match no. 9 pp. 191-207 1980

SUBGROUP-RELATIONS BETWEEN CRYSTALLOGRAPHIC GROUPS

Klaus-Joachim Köhler
Lehrstuhl für Informatik I
RWTH Aachen
5100 Aachen

1. Introduction

This is the second of a series of three papers on constructing crystallographic groups and their subgroups. In the first paper ([9]) partially periodic groups were classified and a dimension-independent algorithm for their construction was derived that can be regarded as a generalization of Zassenhaus' algorithm for space groups ([17]).

In this paper we shall study subgroups of crystallographic groups. During the last years the investigation of phase-transitions has brought along increasing interest in the determination of subgroups of crystallographic groups ([3]). In most cases only such subgroups of space groups have been studied that are themselves space groups. However, there seems to be a growing interest in partially periodic subgroups, as well. Therefore, in this paper the problem of finding the subgroups of a given crystallographic group is discussed in full generality.

We use the terminology and the notations from [9]. In particular,an (n,r)-group C is an n-dimensional crystallographic group with an r-dimensional translation lattice $L(C)$. The corresponding translation subgroup is denoted by $T(C)$, and the linear constituent of C is denoted by $P(C)$.

We show in Chapter 2 that the problem of finding all subgroups of the crystallographic groups of a given crystal system can be reduced to the determination of the maximal subgroups of the following three types.

1.1 Definition: Let C be an (n,r)-group. A subgroup U of C, which must be an (n,s)-group with $s \leq r$, is called of

- type I ("zellengleich", translation-equivalent) if $L(C) = L(U)$, and hence the index $C:U$ is finite,
- type II ("klassengleich", class-equivalent) if $P(C) = P(U)$ and $s = r$, and hence $C:U$ is finite,
- type III if $P(C) = P(U)$ and $L(U)$ is a direct factor of (the $\mathbb{Z}$-module) $L(C)$, and hence $U = C$ or $s < r$ and $C:U$ is infinite. □

The type I-subgroups of a crystallographic group C are in 1-1-correspondence with the subgroups of its finite linear constituent $P(C)$ and thus can easily be found with existing computer programs. Moreover, for $n \leq 4$ the subgroup lattices of the n-dimensional point groups are well-known ([7],[1],[5]). Therefore, we only treat the type II- and type III-subgroups.

In Chapter 3 we derive methods for determining all type II- or type III-subgroups with a given translation lattice. Therefore, all subgroups of a crystallographic group C can be found if one knows the $\mathbb{Z}P(C)$-submodules of L(C).

The $\mathbb{Z}P(C)$-submodules which yield type III-subgroups correspond to $\mathbb{Q}P(C)$-submodules of $\mathbb{Q}L(C)$ and can be determined by classical representation theory.

The $\mathbb{Z}P(C)$-submodules of L(C) which yield type II-subgroups could be determined by methods developed by W.Plesken ([16]).

Instead of determining the type II-subgroups via the $\mathbb{Z}P(C)$-submodules of L(C), we use a method due to J.Neubüser and H.Wondratschek ([13],[14],[15]). Maximal type II-subgroups of an (n,r)-group C are of prime power index p^{α}, $1 \leq \alpha \leq n$, in C. For each integer p^{α} all subgroups U of C of index $C : U = p^{\alpha}$ can be determined by computer programs ([12]). We show in Chapter 4 that for $n \leq 3$ only the prime divisors p of the order of P(C) have to be considered if one neglects the subgroups of C which are affinely equivalent to C.

The "name" of the subgroups, i.e. their affine type, can easily be determined using a method proposed in [9].

In a subsequent paper we shall propose a dimension-independent algorithm for determining all type II- and type III-subgroups of space groups and of partially periodic groups.

I like to thank Professor J. Neubüser and Dr. W. Plesken for their advice, suggestions and corrections.

2. The Types of Subgroups of Crystallographic Groups

We list some more or less trivial properties of the three types of subgroups defined in the introduction.

2.1 Proposition. Let C be an (n,r)-group with $r \geq 1$.

a) The number of type I-subgroups of C is finite.
b) The number of (maximal) type II-subgroups of C is infinite.

Proof: a) follows from the finiteness of P(C).
b) Let $p \in \mathbb{N}$ be a prime number not dividing the order $|P(C)|$ of the linear constituent of C. Then $p \cdot T(C) := \{(p \cdot t, e) \mid (t,e) \in T(C)\}$ is a normal subgroup of C and the factor group $T(C) / p \cdot T(C)$ has a complement $U_p / p \cdot T(C)$ in $C / p \cdot T(C)$ (Schur-Zassenhaus Theorem [6]). Thus U_p is a type II-subgroup of C. As the index

$$C : U_p = T(C) : T(U_p) = T(C) : p \cdot T(C) = p^{\alpha}$$

is finite, there is a maximal type II-subgroup M_p of C containing U_p. For different primes p and q the associated groups M_p and M_q must be different because they have different indices in C. □

2.2 Remark. The number of type III-subgroups of a crystallographic group can be finite or infinite (see Theorem 3.2). □

By the following proposition, which generalizes an observation of C.Hermann ([8]), the problem of finding all subgroups of a crystallographic group is reduced to the determination of (maximal) type I-, II-, and III-subgroups.

2.3 Proposition. Let U be a subgroup of a crystallographic group C. Then there are uniquely determined subgroups V and W of C such that

$$(*) \qquad U \underset{\mathrm{II}}{<} V \underset{\mathrm{III}}{<} W \underset{\mathrm{I}}{<} C$$

i.e.

W is a type I-subgroup of C,
V is a type III-subgroup of W,
U is a type II-subgroup of V.

Proof: The groups

$$W := \langle U, T(C) \rangle$$

and

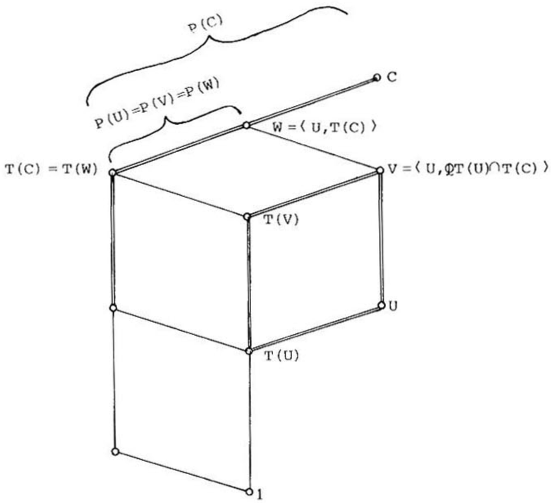
$$\begin{aligned} V &:= \langle U, \mathbb{Q}T(U) \cap T(C) \rangle \\ &:= \langle U, (t,e) \mid t \in \mathbb{Q}L(U) \cap L(C) \rangle \\ &:= \langle U, (t,e) \mid t \in L(C),\ m \cdot t \in L(U) \text{ for a suitable } m \in \mathbb{N} \rangle \end{aligned}$$

trivially fulfill the first and the last condition.

