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A. M. Zamorzaev

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Abstract

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CRYSTALLOGRAPHY

A. M. ZAMORZAEV

DERIVATION OF THREE-DIMENSIONAL SIMILARITY SYMMETRY GROUPS

(Presented by Academician A. V. Shubnikov, May 26, 1967)

1. In 1960 A. V. Shubnikov proposed the idea of similarity symmetry ⁽¹⁾. A refinement of the concept of similarity symmetry groups, the transfer to them of the idea of antisymmetry ⁽²⁾, a description of two-dimensional crystallographic groups of similarity symmetry and antisymmetry, and their generalization with the concept of antisymmetry of various kinds ⁽³⁾ are given in ⁽⁴⁾. Three-dimensional groups of similarity symmetry and antisymmetry have been studied in part ^(5,6).

A group G of similarity transformations in n -dimensional Euclidean space will be called an n -dimensional similarity group (s.g.) if: a) G contains at least one similarity transformation P with coefficient $k \neq 1$; b) at least one point of the space is isolated in the infinite class of its images under all transformations from G ⁽⁵⁾. The point O , fixed under the transformation P , will be called a special point of the group G ; it is fixed under all transformations of the group G ^(4,5).

The derivation of two-dimensional groups of similarity symmetry and antisymmetry in ⁽⁴⁾ is reduced to the consideration of symmetry and antisymmetry groups of rods ⁽⁷⁾. The generalization of these and other groups with the concept of antisymmetry of various kinds was carried out in parallel ^(4,8). Two-dimensional groups of similarity symmetry and antisymmetry have been applied to the description and derivation of a special class of three-dimensional s.g.'s—the so-called conical ones (three-dimensional with a special plane) ^(4,6). Crystallographic conical s.g.'s have been completely generalized with the concept of antisymmetry of various kinds ⁽⁶⁾. The study of noncrystallographic conical and two-dimensional s.g.'s is also reduced to consideration of the better-known noncrystallographic rod groups (symmetry of chain molecules ^(9,10)).

The central content of the present work is the derivation of all three-dimensional s.g.'s. By the method of generalized projections in the spirit of ⁽¹¹⁾, they can be interpreted as point groups of symmetry and antisymmetry ^(2,12) and of color symmetry ⁽¹³⁾. Many general properties of s.g.'s are valid for any dimension n .

2. Let G be an n -dimensional s.g. with special point O . Every transformation g of the group G is uniquely representable as the product of a homothety h , with center O , and a transformation of classical symmetry s , keeping O fixed (a “rotation” about O), which we shall call the components of g . It is easy to see that the collections H and S , respectively, of the homotheties and “rotations” occurring in the transformations of the group G , are also groups.

Construct mappings φ and ψ of the group G onto S and onto H according to the rule $\varphi(g) = s$, $\psi(g) = h$, where $g = hs$ ($g \in G$). Obviously, φ and ψ are homomorphisms, whose kernels are the subgroup H_0 of all homotheties in G ($H_0 = G \cap H$) and the subgroup S_0 of all “rotations” in G ($S_0 = G \cap S$). By the homomorphism theorem ⁽¹⁴⁾, H_0 and S_0 are normal divisors of the group G , and moreover $G/H_0 \cong S$ and $G/S_0 \cong H$.

Theorem 1. *Every s.g. contains a transformation with the least similarity coefficient exceeding unity.*

The given group G , by property a), contains a transformation with coefficient $k > 1$, and by b) there exists a point A (different from O) whose ε -neighborhood which contains no other points of the class of its G -images. Every transformation g from G with coefficient $k' > 1$ carries this ε -neighborhood into an ε' -neighborhood of the point $A' = g(A)$, containing no other points of this class, with $\varepsilon' > \varepsilon$. Therefore, in the layer between the spheres of radii OA and $k \cdot OA$ with center O , the point A' can assume only a finite number of positions; hence the number of such values k' , $1 \leq k' < k$, is finite, and one may choose the smallest of them.

From the theorem just proved it follows that: 1) the group H of homotheties occurring among the transformations of the group G is cyclic (generated by a homothety with the smallest coefficient $k' > 1$); 2) if the subgroup H_0 of homotheties of the group G is nontrivial, then it is cyclic and its index in the group H is finite.

Let us now note that, for $n \geq 3$, the definition given in Section 1 is satisfied not only by discrete groups, but also by groups of semicontinua (for example, the three-dimensional finite group $\{K\}(\infty : m)$ in the notation of ⁽⁶⁾). Therefore we shall replace requirement b) by a stronger one: b') there exist n points not lying in one $(n - 2)$ -dimensional plane, each of which is isolated in the class of its G -images*. In what follows we consider only groups defined by requirements a) and b').

