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Subperiodic Groups as Factor Groups of Reducible Space Groups

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Abstract

Reducible space groups are introduced as those for which the point groups G are Q-reducible. The splitting of the rational space $V(T, Q)$, spanned by the translation subgroup T of the reducible space group, into two G-invariant components is considered. First, it is shown that cases of orthogonal and inclined reductions have to be distinguished. Further, reductions which lead to Z decomposition are distinguished from those which lead to Z reduction. The central point of the paper is the 'factorization theorem' which asserts that factor groups of reducible space groups by their partial G-invariant translation subgroups have the structure of subperiodic groups. The homomorphisms which map the space group onto respective subperiodic groups are analogous to homomorphisms, which map space groups onto respective site-point groups. In analogy with point groups, subperiodic groups are introduced which do not act on the Euclidean space but on a Cartesian product of Euclidean space spanned by their translation subgroup with the vector space spanned by missing translations; it is suggested that these groups are called the contracted subperiodic groups and a formalism is developed in which these groups are geometrically natural representatives of factor groups of reducible space groups.

1. Introduction

Space groups with Q-reducible point groups have several interesting properties, which have been described by a '*separation diagram*' and connected with a '*separation theorem*' (Kopský, 1986, 1988*a*). We shall define here *reducible/irreducible* space groups as those for which the point groups are *Q-reducible/Q-irreducible.* The term reducible space group is justified by the fact that such groups can be expressed as subdirect or multiple subdirect products of space groups in lower dimensions.

The construction, known as subdirect product (sum), was used for the first time by Goursat (1889) in the derivation of four-dimensional point groups and later on numerous occasions in connection with the derivation of various kinds of generalized groups. Its nature has been recognized in the work by Litvin & Opechowski (1974) on spin groups. The subdirect product is well described in the recent book by Opechowski (1986), the multiple subdirect products (and sums) are described by Kopský (1988*b*), where we also prove that reducible space groups are expressible as multiple subdirect products of lower-dimensional space groups. Since this reduction can be extended to irreducible space groups, it is possible to develop crystallography in arbitrary dimensions analogously to the theory of finite groups; namely, to consider the irreducible space groups as basic ones and to set up the rules by which the reducible space groups can be constructed.

In the present paper we shall investigate another interesting property of reducible space groups. If the space group $\mathcal{G}$ with a point group G and a translation subgroup T_G is reducible, then there exist G-invariant subgroups T_{Gi} of T_G which are of lower dimensions than T_G. If such a group also satisfies the condition $T_{Gi} = T_G \cap V(T_{Gi}, R)$, so that it is the group of all translations of T_G in the space it itself spans, we call it the partial translation subgroup of $\mathcal{G}$. As a G-invariant subgroup of T_G it is a normal subgroup of $\mathcal{G}$.

The main result of the present paper is the '*factorization theorem*' which claims that factor groups $\mathcal{G}/T_{Gi}$ of reducible space groups over their partial-translation subgroups are isomorphic to subperiodic groups, the translation subgroups of which lie in a complementary space to $V(T_{Gi}, R)$. We will prove the theorem with the use of homomorphisms which map the space group in question onto certain subperiodic groups acting on the same Euclidean space as the original space group itself. Then we will show that this is not the best way to interpret these factor groups. There is an analogy with the case of point groups which, in their rôle as factor groups of space groups by the complete translation subgroup, are interpreted as operator groups on the space $V(n)$, associated with the Euclidean space $E(n)$, on which the original space group is acting. We show that subperiodic groups as factor groups of space groups by partial translation subgroups should analogously be interpreted as groups which act on Cartesian products of the Euclidean and vector spaces of lower dimensions, which are, in a certain sense, complementary. These groups, called here contracted subperiodic groups also appear in complementary pairs, associated with reductions of vector space under the action of the point group of the reducible space group.

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We start our investigation with consideration of possible reductions of vector spaces over various fields under the action of the point groups and their consequences for the reduction of translation subgroups of space groups. First we distinguish between orthogonal and inclined reductions and between orthogonal- and inclined-reduction classes. Then we show that we have to distinguish cases when reductions of real or rational space spanned over the translation group T_G leads either to Z decomposition into the form of direct sum of partial translation subgroups or to Z reduction into the form of a subdirect sum of these subgroups.

The investigation in the present and subsequent papers, which is in a certain sense inverse to the present one, is performed in a dimension-independent manner and the main results are presented in a compact form which, unfortunately, does not cover all possibilities which occur in cases of inclined-reduction classes. The latter present some problems which require separate investigation.

2. Decomposition pattern of crystallographic point groups

A group G of real orthogonal operators on a real linear orthogonal space $V(n, R)$ of dimension n is said to be an n-dimensional crystallographic point group if it leaves invariant some translation group T_G of rank n which spans the whole $V(n, R)$ over the field of real numbers R. We span also the rational space $V(n, Q) = V(T_G, Q)$ by T_G over the rational field Q and, to get a complete picture, we imbed $V(n, R)$ in a natural way into the complex space $V(n, C)$. The group G is then a group of operators on each of spaces $V(n, K)$, $K = C, R, Q$, as well as on the translation group T_G, which can be considered either as a free Abelian group or as a Z module of rank n. In a unified language (Curtis & Reiner, 1966; Ascher & Janner, 1965, 1968/69; Jarratt, 1980), the spaces $V(n, K)$ and the group T_G are considered as KG modules, where K stands for the fields C, R, Q in $V(n, K)$ and for the ring of integers Z in case of T_G.

The main result concerning reducibility of KG modules for cases when K is a field then reads:

The KG module $V(n, K)$ is either irreducible or completely reducible to the form:

$$V(n, K) = \bigoplus_{\alpha} V_\alpha(n_\alpha d_\alpha, K)$$

$$= \bigoplus_{\alpha} \bigoplus_{a=1}^{n_\alpha} V_{\alpha a}(d_\alpha, K), \qquad (1)$$

where $V_{\alpha a}(d_\alpha, K)$ are irreducible KG modules which realize K-irreducible representations of G of the class $\alpha(K)$, $V_\alpha(n_\alpha d_\alpha, K)$ is the linear envelope of spaces $V_{\alpha a}(d_\alpha, K)$ with the same label $\alpha(K)$ over K, d_α is the dimension of representation $\alpha(K)$, irreducible over K, $n_\alpha(K)$ its multiplicity in G, considered as its own faithful representation.

The first part of this decomposition is unique and the spaces $V_\alpha(n_\alpha d_\alpha, K)$ are mutually orthogonal. It is called the canonical decomposition (see *e.g.* Jarratt, 1980). The second part is the complete decomposition, in which KG submodules $V_{\alpha a}(d_\alpha, K)$ are K-irreducible. The canonical decomposition is complete only if all numbers $n_\alpha(K) = 0$ or 1 for a given field K. Actually, the canonical decomposition is complete for all three fields if it is complete for one of them.

The numbers $n_\alpha(K)$ are uniquely determined by the group G and they depend on the field K, which also defines the labels $\alpha(K)$. As we extend the field from Q to R and further to C, the labels may split according to splitting of representations. The sets $n_\alpha(K)$ will be called here the *decomposition pattern* of the group G. Up to three dimensions we have simple situations, because the decomposition patterns coincide for the fields Q and R, although for cyclic groups of order higher than two the R-irreducible representations split in C. The first cases when decomposition pattern is different in Q and R occur in four dimensions for groups of octagonal, decagonal, and dodecagonal families. A simplified characteristic of decomposition pattern up to four dimensions is given in the book by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978) where only dimensions without labels $\alpha(K)$ are listed.

Our investigation applies to cases when the group G is Q-reducible. As we can again see in the Brown *et al.* (1978) book, this excludes only the groups: (i) $p1$ and $p\bar{1}$ which are all group types in one dimension; (ii) groups of square and hexagonal systems in two dimensions, (iii) cubic groups in three dimensions, and (iv) groups of octagonal, decagonal, dodecagonal, di-isohexagonal orthogonal, icosahedral and hypercubic families in four dimensions, which are irreducible.

3. Orthogonal and inclined reductions

According to decomposition (1), the spaces $V(n, K)$ split generally into many G-invariant K-irreducible subspaces. Here we shall be concerned with cases when the space $V(n, Q)$ splits into a direct sum $V_1(k, Q) \oplus V_2(h, Q)$, $k + h = n$, of two G-invariant subspaces, which can be further reducible. The decomposition pattern determines possible cases of such splitting, which will be called briefly Q reduction. Since the crystallographic point groups are defined in the real space $V(n, R)$ and in practice we shall refer to reduction of this space – the R reduction, it is desirable to see the relationship between R and Q reductions. It is clear that every Q reduction implies R reduction $V(n, R) = V_1(k, R) \oplus V_2(h, R)$, where spaces $V_1(k, R)$, $V_2(h, R)$ are spanned by bases of $V_1(k, Q)$, $V_2(h, Q)$ over the extended field R. The inverse is not always true. To distinguish possible cases, it is suitable to introduce reduction classes:

Definition 1: We say that the K reduction

$$V(n, K) = V_1(k, K) \oplus V_2(h, K) \qquad (2)$$

belongs to the K-reduction class $[n_{\alpha 1}(K), n_{\alpha 2}(K)]$, where $n_{\alpha 1}(K)$, $n_{\alpha 2}(K)$ are multiplicities with which G-invariant K-reducible subspaces $V_{\alpha a}(d_\alpha, K)$ appear in complete decomposition of subspaces $V_1(k, K)$, $V_2(h, K)$.