Since the pure $\mathbb{Z}$-submodule $L(V) = \mathbb{Q}L(U) \cap L(C)$ of $L(C)$ is a direct factor of $L(C)$ ([6,p.100]), V is a type III-subgroup of W.

To prove the uniqueness of V and W, we show that all groups V and W fulfilling (*) coincide with $\langle U, \mathbb{Q}T(U) \cap T(C) \rangle$ and $\langle U, T(C) \rangle$, respectively. Since $L(W) = L(C)$ and $P(W) = P(V) = P(U)$, $W = \langle U, T(C) \rangle$. As U is of finite index in V, $\mathbb{Q}L(U) = \mathbb{Q}L(V)$. Since $L(V)$ is a direct factor of $L(W)$, $L(V) = \mathbb{Q}L(V) \cap L(W) = \mathbb{Q}L(U) \cap L(C)$ ([6,p.100-101]), and therefore $V = \langle U, \mathbb{Q}T(U) \cap T(C) \rangle$. □

The position of these groups in the subgroup lattice of C is represented by the following diagram, the double lines indicating finite indices:



2.4 Corollary. A subgroup U of a crystallographic group C is maximal if and only if U is a maximal type I- or type II-subgroup of C.

Proof: The type III-subgroup V of W in Proposition 2.3 cannot be maximal in W as for $V \neq W$ the group $Z := \langle V, 2 \cdot K \rangle$, where K is a $\mathbb{Z}$-complement of $T(V) = \mathbb{Q}T(U) \cap T(C)$ in T(C), is properly contained in W and Z properly contains V. Therefore, the group U of Proposition 2.3 can be a maximal subgroup of C only if $U = W$ or $C = V$. The converse is obvious. □

Since a type III-subgroup is never maximal, the term *maximal type III- subgroup* denotes a proper type III-subgroup not contained in any other proper type III-subgroup.

As the group W of Proposition 2.3 is of finite index in C, there is only a finite number of subgroups of C containing W. The same holds for the pair of groups V and U. Since, moreover, the dimension of L(W) is finite, every subgroup U of C can be reached from C through a finite chain of subgroups

$$C = U_o > U_1 > \ldots > U_l = U$$

such that for $i = 0 \ldots l-1$ the group U_{i+1} is maximal of type I, II, or III in U_i. Thus, to find all subgroups of the crystallographic groups of $\mathbb{R}^n$, it is sufficient to determine the maximal type I-, II-, and III-subgroups of all (n,r)-groups with $0 \leqslant r \leqslant n$.

2.5 Proposition. Let C and U be crystallographic groups.
a) U is a maximal type I-subgroup of C if and only if U is a type I-subgroup of C and $P(U)$ is a maximal subgroup of $P(C)$.
b) U is a maximal type II-subgroup of C if and only if U is a type II-subgroup of C and its translation lattice $L(U)$ is a maximal $\mathbb{Z}P(C)$-submodule of $L(C)$.
c) U is a maximal type III-subgroup of C if and only if $P(U) = P(C)$ and $\mathbb{Q}L(U) = \{t \in \mathbb{R}^n \mid m \cdot t \in L(U)$ for a suitable $m \in \mathbb{N}\}$ is a maximal $\mathbb{Q}P(C)$-submodule of $\mathbb{Q}L(C)$ and $L(U) = \mathbb{Q}L(U) \cap L(C)$.

The proof is straight-forward. □

We prepare the method for finding the maximal type II-subgroups described in Chapter 4 by the following

2.6 Proposition. Let U be a maximal subgroup of C of type II. Then there exists a prime number p such that

$$p \cdot L(C) < L(U)$$

holds, i.e. the factor group $L(C) / L(U)$ is elementary abelian and

$$C : U = L(C) : L(U) = p^{\alpha} \quad \text{with} \quad 1 \leq \alpha \leq r = \dim L(C) = \dim L(U).$$

Proof: Since U is a maximal type II-subgroup of C, $L(U)$ is a maximal $\mathbb{Z}P(C)$-submodule of $L(C)$. Let $p \in \mathbb{N}$ be a prime divisor of the index $L(C) : L(U)$. Then $p \cdot L(C)$ is a $\mathbb{Z}P$-submodule of $L(C)$ and thus $p \cdot L(C) < L(U)$. By the isomorphism theorem $C / T(C)$ is isomorphic to $U / T(U)$ and hence $C : U = L(C) : L(U)$. □

If one has found a subgroup of a crystallographic group, one usually does not know its "name", i.e. its affine class. This name can be obtained by first determining the $\mathbb{Z} \times \mathbb{Q}$-class of the subgroup and then applying the method of [9, footnote in Chapter 5].

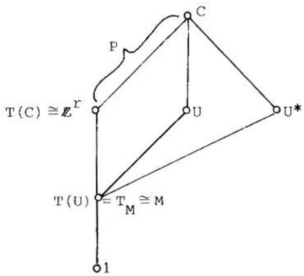
On the other hand, the announced algorithm in [10] automatically yields the affine classes of the subgroups.

3. Finding subgroups with a given translation lattice

Throughout this chapter let $C = \{(v_p + t, p) \mid p \in P,\ t \in \mathbb{Z}^r\}$ be an (n,r)-group and M a $\mathbb{Z}P$-submodule of $\mathbb{Z}^r$ of dimension $s \leq r$ such that either $s = r$ or M is a $\mathbb{Z}$-direct factor of $\mathbb{Z}^r$.

There is a type II- or type III-subgroup U of C with $L(U) = M$ if and only if the factor group $C / T_M := C / \{(t,e) \mid t \in M\}$ is a split extension of $T(C) / T_M$, i.e. there is a complement U / T_M of $T(C) / T_M$ in C / T_M.*)

*) In cohomological terms: The cocycle defining the extension C of T(C) by P induces a coboundary on $T(C) / T_M$.



Different subgroups U and U^* need not be affinely equivalent, but there are only finitely many conjugacy classes because the number of conjugacy classes of complements U/T_M of $T(C)/T_M$ in the factor group C/T_M is finite*) and U is conjugate to U^* in C if and only if U/T_M and U^*/T_M are conjugate subgroups of C/T_M.

3.1 Proposition. The number of subgroups U of the (n,r)-group C with $L(U) = M$ is
a) finite if the dimension s of M equals r,
b) 0,1, or infinite if M is a direct factor of $\mathbb{Z}^r$.

