$$

where

$$\mathfrak{m}_X = \frac{1}{N} \sum_{C \in \mathfrak{F}} \mathfrak{t}_{X,C}$$

and N denotes the order of the factor group $\mathfrak{F}$. The assignment

$$\overline{TS_{\overline{A}}} \mapsto T \cdot (A, \mathfrak{m}_A) = (A, \mathfrak{t} + \mathfrak{m}_A)$$

maps $\overline{\mathfrak{G}}$ isomorphically to an affine group $\mathfrak{G}$. As a condition for homomorphy we find that the equation

$$\overline{TS_{\overline{A}}} \cdot \overline{T'S_{\overline{A}'}} = \overline{TT'^{\overline{S}_{\overline{A}}}}\,\overline{T}_{A,A'}\overline{S}_{\overline{AA}'}$$

must correspond under this map to the equation

$$(A, \mathfrak{t} + \mathfrak{m}_A) \cdot (A', \mathfrak{t}' + \mathfrak{m}_{A'}) = (AA', \mathfrak{t} + A\mathfrak{t}' + \mathfrak{t}_{A,A'} + \mathfrak{m}_{AA'}),$$

which in fact follows from (1). The condition for isomorphy is that

$$T \cdot (A, \mathfrak{m}_A) = (E_n, 0)$$

implies $\overline{TS_{\overline{A}}} = 1$. In fact, we find $A = E_n$, $\overline{S}_{\overline{A}} \in \overline{\mathfrak{T}}$, $\mathfrak{t} + \mathfrak{m}_A = 0$.

But the affine group $\mathfrak{G}$ is affinely equivalent to a space group, for it is discrete and contains n linearly independent translations. So it remains to prove that it can be transformed into a group of motions. By Maschke's Theorem the finite group $\mathfrak{F}$ of real $n \times n$-matrices can be transformed into a group of orthogonal matrices by a real matrix X. So $(X, 0) \cdot \mathfrak{G} \cdot (X, 0)^{-1}$ is a group of motions, and the proof is complete. $\diamond$

Every space group is affinely equivalent to a group of affinities $(A, \mathfrak{S}_A + \mathfrak{g})$, where $\mathfrak{g}$ runs through the module Γ of all integer vectors and

$$\mathfrak{S}_{AB} \equiv \mathfrak{S}_A + A\mathfrak{S}_B \mod \Gamma, \tag{2}$$

whereas A runs through the finite unimodular group $\mathfrak{F}$, and conversely for every group of this kind there exists an affinely equivalent space group. As two space groups are isomorphic if and only if they are affinely equivalent, the same holds for the groups of the aforementioned kind. But which are the conditions for affine equivalence of two groups

$$\begin{gathered}\mathfrak{G} \text{ generated by } \mathfrak{T} \text{ and represantatives } (A, \mathfrak{S}_A) \text{ of } \mathfrak{G} \text{ over } \mathfrak{T}\\ \mathfrak{G}^* \text{ generated by } \mathfrak{T} \text{ and represantatives } (A^*, \mathfrak{S}^*_{A^*}) \text{ of } \mathfrak{G}^* \text{ over } \mathfrak{T}?\end{gathered}$$

So we check when

$$(X, \mathfrak{S}) \cdot \mathfrak{G} \cdot (X, \mathfrak{S})^{-1} = \mathfrak{G}^*$$

holds. As $\mathfrak{T}$ is a maximal abelian normal subgroup,

$$(X, \mathfrak{S}) \cdot \mathfrak{T} \cdot (X, \mathfrak{S})^{-1} = \mathfrak{T}$$

holds. Hence the matrix X is unimodular. Moreover, we obtain the following conditions:

$$\begin{gathered}\mathfrak{G}/\mathfrak{T} \cong \mathfrak{G}^*/\mathfrak{T}\\ \mathfrak{F} \cong \mathfrak{F}^*\end{gathered}$$

even more, with the appropriate notations, it must hold that

$$(X, \mathfrak{S}) \cdot (A, \mathfrak{S}_A) \cdot (X, \mathfrak{S})^{-1} = (A^*, \mathfrak{S}^*_{A^*} + \mathfrak{g}_A)$$

with $\mathfrak{g}_A \in \varGamma$ and

$$\begin{aligned}A^* &= XAX^{-1}\\ \mathfrak{F}^* &= X\mathfrak{F}X^{-1}.\end{aligned}$$

As a consequence, the group $\mathfrak{F}^*$ is unimodularly equivalent to $\mathfrak{F}$, and

$$\mathfrak{S}^*_{A^*} \equiv X\mathfrak{S}_A + (E_n - XAX^{-1})\mathfrak{S} \quad \text{mod } \varGamma.$$

We have now chosen a representative group $\mathfrak{F}$ from each class of arithmetically equivalent finite integral groups of substitutions. If $\mathfrak{G}^*$ is affinely equivalent to $\mathfrak{G}$, then we can affinely transform $\mathfrak{G}^*$ in such a way that the transformed group still belongs to $\mathfrak{F}$. So we are looking for all space groups belonging to $\mathfrak{F}$ which are not isomorphic to each other.

Let $\mathfrak{G}$ and $\mathfrak{G}^*$ beolng to $\mathfrak{F}$. Then the question is, when does

$$(X, \mathfrak{S}) \cdot \mathfrak{G} \cdot (X, \mathfrak{S})^{-1} = \mathfrak{G}^*$$

hold? According to the above, we obtain the neccessary condition

$$X \mathfrak{F} X^{-1} = \mathfrak{F}, \tag{a}$$

that is, X belongs to the group $N_{\mathfrak{F}}$ of all unimodular matrices transforming $\mathfrak{F}$ into itself (the normaliser of $\mathfrak{F}$ in the group of all unimodular substitutions). Moreover,

$$\mathfrak{S}^*_{A^*} \equiv X \mathfrak{S}_A + (E_n - XAX^{-1})\mathfrak{S} \mod \Gamma$$

must hold. In other words, we obtain the condition:

$$\mathfrak{S}^*_{A^*} \equiv X \mathfrak{S}_{A^{X^{-1}}} + (E_n - A)\mathfrak{S} \mod \Gamma. \tag{b}$$

Clearly, the given conditions are also sufficient for the affine equivalence of $\mathfrak{G}$ and $\mathfrak{G}^*$.