The K-reduction class is called *orthogonal* if only one of the multiplicities $n_{\alpha 1}(K)$, $n_{\alpha 2}(K)$ does not vanish for every $\alpha(K)$. Otherwise, the K-reduction class is called *inclined.*

The K reduction (2) itself is *orthogonal*, if the two subspaces are orthogonal, otherwise it is *inclined.*

We can see that the following holds for both fields Q and R: (i) The number of K-reduction classes is finite. (ii) Each orthogonal K-reduction class contains exactly one K reduction which is orthogonal – the class determines the reduction uniquely. (iii) If the canonical decomposition is complete, then all K reductions are orthogonal and uniquely defined by orthogonal K-reduction classes. (iv) The total number of orthogonal K reductions which belong to orthogonal classes is finite.

Inclined reductions present some more problems because: (i) An inclined K-reduction class defines infinitely many K reductions. (ii) An inclined R-reduction class always contains orthogonal reductions, because the subspaces $V_{\alpha a}(d_\alpha, R)$ can always be chosen as orthogonal. (iii) For an inclined Q-reduction class a weaker statement holds: There exist spaces $V(n, Q)$ for which some of the Q reductions of a given inclined Q-reduction class are orthogonal.

The relationship between R- and Q-reduction classes and between the reductions is different for the two situations:

A: *None of the classes $\alpha(Q)$ of Q-irreducible representations of G splits in R.* Then every orthogonal R-reduction class defines uniquely an orthogonal Q-reduction class and the unique R reduction of this class implies unique Q reduction for any space $V(n, Q)$. Each inclined R-reduction class also defines uniquely a Q-reduction class but a certain R reduction implies Q reduction only for certain spaces $V(n, Q)$. On the other hand, a certain R reduction, which implies Q reduction of a given $V(n, Q)$, always exists.

This is exactly the situation in three dimensions, where inclined reductions appear only in triclinic and monoclinic systems. In higher dimensions the following situations may also appear:

B: *Some of the classes $\alpha(Q)$ of Q-irreducible representations of G split in R.* Then the class $\alpha(Q)$ splits into a set of clasees $\alpha_i(R)$, $i = 1, 2, \ldots, p_\alpha$, of the same dimension $d_{\alpha_i} = d_\alpha / p_\alpha$ [see theorem (70.15) in Curtis & Reiner (1966)]. Accordingly, each space $V_{\alpha a}(d_\alpha, Q)$ spans a real space $V_{\alpha a}(d_\alpha, R)$ which reduces into a direct sum of R-irreducible subspaces $V_{\alpha_i a}(d_{\alpha_i}, R)$. An R-reduction class then defines a Q-reduction class if and only if the multiplicities $n_{\alpha_i(R)1}(R)$ and hence also the $n_{\alpha_i(R)2}(R)$ are the same for all indices i belonging to any of $\alpha(Q)$. [The multiplicities $n_{\alpha_i(R)}(R) = n_{\alpha_i(R)1}(R) + n_{\alpha_i(R)2}(R)$ are the same for all i, because G is assumed to be crystallographic.] If the R-reduction class satisfies this condition, it defines the Q-reduction class again uniquely and two situations may appear: (i) The R-reduction class is orthogonal. Then it defines uniquely the R reduction which implies a unique Q reduction for every space $V(n, Q)$. (ii) The R-reduction class is inclined. Then so is the corresponding Q-reduction class, there exist infinitely many R reductions among which are also orthogonal ones and R reductions imply Q reduction only for certain spaces $V(n, Q)$.

4. Z decomposition and Z reduction

A translation group T_G of rank and dimension n in the space $V(n, R)$ spans a rational space $V(n, Q) = V(T_G, Q)$. If T_G is G invariant, then $V(n, Q)$ is G invariant and if G is Q-reducible, then each Q reduction of $V(n, Q)$ implies a certain reduction of T_G. To find the form of this reduction, we introduce projections $\sigma_1: V(n, R) \to V_1(k, R)$, $\sigma_2: V(n, R) \to V_2(h, R)$ of the space $V(n, R)$ onto its G-invariant complementary subspaces $V_1(k, R)$, $V_2(h, R)$, spanned by the same bases as $V_1(k, Q)$, $V_2(h, Q)$. These projections are uniquely defined by Q reduction and they are either orthogonal or skew projections according to whether the Q reduction is orthogonal or inclined. The spaces and the group T_G may also be considered as Abelian groups and the projections as homomorphisms with kernels $\ker \sigma_1 = V_2(h, R)$, $\ker \sigma_2 = V_1(k, R)$ when applied to $V(n, R)$.

Theorem 1: Let T_G be a G-invariant subgroup of $V(n, R)$ of rank and dimension n and G a Q-reducible group on $V(n, R)$. Then with each Q reduction $V(T_G, Q) = V(n, Q) = V_1(k, Q) \oplus V_2(h, Q)$ there is associated a reduction of T_G of the general form:

$$T_G = T_{G1} \oplus T_{G2}[\mathbf{0} \dotplus \mathbf{d}_2 \dotplus \ldots \dotplus \mathbf{d}_p], \qquad (3a)$$

where

$$\begin{aligned} T_{G1} &= \ker \sigma_2(T_G) = T_G \cap V_1(k, R) \\ &= T_G \cap V_1(k, Q), \\ T_{G2} &= \ker \sigma_1(T_G) = T_G \cap V_2(h, R) \\ &= T_G \cap V_2(h, Q) \end{aligned}$$

and p is finite. The projections of T_G are then expressed as

$$\begin{aligned}\sigma_1(T_G) &= T^0_{G1} = T_{G1}[\mathbf{0} \dotplus \mathbf{d}_{21} \dotplus \ldots \dotplus \mathbf{d}_{p1}],\\ \sigma_2(T_G) &= T^0_{G2} = T_{G2}[\mathbf{0} \dotplus \mathbf{d}_{22} \dotplus \ldots \dotplus \mathbf{d}_{p2}],\end{aligned} \quad (3b)$$

where $\mathbf{d}_{ij} = \sigma_j(\mathbf{d}_i)$, $i = 1, 2, \ldots, p$; $j = 1, 2$.

Groups T_{G1}, T^0_{G1}, T_{G2}, T^0_{G2} are G invariant with ranks and dimensions k and h for the first and the following pair, respectively.

Proof: Groups T^0_{G1}, T^0_{G2} are G invariant because for every $\mathbf{t}_i \in T_{Gi} \subset T_G$, the vectors $g\mathbf{t}_i$ must lie simultaneously in V_i and in T_G for every $g \in G$. Since $g\sigma_1(\mathbf{t}) = \sigma_1(g\mathbf{t})$, $g\sigma_2(\mathbf{t}) = \sigma_2(g\mathbf{t})$ holds for every $g \in G$, $\mathbf{t} \in V(n, R)$, we have $GT^0_{Gi} = G\sigma_i(T_G) = \sigma_i(GT_G) = \sigma_i(T_G) = T^0_{Gi}$, so that the groups T^0_{G1}, T^0_{G2} are also G invariant.

The assertion about ranks and dimensions of T_{G1}, T_{G2} follows from the fact that for any vector of $V(n, Q)$ there exists an integer factor which sends this vector to T_G. The rank of the direct sum $T_{G1} \oplus T_{G2}$ is then $h + k = n$, so that this direct sum is a subgroup of finite index p in T_G and T_G is expressed by coset resolution $(3a)$. Formulae $(3b)$ then follow by projections and the groups T_{G1}, T_{G2} are subgroups of T^0_{G1}, T^0_{G2} of the same finite index p. The assertion about ranks and dimensions of T^0_{G1}, T^0_{G2} follows immediately.

Definition 2: We shall refer to $(3a)$ as the *Z reduction* of the group T_G. In the particular case when $p = 1$, which corresponds to the case when intersections and projections of T_G coincide, so that $T_{G1} = T^0_{G1}$, $T_{G2} = T^0_{G2}$, $(3a)$ turns into a direct sum

$$T_G = T_{G1} \oplus T_{G2} = T^0_{G1} \oplus T^0_{G2} \quad (3c)$$

and we shall refer to it as to *Z decomposition* of the group T_G.

We observe that $(3a)$ is a *subdirect sum* of groups T^0_{G1}, T^0_{G2} and the factor groups $T_G/(T_{G1} \oplus T_{G2})$, T^0_{G1}/T_{G1}, T^0_{G2}/T_{G1} are isomorphic groups of order p.

Our R and Q reductions are actually also decompositions, because they are expressed by direct sums (equivalence of reducibility and decomposability of finite groups in fields C, R, Q follows from the theorem of Maschke). Theorem 1 shows that a certain Q reduction ($=Q$ decomposition) may imply either Z reduction or stronger Z decomposition. Notice that, while R or Q reducibility (= decomposability), decomposition pattern and classes of R and Q reductions may be regarded as properties of the group G, the Z reducibility or Z decomposability of the group T_G with respect to a certain Q reduction must be regarded as a property of T_G as ZG module or as a property of the pair (G, T_G). Accordingly, the group G defines a geometric class (Q class), while pairs (G, T_G) define arithmetic classes (Z classes) of space groups. We can see easily that for each Q reduction of $V(T_G, Q)$ there exists a translation group for which Q reduction implies Z decomposition. Indeed, this is the group $T_{G1} \oplus T_{G2}$ itself in $(3a)$.