Proof: a) Since C is finitely generated and M is of finite index in C, there are only finitely many type II-subgroups of C with $L(U) = M$.
b) Let U* be a type III-subgroup of C with $L(U^*) = M$ and let $v^*: P \to \mathbb{Q}^r$ be a vector system of U*. The vector systems of C form a coset $v^* + T := v^* + \{t \mid t: P \to \mathbb{Z}^r\}$ and the vector systems of type III-subgroups U with $L(U) = M$ form a coset $v^* + S$, where S is a subgroup of the free abelian group T. Hence S is free abelian. Different vector systems in $v^* + S$ define the same type III-subgroup U if and only if their difference is a vector system $s \in \{t \mid t: P \to M\} =: R$, i.e. the type III-subgroups U of C with $L(U) = M$ are in 1-1-correspondence to the elements of S/R. Since M is a direct factor of $\mathbb{Z}^r$, R is a direct factor of T and thus a direct factor of S, as well, i.e. S/R is free abelian and its order must be one or infinite. □

The following examples illustrate Proposition 3.1. They show that there need not exist a type III-subgroup U of C with $L(U) = M$ and in case it exists, it need not be unique. Similar examples for type II-subgroups can easily be constructed (see Chapter 4)

3.2 Examples. Let $C = \{(v_p + t, p) \mid p \in P,\ t \in \mathbb{Z}^3\}$ be the space group defined by

---

*) The conjugate classes of complements correspond to the elements of $H^1(P, \mathbb{Z}^r/M)$ and this cohomology group is finite as P is finite and $\mathbb{Z}^r/M$ is finitely generated.

$$P = \left\langle a = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\rangle, \quad v_a = \begin{bmatrix} 1/2 \\ 0 \\ 0 \end{bmatrix} \text{ and } v_e = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

a) There is no type III-subgroup U of C with

$$L(U) = M := \left\{ \begin{bmatrix} 0 \\ x \\ y \end{bmatrix} \;\middle|\; x,y \in \mathbb{Z} \right\},$$

because

$$\left(v_a + \begin{bmatrix} x \\ y \\ z \end{bmatrix}, a \right)^2 = \left(\begin{bmatrix} 2x+1 \\ 2y \\ 0 \end{bmatrix}, e \right) \text{ and } \begin{bmatrix} 2x+1 \\ 2y \\ 0 \end{bmatrix} \notin M \text{ for any } \begin{bmatrix} x \\ y \\ z \end{bmatrix} \in \mathbb{Z}^3.$$

b) For $M := \left\{ \begin{bmatrix} x \\ y \\ 0 \end{bmatrix} \;\middle|\; x,y \in \mathbb{Z} \right\}$ there is an infinite number of (translationally equivalent) type III-subgroups U_i of C with $L(U_i) = M$, namely

$$U_i := \{(v_p^i + t, p) \mid p \in P,\ t \in M\} \text{ with } v_e^i = 0 \text{ and } v_a^i = \begin{bmatrix} 1/2 \\ 0 \\ i \end{bmatrix},\ i \in \mathbb{Z}.$$

c) For $M := \left\{ \begin{bmatrix} x \\ 0 \\ y \end{bmatrix} \;\middle|\; x,y \in \mathbb{Z} \right\}$ the type III-subgroup $U = \{(v_p + t, p) \mid p \in P,\ t \in M\}$ is the only one with $L(U) = M$, because

$$\left(v_a + \begin{bmatrix} x \\ y \\ z \end{bmatrix}, a \right)^2 = \left(\begin{bmatrix} 2x+1 \\ 2y \\ 0 \end{bmatrix}, e \right) \in U \text{ implies } y = 0, \text{ i.e. } \begin{bmatrix} x \\ y \\ z \end{bmatrix} \in M. \quad \square$$

Different type II- or type III-subgroups with the same translation lattice M need not be affinely equivalent, as Example 3.4 shows for type III-subgroups. If, however, M is not only a $\mathbb{Z}$-direct factor but has even a $\mathbb{Z}P$-complement, then we get

3.3 <u>Proposition</u>. Let $C = \{(v_p + t, p) \mid p \in P,\ t \in \mathbb{Z}^r\}$ be an (n,r)-group and let $\mathbb{Z}^r = M \oplus K$ be a decomposition of $\mathbb{Z}^r$ into $\mathbb{Z}P$-submodules M and K. Then all type III-subgroups U of C with $L(U) = M$ are translationally equivalent.

<u>Proof</u>: Let U and U* be type III-subgroups of C with $L(U) = L(U^*) = M$. Since their vector systems v' and v* are defined only up to vectors in M, we can assume that $v'_p - v^*_p \in K$ for all $p \in P$. We have to show that the vector system $t : P \to K$, $t_p := v'_p - v^*_p$, defines a split extension of M by P. From $t_p \in K$ and

$$t_{pq} = v'_{pq} - v^*_{pq} \equiv v'_p + p \cdot v'_q - v^*_p - p \cdot v^*_q \bmod M = t_p + p \cdot t_q \in K$$

for all $p,q \in P$ we obtain

$$t_{pq} = t_p + p \cdot t_q,\quad p,q \in P,$$

i.e. t defines a symmorphic group. □

We reformulate the above results in terms of the generalized Zassenhaus algorithm (see [9] for the following). This will yield algorithms for finding all type II- or type III-subgroups U of C with $L(U) = M$. Let

$P = \langle p_1,\dots,p_k \mid r_1(p_j) = \dots = r_m(p_j) = e\rangle$

be a presentation of $P < GL(r,\mathbb{Z}) \times GL(n-r,\mathbb{Z})$ and let $R \in \mathbb{Z}^{r\cdot m \times r\cdot k}$ be the matrix corresponding to the defining relations $r_1,\dots,r_m$ of P. Then, for the vector $V \in \mathbb{Q}^{r\cdot k}$ consisting of the components $v_{p_1},\dots,v_{p_k} \in \mathbb{Q}^r$ the congruence

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

holds. There exists a subgroup U of C with $P(U) = P$ and $L(U) = M$ if and only if there is a vector system $v+t$, $t : P \to \mathbb{Z}^r$, of C such that for the corresponding vector $V+T$, $T \in \mathbb{Z}^{r\cdot k}$, the congruence

$$R \cdot (V+T) \equiv 0 \bmod M^m$$

holds. The solutions of this system of diophantic equations can be found by methods similar to those used in the Zassenhaus algorithm (see [4]). If there is a solution $V_o = V + T_o$, all solutions form a coset

$$V_o + \{T \in \mathbb{Z}^{r\cdot k} \mid R \cdot T \equiv 0 \bmod M^m\}.$$

Different solutions define the same type II- or type III-subgroup U if their difference lies in M^k, because a vector system of U is determined by U only up to M.

Therefore, the factor group

$$\{T \in \mathbb{Z}^{r\cdot k} \mid R \cdot T \equiv 0 \bmod M^m\} / M^k$$

corresponds to the subgroups U, i.e. for a representative set $\mathcal{T}$ of this factor group the vectors

$$V_o + T,\ T \in \mathcal{T}$$

uniquely define the type II- or type III-subgroups U of C with $L(U) = M$.

If $s = r$, then a representative set $\mathcal{T}$ can easily be calculated by constructing compatible bases of the finitely generated $\mathbb{Z}$-modules $\{T \in \mathbb{Z}^{r\cdot k} \mid R \cdot T \equiv 0 \bmod M^m\}$ and M^k.