Once two groups $\mathfrak{G}$ and $\mathfrak{G}^*$ belonging to the given group $\mathfrak{F}$ are determined by means of the vector systems $(\mathfrak{S}_A)$ and $(\mathfrak{S}^*_{A^*})$, respectively, we have equivalence if and only if the congruence (b) can be solved by a fixed vector $(\mathfrak{S})$ and a matrix X in $N_{\mathfrak{F}}$. Here one needs to take into account that the systems of vectors are not arbitrary, but have to satisfy the congruence conditions

$$\mathfrak{S}_{AB} \equiv \mathfrak{S}_A + A\mathfrak{S}_B \mod \Gamma.$$

In this case we speak of (ordinary) equivalence between (admissible) vector systems. This equivalence clearly has the three usual properties. The same holds for the *strong* equivalence, which we mean when even the congruences

$$\mathfrak{S}^*_{A^*} \equiv \mathfrak{S}_A + (E_n - A)\mathfrak{S} \mod \Gamma$$

can be solved simultaneously. Of course, strong equivalence implies ordinary equivalence, where the converse does not neccessarily hold. It is our task to determine the classes of equivalent vector systems. But at first, we want to determine the classes of strongly equivalent vector systems by explicitely constructing a system of representatives.

§ 2

We choose any system of generators $A_1, \dots, A_\nu$ with a finite number of relations

$$R_j(A_1, \dots, A_\nu) = E_n \quad (j = 1, \dots, r)$$

of the group $\mathfrak{F}$. For example, we could choose the finitely many elements of $\mathfrak{F}$ as generators and the N^2 relations arising from the multiplication table as the defining relations. But to avoid unneccassary computations, it is preferable to choose a system of as few generators as possible with as few defining relations as possible.

At first, let an admissible vector system $(\mathfrak{S}_A)$ be given. We claim that all vectors of the system can be computed mod Γ if the vectors $\mathfrak{S}_{A_1}, \dots, \mathfrak{S}_{A_\nu}$ are known. For it follows from

$$\mathfrak{S}_{E_n} = \mathfrak{S}_{E_n E_n} \equiv \mathfrak{S}_{E_n} + E_n \mathfrak{S}_{E_n} \equiv 2\mathfrak{S}_{E_n} \mod \Gamma$$

that

$$\mathfrak{S}_{E_n} \equiv 0,$$

and from

$$0 \equiv \mathfrak{S}_{E_n} \equiv \mathfrak{S}_{AA^{-1}} \equiv \mathfrak{S}_A + A\mathfrak{S}_{A^{-1}} \mod \Gamma$$

it follows that

$$\mathfrak{S}_{A^{-1}} \equiv -A^{-1}\mathfrak{S}_A \mod \Gamma,$$

in particular

$$\mathfrak{S}_{A_i^{-1}} \equiv -A_i^{-1}\mathfrak{S}_{A_i} \mod \Gamma.$$

If moreover

$$W = A_{i_1}^{\varepsilon_1} A_{i_2}^{\varepsilon_2} \cdots A_{i_s}^{\varepsilon_s} \quad (\varepsilon_i = \pm 1)$$

is a word in powers of the generators $A_1, \dots, A_\nu$, and

$$W_1 = A_{i_2}^{\varepsilon_2} \cdots A_{i_s}^{\varepsilon_s} \quad (\varepsilon_i = \pm 1)$$

denotes the word obtained by omitting the first factor, then

$$\mathfrak{S}_W \equiv \mathfrak{S}_{A_{i_1}^{\varepsilon_1}} + A_{i_1}^{\varepsilon_1}\mathfrak{S}_{W_1} \mod \Gamma, \tag{3}$$

and by induction this implies equations of the form

$$\mathfrak{S}_W = \sum_{i=1}^{\nu} W^{(i)} \mathfrak{S}_{A_i}, \tag{4}$$

where the matrix $W^{(i)}$ depends, aside from the matrices $A_1, \ldots, A_\nu$, only on W and i. One can further show by induction over the word length of W that the construction of $\mathfrak{S}_W$ given above the condition

$$\mathfrak{S}_{WW'} \equiv \mathfrak{S}_W + W\mathfrak{S}_{W'} \mod \Gamma$$

is satisfied. But which conditions have to be satisfied by the vectors $\mathfrak{S}_{A_1}, \ldots, \mathfrak{S}_{A_\nu}$ if we require that they generate an admissible system as in the construction above? Neccassary conditions are

$$\mathfrak{S}_{R_j(A_1,\ldots,A_\nu)} = \sum_{i=1}^{\nu} R_j^{(i)} \mathfrak{S}_{A_i} \equiv 0 \mod \Gamma \quad (j = 1, \ldots, r). \tag{5}$$

These r conditions are also sufficient. For if

$$W(A_1, \ldots, A_\nu) = W'(A_1, \ldots, A_\nu)$$

holds, this is equivalent to

$$W \equiv W' \prod_\lambda W_\lambda R_{j_\lambda}^{\varepsilon_\lambda} W_\lambda^{-1} \mod \Gamma,$$

and here the following holds (mod Γ):

$$\begin{aligned}
\mathfrak{S}_{R_j} &\equiv 0 \\
\mathfrak{S}_{R_j^{-1}} &\equiv -R_j^{-1}\mathfrak{S}_{R_j} \equiv 0 \\
\mathfrak{S}_{W''R_j^\varepsilon W''^{-1}} &\equiv \mathfrak{S}_{W''} + W''\mathfrak{S}_{R_j^\varepsilon} + W''R_j^\varepsilon \mathfrak{S}_{W''^{-1}} \\
&\equiv \mathfrak{S}_{W''} + W''\mathfrak{S}_{R_j^\varepsilon} - W''R_j^\varepsilon W''^{-1}\mathfrak{S}_{W''} \\
&\equiv 0 \\
\mathfrak{S}_W &\equiv \mathfrak{S}_{W'} + W'\mathfrak{S}_{\prod_\lambda W_\lambda R_{j_\lambda}^{\varepsilon_\lambda} W_\lambda^{-1}} \equiv \mathfrak{S}_{W'}.
\end{aligned}$$

