BULETINUL ACADEMIEI DE ŞTIINŢE
A REPUBLICII MOLDOVA. MATEMATICA
Number 2(51), 2006, Pages 106–109
ISSN 1024–7696

Junior spatial groups of $(22'\underline{1})$-symmetry

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Abstract. All junior space groups of $(22'\underline{1})$-symmetry are obtained with the help of junior space groups of the three-fold antisymmetry.

Mathematics subject classification: 52C20, 05B45.
Keywords and phrases: P-symmetry, symmetry, coloursymmetry, antisymmetry.

I. The problem of generalization of 230 spatial Fedorov symmetry groups G_3 with 32 crystallographic P-symmetries ($P \cong G_{30}$) includes junior and middle groups. All the junior groups have already been obtained [1]. Only 2- and 3-middle groups of $(42\underline{1})$- and $(62\underline{1})$-symmetries, respectively, are not known.

Consider the generalization of k symmetry groups of any category $G_{r\ldots}$ with 32 crystallographic P-symmetries in geometric classification. Groups $G^P_{r\ldots}$ are divided in senior ones, among which for 1-symmetry k groups are symmetry groups of the category $G_{r\ldots}$ (generating groups), junior and Q-middle groups. The derivation of senior groups is trivial, as $G = S \times P$, where S is a classical (generating) group, P is the permutation group of indices that characterizes the P-symmetry under consideration, and $\times$ is the symbol of the direct product of groups. The derivation of junior groups of P-symmetry in the case when S has a normal divisor H such that the factor group $P/H \cong P$ must be realized in detail. The calculation of Q-middle groups can be done using the relation between the number of Q-middle groups of some P-symmetries and the number of junior groups of others P-symmetries. To make this relation more precise A. M. Zamorzaev [1] introduced the concept of the strong isomorphism of groups.

Two transformations of a symmetry group S are called undistinguishable if they are of the same geometric type and generate groups of the same order. So, in the symmetry group of a rectangular $2 \cdot m = (1, 2, m_1, m_2)$ the elements m_1 and m_2 are undistinguishable and distinct from the element 2. In the symmetry group of a right parallelepiped $2 : m = (1, 2, m, \widetilde{2})$ all elements are distinct. In the permutation group of indices or indices with signs two elements are called undistinguishable if one of them can go over into the other by means of reindexing. For example, in the group $P_1 = \{(1,2)(3,4),\ (1,3)(2,4)\} = (I,\ (1,2)(3,4),\ (1,3)(2,4),\ (1,4)(2,3))$, which defines (22)-symmetry, all three non-identical permutations, going over into each other cyclically by a cyclic change of the indices 2, 3, 4 (or other three of indices) undistinguishable are, and in the permutation group $P_2 = \{(1+,2+)(1-,2-),\ (1+,1-)(2+,2-)\} = (I,\ (1+,2+)(1-,2-),\ (1+,1-)(2+,2-),$

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$(1+,2-)(1-,2+))$, which defines $(2\underline{1})$-symmetry, there are no undistinguishable elements, as from one of non-identical permutations changes only indices, the other one – only signs, and the third one – both indices and signs. In the factor group S/H or P/Q cosets are undistinguishable (as factor group elements) if they contain undistinguishable elements, respectively. So, in the rotation group of a regular quadrangular prism $S = 4:2 = (1,4,2(=4^2),4^{-1},2_1,2_2,2_3,2_4)$ the subgroup $H = 2 = (1,2)$ is the normal divisor; in the factor group $S/H = (H, 4\cdot H, 2_1\cdot H1, 2_2\cdot H)$ (which is isomorphic to $2:2$) the cosets $2_1\cdot H = (2_1,2_3)$ and $2_2\cdot H = (2_2,2_4)$ are undistinguishable and distinct from the coset $4\cdot H = (4,4^{-1})$.

Two elements of a group are called equally included in this group if there exists an automorphism of the group that maps one element into the other. So, in the group $4:2$ though the elements $2(=4^2)$ and 2_1 are undistinguishable, they are not equally included in this group, and the elements $2_1,2_2,2_3,2_4$ are undistinguishable and are equally included in $4:2$. Equally included elements not necessarily are undistinguishable; so, the elements $2, m$ and $\widetilde{2}$ are equally included in the group $2:m$, but all these elements are distinct.