Theorem 2. *If a subgroup G_0 of the group G is itself an f.s.g., then the index of G_0 in G is finite.*

We give the proof for three-dimensional groups.

By property a), G_0 contains a transformation with coefficient $k > 1$. By b'), for G there exist noncollinear points A, B, C , isolated in the classes of their

G -images; two of them, for example A and B , are noncollinear with O . Every adjacent class gG_0 contains such a transformation g' that

$$\begin{aligned} OA \leq OA' < k \cdot OA, \quad OB \leq OB' < k \cdot OB, \quad \text{where } A' = g'(A), \\ B' = g'(B). \end{aligned} \quad (*)$$

Reasoning with spherical layers, as in Theorem 1, we find that for $g' \in G$ there are only a finite number p of points A' and a finite number q of points B' satisfying condition (*). Consequently, the triangle $OA'B'$ (the g' -image of the triangle OAB) assumes no more than pq positions; but a similarity transformation in space is determined two-valuedly by specifying a triangle and its image⁽¹⁵⁾, and therefore there are no more than $2pq$ distinct g' satisfying (*). Hence the number of adjacent classes gG_0 is finite.

For any $n > 3$ the basic idea of the argument is exactly the same.

From this theorem it follows that: 1) the subgroup S_0 of "rotations" of the group G is finite (if $g' \in S_0$, then it satisfies condition (*)); 2) if G has a nontrivial subgroup of homotheties H_0 , then G/H_0 and the group S of "rotations" occurring among the transformations of G are finite.

3. Let now G be an f.s.g. with a nontrivial subgroup of homotheties H_0 . Then, by Section 2, G/H_0 is finite; $H_0 = \{K\}$, where K is a homothety from G with the smallest coefficient $k > 1$; every adjacent class gH_0 contains the unique transformation g' satisfying condition (*) for any points A and B distinct from O , and its coefficient is equal to one of the numbers $1, k^{1/p}, \dots, k^{p-1/p}$ (p is the index of the subgroup H_0 in H). Choose a sphere of radius R with center O , and on it a point A ; the class of its H_0 -images consists of the intersections of the ray OA with all spheres of radii Rk^l (where l is any integer) having center O ; the points A' satisfying (*) will lie on the concentric spheres of radii $R, Rk^{1/p}, \dots, Rk^{p-1/p}$. Project the points A' and their H_0 -images (and these exhaust all G -images of the point A) from the center O onto the chosen sphere of radius R , and color their projections in p different colors corresponding to the p "spherical levels" of the points A' : to the point $\bar{A}$, which is the projection of the point A' (and of its H_0 -images),

* By virtue of a), these classes are infinite for at least $n - 1$ of these points; therefore for $n \geq 2$, b') implies b).

we assign the j -th color if $OA' = Rk^{j-1/p}$ ($j = 1, 2, \dots, p$). Any transformation from the coset gH_0 maps the class of H_0 -images of the point A into the class of H_0 -images of the point $A' = g'(A)$, where $g' \in gH_0$; therefore, in colored projections onto the sphere the class gH_0 is represented by a transformation of p -colored symmetry in the sense of Belov⁽¹¹⁾ (for $p = 2$, "black-and-white," for $p = 1$, classical), carrying A into $\bar{A}$ and geometrically coinciding with the "rotations"

entering into the transformations of the class gH_0 . The totality $\tilde{S}$ of such transformations is a point group of p -colored symmetry, isomorphic to G/H_0 and obtained from the group S of “rotations” entering into the transformations G ; $\tilde{S}$ is a natural model of G/H_0 and thereby interprets G (cf. the interpretation of the three-dimensional Fedorov groups in the form of colored two-dimensional methods of generalized projections of Belov–Tarkhova ⁽¹¹⁾).

Thus, all s.s.g. containing nontrivial homotheties can be described by means of point groups of p -colored symmetry, well studied for $n = 3$ ^(2,12,13). Therefore the problem of deriving three-dimensional s.s.g. with homotheties is in fact completely solved. All crystallographic s.s.g. (for which S is one of the 32 crystallographic point groups ^(2,12)) are easily written out by means of the corresponding p -colored point groups, assigning to p the values 1, 2, 3, 4, 6. For $p = 1$ there are 32 of them, for $p = 2$ 58 ⁽¹²⁾, for $p = 3, 4, 6$ there are $7+4+7 = 18$ ⁽¹³⁾, and in all 108. Of these, 94 groups are known as 109 conical groups ^(4,6) (in Table 2 of work ⁽⁶⁾, 15 conical groups repeat those derived earlier, if they are regarded as three-dimensional without taking into account a distinguished direction). The remaining 14 s.s.g., associated with the cubic system, do not fall into the conical series. Let us write them in the notation of ^(4,6), using for point groups of symmetry, antisymmetry, and color symmetry the notation of ^(2,13).