Note that when applying relations to a word, for example $W = W_1 W_2 W_2^{-1} W_3 = W_1 W_3$, the vector formed according to (4) does not change mod Γ:

$$\begin{aligned}
\mathfrak{S}_W &\equiv \mathfrak{S}_{W_1} + W_1\mathfrak{S}_{W_2} + W_1W_2\mathfrak{S}_{W_2^{-1}} + W_1W_2W_2^{-1}\mathfrak{S}_{W_3} \\
&\equiv \mathfrak{S}_{W_1} + W_1\mathfrak{S}_{W_3} \\
&\equiv \mathfrak{S}_{W_1W_3} \mod \Gamma.
\end{aligned}$$

Note once more that by virtue of (3) and (4) for every word W we can construct a vector $\mathfrak{S}_W$ from the vectors $\mathfrak{S}_{A_1}, \ldots, \mathfrak{S}_{A_\nu}$, and the condition characterising admissible vectors is satisfied. We just proved that the construction is unique in the sense that the same vector is constructed for two words in the generators $A_1, \ldots, A_\nu$ representing the same element in the group $\mathfrak{F}$.

For example, given the vectors

$$\mathfrak{S}_{A_i} = (E_n - A_i)\mathfrak{S}$$

we find the admissible system of vectors

$$\mathfrak{S}_W = (E_n - W)\mathfrak{S}.$$

This we can prove by induction on the length on W, or by observing that the group generated by the elements

$$\mathfrak{T} \quad \text{and} \quad (A, 0) \quad (A \in \mathfrak{F})$$

is transformed by conjugation with the translation $(E_n, \mathfrak{S})$ into the group generated by the elements

$$\mathfrak{T} \quad \text{and} \quad (A, (E_n - A)\mathfrak{S}) \quad (A \in \mathfrak{F}).$$

The investigation above made it clear that a complete system of admissible vectors $(\mathfrak{S}_A)$ can be replaced by a system consisting of the vectors $\mathfrak{S}_{A_1}, \ldots, \mathfrak{S}_{A_\nu}$ satisfying condition (5). Two of these systems $(\mathfrak{S}_{A_i})$ and $(\mathfrak{S}^*_{A_i^*})$ are ordinarily equivalent if and only if the congruences

$$\mathfrak{S}^*_{A_i^*} \equiv X\mathfrak{S}_{A_i^{X^{-1}}} + (E_n - A_i)\mathfrak{S} \mod \Gamma$$

are solvable for $X \in N_{\mathfrak{F}}$ and a fixed vector $\mathfrak{S}$, whereas they are strongly equivalent if and only if the congruences

$$\mathfrak{S}^*_{A_i^*} \equiv \mathfrak{S}_{A_i} + (E_n - A_i)\mathfrak{S} \mod \Gamma$$

are solvable simultaneously.

First, we consider strong equivalence. All admissible vector systems $(\mathfrak{S}_A)$ form a module M with addition

$$(\mathfrak{S}_A) + (\mathfrak{S}_{A'}) = (\mathfrak{S}_A + \mathfrak{S}_{A'}),$$

because the characteristic congruence relations are linear in the $\mathfrak{S}_A, \ldots$. All vector systems

$$\big((E_n - A)\mathfrak{S} - \mathfrak{g}_A\big) \quad (\mathfrak{g}_A \in \Gamma)$$

form a submodule M_0 of M. Strong equivalence of admissible vector systems is equivalent to the congruence of the vector systems with respect to the submodule M_0. It is our task to determine a system of representatives of M over M_0.

Lemma 1 *M_0 consists of all admissible vector systems $(\mathfrak{S}_A)$ for which there exists a system $(\mathfrak{g}_A)$ of lattice vectors with the property that for all $\lambda \in \mathbb{R}$ the system $\lambda(\mathfrak{S}_A - \mathfrak{g}_A)$ is also admissible.*

PROOF: If

$$\mathfrak{S}_A = (E_n - A)\mathfrak{S} + \mathfrak{g}_A \quad \text{with } \mathfrak{g}_A \in \Gamma,$$

then the vectors

$$\lambda(\mathfrak{S}_A - \mathfrak{g}_A) = (E_n - A)\lambda\mathfrak{S}$$

also form an admissible system. But if the vector system $(\mathfrak{S}_A)$ is admissible and a system of lattice vectors $\mathfrak{g}_A$ exists such that the vector system $8\lambda(\mathfrak{S}_A - \mathfrak{g}_A$ ($\lambda \in \mathbb{R}$ arbitrary) is also admissible, then we set

$$\mathfrak{t}_A = \mathfrak{S}_A - \mathfrak{g}_A$$

and find

$$\lambda\mathfrak{t}_{AB} \equiv \lambda\mathfrak{t}_A + A \cdot \lambda\mathfrak{t}_B \mod \Gamma,$$
$$\lambda(\mathfrak{t}_{AB} - \mathfrak{t}_A - A \cdot \mathfrak{t}_B) \in \Gamma,$$

and as λ is an arbitrary real number, the vector $\mathfrak{t}_{AB} - \mathfrak{t}_A - A\mathfrak{t}_B$ vanishes. Average the resulting equations over all B! If we further set

$$\mathfrak{m} = \frac{1}{N}\sum_{B \in \mathfrak{F}} \mathfrak{t}_B$$

we obtain

$$\mathfrak{m} - \mathfrak{t}_A - A\mathfrak{m} = 0,$$
$$\mathfrak{t}_A = (E_n - A)\mathfrak{m},$$

which was to be shown. ◇

We map the vector system $(\mathfrak{S}_A)$ to a subsystem via

$$(\mathfrak{S}_A) \mapsto (\mathfrak{S}_{A_i})$$

and thereby obtain an isomorphism of M to a different module $\overline{M}$. Here, M_0 is mapped isomorphically to the set $\overline{M}_0$ of vector systems

$$\big((E_n - A_i)\mathfrak{S} + \mathfrak{g}_{A_i}\big) \quad (\mathfrak{g}_{A_i} \in \Gamma).$$