Orthogonal reduction classes

Since a Q reduction of a given orthogonal Q reduction class is unique and orthogonal, the spaces $V_1(k, Q)$, $V_2(h, Q)$ and hence also the projections (homomorphisms) σ_1, σ_2 are uniquely defined by the class and are orthogonal. Also, either of the subspaces already defines uniquely the other one as well as the reduction class and both the homomorphisms σ_1, σ_2. The Z reduction or Z decomposition of T_G still depends on the arithmetic class and generally also on its orientation with respect to the reduction. Comparison with classical crystallographic concepts shows that vectors $\mathbf{d}_i$ in $(3a)$ have the meaning of centring vectors or of additional centring vectors, if T_{G1} or T_{G2} or both are already centred. [See the relationship between subdirect sums and centring vectors (Kopský, 1988b).]

Inclined reduction classes

As stated in the previous section, the number of Q reductions in a given inclined Q-reduction class is infinite. We also need to realize that the choice of one component in an inclined Q reduction, say the $V_1(k, Q)$, does not determine the second one - the $V_2(h, Q)$. Neither of the homomorphisms σ_1, σ_2 is determined only by one of the G-invariant subspaces. Depending on the choice of these subspaces, theorem 1 may lead to various Z reductions or Z decompositions of T_G within one Q-reduction class. It may also happen that a certain Q reduction of a given class leads to Z decomposition, while another leads only to Z reduction.

A remark

Theorem 1 can be extended to arbitrary R reductions with a slight amendment; if the R reduction does not imply corresponding Q reduction, then p is not finite and the groups appearing in the decomposition are not necessarily discrete groups.

5. Reducible space groups and the factorization theorem

The space $V(n, R)$ considered as an Abelian group is a normal subgroup of the full n-dimensional Euclidean motion group $\mathscr{E}(n)$ and the n-dimensional orthogonal group $\mathscr{O}(n)$ is the corresponding factor group. We introduce a homomorphism $\boldsymbol{\sigma}: \mathscr{E}(n) \to \mathscr{O}(n)$ with $\ker \boldsymbol{\sigma} = V(n, R)$, $\operatorname{Im} \boldsymbol{\sigma} = \mathscr{O}(n)$. Then each group of isometries (Euclidean motions) of the n-dimensional Euclidean space $E(n)$ can be expressed by a symbol $\mathscr{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$, where $T_G = \ker \boldsymbol{\sigma}(\mathscr{G}) = \mathscr{G} \cap V(n, R)$ is its G-invariant translation subgroup, $G = \boldsymbol{\sigma}(\mathscr{G}) \subset \mathscr{O}(n)$ is its point group and

$\mathbf{u}_G: G \to V(n, R)$ is its system of nonprimitive translations with respect to the origin P of $E(n)$. In order that $\mathscr{G}$ be a group, $\mathbf{u}_G(g)$ must satisfy Frobenius congruences:

$$\mathbf{w}_G(g, h) = \mathbf{u}_G(g) + g\mathbf{u}_G(h) - \mathbf{u}_G(gh) = \mathbf{0} \pmod{T_G}, \quad (4)$$

where $\mathbf{w}_G: G \times G \to T_G$ is the so-called factor system. The elements of the group $\mathscr{G}$ are then expressed by Seitz symbols $\{g|\mathbf{t}+\mathbf{u}_G(g)\}_P$, where g runs through the group G, $\mathbf{t}$ through the group T_G. As usual, we shall drop the index P for a while on the assumption that the origin P is fixed. The introduced notation is of general validity. The group $\mathscr{G}$ is a space group if the group T_G is of rank and dimension n [some authors use the description of T_G as discrete translation group *large* in $V(n, R)$, *e.g.* Schwarzenberger, 1980)].

Definition 3: The space group $\mathscr{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$ is said to be reducible/irreducible, if its point group G is Q-reducible/Q-irreducible.

Corollary: It follows immediately that the reducibility or irreducibility of space groups is a property common to all space groups of a given geometric (Q) class.

Actually, we can check up to four dimensions from decomposition patterns in the book by Brown, Bülow, Neübüser, Wondratschek & Zassenhaus (1978) that reducibility/irreducibility is a common property of space groups of a crystallographic system or family and the general validity of this statement could also be proved.

Theorem 2 (*Factorization theorem for reducible space groups*): Let $\mathscr{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$ be a reducible space group, $V(T_G, Q) = V(n, Q) = V_1(k, Q) \oplus V_2(h, Q)$, one of the Q reductions of the G-invariant rational space (QG module) $V(T_G, Q)$ into the direct sum of lower-dimensional G-invariant spaces (QG modules) and ($3a$) associated with Z reduction or Z decomposition of T_G. Then the groups T_{G1}, T_{G2} (partial translation subgroups of $\mathscr{G}$) are normal in $\mathscr{G}$ and the factor groups $\mathscr{G}/T_{G2}$, $\mathscr{G}/T_{G1}$ have the structure of subperiodic groups $\mathscr{L} = \{G, T^0_{G1}, P, \mathbf{u}_{G1}(g)\}$ and $\mathscr{R} = \{G, T^0_{G2}, P, \mathbf{u}_{G2}(g)\}$, respectively, where $\mathbf{u}_{Gi}(g) = \sigma_i(\mathbf{u}_G(g))$, $i = 1, 2$.

Proof: The groups T_{G1}, T_{G2} are G invariant and hence normal in $\mathscr{G}$ by theorem 1. Further, we distinguish components of vectors from $V(n, R)$ in subspaces $V_1(k, R) = V(T_{G1}, R)$ and $V_2(h, R) = V(T_{G2}, R)$ by indices 1 and 2, respectively. The components of vectors from T_G lie in T^0_{G1}, T^0_{G2}. We fix the vectors $\{\mathbf{0}, \mathbf{d}_2, \ldots, \mathbf{d}_p\}$. Then every $\mathbf{t} \in T_G$ splits uniquely into $\mathbf{t} = \mathbf{t}^0_1 + \mathbf{t}^0_2 = \mathbf{t}_1 + \mathbf{t}_2 + \mathbf{d}_i$ with $\mathbf{t}_1 \in T_{G1}$, $\mathbf{t}_2 \in T_{G2}$; $\mathbf{t}^0_1 \in T^0_{G1}$, $\mathbf{t}^0_2 \in T^0_{G2}$ and $\mathbf{t}^0_1 = \mathbf{t}_1 + \mathbf{d}_{i1}$, $\mathbf{t}^0_2 = \mathbf{t}_2 + \mathbf{d}_{i2}$. Notice that the components of a general vector $\mathbf{t} \in T_G$ are not entirely independent, unless Z reduction ($3a$) degenerates into Z decomposition ($3c$); they contain independent components $\mathbf{t}_1, \mathbf{t}_2$ but any one of the vectors $\mathbf{d}_i$, $\mathbf{d}_{i1}$, $\mathbf{d}_{i2}$ determines the other two. In particular, for the factor system

$$\mathbf{w}_G(g, h) = \mathbf{w}^0_{G1}(g, h) + \mathbf{w}^0_{G2}(g, h) = \mathbf{w}_{G1}(g, h) + \mathbf{w}_{G2}(g, h) + \mathbf{d}(g, h), \quad (5)$$

where

$$\begin{aligned} \mathbf{w}^0_{G1}(g, h) &= \mathbf{w}_{G1}(g, h) + \mathbf{d}_1(g, h) \in T^0_{G1}, \\ \mathbf{w}^0_{G2}(g, h) &= \mathbf{w}_{G2}(g, h) + \mathbf{d}_2(g, h) \in T^0_{G2}, \end{aligned} \quad (6a)$$

while

$$\mathbf{w}_{G1}(g, h) \in T_{G1}, \ \mathbf{w}_{G2}(g, h) \in T_{G2}. \quad (6b)$$

The system of nonprimitive translations $\mathbf{u}_G: G \to V(n, R)$ also splits into its components $\mathbf{u}_{G1}: G \to V_1(k, R)$, $\mathbf{u}_{G2}: G \to V_2(h, R)$, so that $\mathbf{u}_G(g) = \mathbf{u}_{G1}(g) + \mathbf{u}_{G2}(g)$. Since G acts separately on the components, it is:

$$\begin{aligned} \mathbf{w}^0_{G1}(g, h) &= \mathbf{u}_{G1}(g) + g\mathbf{u}_{G1}(h) - \mathbf{u}_{G1}(gh), \\ \mathbf{w}^0_{G2}(g, h) &= \mathbf{u}_{G2}(g) + g\mathbf{u}_{G2}(h) - \mathbf{u}_{G2}(gh), \end{aligned} \quad (7)$$

and Frobenius congruences (4) split into two sets of congruences, which may be written either as

$$\begin{aligned} \mathbf{w}^0_{G1}(g, h) &= \mathbf{d}_1(g, h) \pmod{T_{G1}}, \\ \mathbf{w}^0_{G2}(g, h) &= \mathbf{d}_2(g, h) \pmod{T_{G2}}, \end{aligned} \quad (8a)$$

or as

$$\begin{aligned} \mathbf{w}^0_{G1}(g, h) &= \mathbf{0} \pmod{T^0_{G1}}, \\ \mathbf{w}^0_{G2}(g, h) &= \mathbf{0} \pmod{T^0_{G2}}, \end{aligned} \quad (8b)$$

with an additional condition that $\mathbf{w}^0_{Gi}(g, h)$ are, for the same pair (g, h), components of the same vector $\mathbf{d}(g, h)$. If the Z reduction ($3a$) turns out to be Z decomposition, then $\mathbf{d}(g, h) = \mathbf{0}$ and congruences ($8a$), ($8b$) are simplified to

$$\begin{aligned} \mathbf{w}_{G1}(g, h) &= \mathbf{0} \pmod{T_{G1}}, \\ \mathbf{w}_{G2}(g, h) &= \mathbf{0} \pmod{T_{G2}}. \end{aligned} \quad (9)$$

