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LETTER TO THE EDITOR

The role of subperiodic and lower-dimensional groups in the structure of space groups

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Abstract. We consider the consequences of $\mathbb{Q}$-reducibility of a point group for the structure of a corresponding space group. First we show that the space group is a subgroup of a direct product of two Euclidean groups of lower dimensions. We introduce the so-called separation diagram from which follows that (i) the space group is a subdirect product of space groups of lower dimensions, (ii) its point group is a subdirect product of point groups of lower-dimensional groups, (iii) the space group has two complementary normal translation subgroups of lower dimensions and the corresponding factor groups are complementary subperiodic groups. The latter conclusion enables us to classify space groups into finer classes than the point classes. The most important fact is that the space groups in higher dimensions can be constructed from $\mathbb{Q}$-irreducible groups of lower dimensions unless they are themselves $\mathbb{Q}$-irreducible.

Among space groups in arbitrary dimensions, we can distinguish those for which the action of the point group on the underlying vector space is $\mathbb{Q}$-irreducible. Up to four dimensions, these groups include (i) both types $\not{p}1$ and $\not{p}\bar{1}$ of one-dimensional space groups, (ii) the groups of square and hexagonal systems (families) in two dimensions, (iii) the cubic groups in three dimensions, (iv) space groups of octagonal, decagonal, dodecagonal, di-isohexagonal orthogonal, icosahedral and hypercubic families. The best but at the same time a very exacting source for consideration of various reducibilities is the book by Curtis and Reiner (1966). We shall just recall here the meaning of $\mathbb{Q}$-reducibility as compared with $\mathbb{R}$-reducibility. The point group action on vector space is said to be a $\mathbb{Q}$-representation if a basis exists in which group operators are expressed by rational ($\mathbb{Q}$) matrices. This is exactly a condition for the point group being crystallographic. The group action is $\mathbb{Q}$-reducible (and decomposable) if the vector space splits into invariant subspaces so that the group operators can be expressed by rational matrices on each of them. Up to three dimensions, the $\mathbb{Q}$-reducibility coincides with $\mathbb{R}$-reducibility. A scheme of reducibilities and decomposabilities is given in the book on four-dimensional space groups (Brown *et al* 1978), from which we also took the information about $\mathbb{Q}$-irreducible families.

Let $\mathscr{E}(n)$ be the n-dimensional Euclidean group—the group of all rigid motions (isometries) of n-dimensional Euclidean space $E(n)$. Then $\mathrm{V}(n)$, the real orthogonal vector space, associated with $E(n)$, is a normal subgroup of $\mathscr{E}(n)$ and the factor group $\mathscr{E}(n)/\mathrm{V}(n)$ is isomorphic to a group $\mathrm{O}(n)$, the real orthogonal group acting on $\mathrm{V}(n)$. We denote by σ: $\mathscr{E}(n)\to\mathrm{O}(n)$ the homomorphism with $\ker\sigma=\mathrm{V}(n)$. Elements of $\mathscr{E}(n)$ are expressed by Seitz symbols $\{g|t\}$, where $g\in\mathrm{O}(n)$, $t\in\mathrm{V}(n)$ and the symbol refers to a certain fixed origin, so that $\{g|0\}$ means the rotation g around this origin. Any space group $\mathscr{G}$ can then be expressed by a symbol $\mathscr{G} = (\mathrm{G}, \mathrm{T_G}, 0, \boldsymbol{u}_\mathrm{G}(g))$, where (i) $\mathrm{T_G} = \mathscr{G} \cap \mathrm{V}(n)$ is the full translation subgroup (the lattice) of $\mathscr{G}$. (ii) $\mathrm{G} = \sigma(\mathscr{G}) \subseteq \mathrm{O}(n)$ is the point group of $\mathscr{G}$. The action of $\mathrm{O}(n)$ on $\mathrm{V}(n)$ determines the action of G on $\mathrm{T_G}$ which is G-invariant. (iii) 0 denotes the origin and $\boldsymbol{u}_\mathrm{G}: \mathrm{G} \to \mathrm{V}(n)$ the system of non-primitive translations. The symbol for $\mathscr{G}$ then denotes the set of all elements of $\mathscr{E}(n)$ of the form $\{g|\boldsymbol{t} + \boldsymbol{u}_\mathrm{G}(g)\}$, where g runs over G, $\boldsymbol{t}$ runs over $\mathrm{T_G}$. In order that this set be a group, the system of non-primitive translations must satisfy Frobenius congruences:

$$\boldsymbol{w}_\mathrm{G}(g, h) = \boldsymbol{u}_\mathrm{G}(g) + g\boldsymbol{u}_\mathrm{G}(h) - \boldsymbol{u}_\mathrm{G}(gh) = 0 \qquad (\mathrm{mod}\ \mathrm{T_G})$$

where $\boldsymbol{w}_\mathrm{G}(g, h)$ is the so-called factor system. According to the definition by Brown *et al* (1978), $\mathscr{G}$ is a space group only if $\mathrm{T_G}$ is a free Abelian group of rank n, large in $\mathrm{V}(n)$, which means that it spans $\mathrm{V}(n)$ over $\mathbb{R}$ (Schwarzenberger 1980).

We assume now that $\mathscr{G} = (\mathrm{G}, \mathrm{T_G}, 0, \boldsymbol{u}_\mathrm{G}(g))$ is a space group for which the action of G on $\mathrm{V}(n)$ is $\mathbb{Q}$-reducible, so that $\mathrm{V}(n)$ splits into a direct sum $\mathrm{V}(n) = \mathrm{V}_1 \oplus \mathrm{V}_2$ of two G-invariant subspaces V_1 and V_2 such that G has a $\mathbb{Q}$-representation on both these subspaces. In crystallographic language this means that both subspaces are spanned by crystallographic directions. For simplicity we also assume that the representations of G on V_1 and V_2 have no irreducible classes in common, so that V_1 and V_2 are mutually orthogonal. The maximal subgroup of $\mathrm{O}(n)$ which leaves both $\mathrm{V}_1, \mathrm{V}_2$ invariant is the direct product $\mathrm{O}_1 \otimes \mathrm{O}_2$ of orthogonal groups on $\mathrm{V}_1, \mathrm{V}_2$. This group is the factor group of the direct product of Euclidean groups $\mathscr{E}_1, \mathscr{E}_2$, which are defined as extensions of $\mathrm{V}_1, \mathrm{V}_2$ by $\mathrm{O}_1, \mathrm{O}_2$, respectively. All basic properties of space groups with $\mathbb{Q}$-reducible point groups can be derived from the following theorem.

Theorem 1. The space group $\mathscr{G}$ is a subgroup of the direct product $\mathscr{E}_1 \otimes \mathscr{E}_2$ only if the space $\mathrm{V}(n)$ splits under the action of the point group G into G-invariant, mutually orthogonal subspaces $\mathrm{V}_1, \mathrm{V}_2$.

Proof. The space $\mathrm{V}(n)$ splits into G-invariant mutually orthogonal subspaces $\mathrm{V}_1, \mathrm{V}_2$ only if G is a subgroup of the direct product $\mathrm{O}_1 \otimes \mathrm{O}_2$. Then each element of G can be written uniquely in the form $g = g_1 g_2 = g_2 g_1$, where $g_1 \in \mathrm{O}_1$, $g_2 \in \mathrm{O}_2$, and g_1, g_2 commute. Any element $\{g|\boldsymbol{t} + \boldsymbol{u}_\mathrm{G}(g)\}$ of the group $\mathscr{G}$ can then be expressed as a product of commuting elements $\{g_1|\boldsymbol{t}_1 + \boldsymbol{u}_{\mathrm{G}1}(g)\}$ and $\{g_2|\boldsymbol{t}_2 + \boldsymbol{u}_{\mathrm{G}2}(g)\}$, where $\boldsymbol{t} = \boldsymbol{t}_1 + \boldsymbol{t}_2$, $\boldsymbol{u}_\mathrm{G}(g) = \boldsymbol{u}_{\mathrm{G}1}(g) + \boldsymbol{u}_{\mathrm{G}2}(g)$ is the unique splitting of $\boldsymbol{t}$, $\boldsymbol{u}_\mathrm{G}(g)$ into their components $\boldsymbol{t}_1$, $\boldsymbol{u}_{\mathrm{G}1}(g) \in \mathrm{V}_1$; $\boldsymbol{t}_2$, $\boldsymbol{u}_{\mathrm{G}2}(g) \in \mathrm{V}_2$. These elements commute because g_1 acts trivially on V_2, g_2 on V_1 and because g_1, g_2 themselves commute. Since one of the elements belongs to $\mathscr{E}_1$ and the other to $\mathscr{E}_2$, the implication is proved in one direction. If $\mathscr{G}$ is a subgroup of $\mathscr{E}_1 \otimes \mathscr{E}_2$, then G is clearly a subgroup of $\mathrm{O}_1 \otimes \mathrm{O}_2$, which proves the implication in the other direction.