Instead of a system of ν vectors with n components, we now introduce a supervector with $n \cdot \nu$ components:

$$S = \begin{pmatrix} \mathfrak{S}_{A_1} \\ \vdots \\ \mathfrak{S}_{A_\nu} \end{pmatrix}.$$

To express the condition for admissibility for this supervector, we introduce the $rn \times \nu n$-matrix

$$\mathfrak{R} = \begin{pmatrix} R_1^{(1)} & \cdots & R_1^{(\nu)} \\ \vdots & \ddots & \vdots \\ R_r^{(1)} & \cdots & R_r^{(\nu)} \end{pmatrix}$$

and obtain the condition:

$$\mathfrak{R} \cdot S \text{ is integral.}$$

The supervectors S with $\mathfrak{R}S$ integral form a module $\overline{\overline{M}}$ isomorphic to $\overline{M}$. In particular, $\overline{\overline{M}}$ contains all integral supervectors. According to Lemma 1, the isomorphism from M to $\overline{\overline{M}}$ maps M_0 to the submodule $\overline{\overline{M}}_0$ of $\overline{\overline{M}}$ consisting of those supervectors S_0 for which an integral supervector G exists with the property that all supervectors $\lambda(S_0 - G)$ with arbitrary real λ are also admissible. This is clearly equivalent to the solvability of the equation

$$\mathfrak{R}(S_0 - G) = 0$$

by an integral supervector G. By elementary operations the matrix $\mathfrak{R}$ is transformed to elementary divisor form:

$$\mathfrak{R} \mapsto \mathfrak{P}\mathfrak{R}\mathfrak{Q} = \begin{pmatrix} e_1 & & & \\ & e_2 & & \\ & & \ddots & \\ & & & e_\varrho \end{pmatrix}, \qquad e_1, \ldots, e_\varrho > 0,$$

where $\mathfrak{P}$ is a unimodular $nr \times nr$-matrix and $\mathfrak{Q}$ is a unimodular $n\nu \times n\nu$-matrix.

This transformation corresponds to the transition from $\overline{\overline{M}}$ to the isomorphic module $\mathfrak{Q}^{-1}\overline{\overline{M}}$. For $\mathfrak{R}S$ being integral implies $\mathfrak{P}\mathfrak{R}\mathfrak{Q}\cdot\mathfrak{Q}^{-1}S$ being integral and vice versa. But $\mathfrak{Q}^{-1}\overline{\overline{M}}$ consists of all supervectors of the form

$$\begin{pmatrix} g_1 e_1^{-1} \\ \vdots \\ g_\varrho e_\varrho^{-1} \\ * \\ \vdots \\ * \end{pmatrix},$$

where the numbers g_i are integers and the stars represent arbitrary real numbers. The module $\mathfrak{Q}^{-1}\overline{\overline{M}}_0$ consists of all vectors which can be expressed as the sum of an integral supervector and a vector in nullspace of $\mathfrak{P}\mathfrak{R}\mathfrak{Q}$, but these are the vectors:

$$\begin{pmatrix} g_1 \\ \vdots \\ g_\varrho \\ * \\ \vdots \\ * \end{pmatrix}.$$

As a system of representatives of $\mathfrak{Q}^{-1}\overline{\overline{M}}$ over $\mathfrak{Q}^{-1}\overline{\overline{M}}_0$ we therefore find the $e_1\cdots e_\varrho$ supervectors

$$P_{l_1,\ldots,l_\varrho} = \begin{pmatrix} l_1 e_1^{-1} \\ \vdots \\ l_\varrho e_\varrho^{-1} \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad l_i = 0,\ldots,e_i-1, \quad i = 1,\ldots,\varrho.$$

Similarly we find as a system of representatives of $\overline{M}$ over $\overline{M}_0$ the vectors

$$\mathfrak{Q}P_{l_1,\ldots,l_\varrho},$$

which can be computed easily, as the elementary operations leading from $\mathfrak{R}$ to $\mathfrak{P}\mathfrak{R}\mathfrak{Q}$ are known. Moreover, it is not strictly neccessary to obtain the elementary divisor form. It is sufficient to know the *monomial form*, where each row and column of $\mathfrak{P}\mathfrak{R}\mathfrak{Q}$ contains at most one number different from 0. The product of these numbers $d_1, \dots, d_\varrho$ different from 0 in the matrix $\mathfrak{P}\mathfrak{R}\mathfrak{Q}$ is precisely the number of cosets of $\overline{M}$ over $\overline{M}_0$, and we obtain the representatives in the form

$$\mathfrak{Q} \cdot \begin{pmatrix} \vdots \\ l_1 d_1^{-1} \\ \vdots \\ l_2 d_2^{-1} \\ \vdots \\ l_\varrho d_\varrho^{-1} \\ \vdots \end{pmatrix}, \quad l_i = 0, \dots, d_i - 1, \quad i = 1, \dots, \varrho,$$

where the dots indicate zeros. The number ϱ equals the rank of the matrix $\mathfrak{R}$. The number $e_1 \cdots e_\varrho = d_1 \cdots d_\varrho$ equals the greatest commond divisor of all $\varrho \times \varrho$-subdeterminants of $\mathfrak{R}$. If there are no elementary divisors different from 0, then $\overline{M} = \overline{M}_0$, and the zero-supervector is the only representative.

§ 3

It is now possible to master the strong equivalence of admissible vector systems by means of elementary operations of a certain matrix. We now consider ordinary equivalence.