Since the components $\mathbf{u}_{G1}(g)$, $\mathbf{u}_{G2}(g)$ satisfy Frobenius congruences ($8b$), it is already clear that they define the groups $\mathscr{L}$ and $\mathscr{R}$. To show that these are the desired factor groups, we introduce mappings:

$$\begin{aligned} \boldsymbol{\sigma}_1\{g|\mathbf{t}\} &= \{g|\sigma_1(\mathbf{t})\} = \{g|\mathbf{t}_1\}, \\ \boldsymbol{\sigma}_2\{g|\mathbf{t}\} &= \{g|\sigma_2(\mathbf{t})\} = \{g|\mathbf{t}_2\}. \end{aligned} \quad (10)$$

Applying them to elements $\{g|\mathbf{t}+\mathbf{u}_G(g)\}$ of $\mathscr{G}$, we get:

$$\begin{aligned} \boldsymbol{\sigma}_1\{g|\mathbf{t}+\mathbf{u}_G(g)\} &= \{g|\mathbf{t}^0_1+\mathbf{u}_{G1}(g)\}, \\ \boldsymbol{\sigma}_2\{g|\mathbf{t}+\mathbf{u}_G(g)\} &= \{g|\mathbf{t}^0_2+\mathbf{u}_{G2}(g)\}, \end{aligned} \quad (11)$$

and, applying them to a product of two elements in

$$\begin{aligned}
&\boldsymbol{\sigma}_i(\{g\,|\,\mathbf{t}+\mathbf{u}_G(g)\}\{h\,|\,\mathbf{t}'+\mathbf{u}_G(h)\})\\
&\quad=\boldsymbol{\sigma}_i(\{gh\,|\,\mathbf{t}+g\mathbf{t}'+\mathbf{u}_G(gh)+\mathbf{w}_G(g,h)\})\\
&\quad\left\{\begin{aligned}&=\{gh\,|\,\mathbf{t}_i^0+g\mathbf{t}_i^{0\prime}+\mathbf{u}_{Gi}(gh)+\mathbf{w}_{Gi}^0(g,h)\}\\ &=\{g\,|\,\mathbf{t}_i^0+\mathbf{u}_{Gi}(g)\}\{h\,|\,\mathbf{t}_i^{0\prime}+\mathbf{u}_{Gi}(h)\}\end{aligned}\right\}\\
&\quad=\boldsymbol{\sigma}_i(\{g\,|\,\mathbf{t}+\mathbf{u}_G(g)\})\boldsymbol{\sigma}_i(\{h\,|\,\mathbf{t}'+\mathbf{u}_G(h)\}),
\end{aligned}\tag{12}$$

we see that the mappings are homomorphisms which map the group $\mathscr{G}$ onto the groups $\mathscr{L}$, $\mathscr{R}$. Indeed, as g runs through G, $\mathbf{t}$ through T_G, the elements on the right-hand sides of (11) run through the elements of $\mathscr{L}$, $\mathscr{R}$, respectively. The part of (12) set in braces is the multiplication law on groups $\mathscr{L}$, $\mathscr{R}$. From (11) we also see that kernels of these homomorphisms, as applied to $\mathscr{G}$, are $\ker\boldsymbol{\sigma}_1(\mathscr{G})=T_{G2}$, $\ker\boldsymbol{\sigma}_2(\mathscr{G})=T_{G1}$. Existence of the homomorphisms with these kernels and with images $\boldsymbol{\sigma}_1(\mathscr{G})=\mathscr{L}$, $\boldsymbol{\sigma}_2(\mathscr{G})=\mathscr{R}$ is exactly what we wanted to prove.

Definition 4: We shall say that two subperiodic groups are *complementary* if they have the same point group G and if their translation subgroups T_{G1}^0, T_{G2}^0 span complementary subspaces of $V(n,R)$.

Thus the factorization theorem shows that factor groups of a reducible space group by partial translation subgroups T_{G1}, T_{G2}, corresponding to a certain Q reduction, are isomorphic to a pair of complementary subperiodic groups. We use the letters $\mathscr{L}$ and $\mathscr{R}$ for these groups to indicate an analogy and anticipate the use of factorization theorem in three dimensions where the complementary groups are the layer and rod groups.

6. Origin dependence of homomorphisms $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$

The homomorphisms $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ and the groups $\mathscr{L}$, $\mathscr{R}$ are related to the choice of origin as well as the Seitz symbols. This is innocuously hidden in (10), where Seitz symbols refer to a certain origin P. Let us see how the picture changes if we choose another origin $S=P+\boldsymbol{\tau}$. The Seitz symbols for the two origins are related by

$$\{g\,|\,\mathbf{t}\}_S=\{g\,|\,\mathbf{t}+\boldsymbol{\varphi}(g,\boldsymbol{\tau})\}_P,$$
$$\{g\,|\,\mathbf{t}\}_P=\{g\,|\,\mathbf{t}-\boldsymbol{\varphi}(g,\boldsymbol{\tau})\}_S,$$

where $\boldsymbol{\varphi}(g,\boldsymbol{\tau})=\boldsymbol{\tau}-g\boldsymbol{\tau}$ is the *shift function.* Hence the group $\mathscr{G}$ can be equivalently expressed with respect to two origins as

$$\begin{aligned}\mathscr{G}&=\{G,T_G,P,\mathbf{u}_G(g)\}\\&=\{G,T_G,S,\mathbf{u}_G(g)-\boldsymbol{\varphi}(g,\boldsymbol{\tau})\},\end{aligned}\tag{13a}$$

while

$$\begin{aligned}\mathscr{G}(\boldsymbol{\tau})&=\{G,T_G,P,\mathbf{u}_G(g)+\boldsymbol{\varphi}(g,\boldsymbol{\tau})\}\\&=\{G,T,S,\mathbf{u}_G(g)\}\end{aligned}\tag{13b}$$

is a space group, obtained by a 'shift' of $\mathscr{G}$ on $\boldsymbol{\tau}$.

The homomorphisms σ_1, σ_2 are not influenced by the choice of origin, while homomorphisms $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ defined by (10) depend on the choice of origin and should therefore be distinguished for its distinct choices. Hence we amend (10) to

$$\begin{aligned}\boldsymbol{\sigma}_{Pi}\{g\,|\,\mathbf{t}\}_P&=\{g\,|\,\mathbf{t}_i\}_P\\ \boldsymbol{\sigma}_{Si}\{g\,|\,\mathbf{t}\}_S&=\{g\,|\,\mathbf{t}_i\}_S.\end{aligned}\tag{10a}$$

Accordingly, we have to distinguish also the subperiodic groups, obtained by mappings $\boldsymbol{\sigma}_{Pi}$, $\boldsymbol{\sigma}_{Si}$, by indices P and S. We get

$$\begin{aligned}\mathscr{L}_P&=\boldsymbol{\sigma}_{P1}(\mathscr{G})=\{G,T_{G1}^0,P,\mathbf{u}_{G1}(g)\},\\ \mathscr{R}_P&=\boldsymbol{\sigma}_{P2}(\mathscr{G})=\{G,T_{G2}^0,P,\mathbf{u}_{G2}(g)\}.\end{aligned}\tag{14a}$$

Taking into account that the shift function satisfies $\boldsymbol{\sigma}_i(\boldsymbol{\varphi}(g,\boldsymbol{\tau}))=\boldsymbol{\varphi}(g,\sigma_i(\boldsymbol{\tau}))=\boldsymbol{\varphi}(g,\boldsymbol{\tau}_i)$ we get

$$\begin{aligned}\mathscr{L}_S&=\boldsymbol{\sigma}_{S1}(\mathscr{G})=\{G,T_{G1}^0,S,\mathbf{u}_{G1}(g)-\boldsymbol{\varphi}(g,\boldsymbol{\tau}_1)\}\\&=\{G,T_{G1}^0,P+\boldsymbol{\tau}_2,\mathbf{u}_{G1}(g)\},\\ \mathscr{R}_S&=\boldsymbol{\sigma}_{S2}(\mathscr{G})=\{G,T_{G2}^0,S,\mathbf{u}_{G2}(g)-\boldsymbol{\varphi}(g,\boldsymbol{\tau}_2)\}\\&=\{G,T_{G2}^0,P+\boldsymbol{\tau}_1,\mathbf{u}_{G2}(g)\}.\end{aligned}\tag{14b}$$

In view of (13b), we can also write the latter groups as $\mathscr{L}_S=\mathscr{L}_P(\boldsymbol{\tau}_2)$, $\mathscr{R}_S=\mathscr{R}_P(\boldsymbol{\tau}_1)$ and interpret them as the groups $\mathscr{L}_P$, $\mathscr{R}_P$, shifted in space by vectors $\boldsymbol{\tau}_2=\sigma_2(\boldsymbol{\tau})$, $\boldsymbol{\tau}_1=\sigma_1(\boldsymbol{\tau})$, respectively. The groups $\mathscr{L}_P$, $\mathscr{R}_P$ leave invariant hyperplanes $(P,V_1(k,R))$ and $(P,V_2(h,R))$, while $\mathscr{L}_S$, $\mathscr{R}_S$ leave invariant hyperplanes $(S,V_1(k,R))$, $(S,V_2(h,R))$, respectively.