For $s < r$ a set $\mathcal{T}$ can be determined as follows. As $\mathbb{Z}^r$ is a direct sum of M and a complement K, say, we can assume that the elements of P are of the reduced form

$$p = \begin{pmatrix} p^M & p^* & 0 \\ 0 & p^K & 0 \\ 0 & 0 & p'' \end{pmatrix}, \quad \begin{array}{l} p^M \in GL(s,\mathbb{Z}),\ p^* \in \mathbb{Z}^{s\times(r-s)}, \\ p^K \in GL(r-s,\mathbb{Z}),\ p'' \in GL(n-r,\mathbb{Z}). \end{array}$$

Now the condition $R \cdot T \equiv 0 \bmod M^m$ is equivalent to $R' \cdot T' = 0$, where $R' \in \mathbb{Z}^{(r-s)\cdot m \times (r-s)\cdot k}$ and $T' \in \mathbb{Z}^{(r-s)\cdot k}$ are obtained from R and T, respectively, by cancelling the rows and columns corresponding to M (see Example 3.4). The set $\mathcal{T}$ is in 1-1-correspondence to

$$\mathcal{T}' := \{T' \in \mathbb{Z}^{(r-s)\cdot k} \mid R' \cdot T' = 0\}.$$

3.4 <u>Example</u>. Let $n = r = 2$, $s = 1$,

$P = \left\langle p = \begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix} \mid r(p) = p^2 = e \right\rangle$, and C the symmorphic (n,r)-group with linear constituent P and vector system $v : P \to \langle 0 \rangle$, i.e. $V = v_p = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. The lattice $M = \left\langle \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right\rangle$ is a $\mathbb{Z}P$-submodule of $\mathbb{Z}^2$, and $K = \left\langle \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\rangle$ is a $\mathbb{Z}$-complement of M. As C is symmorphic, there is a type III-subgroup U of C with $L(U) = M$, and we have only to determine the set $\mathcal{T}'$ to get all such subgroups. We get $R = (e+p) = \begin{pmatrix} 2 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 0 & R' \end{pmatrix}$ and $T = \begin{bmatrix} T' \\ t \end{bmatrix} \in \mathbb{Z}^{r \cdot k} = \mathbb{Z}^2$. Now

$$\mathcal{T}' = \{T' \in \mathbb{Z}^1 \mid R' \cdot T' = 0\} = \{T' \in \mathbb{Z} \mid 0 \cdot T' = 0\} = \mathbb{Z},$$

and $\mathcal{T}'$ corresponds to

$$\mathcal{T} = \{ \begin{bmatrix} 0 \\ T' \end{bmatrix} \in \mathbb{Z}^2 \mid T' \in \mathcal{T}'\}.$$

The type III-subgroups U_i defined by $v_p^i = v_p + \begin{bmatrix} 0 \\ i \end{bmatrix}$, $i \in \mathcal{T}' = \mathbb{Z}$, are symmorphic if and only if i is even, i.e. we have two affine classes of subgroups. □

The above derived methods reduce the problem of finding all type II- and type III-subgroups of C to the problem of determining the maximal $\mathbb{Z}P$-submodules of $\mathbb{Z}^r$ (of dimension $s = r$) and the $\mathbb{Z}P$-submodules of $\mathbb{Z}^r$ that are direct factors of $\mathbb{Z}^r$. The maximal $\mathbb{Z}P$-submodules can be determined by methods developed in [16], while the direct factors M of $\mathbb{Z}^r$ are in 1-1-correspondence to the $\mathbb{Q}P$-submodules Q of $\mathbb{Q}^r$ via

$$M = Q \cap \mathbb{Z}^r, \quad Q = \mathbb{Q}M$$

(Proposition 2.5c).

The number of $\mathbb{Q}P$-submodules of $\mathbb{Q}^r$ is finite if and only if the homogeneous components of $\mathbb{Q}^r$ are irreducible ([6]). The homogeneous components can be determined by means of representation theory. Therefore, all $\mathbb{Q}P$-submodules of $\mathbb{Q}^r$ can easily be found if the homogeneous components are irreducible, while the problem of finding all irreducible constituents of a reducible homogeneous component need not be trivial.

For $r \leq 3$, however, all non-trivial $\mathbb{Q}P$-submodules of $\mathbb{Q}^r$ can easily be found, as they must be of dimension one or two, and thus they are $\mathbb{Q}$-subspaces of the intersection of eigenspaces of all elements of P or orthogonal complements of these intersections.

4. Maximal Type II-Subgroups

We propose a method for deriving maximal type II-subgroups of a crystallographic group which is essentially due to J.Neubüser and H.Wondratschek ([13], [14], [15]).

Let C be an (n,r)-group. To obtain all maximal type II-subgroups of C, one only has to find all subgroups of index p^α for each prime number p and $1 \leq \alpha \leq r$ and select the maximal type II-subgroups from this set (Proposition 2.6). For each fixed prime p this can be done by existing computer programs ([12]).

By the proof of Proposition 2.1b) there is a maximal type II-subgroup of index p^α for every prime p not dividing $|P(C)|$. So we really have to take into account all primes. However, concentrating on the maximal type II-subgroups that are affinely inequivalent to C, we have to consider - at least for $n \leq 3$ - only the prime divisors of $|P(C)|$ because of

4.1 Theorem. Let U be a maximal type II-subgroup of the (n,r)-group C with index

$C:U=p^{\alpha}$. If $n\leqslant 3$ and p does not divide $|P(C)|$, then C and U are affinely equivalent.

The rest of the paper is essentially the proof of this theorem, that was conjectured and partially proved by J.Neubüser and H.Wondratschek. They observed that for $n\leqslant 4$ a maximal type II-subgroup U of a space group C whose index $C:U=p^{\alpha}$ is relatively prime to $|P(C)|$ is always arithmetically equivalent to C ([5]). In other words, a maximal $\mathbb{Z}P(C)$-submodule M of L(C) with $L(C):M$ relatively prime to $|P(C)|$ is $\mathbb{Z}$-equivalent to L(C). Of course, this observation holds also for (n,r)-groups with $1\leqslant r<n\leqslant 4$, i.e. if $C:U$ is relatively prime to $|P(C)|$ then P(C) is $\mathbb{Z}\times\mathbb{Q}$-equivalent to $P(U^*)$, where U^* is the natural representation of U with $L(U^*)=\mathbb{Z}^r$. Therefore, we can assume that the subgroup U of Theorem 4.1 has a translation lattice L(U) which is $\mathbb{Z}$-equivalent to the $\mathbb{Z}P$-module L(C).

We shall prove Theorem 4.1 by deriving a series of sufficient conditions which, when imposed upon C, yield the affine equivalence of C and U. For $n\leqslant 3$ every (n,r)-group C fulfills at least one of these conditions.

Before we prove Theorem 4.1, we cite two counterexamples which show that it does not hold for arbitrary n.

First, an example by W.Gaschütz ([5]) shows, that for $n=22$ L(C) and L(U) need not be $\mathbb{Z}$-equivalent $\mathbb{Z}P$-modules.

Second, C and U can be affinely inequivalent even if their linear constituents are $\mathbb{Z}\times\mathbb{Q}$-equivalent as the following unpublished example by W.Plesken shows for $n=11$.

