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On Crystallography in Higher Dimensions. II. Procedure of Computation in R_4.

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(*Dedicated to Wolfgang Gaschütz on the occasion of his* 50*th birthday*)

The mathematical background and the computing methods applied to the classification of lattices and crystallographic groups of 4-dimensional space R_4 are described.

This paper is a direct continuation of the preceding one (Neubüser, Wondratschek & Bülow, 1971) to which we refer as I. We shall use the definitions explained there. In this paper we describe the methods we used to derive all Bravais types of lattices of R_4 and to order these, as well as the arithmetic and geometric classes, by means of crystal families and crystal systems.

Our approach started from Bülow's (1967; *cf.* also Bülow & Neubüser, 1970) determination of the 710 arithmetic crystal classes of R_4, which has since been reconfirmed.

1. The determination of the arithmetic classes of R_4

The computation started from a result of Dade (1965). He proved that the maximal finite groups of integral 4×4 matrices fall into 9 classes under transformation with integral unimodular matrices and he determined one group from each of these classes. We shall call these 9 groups the Dade groups of R_4. As each finite integral 4×4 matrix group is contained in a maximal one, each arithmetic crystal class is represented by at least one of the subgroups of the Dade groups. The task of finding all arithmetic crystal classes can therefore be split into two steps:

(i) Find all subgroups of the 9 Dade groups.
(ii) Classify the set, so obtained, under transformation with integral unimodular matrices.

The first step was performed using computer programs (Felsch & Neubüser, 1963) that determine – among other things – all subgroups of a group given by a set of generating elements. Altogether, the 9 Dade groups contain 11072 subgroups belonging to 1361 classes of conjugate subgroups. As conjugate subgroups of the Dade groups are arithmetically equivalent, it suffices for the determination of all arithmetic classes of R_4 to choose one representative from each of the 1361 classes of conjugate subgroups. Before these representatives were sorted into arithmetic crystal classes further groups were added to their list. These further groups came from hand-computations of Zassenhaus & Falk (1967) who had started to determine by direct methods all arithmetic crystal classes consisting of rationally reducible groups of integral matrices, of Janssen (1967, 1969) who had tried to determine all arithmetic crystal classes of (3,1)-reducible groups, and of Wondratschek, who had found arithmetic crystal classes by representing groups of Hurley's (1951) geometric crystal classes on different lattices. These further groups were added to the list of groups obtained as subgroups of the Dade groups merely as a further check to reduce the possibility of computational errors. It was found, however – as was to be expected in absence of programming errors – that each of the groups thus added was arithmetically equivalent to one of the subgroups of the Dade groups. The way of sorting the whole list of groups into arithmetic classes was very similar to the one described by Bülow (1967) and by Bülow & Neubüser (1970) for Bülow's first computation, except that any human error in sorting was avoided by the use of magnetic tapes as backing store. We refer to those papers for details. The result confirmed Bülow's first computation: there are 710 arithmetic crystal classes in R_4 which fall into 227 geometric ones. For each of the 710 classes all those groups of the list that belong to this class were noted, also for each of the subgroups of the Dade groups all its maximal subgroups. We used this information to derive a complete list of the Bravais types of R_4.

2. Another characterization of Bravais groups

As explained in I the Bravais types of lattices are in a natural $1-1$ correspondence with the Bravais classes, which are special arithmetic crystal classes. In order to select the Bravais classes from the set of all arithmetic crystal classes we derive from the definition given in I another characterization of Bravais classes due to Zassenhaus (1966), applying some linear algebra.

To each lattice basis $\boldsymbol{B}=\{\mathbf{b}_1,\cdots,\mathbf{b}_n\}$ of a lattice L in R_n we can assign the $n\times n$ matrix $B=(\mathbf{b}_i\cdot\mathbf{b}_j)$ of the scalar products $\mathbf{b}_i\cdot\mathbf{b}_j$ of the basis vectors of $\boldsymbol{B}$. This matrix is symmetric and positive definite. Conversely each symmetric positive definite matrix can be thus obtained from some lattice.

Let $\mathscr{B}(L)$ be the group of all linear mappings (implying *e. g.* that they leave the origin fixed) of R_n which

(i) map L onto L,
(ii) are motions, *i. e.* they are linear mappings that leave the lengths of all vectors unchanged.