Notice now an important point. The shift of the group $\mathscr{G}$ in space by $\boldsymbol{\tau}$ leads to the shift of factor groups by projections of $\boldsymbol{\tau}$ onto $V_1(k,R)$, $V_2(h,R)$ which are the vectors $\boldsymbol{\tau}_1=\sigma_1(\boldsymbol{\tau})$, $\boldsymbol{\tau}_2=\sigma_2(\boldsymbol{\tau})$ and the shift by $\boldsymbol{\tau}_1$ applies to the group $\mathscr{L}_P$, while the shift by $\boldsymbol{\tau}_2$ applies to $\mathscr{R}_P$, so that:

$$\begin{aligned}\boldsymbol{\sigma}_{P1}(\mathscr{G}(\boldsymbol{\tau}))&=\mathscr{L}_P(\sigma_1(\boldsymbol{\tau}))=\mathscr{L}_P(\boldsymbol{\tau}_1),\\ \boldsymbol{\sigma}_{P2}(\mathscr{G}(\boldsymbol{\tau}))&=\mathscr{R}_P(\sigma_2(\boldsymbol{\tau}))=\mathscr{R}_P(\boldsymbol{\tau}_2).\end{aligned}\tag{15}$$

This should be distinguished from the shifts caused by the change of the origin. The shift of origin P by $\boldsymbol{\tau}$ does not change the subperiodic group $\mathscr{L}_P$ if it lies in the subspace $V_1(k,R)$, and it does not change the subperiodic group $\mathscr{R}_P$ if it lies in the subspace $V_2(h,R)$. Such shifts change the systems of nonprimitive translations in the group $\mathscr{G}$ as well as in the groups $\mathscr{L}_P$ or $\mathscr{R}_P$. The shift by $\boldsymbol{\tau}_1\in V_1(k,R)$ does not change the group $\mathscr{L}_P$ but applies to the group $\mathscr{R}_P$, while the shift $\boldsymbol{\tau}_2\in V_2(h,R)$ does not change the group $\mathscr{R}_P$ but applies to the group $\mathscr{L}_P$.

Further, the shifts $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_2$ depend on both homomorphisms σ_1, σ_2. The hyperplane $(P,V_1(k,R))$ itself may be considered as the hyperplane onto which we 'project' the group $\mathscr{G}$ in the factorization procedure, while the orientation $V_2(h,R)$ of the second set of hyperplanes determines the direction of the projection and *vice versa*. The homomorphisms σ_1, σ_2 themselves are determined by the pair of complementary subspaces $V_1(k, R)$, $V_2(h, R)$, which must be G invariant. Now, the specification of any one of these subspaces already determines the reduction class. If this reduction class is orthogonal, then either one of the subspaces already determines the second one and hence also both homomorphisms σ_1, σ_2 uniquely. If the reduction class is inclined, then the choice of one of the subspaces, say of the $V_1(k, R)$, determines only an orientation of hyperplanes onto which we project and there is still a certain freedom in the choice of the direction of the projection, which is correlated with the choice of the complementary subspace $V_2(h, R)$ and hence of the second set of hyperplanes onto which we project the group $\mathscr{G}$.

7. The general subperiodic groups

We have proved the factorization theorem for crystallographic space groups with the use of homomorphisms which correspond to crystallographic directions. The theorem actually holds for a wider class of groups of Euclidean motions and there is also generally no necessity to restrict the reductions to Q reductions. As we have pointed out at the beginning of § 5, the symbol $\{G, T_G, P, \mathbf{u}_G(g)\}$ can be used for any subgroup $\mathscr{G}$ of $\mathscr{E}(n)$. We shall further say that $\mathscr{G}$ is a space group (perhaps noncrystallographic) if its translation subgroup T_G (which is now not necessarily discrete) spans the whole $V(n, R)$, otherwise we say that $\mathscr{G}$ is subperiodic. In other words, the group is subperiodic if its translation subgroup spans a proper (or trivial) subspace of $V(n, R)$. With the exception of site-point groups which correspond to the case of trivial subspace, the point groups of subperiodic groups are necessarily reducible, because the linear envelope of T_G is a proper subspace $V_1(k, R)$ of $V(n, R)$.

Each subspace $V_1(k, R)$ defines a set of parallel hyperplanes $(P+\boldsymbol{\tau}_2, V_1(k, R))$, where $\boldsymbol{\tau}_2$ runs through coset representatives in coset resolution of $V(n, R)$ with respect to its subgroup $V_1(k, R)$. We can choose these representatives in such a way that they will form a complementary subspace $V_2(h, R)$ to $V_1(k, R)$ in $V(n, R)$. At this point we have again to distinguish cases when $V_2(h, R)$ is chosen either as an orthogonal or as an inclined complement. The choice of an orthogonal complement provides a particularly clear picture which enabled us to formulate the main results of reducibility theory for space groups in a compact manner (Kopský, 1986, 1988*a*). Let us first elaborate this case.

Orthogonal reductions

If we choose the complement $V_2(h, R)$ as an orthogonal one, then we have a second set of hyperplanes $(P+\boldsymbol{\tau}_1, V_2(h, R))$, orthogonal to the first one. The greatest point group which leaves the subspace $V_1(k, R)$ invariant is the direct product $\mathscr{O}_{12} = \mathscr{O}_1(k)\times\mathscr{O}_2(h)$ of orthogonal groups on $V_1(k, R)$ and on its orthogonal complement $V_2(h, R)$. This is at the same time also the greatest subgroup of $\mathscr{O}(n)$, which leaves the orthogonal complement $V_2(h, R)$ invariant. To this group there corresponds a subgroup (space group)

$$\begin{aligned}\mathscr{E}_{12} &= \mathscr{E}_1(k)\times\mathscr{E}_2(h)\\ &= \{\mathscr{O}_1(k)\times\mathscr{O}_2(h),\ V(n, R),\ P, \mathbf{u}=\mathbf{0}\} \end{aligned}\tag{16a}$$

of $\mathscr{E}(n)$, which is a direct product of groups

$$\begin{aligned}\mathscr{E}_1(k) &= \{\mathscr{O}_1(k)\times\{e_2\},\ V_1(k, R),\ P, \mathbf{u}=\mathbf{0}\},\\ \mathscr{E}_2(k) &= \{\{e_1\}\times\mathscr{O}_2(h),\ V_2(h, R),\ P, \mathbf{u}=\mathbf{0}\}.\end{aligned}\tag{16b}$$

Indeed, each element of $\mathscr{E}_1(k)\times\mathscr{E}_2(h)$ can be uniquely expressed as a pair (g_1, g_2), where $g_1\in\mathscr{O}_1(k)$, $g_2\in\mathscr{O}_2(h)$ and

$$\begin{aligned}\{g|\mathbf{t}\}_P &= \{(g_1, g_2)|\mathbf{t}\}_P = \{g_1|\mathbf{t}_1\}_P\{g_2|\mathbf{t}_2\}_P\\ &= \{g_2|\mathbf{t}_2\}_P\{g_1|\mathbf{t}_1\}_P\end{aligned}$$

because g_1 acts trivially on $\mathbf{t}_2\in V_2(h, R)$, g_2 on $\mathbf{t}_1\in V_1(k, R)$. Elements $\{g_1|\mathbf{t}_1\}_P$ of $\mathscr{E}_1(k)$ act in a concerted manner on hyperplanes $(P+\boldsymbol{\tau}_2, V_1(k, R))$, moving the points $(P+\boldsymbol{\tau}_2)+\mathbf{x}_1$ to points $(P+\boldsymbol{\tau}_2)+g_1\mathbf{x}_1+\mathbf{t}_1$. Further, they act on the set of hyperplanes $(P+\boldsymbol{\tau}_1, V_2(h, R))$ as on the points of the k-dimensional Euclidean space with points $P+\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_1\in V_1(k, R)$. Indeed, it is $\{g_1|\mathbf{t}_1\}_P(P+\boldsymbol{\tau}_1, V_2(h, R)) = (P+g_1\boldsymbol{\tau}_1+\mathbf{t}_1, V_2(h, R))$ and the point $(P+\boldsymbol{\tau}_1)+\mathbf{x}_2$ of the hyperplane $(P+\boldsymbol{\tau}_1, V_2(h, R))$ is sent to the point $(P+g_1\boldsymbol{\tau}_1+\mathbf{t}_1)+\mathbf{x}_2$ of the hyperplane $(P+g_1\boldsymbol{\tau}_1+\mathbf{t}_1, V_2(h, R))$. The reader will doubtlessly see himself the action of elements $\{g_2|\mathbf{t}_2\}_P$ in analogy with this consideration.