An isomorphism of the group G_1 onto G_2 is called strong if under this isomorphism to any undistinguishable and equally included in G_1 elements undistinguishable elements correspond, and to distinct and equally included in G_1 elements distinct elements correspond. In this case the groups G_1 and G_2 are called strong isomorphic (the designation: $G_1 \cong G_2$).

P_1-symmetry and P_2-symmetry are called isomorphic if the permutation groups P_1 and P_2, defining these P-symmetries, are strong isomorphic (the designation: $P_1 \cong P_2$).

Among 32 crystallographic P-symmetries in geometric classification only 22 are not isomorphic. Let enumerate permutation groups that define these P-symmetries, grouping them by strong isomorphism: 1)1; 2)$2 \cong \underline{1} \cong \underline{2}$; 3)3; 4)$4 \cong \underline{4}$; 5)$6 \cong 3\underline{1} \cong \underline{6}$; 6)22; 7)$2\underline{1}$; 8)$2\underline{2}$; 9)$32 \cong 3\underline{2}$; 10)$42 \cong 4\underline{2}$; 11)$\underline{4}2$; 12)$62 \cong 6\underline{2}$; 13)$32\underline{1} \cong \underline{6}2$; 14)$4\underline{1}$; 15)$6\underline{1}$; 16)$22\underline{1}$; 17)$42\underline{1}$; 18)$62\underline{1}$; 19)23; 20)$43 \cong \underline{4}3$; 21)$23\underline{1}$; 22)$43\underline{1}$.

In [1] the following affirmations are proved: 1) The number of different Q-middle groups of P-symmetry in the family is equal to the number of different junior groups of P'-symmetry with the same generating group if $P/Q \cong P'$; 2) If $P_1 \cong P_2$, then the numbers of different junior groups of P_1-symmetry and P_2-symmetry with the same generating group are equal. Hence, to calculate the number of junior and Q-middle groups of all 32 crystallographic P-symmetries by the generalization of any category of classical groups it is enough to study the groups of $2-, 3-, 4-, 6-, (22)-, (2\underline{1})-, (2\underline{2})-, (32)-, (\underline{4}2)-, (42)-, (62)-, (\underline{6}2)-, (4\underline{1})-, (6\underline{1})-,$ $(22\underline{1})-, (42\underline{1})-, (62\underline{1})-, (23)-, (43), (23\underline{1})$- and $(43\underline{1})$-symmetry.

To finish this task it is necessary to study different junior groups of hypercrystallographic $(22'\underline{1})$-symmetry ($P \cong G_{430}$), as by means of these groups we can calculate 2-middle groups of $(42\underline{1})$-symmetry and 3-middle groups of $(62\underline{1})$-symmetry, because $42\underline{1}/2 \cong 62\underline{1}/3 \cong 22'\underline{1}$.

II. The symbol $22'\underline{1}$ is a symbol of three-dimensional point group of the CM kind generated by rotations around two two-fold antirotational and one two-fold rotational axes which are pairwise orthogonal and by antiidentical transformation $\underline{1}$. One of the hypercrystallographic P-symmetries that models junior symmetry and antisymmetry group $mm'm'$ ($22'\underline{1} \approx 22'2'\underline{1} \approx mm'\,m'$), generated by reflections in three pairwise orthogonal planes (one reflection plane and two antireflection planes), is denoted by this symbol ($\underline{1}$ is interpreted as reflection in a point, i.e. as an inversion).

The groups $mm'm'$ and $E_3 = \{1\} \times \{1'\} \times \{{}^*1\}$ are isomorphic, where the group E_3 is the direct product of three groups of order 2, generated by antiidentical transformations of kind 1, kind 2 and kind 3, respectively. The existence of such isomorphism makes it possible to reduce the problem of searching junior space groups of $(22'\underline{1})$-symmetry to the problem of searching junior space groups of three-fold antisymmetry.

However, to different received junior space groups of the type M^3 from one family correspond the same groups of $(22'\underline{1})$-symmetry, as the group $E_3 = (e,\ \underline{1},\ 1',\ {}^*1,\ \underline{1}',\ {}^*\underline{1},\ {}^*1',\ {}^*\underline{1}')$ contains 7 different kinds of antisymmetry transformations, and in the group $mm'm' = m_1m_2'm_3' = (e, m_1, m_2',\ m_3',\ m_1m_2' = 2_{12}',\ m_1m_3' = 2_{13}',\ m_2'm_3' = 2_{23},\ m_1m_2'm_3' = i_{123})$ only five transformations are essentially different, for example, $m_1, m_2', 2_{12}', 2_{23}, i_{123}$, as the transformations m_2', m_3' and $2_{12}', 2_{13}'$ play the same geometric role, respectively.