The Bravais group $\mathscr{B}(L,\boldsymbol{B})$ is then the group of matrices representing $\mathscr{B}(L)$ with respect to the basis $\boldsymbol{B}$.

Hence the two conditions translate into the following: $\mathscr{B}(L,\boldsymbol{B})$ is the group of all $n\times n$ matrices X which

(i) are integral unimodular,
(ii) fulfil the condition $XBX^t=B$, where X^t denotes the transpose of X.

As each group in a Bravais class is a group $\mathscr{B}(L,\boldsymbol{B})$ for some lattice L and some lattice basis $\boldsymbol{B}$ of L, we see:

2·1. If we want to know whether a certain arithmetic class, given to us by one of its groups $\mathscr{H}$, is a Bravais class, we have to decide whether there exists a symmetric positive definite matrix B such that $\mathscr{H}$ consists of *all* unimodular matrices X with $XBX^t=B$.

We can do this with the help of the following consideration (which will be illustrated by an example in §3): Let $\mathscr{H}$ be a group of integral $n\times n$ matrices. Then the set of all symmetric matrices S such that $XSX^t=S$ for all $X\in\mathscr{H}$ forms a subspace of the $n(n+1)/2$-dimensional vector space Φ of all symmetric $n\times n$ matrices. We denote this subspace by $\Omega(\mathscr{H})$.

On the other hand, let a subset $Y\subseteq\Phi$ be given. The set of all unimodular matrices X with $XSX^t=S$ for all $S\in Y$ is a group, which we denote by $\mathscr{G}(Y)$. If Y consists of one element only, say B, we shall write $\mathscr{G}(\{B\})$.

2·2. Clearly for any group $\mathscr{H}$ of integral matrices we have $\mathscr{H}\subseteq\mathscr{G}[\Omega(\mathscr{H})]$.

Let $Y\subseteq Y'\subseteq\Phi$. $X\in\mathscr{G}(Y')$ means $XSX^t=S$ for all $S\in Y'$ and in particular $XSX^t=S$ for all $S\in Y\subseteq Y'$, hence $X\in\mathscr{G}(Y)$.
This means:

2·3. $Y\subseteq Y'$ implies $\mathscr{G}(Y')\subseteq\mathscr{G}(Y)$.

Now let $\mathscr{B}$ be a group from a Bravais class. Then by 2·1 there exists a symmetric positive definite matrix B such that $\mathscr{B}=\mathscr{G}(\{B\})$. Consider $\Omega(\mathscr{B})$. Then by 2·2 we have $\mathscr{B}\subseteq\mathscr{G}[\Omega(\mathscr{B})]$. As $B\in\Omega(\mathscr{B})$ by 2·3 we have

$$\mathscr{B}=\mathscr{G}(\{B\})\supseteq\mathscr{G}[\Omega(\mathscr{B})].$$

Hence $\mathscr{B}=\mathscr{G}[\Omega(\mathscr{B})]$. So we arrive at the following characterization:

> The arithmetic class of a finite group $\mathscr{H}$ of integral matrices is a Bravais class if and only if $\mathscr{H}=\mathscr{G}[\Omega(\mathscr{H})]$.

This, however, is a characterization we can utilize with the data at our disposal.

Any subspace of Φ can be given by a finite set of linear equations and the dimension of such a subspace can be determined from these equations by well-known techniques. In particular the subspace $\Omega(\mathscr{H})$ is given by the finite set of linear equations

$$XSX^t=S\,,$$

where S is a symmetric matrix of $n(n+1)/2$ indeterminates, and where X runs through all elements of $\mathscr{H}$. So it is easy to find $\Omega(\mathscr{H})$ for a given $\mathscr{H}$.

It is a much more difficult task to find $\mathscr{G}(Y)$ for a subspace Y of Φ given by a set of linear equations. However, using all that has been determined with the computer we can avoid such computations by the procedure described in § 4.

3. An example

We now give an example to illustrate the concepts used in § 2.