The group $\mathscr{E}_{12} = \mathscr{E}_1(k)\times\mathscr{E}_2(h)$ is the greatest subgroup of $\mathscr{E}(n)$ which transforms both sets of hyperplanes only among themselves. This group contains all space groups, the point groups of which admit the reduction $V(n, R) = V_1(k, R)\oplus V_2(h, R)$. It contains subspaces $V_1(k, R)$, $V_2(h, R)$ as normal subgroups and it is easy to see that the factorization theorem applies to it. The homomorphisms $\boldsymbol{\sigma}_{P1}, \boldsymbol{\sigma}_{P2}$, defined by (10*a*), send it to groups

$$\begin{aligned}\boldsymbol{\sigma}_{P1}(\mathscr{E}_{12}) &= \mathscr{E}_1(k)\times\mathscr{O}_{P2}(h) = \mathscr{L}(P, V_1(k, R))\\ &= \{\mathscr{O}_1(k)\times\mathscr{O}_2(h),\ V_1(k, R),\ P, \mathbf{u}=\mathbf{0}\},\\ \boldsymbol{\sigma}_{P2}(\mathscr{E}_{12}) &= \mathscr{O}_{P1}(k)\times\mathscr{E}_2(h) = \mathscr{R}(P, V_2(h, R))\\ &= \{\mathscr{O}_1(k)\times\mathscr{O}_2(h),\ V_2(h, R),\ P, \mathbf{u}=\mathbf{0}\}.\end{aligned}\tag{17a}$$

Let us again analyse at least the first of these groups. Its elements are commuting products of $\{g_1|\mathbf{t}_1\}_P\in\mathscr{E}_1(k)$ and of $\{g_2|\mathbf{0}\}_P\in\mathscr{O}_{P2}(h)$. We have seen above the action of the first of these elements on the hyperplanes. The second element leaves the hyperplane

$(P, V_1(k, R))$ pointwise invariant and sends the hyperplanes $(P+\boldsymbol{\tau}_2, V_1(k, R))$ to $(P+g_2\boldsymbol{\tau}_2, V_1(k, R))$ in such a way that it sends the point $(P+\boldsymbol{\tau}_2)+\mathbf{x}_1$ to the point $(P+g_2\boldsymbol{\tau}_2)+\mathbf{x}_1$. The group $\mathscr{E}_1(k)\times\mathscr{O}_{P2}(h)$ is the greatest subgroup of $\mathscr{E}(n)$, which leaves the hyperplane $(P, V_1(k, R))$ invariant.

Definition 5: The set of all elements of $\mathscr{E}(n)$ which leave a hyperplane $(P, V_1(k, R))$ invariant is called the *general subperiodic group* of this hyperplane. Two general subperiodic groups are called *complementary* if the orientations of their hyperplanes are orthogonal complements.

The groups $\mathscr{L}(P, V_1(k, R))$ and $\mathscr{R}(P, V_2(h, R))$ in (17*a*) are the complementary general subperiodic groups which realize factor groups of $\mathscr{E}_{12}$ over $V_2(h, R)$, $V_1(k, R)$, respectively. Accordingly, $\ker \boldsymbol{\sigma}_{P1} = V_2(h, R)$, $\ker \boldsymbol{\sigma}_{P2} = V_1(k, R)$.

The homomorphisms $\boldsymbol{\sigma}_{P1}, \boldsymbol{\sigma}_{P2}$ can now be applied to any subgroup $\mathscr{G}=\{G, T_G, P, \mathbf{u}_G(g)\}$ of $\mathscr{E}_{12}$ and here $\mathscr{G}$ needs to be neither crystallographic nor space group. As a result of homomorphic mappings, we get the groups

$$\begin{aligned}\boldsymbol{\sigma}_{P1}(\mathscr{G}) &= \{G, \sigma_1(T_G), P, \sigma_1\mathbf{u}_G(g)\}\\ &= \{G, T^0_{G1}, P, \mathbf{u}_{G1}(G)\},\\ \boldsymbol{\sigma}_{P2}(\mathscr{G}) &= \{G, \sigma_2(T_G), P, \sigma_2\mathbf{u}_G(g)\}\\ &= \{G, T^0_{G2}, P, \mathbf{u}_{G2}(G)\},\end{aligned} \tag{18}$$

which will be isomorphic to factor groups $\mathscr{G}/T_{G2}$, $\mathscr{G}/T_{G1}$, respectively, where:

$$\begin{aligned}T_{G1} &= \ker \boldsymbol{\sigma}_{P2}(\mathscr{G}) = \ker \sigma_2(T_G)\\ &= \mathscr{G}\cap V_1(k, R),\\ T_{G2} &= \ker \boldsymbol{\sigma}_{P1}(\mathscr{G}) = \ker \sigma_1(T_G)\\ &= \mathscr{G}\cap V_2(h, R).\end{aligned} \tag{19}$$

This gives a slightly different (and more general) picture from the factorization theorem as we have formulated it here. The reduction $V(n, R) = V_1(k, R)\oplus V_2(h, R)$ is orthogonal but it does not necessarily imply Q reduction; actually, the action of G on $V(n, R)$ is not necessarily a Q representation (T_G is not necessarily a discrete translation group). If $\mathscr{G}$ is a crystallographic space group and the reduction is of orthogonal class for its point group G, then the present result coincides with that of our factorization theorem. The same holds in cases of inclined-reduction classes if the R reduction above is accidentally also a Q reduction. Otherwise either one or both of the homomorphisms σ_1, σ_2 result in groups T^0_{G1}, T^0_{G2} which are not discrete; accordingly the groups T_{G1}, T_{G2} do not necessarily span the subspaces $V_1(k, R)$, $V_2(h, R)$. These situations may be of interest in the theory of quasicrystals and it would be desirable to perform an analysis of their relationship to the recently introduced concept of quasicrystalline space groups (Rokhsar, Wright & Mermin, 1988*a*, *b*). We shall stay for the moment with crystallographic space groups.

Inclined reductions

If the point group G admits an inclined reduction $V(n, R) = V_1(k, R)\oplus V_2(h, R)$, which implies a Q reduction, then not only the spaces $V_1(k, R)$, $V_2(h, R)$, but also their orthogonal complements $\hat{V}_2(h, R)$, $\hat{V}_1(k, R)$ are G invariant. Accordingly, the point group G is a subgroup of direct products of orthogonal groups $\hat{\mathscr{O}}_{12} = \mathscr{O}_1(k)\times\hat{\mathscr{O}}_2(h)$, $\hat{\mathscr{O}}_{21} = \hat{\mathscr{O}}_1(k)\times\mathscr{O}_2(h)$ and space groups with point group G are subgroups of space groups $\hat{\mathscr{E}}_{12} = \{\hat{\mathscr{O}}_{12}, V(n, R), P, \mathbf{u}=\mathbf{0}\}$, $\hat{\mathscr{E}}_{21} = \{\hat{\mathscr{O}}_{21}, V(n, R), P, \mathbf{u}=\mathbf{0}\}$. Hence the point group G is a subgroup of an intersection $\mathscr{O}_{12} = \hat{\mathscr{O}}_{12}\cap\hat{\mathscr{O}}_{21}$ and all Euclidean motion groups with this point group are subgroups of the intersection

$$\begin{aligned}\mathscr{E}_{12} &= \hat{\mathscr{E}}_{12}\cap\hat{\mathscr{E}}_{21}\\ &= \{\mathscr{O}_{12}, V(n, R), P, \mathbf{u}=\mathbf{0}\}.\end{aligned} \tag{20}$$

The subspaces $V_1(k, R)$, $V_2(h, R)$ considered as translation groups are already normal subgroups of this group because they are simultaneously $\mathscr{O}_{12}$ invariant. Notice that while $V_1(k, R)$ is normal in $\hat{\mathscr{E}}_{12}$, $V_2(h, R)$ in $\hat{\mathscr{E}}_{21}$, the group $\mathscr{E}_{12}$ is the greatest subgroup of $\mathscr{E}(n)$ in which both of these subspaces are normal subgroups. The projections σ_1, σ_2 and the choice of origin again define homomorphisms $\boldsymbol{\sigma}_{P1}$, $\boldsymbol{\sigma}_{P2}$ by (10*a*) and these homomorphisms send the group $\mathscr{E}_{12}$ onto subgroups

$$\begin{aligned}\boldsymbol{\sigma}_{P1}(\mathscr{E}_{12}) &= \mathscr{L}(P, V_1(k, R);\ V_2(h, R))\\ &= \{\mathscr{O}_{12}, V_1(k, R), P, \mathbf{u}=\mathbf{0}\},\\ \boldsymbol{\sigma}_{P2}(\mathscr{E}_{12}) &= \mathscr{R}(P, V_2(h, R);\ V_1(k, R))\\ &= \{\mathscr{O}_{12}, V_2(k, R), P, \mathbf{u}=\mathbf{0}\}\end{aligned} \tag{21}$$

of general subperiodic groups $\mathscr{L}(P, V_1(k, R))$, $\mathscr{R}(P, V_2(h, R))$.