The group $N_{\mathfrak{F}}$ consisting of all unimodular matrices X satisfying $X\mathfrak{F}X^{-1} = \mathfrak{F}$ contains the normal subgroup $Z_{\mathfrak{F}}$ consisting of those unimodular matrices even satisfying $XAX^{-1} = A$ for all $A \in \mathfrak{F}$. But $Z_{\mathfrak{F}}$ is precisely the group of units in the ring $V_{\mathfrak{F}}$ of all integral $n \times n$-matrices commuting with the elements of $\mathfrak{F}$. $V_{\mathfrak{F}}$ contains a basis over the ring $\mathbb{Z}$ of integer numbers. This basis is also a basis of the ring V of all rational matrices commuting with all elements of $\mathfrak{F}$ with respect to the field $\mathbb{Q}$ of rational numbers. Therefore, $V_{\mathfrak{F}}$ is an ordering of the hypercomplex system V over $\mathbb{Q}$. As V is at the same time the ring commuting with all elements of the skew $\mathbb{Q}$-ring $\mathfrak{F}^*$ generated by the matrices in $\mathfrak{F}$, and $\mathfrak{F}^*$ is fully reducible over $\mathbb{Q}$, it follows that $\mathfrak{F}^*$ is semisimple. Then the ring V is also semisimple by a well-known theorem due to E. Noether. So $Z_{\mathfrak{F}}$ is the group of units in an ordering of a semisimple system over $\mathbb{Q}$. Siegel [8] sketched a method to construct a system of finitely many generators $X_1, \dots, X_\lambda$ of $Z_{\mathfrak{F}}$. Moreover, this can be done in a very simple way in case $n \leq 3$.

Transforming $\mathfrak{F}$ by $X \in N_{\mathfrak{F}}$ gives rise to the automorphism

$$A \mapsto A^X$$

of $\mathfrak{F}$. The map

$$X \mapsto \left(A \mapsto A^X\right)$$

yields a homomorphic mapping of $N_{\mathfrak{F}}$ to a subgroup $\mathfrak{U}$ of the group of automorphisms of $\mathfrak{F}$, which contains the group $\mathfrak{I}$ of inner automorphisms of $\mathfrak{F}$ because $\mathfrak{F}$ is contained in $N_{\mathfrak{F}}$. Under this map, the identity automorphism of $\mathfrak{F}$ corresponds precisely to the elements of $Z_{\mathfrak{F}}$. According to the First Isomorphism Theorem, $Z_{\mathfrak{F}}$ is a normal subgroup in $N_{\mathfrak{F}}$ and the factor group is isomorphic to $\mathfrak{U}$:

$$N_{\mathfrak{F}}/Z_{\mathfrak{F}} \cong \mathfrak{U}.$$

As $\mathfrak{F}$ is finite, $\mathfrak{U}$ is finite as well. So there exist finitely many matrices $X_{\lambda+1}, \ldots, X_\mu$ in $N_{\mathfrak{F}}$ which together with $Z_{\mathfrak{F}}$ generate all of $N_{\mathfrak{F}}$:

$$N_{\mathfrak{F}} = \langle X_1, \ldots, X_\mu \rangle.$$

We can find a system of representatives of $N_{\mathfrak{F}}$ over $Z_{\mathfrak{F}}$ by studying the arithmetic equivalence of the integral representations $A \mapsto A = \Delta(A)$ and $A \mapsto A^\alpha = \Delta^\alpha(A)$ (α an abritrary automorphism of $\mathfrak{F}$) of the abstract group given by $\mathfrak{F}$. Whenever Δ and Δ^α are arithmetically equivalent, we find a matrix $X \in N_{\mathfrak{F}}$ according to the equation

$$\Delta^\alpha(A) = X \cdot \Delta(A) \cdot X^{-1}$$

holding in this case. All these matrices form a system of representatives.

Lemma 2 *The map*

$$(\mathfrak{S}_A) \mapsto (X\mathfrak{S}_{A^{X^{-1}}}) \quad (X \in N_{\mathfrak{F}})$$

is an automorphism of the module M of admissible vector systems which maps the submodule M_0 to itself.

PROOF: It holds that

$$X\mathfrak{S}_{(AB)^{X^{-1}}} = X\mathfrak{S}_{A^{X^{-1}}B^{X^{-1}}} \equiv X(\mathfrak{S}_{A^{X^{-1}}} + A^{X^{-1}}\mathfrak{S}_{B^{X^{-1}}}) \equiv X\mathfrak{S}_{A^{X^{-1}}} + AX\mathfrak{S}_{B^{X^{-1}}}$$
$$X(\mathfrak{S}_{A^{X^{-1}}} + \mathfrak{S}'_{A^{X^{-1}}}) = X\mathfrak{S}_{A^{X^{-1}}} + X\mathfrak{S}'_{A^{X^{-1}}}$$
$$X^{-1}(X\mathfrak{S}_{(A^{X^{-1}})^X}) = \mathfrak{S}_A$$
$$X\big((E_n - A^{X^{-1}})\mathfrak{S} + \mathfrak{g}_{A^{X^{-1}}}\big) = \big((E_n - A)X\mathfrak{S} + X\mathfrak{g}_{A^{X^{-1}}}\big) \in M_0,$$

which proves everything. $\diamond$

So for the ordinary equivalence those strongly equivalent classes are identified which arise from the strong equivalence class of $(\mathfrak{S}_A)$ by one of the maps $(\mathfrak{S}_A) \mapsto (X\mathfrak{S}_{A^{X^{-1}}})$ with $X \in N_{\mathfrak{F}}$. In other words, every matrix $X \in N_{\mathfrak{F}}$ corresponds to a permutation X^* of the finitely many strong equivalence classes, so that all these permutations together form a permutation group $N^*_{\mathfrak{F}}$ homomorphic to $N_{\mathfrak{F}}$, and the ordinary equivalence classes simply consist of the system of strong equivalence classes conjugate under $N_{\mathfrak{F}}$.