4.2 <u>Example</u>. For $i=1,\dots,10$ let $e_i\in\mathbb{Z}^{10}$ be the column with 1 in the i-th row and 0 otherwise, and let $e_{11}:=-\sum_{i=1}^{10}e_i$. Let $p_1'',p_2''\in GL(10,\mathbb{Z})$ be matrices composed of the columns $e_i\in\mathbb{Z}^{10}$ as follows

$$p_1''=(e_2\dots e_{11}),\quad p_2''=(e_1e_4e_7e_{10}e_2e_5e_8e_{11}e_3e_6).$$

(The matrices p_1'' and p_2'' correspond via a group isomorphism to the permutations $\begin{pmatrix}1&2&3&4&5&6&7&8&9&10&11\\2&3&4&5&6&7&8&9&10&11&1\end{pmatrix}$ and $\begin{pmatrix}1&2&3&4&5&6&7&8&9&10&11\\1&4&7&10&2&5&8&11&3&6&9\end{pmatrix}$.) The group

$$P=\langle p_1,p_2\rangle,\quad p_1=\begin{pmatrix}1&0\\0&p_1''\end{pmatrix},\quad p_2=\begin{pmatrix}1&0\\0&p_2''\end{pmatrix}\in GL(1,\mathbb{Z})\times GL(10,\mathbb{Z}),$$

is a semidirect product of $\langle p_1\rangle$ and $\langle p_2\rangle$ defined by the relations

$$p_1^{11}=1,\quad p_2^5=1,\quad p_2^{-1}p_1p_2=p_1^4$$

and thus $|P|=11\cdot 5=55$.

The (11,1)-group

$$C=\langle([0],p_1),\ ([1/5],p_2)\rangle\quad\text{with}\quad L(C)=\mathbb{Z}$$

has a maximal type II-subgroup

$$U=\langle([0],p_1),\ ([6/5],p_2),\ ([2],e)\rangle\quad\text{with}\quad L(U)=2\mathbb{Z}$$

of index $C:U=2$ relatively prime to $|P|=55$. Obviously, U is affinely equivalent to

$$U^* := (0, \begin{pmatrix}2 & 0\\ 0 & e\end{pmatrix})^{-1} \cdot U \cdot (0, \begin{pmatrix}2 & 0\\ 0 & e\end{pmatrix}) = \langle ([0],p_1),([3/5],p_2),([1],e)\rangle \text{ with } L(U^*)=\mathbb{Z}.$$

Although $P(C)=P(U^*)=P$ and $L(C)=L(U^*)=\mathbb{Z}$, C and U^* are not affinely equivalent as we shall show now.

By the generalized Zassenhaus algorithm ([9]) the vector systems $v^i : P\to\mathbb{Q}$ defined by

$$v^i_{p_1}=0, \quad v^i_{p_2}=i/5, \quad i=0,\dots,4,$$

represent the classes of translationally equivalent (11,1)-groups U_i with linear constituent P.

The centralizer $C_{\mathbb{Z}\times 1}(P) = \left\langle \begin{pmatrix}-1 & 0\\ 0 & e\end{pmatrix}\right\rangle$ yields the orbits

$$\{v^o\},\ \{v^1,v^4\},\ \text{and } \{v^2,v^3\},$$

i.e. v^1 and v^4 define affinely equivalent groups and so do v^2 and v^3.

The automorphism group of P is generated by

$$\varphi : \begin{matrix} p_1\to p_1^2 \\ p_2\to p_2\end{matrix} \quad \text{and} \quad \psi : \begin{matrix} p_1\to p_1 \\ p_2\to p_2\cdot p_1^3 = p_1\cdot p_2\cdot p_1^{-1}.\end{matrix}$$

This can be shown by group theoretic methods.

The automorphisms ψ and φ are induced by the matrices p_1^{-1} and $x=\begin{pmatrix}1 & 0\\ 0 & x''\end{pmatrix} \in N_{\mathbb{Z}\times\mathbb{Q}}(P)$ with $x''=(e_1e_7e_2e_8e_3e_9e_4e_{10}e_5e_{11})$. ($x''$ corresponds to the permutation $\begin{pmatrix}1&2&3&4&5&6&7&8&9&10&11\\ 1&7&2&8&3&9&4&10&5&11&6\end{pmatrix}$.) As ψ is an inner automorphism and φ fixes p_2, the corresponding matrices p_1^{-1} and x act trivially on the vector systems v^i.

Therefore v^1 and v^3 define affinely inequivalent groups, i.e. C and U^* are not affinely equivalent.

The same arguments hold for the space group $C^* := \langle C,(t,e)\mid t\in\mathbb{Z}^{11}\rangle$. □

We prepare the proof of Theorem 4.1 by a definition and some remarks.

4.3 Definition. Let P be a finite subgroup of $GL(r,\mathbb{Z})\times GL(n-r,\mathbb{Z})$.

a) The number of classes of translationally equivalent (n,r)-groups with linear constituent P and translation lattice L is denoted by $h(P,L)$.

b) Let $C=\{v_p+t,p)\mid p\in P,\ t\in\mathbb{Z}^r\}$ be an (n,r)-group.
The *order* $|v|$ of its vector system $v:P\to\mathbb{R}^r$ is defined by the least positive integer $i\in\mathbb{N}$ such that the (n,r)-group $\{(i\cdot v_p+t,p)\mid p\in P,\ t\in\mathbb{Z}^r\}$ is symmorphic.*) □

---

*) The vector system $v:P\to\mathbb{R}^r$ induces a 1-cocycle $\bar v : P\to\mathbb{R}^r/L$ which maps p onto $\bar v_p := v_p+L$. The 1-cocycles, i.e. functions $\bar v : P\to\mathbb{R}^r/L$ with $\bar v_{p\cdot q}=\bar v_p+p\cdot\bar v_q$, form an abelian group $C^1(P,\mathbb{R}^r/L)$. The cocycles of symmorphic groups form the subgroup of coboundaries $B^1(P,\mathbb{R}^r/L)$. The factor group $H^1(P,\mathbb{R}^r/L) := C^1(P,\mathbb{R}^r/L)\,/\,B^1(P,\mathbb{R}^r/L)$ is called cohomology group. The elements of $H^1(P,\mathbb{R}^r/L)$ are in 1-1-correspondence to the classes of translationally equivalent (n,r)-groups with linear constituent P and translation lattice L. So $h(P,L)$ is the order of the abelian group $H^1(P,\mathbb{R}^r/L)$ and $|v|$ is the order of the element $\bar v+B^1(P,\mathbb{R}^r/L)$ of $H^1(P,\mathbb{R}^r/L)$ (see e.g. [2]).

The order $|v|$ divides $h(P,\mathbb{Z}^r)$ as well as $|P|$, and each prime divisor of $h(P,\mathbb{Z}^r)$ is also a divisor of $|P|$ ([9]).

By Proposition 2.5 a type II-subgroup U of an (n,r)-group C is maximal if and only if $M := L(U)$ is a maximal $\mathbb{Z}P$-submodule of $\mathbb{Z}^r$.