Notice that the latter two general subperiodic groups are not complementary in the sense of definition 4 (as it is reflected in definition 5) because they correspond to different point groups $\hat{\mathscr{O}}_{12}, \hat{\mathscr{O}}_{21}$; now

$$\begin{aligned}\mathscr{L}(P, V_1(k, R)) &= \{\hat{\mathscr{O}}_{12}, V_1(k, R), P, \mathbf{u}=\mathbf{0}\},\\ \mathscr{R}(P, V_2(k, R)) &= \{\hat{\mathscr{O}}_{21}, V_2(k, R), P, \mathbf{u}=\mathbf{0}\}.\end{aligned} \tag{22}$$

The greatest complementary subperiodic groups which correspond to the inclined reduction are now the groups (21).

The groups $\mathscr{O}_{12}$, $\mathscr{E}_{12}$ play here the same rôle as the groups denoted before by the same symbols for orthogonal reductions. The group $\mathscr{O}_{12}$ is the greatest subgroup of $\mathscr{O}(n)$ which leaves both subspaces $V_1(k, R)$, $V_2(h, R)$ invariant and $\mathscr{E}_{12}$ is the greatest subgroup of $\mathscr{E}(n)$ which transforms the sets of hyperplanes $(P+\boldsymbol{\tau}_2, V_1(k, R))$, $(P+\boldsymbol{\tau}_1, V_2(h, R))$ among themselves. Orthogonal reductions are particular cases of inclined ones and they occur when $V_1(k, R) = \hat{V}_1(k, R)$, $V_2(h, R) = \hat{V}_2(h, R)$, $\mathscr{O}_{12} = \hat{\mathscr{O}}_{12} = \hat{\mathscr{O}}_{21}$, $\mathscr{E}_{12} = \hat{\mathscr{E}}_{12} = \hat{\mathscr{E}}_{21}$.

Summary

The origin of the ambiguity in factor groups $\mathscr{L}_P$, $\mathscr{R}_P$ is now quite transparent; according to the choice of origin P we map the groups $\mathscr{G}$ into various general subperiodic groups which differ only by a shift in space and which correspond to various hyperplanes of the same orientation but of different location in the space. This location is determined by the point P through which the corresponding hyperplanes pass.

We have also established the following: If a subspace $V_1(k, R)$ of $V(n, R)$ is G invariant, then there exist homomorphisms, which map the groups of geometric class G into the general subperiodic groups $\mathscr{L}(P+\boldsymbol{\tau}_2, V_1(k, R))$. If the reduction class of G determined by $V_1(k, R)$ is orthogonal, then there is only one such homomorphism for each of these general subperiodic groups. Otherwise there is also a certain further freedom in the choice of the 'direction' of these homomorphisms, related to the choice of the direction of the complementary space. In the case of crystallographic groups we must set further restrictions on the choice of subspaces if we want to get crystallographic subperiodic groups as the projections. This is, for example, the reason for which we cannot guarantee that an orthogonal projection of a crystallographic space group will be a crystallographic subperiodic group if the corresponding reduction belongs to an inclined class.

8. The contracted subperiodic groups

The remedy for the ambiguity in '*location*' of resulting subperiodic groups is provided by introduction of groups for which we suggest the name '*contracted subperiodic groups*'. The basic idea and the difference between ordinary and contracted subperiodic groups can best be illustrated by consideration of the point groups and their relationship to site-point groups. With each point P of $E(n)$ there is associated a group $\mathscr{O}_P(n) = \{\mathscr{O}(n), T = (\mathbf{0}), P, \mathbf{u} = \mathbf{0}\}$, the group of all n-dimensional rotations which leave the point P invariant. The homomorphism $\boldsymbol{\sigma}: \mathscr{E}(n) \to \mathscr{O}(n)$ introduced at the beginning of § 5 sends each subgroup $\mathscr{G} = \{G, T_G, P, \mathbf{u}(g)\}$ of $\mathscr{E}(n)$ onto its point group $G = \boldsymbol{\sigma}(\mathscr{G})$, the subgroup of $\mathscr{O}(n)$ which acts on $V(n, R)$. We can associate with each point P a homomorphism $\boldsymbol{\sigma}_P: \mathscr{E}(n) \to \mathscr{O}_P(n)$ by $\boldsymbol{\sigma}_P\{g|\mathbf{t}\}_P = \{g|\mathbf{0}\}_P$. Such homomorphisms will send the group $\mathscr{G}$ to site-point groups $G_P = \{G, (\mathbf{0}), P, \mathbf{u} = \mathbf{0}\}$, which, as groups acting on $E(n)$, differ from G by their location in $E(n)$. These site-point groups can be considered as factor groups of the group $\mathscr{G}$ over its translation subgroup T_G as well as the group G. It is, however, a better practice to consider the point group G, which is deprived of any location in $E(n)$, as the representative of the factor group; the group G is at the same time an operator group on $V(n, R)$ and hence on T_G.

The contracted subperiodic groups play an analogous role with respect to partial translation subgroups as the point groups with respect to the full translation subgroups. We shall introduce them quite formally as groups acting on Cartesian products of Euclidean and orthogonal vector spaces. Let us first consider a Cartesian product $E_1(k) \times V_2(h, R)$ of k-dimensional Euclidean space $E_1(k)$ and h-dimensional real orthogonal vector space $V_2(h, R)$. The elements of this product are pairs $(P_1 + \mathbf{x}_1, \mathbf{x}_2)$ of a point $P_1 + \mathbf{x}_1$ of $E_1(k)$ and of a vector $\mathbf{x}_2 \in V_2(h, R)$, where P_1 is an arbitrary but fixed point of $E_1(k)$ and $V_1(k, R)$ its difference space. Further we introduce a direct product $\mathscr{E}_1(k) \times \mathscr{O}_2(h)$ of a Euclidean group acting on $E_1(k)$ and an orthogonal group acting on $V_2(h, R)$. We shall write elements of this group in the form $[(g_1, g_2)|\mathbf{t}_1]_{P_1}$ and their action on elements of the Cartesian product will be defined by

$$[(g_1, g_2)|\mathbf{t}_1]_{P_1}(P_1 + \mathbf{x}_1, \mathbf{x}_2) = (P_1 + g_1\mathbf{x}_1 + t_1, g_2\mathbf{x}_2). \tag{23a}$$

Though both the Cartesian product and the group acting on it may be introduced independently of any space $E(n)$, it is of advantage for our purposes to identify the spaces $V_1(k, R)$, $V_2(h, R)$ with orthogonal complements in the difference space $V(n, R)$ of $E(n)$. We shall further introduce a Cartesian product $V_1(k, R) \times E_2(h)$, the elements of which are pairs $(\mathbf{x}_1, P_2 + \mathbf{x}_2)$ of a vector $\mathbf{x}_1$ from $V_1(k, R)$ and of a point $P_2 + \mathbf{x}_2$ from $E_2(h)$, where P_2 is an arbitrary but fixed point of $E_2(h)$ and $\mathbf{x}_2 \in V_2(h, R)$. Again we introduce the direct product $\mathscr{O}_1(k) \times \mathscr{E}_2(h)$ of an orthogonal group on $V_1(k, R)$ with Euclidean group on $E_2(h)$. To distinguish the elements of this group formally from the previous one, we shall write them in the form $\langle (g_1, g_2)|\mathbf{t}_2\rangle_{P_2}$ and define their action on the Cartesian product by

$$\langle (g_1, g_2)|\mathbf{t}_2\rangle_{P_2}(\mathbf{x}_1, P_2 + \mathbf{x}_2) = (g_1\mathbf{x}_1, P_2 + g_2\mathbf{x}_2 + \mathbf{t}_2). \tag{23b}$$

Now we can introduce homomorphisms $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$ as

$$\begin{aligned} \boldsymbol{\sigma}_1\{g|\mathbf{t}\}_P &= [g|\sigma_1(\mathbf{t})]_{P_1} = [g|\mathbf{t}_1]_{P_1}, \\ \boldsymbol{\sigma}_2\{g|\mathbf{t}\}_P &= \langle g|\sigma_2(\mathbf{t})\rangle_{P_2} = \langle g|\mathbf{t}_2\rangle_{P_2}, \end{aligned} \tag{10b}$$

which map the group $\mathscr{E}_{12}$ onto the direct products

$$\begin{aligned} \boldsymbol{\sigma}_1(\mathscr{E}_{12}) &= \mathscr{E}_1(k) \times \mathscr{O}_2(h) = \mathscr{L}(V_1(k, R)) \\ &= [\mathscr{O}_1(k) \times \mathscr{O}_2(h), V_1(k, R), P_1, \mathbf{u}_1 = \mathbf{0}], \\ \boldsymbol{\sigma}_2(\mathscr{E}_{12}) &= \mathscr{O}_1(k) \times \mathscr{E}_2(h) = \mathscr{R}(V_2(h, R)) \\ &= \langle \mathscr{O}_1(k) \times \mathscr{O}_2(h), V_2(h, R), P_2, \mathbf{u}_2 = \mathbf{0}\rangle. \end{aligned} \tag{17b}$$

We suggest the names '*general contracted subperiodic groups*' with translation spaces $V_1(k, R)$, $V_2(h, R)$ for the last two groups and '*contracted subperiodic groups*' for their subgroups. We shall now briefly outline the use of contracted subperiodic groups in the factorization procedure.