The groups $\mathrm{V}_1, \mathrm{V}_2$ are evidently normal subgroups of $\mathscr{E}_1 \otimes \mathscr{E}_2$ and so also is the whole $\mathrm{V}(n)$. Further, each of the groups $\mathscr{E}_1, \mathscr{E}_2$ is itself normal in its direct product, the other being the corresponding factor group. We introduce several homomorphisms of $\mathscr{E}_1 \otimes \mathscr{E}_2$ defined by their kernels onto corresponding factor groups and present them in a commutative diagram for which we suggest the name of 'separation diagram'. From this diagram we can easily see the properties of a group $\mathscr{G} \subseteq \mathscr{E}_1 \otimes \mathscr{E}_2$.

Theorem 2. If $\mathscr{G} \subseteq \mathscr{E}_1 \otimes \mathscr{E}_2$, then:

(i) $\mathscr{G}$ is a subdirect product of subgroups $\mu_1(\mathscr{G}) = \mathscr{G}_1$ and $\mu_2(\mathscr{G}) = \mathscr{G}_2$ of $\mathscr{E}_1, \mathscr{E}_2$, respectively.

(ii) The point group G is a subdirect product of subgroups $\sigma_1\mu_1(\mathscr{G}) = \rho_1\sigma(\mathscr{G}) = G_1$ and $\sigma_2\mu_2(\mathscr{G}) = \rho_2\sigma(\mathscr{G}) = G_2$ of O_1, O_2, respectively.

(iii) The group $\mathscr{G}$ has normal subgroups $T_{G1} = \ker \sigma_1(\mathscr{G}) = V_1 \cap \mathscr{G}$, $T_{G2} = \ker \sigma_2(\mathscr{G}) = V_2 \cap \mathscr{G}$ and the corresponding factor groups are isomorphic to subgroups of $O_1 \otimes \mathscr{E}_2$, $\mathscr{E}_1 \otimes O_2$, respectively.

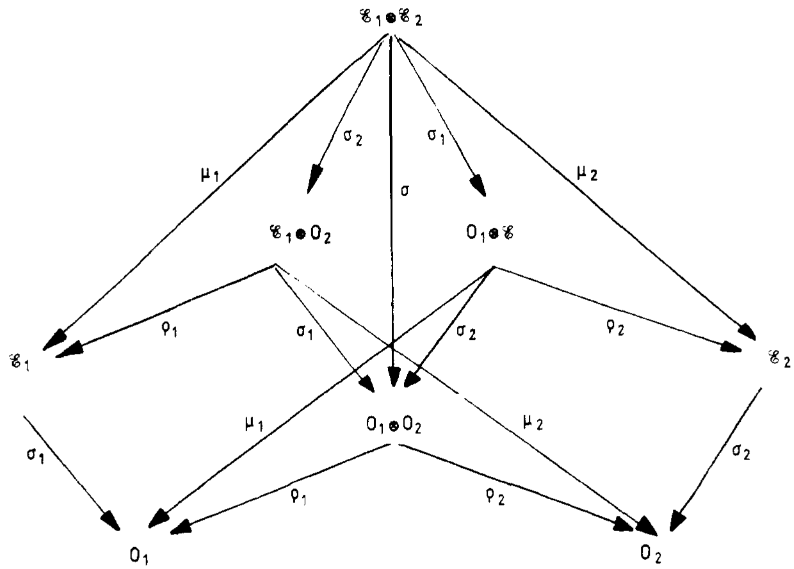

Figure 1. The separation diagram: $\ker \sigma = V(n)$, $\ker \sigma_1 = V_1$, $\ker \sigma_2 = V_2$; $\ker \mu_1 = \mathscr{E}_2$, $\ker \mu_2 = \mathscr{E}_1$, $\ker \rho_1 = O_2$, $\ker \rho_2 = O_1$.