Under the isomorphism of M and $\overline{\overline{M}}$, the automorphism

$$(\mathfrak{S}_A) \mapsto (X\mathfrak{S}_{A^{X^{-1}}})$$

of M corresponds to the automorphism

$$S = \begin{pmatrix} \mathfrak{S}_{A_1} \\ \vdots \\ \mathfrak{S}_{A_\nu} \end{pmatrix} \mapsto \begin{pmatrix} X\mathfrak{S}_{A_1^{X^{-1}}} \\ \vdots \\ X\mathfrak{S}_{A_\nu^{X^{-1}}} \end{pmatrix} = \mathfrak{X}S$$

of $\overline{\overline{M}}$, where the $n\nu \times n\nu$-matrix

$$\mathfrak{X} = \begin{pmatrix} X[A_1^{X^{-1}}]^{(1)} & \cdots & X[A_1^{X^{-1}}]^{(\nu)} \\ \vdots & \ddots & \vdots \\ X[A_\nu^{X^{-1}}]^{(1)} & \cdots & X[A_\nu^{X^{-1}}]^{(\nu)} \end{pmatrix}$$

is assigned to X. When going from $\overline{\overline{M}}$ to $\mathfrak{Q}^{-1}\overline{\overline{M}}$, the autmorphism $S \mapsto \mathfrak{X}S$ of $\overline{\overline{M}}$ corresponds to the automorphism

$$\mathfrak{Q}^{-1}S \mapsto \mathfrak{Q}^{-1}\mathfrak{X}\mathfrak{Q} \cdot \mathfrak{Q}^{-1}S \tag{6}$$

of $\mathfrak{Q}^{-1}\overline{\overline{M}}$. This autmorphism map $\mathfrak{Q}^{-1}\overline{\overline{M}}_0$ to itself. From the matrix

$$\mathfrak{Q}^{-1}\mathfrak{X}\mathfrak{Q} = (\gamma_{ik}(X)) = (\gamma_{ik})$$

we immediately obtain the permutation of cosets of $\mathfrak{Q}^{-1}\overline{\overline{M}}$ over $\mathfrak{Q}^{-1}\overline{\overline{M}}_0$ associated to (6).

If $\mathfrak{P}\mathfrak{R}\mathfrak{Q}$ is assumed to be in elementary divisor form, then, in our previous notation,

$$\mathfrak{Q}^{-1}\mathfrak{X}\mathfrak{Q}\cdot P_{l_1,\dots,l_\varrho} = \begin{pmatrix} \sum_{k=1}^{\varrho} \gamma_{1k} l_k e_k^{-1} \\ \vdots \\ \sum_{k=1}^{\varrho} \gamma_{\varrho k} l_k e_k^{-1} \\ * \\ \vdots \\ * \end{pmatrix},$$

and this supervector is strongly equivalent to $P_{l'_1,\dots,l'_\varrho}$, where the numbers l'_i are uniquely determined by the congruence

$$l'_i \equiv e_i \cdot \sum_{k=1}^{\varrho} \gamma_{ik} l_k e_k^{-1} \mod e_i$$

and the inequality

$$0 \le l'_i < e_i \quad (i = 1, \dots, \varrho).$$

We thus find the associated permutation:

$$\pi_{\mathfrak{X}} = \begin{pmatrix} \mathfrak{Q} P_{l_1,\dots,l_\varrho} \\ \mathfrak{Q} P_{l'_1,\dots,l'_\varrho} \end{pmatrix}.$$

Here it is sufficient to consider the finitely many matrices $X_1, \dots, X_\mu$ generating $N_{\mathfrak{F}}$, because all permutations $\pi_{\mathfrak{X}}$ arise as finite products of the permutations $\pi_{X_1}, \dots, \pi_{\mathfrak{X}_\mu}$. Given a strong equivalence class represented by the supervector $\mathfrak{Q} P_{l_1,\dots,l_\varrho}$, we combine all strong equivalence classes obtained from it by repeatedly applying the permutations $\pi_{X_1}, \dots, \pi_{\mathfrak{X}_\mu}$ into an ordinary equivalence class. The ordinary equivalence classes precisely represent all types of non-isomorphic space groups belonging to $\mathfrak{F}$. Thereby, Speiser's problem is solved.

§ 4

For the practical application it is remarkable that the automorphisms

$$(\mathfrak{S}_A) \mapsto (X\mathfrak{S}_{AX^{-1}})$$

of M associated to the elements $X \in \mathfrak{F}$ fix the strong equivalence classes. For in this case

$$\begin{aligned} X\mathfrak{S}_{AX^{-1}} = X\mathfrak{S}_{X^{-1}AX} &\equiv X(\mathfrak{S}_{X^{-1}} + X^{-1}\mathfrak{S}_A + X^{-1}A\mathfrak{S}_X) \\ &\equiv X\mathfrak{S}_{X^{-1}} + \mathfrak{S}_A + A\mathfrak{S}_X \\ &\equiv \mathfrak{S}_A + A\mathfrak{S}_X - \mathfrak{S}_X \\ &\equiv \mathfrak{S}_A + (E_n - A)\cdot(-\mathfrak{S}_X) \mod \Gamma. \end{aligned}$$

So $(X\mathfrak{S}_{AX^{-1}})$ is strongly equivalent to $(\mathfrak{S}_A)$. From this remark we deduce the useful obervation that those generators of $N_{\mathfrak{F}}$ contained in $\mathfrak{F}$ need not be considered in the reduction algorithm described in § 3.

Moreover, the existence of $-E_n$ in $N_{\mathfrak{F}}$ is reflected in the fact that the supervector $\mathfrak{Q}P_{l_1,\dots,l_\varrho}$ is equivalent to the supervector $\mathfrak{Q}P_{-l_1,\dots,-l_\varrho}$.

As an example we study the plane groups. We assume the knowledge of all finite unimodular groups of substitutions in two variables. By the alogrithm presented here we find 17 types, as was to be expected.

Two general remarks beforehand.

The strong equivalence class of $\mathfrak{Q}P_{0,\dots,0}$ is also an ordinary equivalence class.