Consequently, for example, to the group $\{\underline{a}, b, c\}(2' \cdot^* m : 2)$ and to five groups, received from this group by all permutations of signs –, /, * (which mean the transformations of antisymmetry of kind 1, kind 2 and kind 3, respectively),

$$\{\underline{a}, b, c\}({}^*2 \cdot m' : 2) \quad \{a', b, c\}(\underline{2} \cdot {}^*m : 2)$$

$$\{a', b, c\}({}^*2 \cdot \underline{m} : 2) \quad \{{}^*a, b, c\}(\underline{2} \cdot m' : 2) \quad \{{}^*a, b, c\}(2' \cdot \underline{m} : 2),$$

i.e. to six different junior groups of three-fold antisymmetry from family $18s$ correspond three different groups of $(22'\underline{1})$-symmetry:

$$\{a^1, b, c\}(2^3 \cdot m^2 : 2) \qquad \{a^3, b, c\}(2^1 \cdot m^2 : 2) \qquad \{a^3, b, c\}(2^2 \cdot m^1 : 2).$$

To the group $\{\underline{a}, b, c\}({}^*2 \cdot m :\ {}^*2')$ and to two groups, received from this group by all even permutations of signs –, /, * (which mean the transformations of antisymmetry of kind 1, kind 2 and kind 3, respectively),

$$\{a', b, c\}(\underline{2} \cdot m :\ {}^*\underline{2}) \quad \{{}^*a, b, c\}(2' \cdot m : \underline{2}'),$$

i.e. to three different junior groups of three-fold antisymmetry from family $18s$ correspond two different groups of $(22'\underline{1})$-symmetry:

$$\{a^1, b, c\}(2^3 \cdot m : 2^{23}) \qquad \{a^2, b, c\}(2^1 \cdot m : 2^{13}).$$

To the groups

$$\left\{a, b, \frac{a+b+c}{2}\right\}\left(\frac{c}{2}\,{}^*\underline{2} \cdot \frac{b}{2}\,\underline{m} : \frac{a}{2}\,{}^*2'_{\frac{b}{4}}\right)$$

and

$$\left\{a, b, \frac{a+b+c}{2}\right\}\left(\frac{c}{2}{}^{*}\underline{2} \cdot \frac{b}{2}{}^{*}m : \frac{a}{2}\underline{2}'_{\frac{b}{4}}\right),$$

i.e. to two different junior groups of three-fold antisymmetry from family $21a$ there corresponds one group of $(22'\underline{1})$-symmetry:

$$\left\{a, b, \frac{a+b+c}{2}\right\}\left(\frac{c}{2}2^{13} \cdot \frac{b}{2}m^{1} : \frac{a}{2}2^{12}{}_{\frac{b}{4}}\right).$$

Consequently, to receive all different junior groups of $(22'\underline{1})$-symmetry it is necessary to receive all different junior groups of three-fold antisymmetry, to collect them in nests and to replace 6 by 3, 3 by 2, 2 by 1 and 1 by 1.

Hence, as the number of different junior groups of three-fold antisymmetry is equal to $16937*6+2490*3+5*2+37*1 = 109139$, then the number of different junior space groups of $(22'\underline{1})$-symmetry is equal to $16937*3+2490*2+5*1+37*1 = 55833$.

To be sure of this result it is enough to use the numeric table from the work [1] in which in the second column the quantity of groups in the corresponding equivalence class (including a group-representative) is given, and in the third column – the numeric distribution of groups of type M^3 (obtained from the given group-representative) in 6, 3, 2 and 1 group.

As the number of different junior space groups of $(22'\underline{1})$-symmetry gives us the number of 2- and 3-middle groups of $(42\underline{1})$- and $(62\underline{1})$-symmetries respectively, then we obtain 55833 2-middle groups of $(42\underline{1})$-symmetry and 55833 3-middle groups of $(62\underline{1})$-symmetry.

Thus, for $(42\underline{1})$-symmetry 55833+52761=108594 groups, and for $(62\underline{1})$-symmetry 55833+55637=111470 groups are derived.

So, the number of all possible space groups G_3^P of complete 32 crystallographic P-symmetries in geometric classification is equal to 436011.

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Received October 28, 2005