Both theorems 1 and 2 are valid and the separation diagram can be constructed if the point group G is at least $\mathbb{R}$-reducible. In this case, however, the linear envelopes of translation groups T_{G1}, T_{G2} are not necessarily the whole spaces V_1, V_2. If the reducibility of G is $\mathbb{Q}$-reducibility, then the linear envelopes of T_{G1}, T_{G2} over the reals are the spaces V_1, V_2, the groups G_1, G_2 are crystallographic groups and the translation group T_G is a subdirect sum of groups T^0_{G1}, T^0_{G2}, the projections of T_G onto V_1, V_2. More precisely, T_G is expressible as

$$T_G = T_{G1} \oplus T_{G2}(0 \dot{+} d_2 \dot{+} d_3 \dot{+} \ldots \dot{+} d_p)$$

and

$$T^0_{G1} = T_{G1}(0 \dot{+} d_{21} \dot{+} d_{31} \dot{+} \ldots \dot{+} d_{p1})$$

$$T^0_{G2} = T_{G2}(0 \dot{+} d_{22} \dot{+} d_{32} \dot{+} \ldots \dot{+} d_{p2})$$

where d_{ji} are the components of d_j in V_i, $i = 1, 2$. The factor groups $T_G/(T_{G1} \oplus T_{G2})$, T^0_{G1}/T_{G1} and T^0_{G2}/T_{G2} are isomorphic according to the construction of subdirect sums or products (Hall 1959, Litvin and Opechowski 1974).

We observe that the factor groups $\mathscr{G}/T_{G1}$, $\mathscr{G}/T_{G2}$ can be considered as subperiodic groups with translation subgroups T^0_{G2} and T^0_{G1}, respectively. These are, however, not the ordinary subperiodic groups in n-dimensional space but rather their isomorphs which are deprived of the position in the direction of missing translations. The situation is analogous to the relation between site point groups and point groups considered as factor groups of space groups with respect to the whole translation subgroup. The space group can be considered as an extension of the group of missing translations T_{G1} or T_{G2} by the corresponding subperiodic group. Consequently, the space groups can be distributed into classes of these factor groups, which provides finer classification than the ordinary geometric or arithmetic classes.

We have applied part (iii) of theorem 2 to investigation of plane (Litvin and Kopsky 1986) and space (Fuksa and Kopský 1986a) groups with Q-reducible point groups. The situation is simple but very interesting. In the first case we obtain the frieze groups, in the second case we obtain layer and rod groups as factor groups. In analogy with Wyckoff positions, we can analyse subperiodic symmetries along missing directions; we call this procedure the scanning of subperiodic groups. This analysis has applications in the theory of domain walls and twin boundaries. The occurrence of subperiodic groups as factor groups is also important in consideration of lattices of subgroups, especially of normal subgroups, of space groups and can be used to develop representation theory of space groups by ascent from lower to higher dimensions. We consider this situation in more detail in our study of lattices of normal subgroups of space groups up to three dimensions (Fuksa and Kopský 1986b).

Consecutive use of theorem 2 gives one an insight into the structure of space groups with Q-reducible point groups and can be used for derivation of higher-dimensional space or subperiodic groups as well as for introduction of hierarchy of these groups. This problem has already been considered by Jarrat (1980) for space group families. The point group G can be ultimately reduced to its Q-irreducible components of which it is a multiple subdirect product. Corresponding space groups are then multiple subdirect products of space groups of lower dimensions. Theorem 2 can be used in each step of 'canonical decomposition' (see Jarrat 1980). Its modification holds also in cases of decomposition within the same representation class, when G-invariant subspaces V_1 and V_2 transform by the same law as well as in cases of subperiodic groups.

Reducibility of space groups is evidently worthy of more detailed investigation. This will give us a better understanding of space and subperiodic groups which at present are known up to four dimensions. On the other hand, it will enable us to construct particular reducible groups in such dimensions in which it is hopeless to expect lists of all groups.

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