Let $\mathscr{H}$ be the group consisting of the matrices:

$$I=\begin{pmatrix}1&0\\0&1\end{pmatrix}\ ;\quad X_1=\begin{pmatrix}\bar{1}&\bar{1}\\1&0\end{pmatrix}\ ;\quad X_2=\begin{pmatrix}0&1\\\bar{1}&\bar{1}\end{pmatrix}.^*$$

$\Omega(\mathscr{H})$ is determined by the equations $XSX^t=S$ where X runs through all elements of $\mathscr{H}$. Instead we use the equivalent equations $SX^t=X^{-1}S$. Further it is clear that it suffices to restrict X to a set of generators of $\mathscr{H}$. As in our case X_1 (or X_2) generates $\mathscr{H}$, we have the equation

$$SX_1^t=X_1^{-1}S.$$

$$X_1^{-1}=\begin{pmatrix}0&1\\\bar{1}&\bar{1}\end{pmatrix},\quad X_1^t=\begin{pmatrix}\bar{1}&1\\\bar{1}&0\end{pmatrix},\quad S=\begin{pmatrix}s_{11}&s_{12}\\s_{12}&s_{22}\end{pmatrix},\ \text{so we}$$

have

$$\begin{pmatrix}-s_{11}-s_{12}&s_{11}\\-s_{12}-s_{22}&s_{12}\end{pmatrix}=\begin{pmatrix}s_{12}&s_{22}\\-s_{11}-s_{12}&-s_{12}-s_{22}\end{pmatrix}$$

or

$$\begin{aligned}-s_{11}-s_{12}&=s_{12}\\ s_{11}&=s_{22}\\ -s_{12}-s_{22}&=-s_{11}-s_{12}\\ s_{12}&=-s_{12}-s_{22}.\end{aligned}$$

It follows that $\Omega(\mathscr{H})$ consists of all matrices

$$S=\begin{pmatrix}s_{11}&-\tfrac{1}{2}s_{11}\\-\tfrac{1}{2}s_{11}&s_{11}\end{pmatrix}$$

with s_{11} any real number.

Clearly $\mathscr{G}[\Omega(\mathscr{H})]$ contains both $\mathscr{H}$ and I'. However, also $Y=\begin{pmatrix}0&1\\1&0\end{pmatrix}$ fulfils the equations $YSY^t=S$ with $S\in\Omega(\mathscr{H})$. The group $\mathscr{F}$ generated by X_1, I', and Y is of order 12. This is the maximal order which a finite group of 2×2 integral matrices can have. Hence we can conclude that $\mathscr{F}=\mathscr{G}[\Omega(\mathscr{H})]$. We may therefore say that the arithmetic class defined by $\mathscr{H}$ belongs to the Bravais type defined by $\mathscr{F}=\mathscr{G}[\Omega(\mathscr{H})]$.

4. Determination of the Bravais groups

The computer programs mentioned already in § 1 of this paper produce a list Λ_0 of all subgroups of the Dade groups. Furthermore, for each of these subgroups all its maximal subgroups are noted.

The program to be described here will build up from Λ_0 a list B which will contain one representative group $\mathscr{H}$ from each Bravais class. Also for each such $\mathscr{H}$ it will build up a list $A\ (\mathscr{H})$ which will contain one representative group from each arithmetic class belonging to the Bravais type defined by $\mathscr{H}$.

The program uses a certain procedure recursively. In the following description of a general run of this procedure we will denote by Λ the actual state of a list which at the beginning of the whole program is identical with Λ_0 and is changed in each run by removing all groups belonging to arithmetic classes that belong to a certain Bravais type.

(*)The program selects from the groups in Λ one of highest order (*e.g.* the first one of highest order with respect to the ordering in Λ), let this be $\mathscr{H}$.

$\mathscr{H}$ and all groups in Λ, which are arithmetically equivalent to $\mathscr{H}$ are removed from Λ. Then $\Omega(\mathscr{H})$ is computed, *i.e.* a finite system of linear equations defining $\Omega(\mathscr{H})$ is derived from the matrices of $\mathscr{H}$. $\mathscr{H}$ is added to the list B. A list $A(\mathscr{H})$ is started, into which $\mathscr{H}$ and all its maximal subgroups are put. The program works through the list $A(\mathscr{H})$ starting with the first maximal subgroup of $\mathscr{H}$ in $A(\mathscr{H})$, removing groups from it and possibly adding more groups to it, by a subroutine the general run of which will be described now:

Let $\mathscr{V}$ be the group in $A(\mathscr{H})$ to be investigated. Then $\Omega(\mathscr{V})$ is computed in the same way as $\Omega(\mathscr{H})$.