From now on let $C = \{(v_p + t,p) \mid p\in P,\ t\in\mathbb{Z}^r\}$ be an (n,r)-group with vector system $v : P\to\mathbb{Q}^r$ and let M be a maximal $\mathbb{Z}P$-submodule of $\mathbb{Z}^r$.

There need not exist a type II-subgroup U of C with $L(U) = M$, as Example 3.2 with $M = M_1 := \left\{ \begin{bmatrix} 2x \\ y \\ z \end{bmatrix} \middle|\ x,y,z\in\mathbb{Z} \right\}$ shows. Moreover, two type II-subgroups U and U* of C with $L(U) = L(U^*) = M$ need not be affinely equivalent, as Example 3.2 shows for

$$U = \langle (v_a + t,a) \mid t\in M_2\rangle, \quad U^* = \langle (v_a + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + t,a) \mid t\in M_2\rangle,$$

and $M_2 := \left\{ \begin{bmatrix} x \\ 2y \\ z \end{bmatrix} \middle|\ x,y,z\in\mathbb{Z} \right\}$. We get, however,

4.4 Lemma. Let U and U* be type II-subgroups of C with $L(U) = L(U^*) = M$. If $h(P,M)$ and the index $\mathbb{Z}^r : M$ are relatively prime, then U and U* are translationally equivalent.

Proof: Since the vector systems of U and U* are vector systems of C, as well, their difference is a vector system $s : P\to\mathbb{Z}^r$ of P with respect to M. The subgroups U and U* are translationally equivalent if and only if s defines a split extension of M by P (see [9]). So we only have to show that $|s| = 1$. Since $(\mathbb{Z}^r : M)\cdot s_p \in M$ for all $p\in P$, $|s|$ divides $\mathbb{Z}^r : M$. As s is a vector system of P with respect to M, $|s|$ divides $h(P,M)$, too, and thus $|s| = 1$. □

The following special case of our main Theorem 4.1 is due to J.Neubüser.

4.5 Proposition. Let C be symmorphic, i.e. a split extension of $\mathbb{Z}^r$ by P, and let M be a $\mathbb{Z}$-equivalent $\mathbb{Z}P$-submodule of $\mathbb{Z}^r$. If $h(P,\mathbb{Z}^r)$ and $\mathbb{Z}^r : M$ are relatively prime, then every type II-subgroup U of C with $L(U) = M$ is affinely equivalent to C.

Proof. Since C splits, we can assume that $v_p = 0$ for all $p\in P$. Therefore, the split extension

$$U^* = \{(t,p) \mid p\in P,\ t\in M\}$$

is a type II-subgroup of C with $L(U^*) = M$. Being split extensions of $\mathbb{Z}$-equivalent $\mathbb{Z}P$-modules $\mathbb{Z}^r$ and M, respectively, C and U* must be affinely equivalent. Any other subgroups U of C with $L(U) = M$ must be translationally equivalent to U* by Lemma 4.4 as $h(P,\mathbb{Z}^r) = h(P,M)$. □

To prove our main Theorem 4.1, we only have to show that for $n\leqslant 3$ Proposition 4.5 holds even for non-symmorphic groups C, because for $n\leqslant 3$ M is always $\mathbb{Z}$-equivalent to $\mathbb{Z}^r$ if $\mathbb{Z}^r : M$ is relatively prime to $|P|$ and hence relatively prime to $h(P,\mathbb{Z}^r)$. We show this generalization of Proposition 4.5 via a series of technical lemmata. The main idea is as follows: Let U be a type II-subgroup of C with $L(U) = M$. Since $\mathbb{Z}^r$ and M are

$\mathbb{Z}$-equivalent $\mathbb{Z}P$-modules, there is a $\mathbb{Z}P$-endomorphism $\varphi: \mathbb{Z}^r \to \mathbb{Z}^r$ mapping $\mathbb{Z}^r$ onto M. Conjugation of C with the natural extension $\varphi^*: \mathbb{R}^n \to \mathbb{R}^n$ of φ yields an affinely equivalent (n,r)-group $C^* := \varphi^* \cdot C \cdot \varphi^{*-1}$ with $L(C^*) = M$. If C^* is a subgroup of C, then by Lemma 4.4 U and C^* are translationally equivalent, and hence U is affinely equivalent to C. The following lemmata yield sufficient conditions for the existence of $\varphi \in \mathrm{End}_{\mathbb{Z}P}(\mathbb{Z}^r)$ with $\varphi(\mathbb{Z}^r) = M$ such that the corresponding (n,r)-group C^* is a subgroup of C. For $n \leqslant 3$ every (n,r)-group C fulfills at least one of these conditions.

4.6 Lemma. Let $h(P,\mathbb{Z}^r)$ and $\mathbb{Z}^r : M$ be relatively prime. If there is a $\mathbb{Z}P$-endomorphism $\varphi \in \mathrm{End}_{\mathbb{Z}P}(\mathbb{Z}^r)$ mapping $\mathbb{Z}^r$ onto M such that (for its natural extension to $\mathbb{Q}^r$, which we denote by φ again)

$$\varphi(v_p) \equiv v_p \bmod \mathbb{Z}^r \text{ for all } p \in P,$$

then every type II-subgroup U of C with $L(U) = M$ is affinely equivalent to C.

Proof. Let φ^* be the natural extension of φ onto $\mathbb{R}^n$ acting on the orthogonal complement of $\mathbb{R}^r$ as identity. Then the group

$$C^* := \varphi^* \cdot C \cdot \varphi^{*-1} := \{(\varphi^*(v_p) + t, p) \mid p \in P,\ t \in \varphi^*(\mathbb{Z}^r) = M\}$$

is a subgroup of C affinely equivalent to C by construction. As $\mathbb{Z}^r : M$ and $h(P,\mathbb{Z}^r) = h(P,M)$ are relatively prime, every type II-subgroup U of C with $L(U) = M$ is translationally equivalent to C^* by Lemma 4.4 and thus affinely equivalent to C. □

For the next lemma we need some definitions and notations.

We define $\mathbb{Q}(v)$ to be the smallest $\mathbb{Q}P$-submodule of $\mathbb{Q}^r$ containing all v_p, $p \in P$. (Note that $\mathbb{Q}(v)$ is not uniquely determined by C since v is determined by C only up to vectors in $\mathbb{Z}^r$.)

By Maschke's theorem ([6]) there is a $\mathbb{Q}P$-complement Q_o of $\mathbb{Q}(v)$ in $\mathbb{Q}^r$.

Let

$$\mathbb{Q}^r = H_1 \oplus \ldots \oplus H_m$$

be the decomposition of the $\mathbb{Q}P$-module $\mathbb{Q}^r$ into its homogeneous components and let

$$Q_i := H_i \cap \mathbb{Q}(v) \text{ for } i = 1,\ldots,m.$$

Changing the indices, we can assume that for a suitable $s \leqslant m$

$$\mathbb{Q}(v) = Q_1 \oplus \ldots \oplus Q_s$$

is the decomposition of $\mathbb{Q}(v)$ into its homogeneous components.