We have now a unique general contracted subperiodic group $\mathscr{L}(V_1(k, R))$ for each subspace $V_1(k, R)$. The orthogonal group $\mathscr{O}(n)$ can be considered on the same basis as the contracted subperiodic group corresponding to trivial subspace $(\mathbf{0})$. We shall again say that the groups $\mathscr{L}(V_1(k, R))$, $\mathscr{R}(V_2(h, R))$ are complementary if the subspaces $V_1(k, R)$, $V_2(h, R)$ are orthogonal complements in $V(n, R)$. To include inclined reductions into the scheme, we have to consider also the Cartesian products $E_1(k)\times V_2(h, R)$ and their partners $V_1(k, R)\times E_2(h)$ for which the subspaces $V_1(k, R)$, $V_2(h, R)$, playing the rôles of difference spaces or of components in products, are not orthogonal. Such products are then subject to action of those subgroups $\mathscr{L}(V_1(k, R);\ V_2(h, R))$, $\mathscr{R}(V_2(h, R);\ V_1(k, R))$ of the general contracted subperiodic groups (17*b*) which correspond to the point group $\mathscr{O}_{12}=\hat{\mathscr{O}}_{12}\cap\hat{\mathscr{O}}_{21}$ [*cf.* (21), (22)]. In these cases the latter contracted subperiodic groups are again not general but they are complementary and we can introduce homomorphisms $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ by the same relations (10*b*) as for the orthogonal case. The domain for the action of these homomorphisms will again be the group $\mathscr{E}_{12}=\hat{\mathscr{E}}_{12}\cap\hat{\mathscr{E}}_{21}$.

Hence the contracted groups into which we project the reducible subgroups of $\mathscr{E}(n)$ are now defined uniquely. The homomorphisms $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$, defined by (10*b*), are still not unique; they depend on pairs of points P, P_1 and P, P_2. This dependence has, however, a clear geometrical meaning. With original homomorphisms $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$, we can associate projections of $E(n)$ onto hyperplanes $(P+\boldsymbol{\tau}_2,\ V_1(k, R))$, $(P+\boldsymbol{\tau}_1,\ V_2(h, R))$ or projections onto single spaces $E_1(k)$, $E_2(h)$ which represent the whole set of hyperplanes. The projections onto hyperplanes do not need any further specification of origin because these hyperplanes are part of the space $E(n)$. On the other hand, to make the projections onto $E_1(k)$, $E_2(h)$ unique, we have to choose a point P in $E(n)$ and specify its projections P_1 onto $E_1(k)$ and P_2 onto $E_2(h)$. The homomorphisms $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ become unique if this relationship is fixed and they do not further change if we assign to the shift of origin P on $\boldsymbol{\tau}$ to $P+\boldsymbol{\tau}$ the corresponding shifts of origins P_1, P_2 on projections $\boldsymbol{\tau}_1=\sigma_1(\boldsymbol{\tau})$, $\boldsymbol{\tau}_2=\sigma_2(\boldsymbol{\tau})$. Assuming that we keep the points P, P_1, P_2 fixed, we can also drop the subscripts at Seitz symbols.

Let us finally see the effect of homomorphisms $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ on ordinary subperiodic groups. All groups $\mathscr{L}(\boldsymbol{\tau}_2)$, $\mathscr{R}(\boldsymbol{\tau}_1)$ with $\boldsymbol{\tau}_2\in V_2(h, R)$, $\boldsymbol{\tau}_1\in V_1(k, R)$ are sent to a pair of single contracted groups according to

$$\begin{aligned}
\boldsymbol{\sigma}_1:\quad & \mathscr{L}(\boldsymbol{\tau}_2)=\{G,\ T^0_{G1},\ P+\boldsymbol{\tau}_2,\ \mathbf{u}_{G1}(g)\}\to\boldsymbol{\mathscr{L}}\\
&\qquad=[G,\ T^0_{G1},\ P_1,\ \mathbf{u}_{G1}(g)],\\
\boldsymbol{\sigma}_2:\quad & \mathscr{R}(\boldsymbol{\tau}_1)=\{G,\ T^0_{G2},\ P+\boldsymbol{\tau}_1,\ \mathbf{u}_{G2}(g)\}\to\boldsymbol{\mathscr{R}}\\
&\qquad=\langle G,\ T^0_{G2},\ P_2,\ \mathbf{u}_{G2}(g)\rangle.
\end{aligned}\tag{24}$$

This relationship holds for orthogonal as well as for inclined reductions. Notice that the groups $\mathscr{L}(\boldsymbol{\tau}_2)$ which are mapped by these homomorphisms onto the group $\boldsymbol{\mathscr{L}}$ differ for different choices of the space $V_2(h, R)$, which are possible if $V_1(k, R)$ defines an inclined reduction class under the action of G, and the same holds for the second set of groups. This can be expressed in the following way: The shift of the group $\mathscr{L}(\mathbf{0})=\{G,\ T^0_{G1},\ P,\ \mathbf{u}_{G1}(g)\}$ along $V_2(h, R)$ as well as the shift of the group $\mathscr{R}(\mathbf{0})=\{G,\ T^0_{G2},\ P,\ \mathbf{u}_{G2}(g)\}$ along $V_1(k, R)$ does not change its image under homomorphisms $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$ which are determined by the reduction $V(n, R)=V_1(k, R)\oplus V_2(h, R)$.

Finally, if $\boldsymbol{\sigma}_1(\mathscr{G})=\boldsymbol{\mathscr{L}}$, $\boldsymbol{\sigma}_2(\mathscr{G})=\boldsymbol{\mathscr{R}}$, then $\boldsymbol{\sigma}_1(\mathscr{G}(\boldsymbol{\tau}))=\mathscr{L}(\boldsymbol{\tau}_1)$, $\boldsymbol{\sigma}_2(\mathscr{G}(\boldsymbol{\tau}))=\mathscr{R}(\boldsymbol{\tau}_2)$, where $\boldsymbol{\tau}_1=\sigma_1(\boldsymbol{\tau})$, $\boldsymbol{\tau}_2=\sigma_2(\boldsymbol{\tau})$; compare this with (15). In other words, the shift of the group $\mathscr{G}$ on $\boldsymbol{\tau}$ leads to the shift of its images on the projections of $\boldsymbol{\tau}$ onto the subspaces $V_1(k, R)$, $V_2(h, R)$, respectively.

Discussion

We have seen that factorization of reducible space groups by their partial translation subgroups leads to groups which have the structure of subperiodic groups. There are generally many possibilities of how to represent such groups and many ways of choosing the corresponding homomorphisms. We investigated only those homomorphisms which can be suitably geometrically interpreted. Our considerations have been concentrated from the beginning on applications to crystallographic space groups. As we have seen, the factorization theorem has more general validity; there is a way open for its generalization to noncrystallographic cases or to cases when crystallographic groups can be factorized to noncrystallographic ones. The original homomorphisms σ_1, σ_2 are just ordinary projections of vector space onto spaces of lower dimensions; the homomorphisms written in boldface can be interpreted as projections of groups. We believe that this point is of interest in connection with the theory of quasicrystalline structures.

The idea to distinguish the ordinary and contracted subperiodic groups is not quite new, although we have given it a rather general character here. The 'sectional groups' and groups of a 'two sided plane' used by Holser (1958) correspond to layer groups of three-dimensional space and to contracted layer groups, respectively. The idea is also close to so-called 'spin groups' (Litvin & Opechowski, 1974), if that were to be extended from point to space groups, and the contracted groups have some common features with the 'P-symmetry groups' of Zamorzaev (1967). Let us also mention the classification work of Bohm & Dornberger-Schiff (1967) in which the augmented matrices represent either the contracted groups or ordinary subperiodic groups with respect to an origin which lies in the hyperplane they leave invariant [the matrices given in that work are not general enough to express subperiodic groups with respect to any chosen origin in $E(n)$].

The site-point groups of the Euclidean space may be also considered as the simplest kind of subperiodic group - groups with trivial translation subgroup. It is well known that space groups may be considered as extensions of translation subgroups by point groups (Ascher & Janner, 1965; 1968/69). Analogously, reducible space groups may be considered as extensions of their partial translation subgroups by the corresponding factor groups - the subperiodic groups. It is again an advantage to use the contracted subperiodic groups in such an approach. There are far-reaching analogies in the consideration of space groups as extensions by subperiodic groups with the ordinary consideration of these groups as extensions by point groups.

The first immediate consequence of the factorization theorem is, however, the fact that we can classify reducible space groups into subperiodic classes. This will be the subject of our subsequent paper.

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Subperiodic Classes of Reducible Space Groups

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Abstract

Classification of reducible space groups into pairs of complementary subperiodic classes with respect to various reductions is introduced and analysed. This classification is finer than the classification into geometric classes and it intersects with the classification into arithmetic classes. It is proved that an intersection theorem holds for those classes which correspond to Z decomposition of the translation subgroups of the reducible space groups and then symmorphic representatives of subperiodic classes of reducible space groups are introduced in analogy with the ordinary concept of symmorphic space groups. In particular, it is shown that the symmorphic space group is a symmorphic representative of subperiodic classes, defined by complementary symmorphic subperiodic groups. In cases of Z reductions it is shown that the pair of complementary subperiodic classes may define none, one or several space groups; if one such group belongs to these classes, then also a set of groups which differ by shifts in space does. These shifts are determined with translation normalizers. Further ramifications and possible use of the theory are discussed.

1. Introduction

As we have shown in a previous paper (Kopský, 1989), reducible space groups can be factorized by their partial translation subgroups and the resulting groups can be interpreted as subperiodic groups. *Vice*

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