Two cases can occur:

(i) $\Omega(\mathscr{V})\neq\Omega(\mathscr{H})$. Then $\mathscr{V}$ remains in Λ, but is removed from $A(\mathscr{H})$.

(ii) $\Omega(\mathscr{V})=\Omega(\mathscr{H})$. Then $\mathscr{V}$ and all groups that are arithmetically equivalent to $\mathscr{V}$ are removed from Λ. Further all maximal subgroups of $\mathscr{V}$ are added to the list $A(\mathscr{H})$ and all groups in $A(\mathscr{H})$ that are arithmetically equivalent to $\mathscr{V}$, but $\neq\mathscr{V}$, are removed from it.

In both cases the program then continues with the next group in $A(\mathscr{H})$, if any. If there is no further group in $A(\mathscr{H})$, the program tests whether Λ is already empty. If this is the case, the program stops. Otherwise it starts again with the part described above at (*).

Obviously, as there are only finitely many subgroups of the Dade groups, the whole procedure will eventually stop.

From the definitions given in I and from the characterization of the Bravais classes in § 2. of this paper it is then clear, that the list B contains exactly one group from each Bravais class. For each group $\mathscr{H}$ from B groups remaining in $A(\mathscr{H})$ represent all different arithmetic classes belonging to the Bravais type defined by the Bravais class of $\mathscr{H}$.

As mentioned above, the distribution of the arithmetic classes into geometric ones had already been determined before. Using this distribution and the lists $A(\mathscr{H})$, the crystal families and crystal systems were easily found, following exactly the definitions 2·7 and 2·9 in I.

In this section only a simplified version of the actual program has been described. The real program makes

* The crystallographer sees at once that this group cannot be a Bravais group of any lattice, as it does not contain $I'=\begin{pmatrix}\bar{1}&0\\0&\bar{1}\end{pmatrix}$.

more sophisticated use of the data available and is far more efficient.

All the computations were executed on the Electrologica EL X1/EL X8 at the Rechenzentrum der Universität Kiel.

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On Crystallography in Higher Dimensions. III. Results in R_4

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An explicit classification of lattices and crystallographic groups of 4-dimensional space R_4 is given. There are (in R_4): 710 arithmetic crystal classes; 227 geometric crystal classes belonging to 118 isomorphism types of groups; 64 Bravais classes corresponding to 64 Bravais types of lattices; 33 crystal systems; 23 crystal families.

This paper presents some of the results obtained by the methods, explained in Bülow, Neubüser & Wondratschek (1971) (referred to as II). The definitions used are found in Neubüser, Wondratschek & Bülow (1971) (referred to as I).

1. Crystal classes and crystal systems

The 710 arithmetic crystal classes are not explicitly given. For each (geometric) crystal class the number of arithmetic crystal classes contained in it is included in Table 1.

The 227 (geometric) crystal classes, derived by Hurley (1951) (*cf.* also Hurley, Neubüser & Wondratschek, 1967), have been ordered into the 33 crystal systems in Table 1.

Within a crystal system the crystal classes are ordered by the following characteristics (common to all groups in a crystal class) which apply in the sequence listed below:*

(*a*) Group order. Smaller order precedes larger one.
(*b*) Determinants. Determinants only positive precede determinants both positive and negative.
(*c*) Crystal classes of groups containing I' precede those of groups not containing I'.
(*d*) Highest order of elements: Smaller order precedes higher order.

* Of course there are other ordering schemes; this one seemed convenient to us. A nomenclature for the crystal classes corresponding to that of Hermann–Mauguin in R_2 and R_3 has not yet been developed. There are some difficulties in introducing such a nomenclature, as in R_4 there are no symmetry axes in most cases and, therefore, the description of 'symmetry in certain directions' is not as easily used as in R_2 and R_3.