Combine the matrix $\mathfrak{R}$ and the matrices $\mathfrak{X}_1, \dots, \mathfrak{X}_\mu$ into a matrix with upper part $\mathfrak{R}$ and lower part

$$\begin{pmatrix} \mathfrak{X}_1 \\ \vdots \\ \mathfrak{X}_\mu \end{pmatrix}.$$

Transform the matrix $\mathfrak{R}$ into monomial form by elementary operations, and simultaneously apply these operations to the lower part of the combined matrix. So if in the upper part a times the jth column is added to the kth column, the same is to happen in the lower part of the matrix. But afterwards, in each of the μ parts of the lower part, a times the kth row is to be subtracted from the jth row. List these these row operations in their order of appearance, say $A^{a_1}_{k_1,j_1}, \dots, A^{a_s}_{k_s,j_s}$. Consult the system of representatives of the $P_{l_1,\dots,l_\varrho}$. Determine the permutations $\pi_{\mathfrak{X}_1}, \dots, \pi_{\mathfrak{X}_\mu}$ via the lower part of the transformed combined matrix, which by construction is precisely

$$\begin{pmatrix} \mathfrak{Q}^{-1}\mathfrak{X}_1\mathfrak{Q} \\ \vdots \\ \mathfrak{Q}^{-1}\mathfrak{X}_\mu\mathfrak{Q} \end{pmatrix}.$$

Collect the representatives $\mathfrak{Q}P_{l_1,\ldots,l_\varrho}$ of the strong equivalence classes in systems invariant under $\langle \pi_{\mathfrak{X}_1}, \ldots, \pi_{\mathfrak{X}_\mu}\rangle$, up to strong equivalence. From each of these systems, choose a supervector. The supervectors obtained in this manner comprise a complete system of non-equivalent, admissible vector systems belonging to $\mathfrak{F}$. Note that the path from $P_{l_1,\ldots,l_\varrho}$ to $\mathfrak{Q}P_{l_1,\ldots,l_\varrho}$ leads through the row operations listed before, but in reversed order and with opposite sign in the exponent, that is,

$$A_{k_s,j_s}^{-a_s}, \ldots, A_{k_1,j_1}^{-a_1}.$$

Example 1 Consider

$$\mathfrak{F} = \langle A_1, A_2\rangle$$

with generators

$$A_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

and relations

$$R_1 = A_1^2 = E_2, \quad R_2 = A_2^2 = E_2, \quad R_3 = (A_1A_2)^2 = E_2,$$

$$\mathfrak{R} = \begin{pmatrix} A_1 + E_2 & 0 \\ 0 & A_2 + E_2 \\ A_1A_2 + E_2 & A_1 + A_2 \end{pmatrix}.$$

As $A_2 + E_2 = 0$, there are two zero rows in $\mathfrak{R}$. Zero rows can be omitted, so that a matrix

$$\mathfrak{R}' = \begin{pmatrix} A_1 + E_2 & 0 \\ A_1A_2 + E_2 & A_1 + A_2 \end{pmatrix}$$

with only four rows remains. Moreover,

$$N_{\mathfrak{F}} = \langle X, \mathfrak{F}\rangle, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$XA_1X^{-1} = A_1A_2, \quad XA_2X^{-1} = A_2, \quad X\mathfrak{S}_{A_1A_2} = X\mathfrak{S}_{A_1} + XA_1\mathfrak{S}_{A_2},$$

$$\mathfrak{X} = \begin{pmatrix} X & XA_1 \\ 0 & X \end{pmatrix},$$

$$\frac{\mathfrak{R}'}{\mathfrak{X}} = \left(\begin{array}{cccc} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & -2 \\ \hline 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array}\right) \rightsquigarrow \left(\begin{array}{cccc} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \\ \hline 0 & 0 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -1 & 0 & 0 & 0 \end{array}\right)$$

Add the fourth row to the second row and note the column operation $A_{2,4}^{-1}$ of $\mathfrak{X}$. We find

$$P_{l_1,l_2} = \mathfrak{Q}\,P_{l_1,l_2} = \begin{pmatrix} \frac{1}{2}l_1 \\ 0 \\ 0 \\ \frac{1}{2}l_2 \end{pmatrix}, \quad \mathfrak{Q}^{-1}\mathfrak{X}\mathfrak{Q}\cdot P_{l_1,l_2} = \begin{pmatrix} -\frac{1}{2}l_2 \\ \frac{1}{2}l_1 \\ \frac{1}{2}l_2 \\ -\frac{1}{2}l_1 \end{pmatrix}, \; 0 \le l_i < 2 \text{ and } i = 1, 2.$$

$$\pi_{\mathfrak{X}} = (P_{00})(P_{11})(P_{10}P_{01}), \quad P_{01} \text{ is discarded.}$$

The three plane groups associated to $\mathfrak{F}$ are generated by $\mathfrak{T}_2$ and

(a) $(A_1, 0), (A_2, 0)$,

(b) $(A_1, \frac{1}{2}\mathfrak{e}_1), (A_2, 0)$,

(c) $(A_1, \frac{1}{2}\mathfrak{e}_1), (A_2, \frac{1}{2}\mathfrak{e}_2)$,

respectively, where $\mathfrak{e}_1 = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$, $\mathfrak{e}_2 = \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$. ◇

In order to derive the groups of motions of the plane with finite fundamental domain (the symmetry groups of plane ornamentations) we use the following unimodular matrices:

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

We use SPEISER's [6] § 29 notation for the groups and list the generators of the groups additional to $\mathfrak{T}_2$.

I. *General planar lattice:*

(1) $A_1 = E; \quad A_1^1 = E, \mathfrak{R} = (E)$;
$\mathfrak{C}_1 : (E, 0)$

(2) $A_1 = -E; \quad A_1^2 = E, \mathfrak{R} = (A_1 + E) = 0$;
$\mathfrak{C}_2 : (-E, 0)$

II. *Rectangular lattice:*

(3), (4) $A_1 = B; \quad A_1^2 = E, \mathfrak{R} = (A_1 + E) = \left(\begin{smallmatrix} 2 & 0 \\ 0 & 0 \end{smallmatrix}\right)$;
$\mathfrak{C}_s^{\mathrm{I}} : (B, 0)$
$\mathfrak{C}_s^{\mathrm{II}} : (B, \frac{1}{2}\mathfrak{e}_1)$

(5), (6), (7) $A_1 = B$, $A_2 = -E$ (see Example 1);

$\mathfrak{C}_{2v}^{\mathrm{I}} : (B, 0), (-E, 0)$

$\mathfrak{C}_{2v}^{\mathrm{II}} : (B, \frac{1}{2}e_1), (-E, 0)$

$\mathfrak{C}_{2v}^{\mathrm{III}} : (B, \frac{1}{2}e_1), (-E, \frac{1}{2}e_2)$

III. *Rhombic lattice:*

(8) $A_1 = A$; $\quad A_1^2 = E, \mathfrak{R} = (A_1 + E) = \left(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix}\right)$;