We define $\mathbb{Z}P$-submodules of $\mathbb{Z}^r$ by

$$L_i := \mathbb{Z}^r \cap Q_i \quad \text{for } i = 0,1,\ldots,s.$$

Let $a \in \mathbb{N}$ be the least positive integer such that

$$a \cdot \mathbb{Z}^r < L_o \oplus L_1 \oplus \ldots \oplus L_s,$$

i.e.

$$a = \exp(\mathbb{Z}^r / (L_o \oplus \ldots \oplus L_s)),$$

the exponent of the abelian group $\mathbb{Z}^r / (L_o \oplus \ldots \oplus L_s)$.

4.7 Lemma. Let $h(P,\mathbb{Z}^r)$ and $\mathbb{Z}^r : M$ be relatively prime. Let $\varphi \in \mathrm{End}_{\mathbb{Z}P}(\mathbb{Z}^r)$ be a $\mathbb{Z}P$-

endomorphism mapping $\mathbb{Z}^r$ onto M such that the natural extension of φ onto $\mathbb{Q}^r$ has eigenvalues

$a_i \equiv 1 \bmod a \cdot |v|$

and the homogeneous components Q_i of $\mathbb{Q}(v)$ lie in corresponding eigenspaces. Then every type II-subgroup U of C with $L(U) = M$ is affinely equivalent to C.

Proof: The restriction of φ onto the homogeneous components of $\mathbb{Q}(v)$ is

$\varphi|_{Q_i} = a_i \cdot \mathrm{id} = (1 + x_i \cdot a \cdot |v|) \cdot \mathrm{id}, \ i = 1,\dots,s,$

for suitable $x_i \in \mathbb{Z}$. (We do not claim that $a_i \neq a_j$ for $i \neq j$.) Representing v_p, $p \in P$, with respect to a lattice basis of

$L_1 \oplus \dots \oplus L_s$

we see that

$\varphi(v_p) \equiv v_p \bmod \mathbb{Z}^r$ for all $p \in P$.

Thus we can apply Lemma 4.6. □

We now derive some sufficient conditions for the existence of an endomorphism φ as in Lemma 4.7.

4.8 Lemma. Let $\mathbb{Z}^r$ and M be $\mathbb{Z}$-equivalent $\mathbb{Z}P$-modules and let $h(P,\mathbb{Z}^r)$ and $\mathbb{Z}^r : M$ be relatively prime. Then a type II-subgroup U of C with $L(U) = M$ is affinely equivalent to C if one of the following conditions a)...d) holds:

a) - $\mathbb{Z}^r = L_o \oplus \dots \oplus L_s$ (i.e. $a = 1$),
- L_i is absolutely irreducible for $i = 1,\dots,s$ (i.e. $\mathbb{Z}^r \cap \mathbb{Q}(v)$ is the direct sum of mutually inequivalent absolutely irreducible $\mathbb{Z}P$-modules $L_1,\dots,L_s$),
- the $\mathbb{Q}P$-module $\mathbb{Q}(v) = Q_1 \oplus \dots \oplus Q_s$ and its complement Q_o have no common constituents,
- $\exp(\mathbb{Z}^r/M) \equiv \pm 1 \bmod |v|$.

b) - $2 \cdot \mathbb{Z}^r < L_o \oplus \dots \oplus L_s$ (i.e. $a \leq 2$),
- L_i is absolutely irreducible for $i = 1,\dots,s$.
- $\mathbb{Q}(v)$ and Q_o have no common constituents,
- $\exp(\mathbb{Z}^r/M) \equiv \pm 1 \bmod 2 \cdot |v|$.

c) - $\mathbb{Z}^r$ is a direct sum of 1-dimensional $\mathbb{Z}P$-submodules,
- $\exp(\mathbb{Z}^r/M) \equiv \pm 1 \bmod |v|$.

d) - There are at most two affine classes of (n,r)-groups with translation lattice $\mathbb{Z}^r$ and linear constituent P.

Proof: The conditions of a) and b) can be restated as follows:

- $a \in \{1,2\}$
- L_i absolutely irreducible for $i = 1,\dots,s$,
- $\mathbb{Q}(v)$ and Q_o have no common constituents,
- $\exp(\mathbb{Z}^r/M) \equiv \pm 1 \bmod a \cdot |v|$.

To apply Lemma 4.7, we have to construct $\varphi \in \mathrm{End}_{\mathbb{Z}P}(\mathbb{Z}^r)$ such that

$\varphi(\mathbb{Z}^r) = M$ and $\varphi|_{L_i} = a_i \cdot \mathrm{id}$ with $a_i \equiv 1 \bmod a \cdot |v|$.

Since $\mathbb{Z}^r$ and M are $\mathbb{Z}$-equivalent, there is a $\mathbb{Z}P$-endomorphism $\varphi' \in \mathrm{End}_{\mathbb{Z}P}(\mathbb{Z}^r)$ with $\varphi'(\mathbb{Z}^r) = M$. The endomorphism φ' maps L_i into L_i for $i = 0,\ldots,s$, as neither $\langle v \rangle$ and Q_o nor L_i and L_j, $i \neq j$, have common constituents. Schur's Lemma ([6]) applied to the absolutely irreducible $\mathbb{Z}P$-modules $L_i, i = 1,\ldots,s$, yields

$$\varphi'|_{L_i} = a_i \cdot \mathrm{id},\ a_i \in \{\pm 1, \pm \exp(\mathbb{Z}^r/M)\}$$

as $\exp(\mathbb{Z}^r/M)$ is prime.

We shall show that replacing a_i by $-a_i$ again yields a $\mathbb{Z}P$-endomorphism φ with $\varphi(\mathbb{Z}^r) = M$ and thus we can assume that

$$a_i \equiv 1 \bmod a \cdot |v| \text{ for } 1 = 1,\ldots,s$$

and the assertion follows from Lemma 4.7.

The mapping φ can be described as

$$\varphi := \varphi' \cdot \sum_j \psi_j$$

where ψ_j acts as inversion $-\mathrm{id}_{Q_j}$ on Q_j and trivial on Q_i for $i \neq j$, i.e.

$$\psi_j := \mathrm{id}_{Q_o} \oplus \ldots \oplus \mathrm{id}_{Q_{j-1}} \oplus -\mathrm{id}_{Q_j} \oplus \mathrm{id}_{Q_{j+1}} \oplus \ldots \oplus \mathrm{id}_{Q_s}|_{\mathbb{Z}^r},$$

and j runs through the set

$$\{j \in \mathbb{N} \mid 1 \leq j \leq s,\ a_j \equiv -1 \bmod a \cdot |v|\}.$$

As

$$2 \cdot \mathbb{Z}^r < L_o \oplus \ldots \oplus L_s < \mathbb{Z}^r,$$

each ψ_j is a $\mathbb{Z}P$-automorphism of $\mathbb{Z}^r$ and thus $\varphi \in \mathrm{End}_{\mathbb{Z}P}(\mathbb{Z}^r)$ and $\varphi(\mathbb{Z}^r) = M$.