The groups $3/2$ and $\bar{3}^{(3)}/2$ are interpreted by the s.s.g. $\{K\}(3/2)$ and $\{K\}(K'^{1/3}\bar{3}/2)$; the groups $\bar{6}/2$, $\bar{6}/2$, $\bar{6}^{(3)}/2$, and $\bar{6}^{(6)}/2$ —by the s.s.g. $\{K\}(\bar{6}/2)$, $\{K\}(K'^{1/2}\bar{6}/2)$, $\{K\}(K'^{1/3}\bar{6}/2)$, and $\{K\}(K'^{1/6}\bar{6}/2)$; the groups $3/\bar{4}$, $3/\bar{4}$, $3/4$, and $3/\bar{4}-\{K\}(3/\bar{4})$, $\{K\}(3/K'^{1/2}\bar{4})$, $\{K\}(3/4)$, and $\{K\}(3/K'^{1/2}4)$; the groups $\bar{6}/4$, $\bar{6}/4$, $\bar{6}/4$, and $\bar{6}/4-\{K\}(\bar{6}/4)$, $\{K\}(K'^{1/2}\bar{6}/4)$, $\{K\}(\bar{6}/K'^{1/2}4)$, and $\{K\}(K'^{1/2}\bar{6}/K'^{1/2}4)$.

Among noncrystallographic three-dimensional s.s.g. with homotheties, three are not conical: $\{K\}(3/5)$, $\{K\}(3/10)$, and $\{K\}(3/K'^{1/2}\bar{10})$ (they are interpreted by the groups $3/5$, $3/\bar{10}$, and $3/\bar{10}$ ⁽²⁾; for $p > 2$ colored groups from $3/5$ and $3/\bar{10}$ are not derived). All the remaining three-dimensional groups with homotheties are conical, since the remaining three-dimensional point groups have a plane invariant under all their transformations (distinguished).

4. We shall now show that all three-dimensional s.s.g., with the exception of the 17 listed above, are conical. It remains to consider only groups that do not contain nontrivial homotheties (and, consequently, also homothetic reflections ^(4–6), and screw motions or reflections ^(4–6) with rotation angles, and mirror rotations entering into them, rational with respect to π).

Theorem 3. *A three-dimensional s.s.g. without nontrivial homotheties is conical.*

Let G be a three-dimensional s.s.g. without homotheties, and P a transforma-

tion contained in it with coefficient $k \neq 1$. In this case P can only be a screw motion (or screw reflection) ⁽⁴⁻⁶⁾ with an angle of rotation (or mirror rotation) φ irrational with respect to π ; it leaves invariant exactly one line d (axis). We shall show that d is a distinguished line of the group G , i.e., invariant under its transformations.

Suppose that G contains a transformation g carrying d into another line d_1 . The transformation $P_1 = gPg^{-1}$ is a screw motion (reflection) with coefficient k and angle φ , but with axis d_1 , and the transformations $P_2 = PP_1P^{-1}, \dots, P_n = P^{n-1}P_1P^{1-n}, \dots$ are screw motions (reflections)

with coefficient k , angle φ , and axes $d_2 = P(d_1), \dots, d_n = P^{n-1}(d_1), \dots$. Since φ/π is irrational, all the lines d_i ($i = 1, 2, \dots$) are distinct; therefore the transformations P_i are also distinct, and hence so are all $s_i = P^{-1}P_i$, belonging to the subgroup S_0 of "rotations" of the group G . But this contradicts the finiteness of the group S_0 (Corollary 1 to Theorem 2).

Consequently, d is a special line. But then the plane perpendicular to it and passing through the point O is also special, i.e., the group G is finite.

All finite s.s.g., as was already noted in § 1, can be described by means of rod groups of symmetry and antisymmetry, whose survey presents no fundamental difficulty. The problem of deriving three-dimensional s.s.g. may be regarded as completely solved.

5. From §§ 2, 3 it follows that the problem of deriving n -dimensional s.s.g. with homotheties (in particular, crystallographic ones) comes down directly to the study of n -dimensional point groups of symmetry and the derivation from them of color groups. The case $n = 4$ is facilitated by the fact that the point crystallographic groups have already been found ⁽¹⁶⁾.

In ⁽⁵⁾ it was noted that the derivation of n -dimensional s.s.g. makes it possible at once to describe $(n+1)$ -dimensional linear groups of symmetry with an invariant directed line (symmetry groups of $(n+1)$ -dimensional directed rods). Thus, in the present work the problem of deriving the symmetry groups of directed 4-dimensional rods has also been solved; there are 108 crystallographic groups among them. For the description of all 4-dimensional rod groups, however, an extension of three-dimensional s.s.g. to the so-called groups of conformal symmetry (§ 5 ⁽⁴⁾) is required.

Kishinev State University

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