$\mathfrak{C}_s^{\mathrm{III}} : (A, 0)$

(9) $A_1 = A$, $A_2 = -E$; $\quad$ relations and $\mathfrak{R}$ as in (5) to (7)

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

$\mathfrak{C}_{2v}^{\mathrm{IV}} : (A, 0), (-E, 0)$

IV. *Square lattice:*

(10) $A_1 = D$; $\quad A_1^4 = E, \mathfrak{R} = (A_1^3 + A_1^2 + A_1 + E) = 0$

$\mathfrak{C}_4 : (D, 0)$

(11), (12) $A_1 = D$, $A_2 = B$; $\quad A_1^4 = E$, $A_2^2 = E$, $(A_1 A_2)^2 = E$,

$$\mathfrak{R} = \begin{pmatrix} A_1^3 + A + 1^2 + A_1 + E & 0 \\ 0 & A_2 + E \\ A_1 A_2 + E & A_1 + A_2 \end{pmatrix},$$

note that $A_1^3 + A + 1^2 + A_1 + E$ vanishes. Omit the first two rows, which are zero rows,

$$\mathfrak{R}' = \begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \end{pmatrix} \rightsquigarrow \begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and note $A_{2,1}$, $A_{3,1}$, $A_{4,1}^{-1}$.

$$P_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2}l \\ 0 \end{pmatrix}, \quad l = 0, 1.$$

Apply $A_{4,1}$, $A_{3,1}^{-1}$, $A_{2,1}^{-1}$ in this order.

$\mathfrak{C}_{4v}^{\mathrm{I}} : (D, 0), (B, 0)$

$\mathfrak{C}_{4v}^{\mathrm{II}} : (D, -\frac{1}{2}\mathrm{e}_1), (B, \frac{1}{2}\mathrm{e}_1)$

V. *Hexagonal lattice:*

(13) $A_1 = C;\quad A_1^3 = E, \mathfrak{R} = (A_1^2 + A + 1 + E) = 0;$

$\mathfrak{C}_3 : (C, 0)$

(14) $A_1 = C, A_2 = A;\quad A_1^3 = E, A_2^2 = E, (A_1A_2)^2 = E,$

$$\mathfrak{R} = \begin{pmatrix} A_1^2 + A_1 + E & 0 \\ 0 & A_2 + E \\ A_1A_2 + E & A_1 + A_2 \end{pmatrix},$$

omit the first two (zero) rows,

$$\mathfrak{R}' = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ -1 & 2 & 2 & -1 \end{pmatrix} \rightsquigarrow \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix};$$

$\mathfrak{C}_{3v}^{\mathrm{I}} : (C, 0), (A, 0)$

(15) $A_1 = C, A_2 = -A;$ relations and $\mathfrak{R}$, $\mathfrak{R}'$ as in (14),

$$\mathfrak{R}' = \begin{pmatrix} 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \\ 2 & 0 & 0 & -2 \\ 1 & 0 & 0 & -1 \end{pmatrix} \rightsquigarrow \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix};$$

$\mathfrak{C}_{3v}^{\mathrm{II}} : (C, 0), (-A, 0)$

(16) $A_1 = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 1 \end{smallmatrix}\right) = -C;\quad A_1^6 = E, \mathfrak{R} = (A_1^5 + A_1^4 + A_1^3 + A_1^2 + A_1 + E) = 0;$

$\mathfrak{C}_6 : (C, 0)$

(17) $A_1 = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 1 \end{smallmatrix}\right) = -C, A_2 = A;\quad A_1^6 = E, A_2^2 = E, (A_1A_2)^2 = E,$

$$\mathfrak{R} = \begin{pmatrix} A_1^5 + A_1^4 + A_1^3 + A_1^2 + A_1 + E & 0 \\ 0 & A_2 + E \\ A_1A_2 + E & A_1 + A_2 \end{pmatrix},$$

omit the two zero rows,

$$\mathfrak{R}' = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 2 & 0 & 0 & 2 \\ 1 & 0 & 0 & 1 \end{pmatrix} \rightsquigarrow \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix};$$

$\mathfrak{C}_{6v} : (-C, 0), (A, 0)$

References

[1] A. SCHOENFLIESS, *Kristallsysteme und Kristallstruktur*, Teubner, 1981.

[2] L. BIEBERBACH, *Über die Bewegungsgruppen des n-dimensionalen euklidischen Raumes mit einem endlichen Fundamentalbereich*, Gött. Nachr., 1910, 75-84.

[3] —, *Über die Bewegungsgruppen der Euklidischen Räume I*, Math. Ann. 70, 1911, 297-336.

—, *Über die Bewegungsgruppen der Euklidischen Räume II*, Die Gruppen mit endlichem Fundamentalbereich, Math. Ann. 72, 1912, 400-412.

[4] —, *Über die Minkowskische Reduktion der positiven quadratischen Formen und die endlichen Gruppen linearer ganzzahliger Substitutionen*, Gött. Nachr., 1912, 207-216.

[5] F.G. FROBENIUS, *Über die unzerlegbaren diskreten Bewegungsgruppen*, Sitzungsber. Akad. Wiss. Berlin 29, 1911, 654-665.

[6] A. SPEISER, *Theorie der Gruppen von endlicher Ordnung*, 3. Aufl., Springer, 1937.

[7] H. ZASSENHAUS, *Beweis eines Satzes über diskrete Gruppen*, Hamb. Abh. 12, 1938, 298-312.

[8] C.L. SIEGEL, *Discontinuous Groups*, Ann. Math. 44, 1943, 674-689.

Added in proof: The book *Die Bewegungsgruppen der Kristallographie* by J.J. BURCKHARDT, Birkhäuser Basel, 1947, essentially employs the same algorithm as presented here to determine the space group of $\mathbb{R}^3$. – ZASSENHAUS

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Original: *Über einen Algorithmus zur Bestimmung der Raumgruppen*, Commentarii Mathematici Helvetici 21, 1948, 117-141.

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