c) We shall deal with the homogeneous components $H_1,\ldots,H_m$ of $\mathbb{Q}^r$ instead of using Q_i and L_i. Note that Lemma 4.7 remains valid when we replace $\mathbb{Q}(v)$ by $\mathbb{Q}^r$ and Q_i by H_i for $i > 0$.

$$\mathbb{Z}^r = (\mathbb{Z}^r \cap H_1) \oplus \ldots \oplus (\mathbb{Z}^r \cap H_m)$$

as $\mathbb{Z}^r$ decomposes into a direct sum of irreducible $\mathbb{Z}P$-modules. Since M is a maximal and $\mathbb{Z}$-equivalent $\mathbb{Z}P$-submodule of $\mathbb{Z}^r$,

$$M = (\mathbb{Z}^r \cap H_1) \oplus \ldots \oplus (\mathbb{Z}^r \cap H_{j-1}) \oplus M^* \oplus (\mathbb{Z}^r \cap H_{j+1}) \oplus \ldots \oplus (\mathbb{Z}^r \cap H_m)$$

for a suitable j and a maximal $\mathbb{Z}P$-submodule M^* of $\mathbb{Z}^r \cap H_j$. Each $\mathbb{Z}$-submodule of $\mathbb{Z}^r \cap H_j$ is even a $\mathbb{Z}P$-submodule because $\mathbb{Z}^r \cap H_j$ consists of similar one-dimensional constituents.

Now $\mathbb{Z}^r \cap H_j$ can be decomposed into a direct sum of $\mathbb{Z}$-submodules (and thus $\mathbb{Z}P$-submodules) $M' \neq 0$ and M'' such that

$$\mathbb{Z}^r \cap H_j = M' \oplus M'' \text{ and } M^* = q \cdot M' \oplus M'',\ q := \exp(\mathbb{Z}^r/M).$$

The $\mathbb{Z}P$-endomorphism $\varphi \in \mathrm{End}_{\mathbb{Z}P}(\mathbb{Z}^r)$, defined by

$$\varphi|_{\mathbb{Z}^r \cap H_i} = \mathrm{id} \text{ for } i \neq j,\ \varphi|_{M''} = \mathrm{id},\ \varphi|_{M'} = \begin{cases} q \cdot \mathrm{id} \text{ for } q \equiv 1 \bmod |v| \\ -q \cdot \mathrm{id} \text{ for } q \equiv -1 \bmod |v| \end{cases}$$

is suitable to apply Lemma 4.7.

d) If U is a split extension, then C must split. If C splits, apply Proposition 4.5. □

4.9 Proposition. Let U be a maximal type II-subgroup of C with $L(U) = M$. If $n \leq 3$ and if $\mathbb{Z}^r$ and M are $\mathbb{Z}$-equivalent $\mathbb{Z}P$-modules and if $h(P,\mathbb{Z}^r)$ and $\mathbb{Z}^r : M$ are relatively prime, then U is affinely equivalent to C.

Proof: All but two (n,r)-groups with $n \leqslant 3$ fulfill at least one of the sufficient conditions of Lemma 4.8. For the two exceptional space groups P 4/n and P 4_2/n Lemma 4.6 can be applied.

We do not discuss all 219 + 80 + 67 + 17 + 7 3- and 2-dimensional groups but only give an idea of how to derive the congruence

$$\exp(\mathbb{Z}^r/M) \equiv \pm 1 \bmod a \cdot |v|.$$

We observed that for $n \leqslant 3$

- $|v| \in \{1,2,3,4,6\}$ for the vector systems v of all (n,r)-groups C with P(C) = C and $L(C) = \mathbb{Z}^r$,
- $a \leqslant 3$,
- if 3 or 4 divides $|v|$ for the vector system v of some (n,r)-group C with P(C) = P and $L(C) = \mathbb{Z}^r$, then a = 1,
- if a = 3 and $|v| \leqslant 2$ for the vector systems v of all (n,r)-groups C with P(C) = P and $L(C) = \mathbb{Z}^r$, then $h(P,\mathbb{Z}^r) = 2$.

By straight forward calculations we find

$$\exp(\mathbb{Z}^r/M) \equiv \pm 1 \bmod a \cdot |v|$$

if $\mathbb{Z}^r : M$ and $h(P,\mathbb{Z}^r)$ are relatively prime and $h(P,\mathbb{Z}^r) \neq 2$. (For $h(P,\mathbb{Z}^r) = 2$ we can apply Lemma 4.8 d).) □

[1] Ascher,E., Lattices of Equi-Translation Subgroups of Space Groups, Report Battelle Institute, 1968.

[2] Ascher,E., Janner,A., Algebraic Aspects of Crystallography. II. Non-primitive Translations in Space Groups, Commun. math. Phys. 11 (1968), 138 - 167.

[3] Bäringhausen,H., Group-subgroup relations between space groups as ordering principle in crystal chemistry: The "family tree" of perovskite-like structures, Acta Cryst. A31 (1975), 3.

[4] Brown,H., An algorithm for the determination of space groups, Math.Comp. 23 (1969), 499 - 514.

[5] Bülow,R., Eine Ableitung der Kristallklassen im R_4 mit Hilfe gruppentheoretischer Programme, Diplomarbeit, Kiel, 1967.

[6] Curtis,C.W., Reiner,J., Representation theory of finite groups and associative algebras, Wiley (Interscience), New York, 1962.

[7] Henry,N.F.M., Lonsdale,K. (Ed.), International Tables for X-Ray Crystallography, Vol. I, Symmetry Groups, Birmingham, The Kynoch Press, 1969.

[8] Hermann,C., Zur systematischen Strukturtheorie, IV. Untergruppen, Z. Krist. 69 (1929), 533 - 555.

[9] Köhler,K.-J., On the Structure and the Determination of n-Dimensional Partially Periodic Crystallographic Groups, to appear.

[10] Köhler,K.-J., An Algorithm for Finding the Subgroups of n-Dimensional Crystallographic Groups, to appear.

[11] Köhler,K.-J., Untergruppen kristallographischer Gruppen, Dissertation Aachen, 1977.

[12] Lepique,E., Ein Programm zur Berechnung der Untergruppen von vorgegebenem Index in endlich präsentierten Gruppen, Diplomarbeit, Aachen, 1972.

[13] Neubüser,J., Wondratschek,H., Untergruppen der Raumgruppen, Kristall und Technik 1 (1966), 529 - 543.

[14] Neubüser,J., Wondratschek,H., Maximal subgroups of the space groups, Report, 1969.

[15] Neubüser,J., Wondratschek,H., Minimal supergroups of the space groups, Report, 1970.

[16] Plesken,W., Pohst,M., On Maximal Finite Irreducible Subgroups of GL(n,$\mathbb{Z}$), I. The Five and Seven Dimensional Cases, Math.Comp. 31 (1977), 536 - 551.

[17] Zassenhaus,H., Über einen Algorithmus zur Bestimmung der Raumgruppen, Comment. Math. Helv. 21 (1948), 117 - 141.