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1978 J. Phys. A: Math. Gen. 11 805

(http://iopscience.iop.org/0305-4470/11/5/010)

J. Phys. A: Math. Gen., Vol. 11, No. 5, 1978. Printed in Great Britain

On quasisymmetry (*P*-symmetry) groups

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Received 20 June 1977, in final form 23 November 1977

Abstract. A general method of obtaining quasisymmetry (P-symmetry) groups, using the concept of semi-direct products, is established. Using the ideas of little groups and their allowable irreducible representations, a new method of association of minor quasisymmetry groups with the irreducible representations of the generator groups is developed. Two concrete examples of diagrammatic representations of objects possessing the symmetry of minor quasisymmetry groups, when viewed as coloured groups, are given.

1. Introduction

The concept of antisymmetry was introduced into the study of crystallographic point groups and space groups by Shubnikov (1951) translated in Shubnikov and Belov (1964). The interpretation of antisymmetry as two-colour symmetry has led to the idea of polychromatic symmetry (Belov and Tarkhova 1956). Many extensions of this concept of antisymmetry were made, among which cryptosymmetry (Niggli and Wondratschek 1960, Wondratschek and Niggli 1961, Wittke 1962) is a fundamental one. Zamorzaev (1967) introduced the concept of quasisymmetry (or P-symmetry) and brought all the important earlier generalisations of antisymmetry, including cryptosymmetry, into its fold. Through his fundamental quasisymmetry theorem, Zamorzaev (1967) gave a method of deriving all groups of quasisymmetry from the generating groups. The 58 double coloured groups and the 18 polychromatic groups are just full P-symmetry minor groups with appropriate crystallographic point groups as generators and suitable cyclic groups (of permutations) of orders 2, 3, 4 and 6 as the permutation group P.

It is well known that the 58 double coloured groups are associated with the 58 distinct one-dimensional alternating representations of the 32 crystallographic point groups (Indenbom 1959, Niggli and Wondratschek 1960, Bertaut 1968, Krishnamurty and Gopala Krishna Murty 1969). The 18 polychromatic groups are associated with the 18 pairs of one-dimensional complex representations of the crystallographic point groups (Niggli and Wondratschek 1960, Indenbom *et al* 1960, Krishnamurty and Applanarasimham 1972). Niggli and Wondratschek (1960) derived some more simple cryptosymmetries and associated them with the degenerate irreducible representations (IR) of the crystallographic point groups using the concept of kernel. Recently a method of constructing multicoloured groups to be associated with the two-dimensional IR of the crystallographic point groups was suggested (Krishnamurty and Applanarasimham 1975), considering various subgroups of index 2, such that the chosen subgroups contain a pair of one-dimensional complex

0305-4770/78/0005-0805$01.00

representations. But on verification of the coloured elements obtained by them, it was found that they do not form a group. This defect has been rectified later by Appalanarasimham (1975).

In § 2 of this paper, a general method of obtaining quasisymmetry (P-symmetry) groups using the concept of semi-direct products is established. If G can be written as the semi-direct product of two groups S and $T (G = S \wedge T)$ and if S' and T' are two quasisymmetry groups with S and T as generators respectively, then $G' = S' \wedge T'$ (if S' and T' satisfy all the requirements of the semi-direct product) is shown to be a quasisymmetry group with G as the generator. It is also shown that the nature of G' (whether it is a major or minor or intermediate group) depends upon the nature of S' and T'. In § 3, using the little groups and their one-dimensional allowable irreducible representations (AIR) that induce the various IR of the crystallographic point groups, we associated the quasisymmetry minor groups with the IR of the generator groups. This method of obtaining the quasisymmetry groups and associating them with the IR of the generator groups differs from those of earlier investigators. We also give two concrete examples, by means of diagrammatic representations, of objects possessing the symmetry of minor quasisymmetry groups, when they are viewed as coloured groups. The notation adopted herein is mostly that of Bradley and Cracknell (1972).

2. Construction of quasisymmetry groups as semi-direct products

In this section we establish a general method of obtaining P-symmetry groups using the concept of semi-direct products and the fundamental quasisymmetry theorem of Zamorzaev (1967). In what follows, we outline the proofs for two cases only. The proofs for the remaining cases follow either in a similar way or they are essentially trivial.

Theorem 1. Let $G = S \wedge T$, S' be a full P-symmetry group with S as the generator and T' be a full Q-symmetry group† with T as the generator, where $P \neq Q \neq \{I\} \neq P$. If $G' = S' \wedge T'$ and if S' and T' are of the same category (both major or both minor or both intermediate), then G' is a full PQ-symmetry group of the same category with G as the generator. If $G' = S' \wedge T'$ and if S' and T' are of different categories, then G' is a full PQ-symmetry intermediate group with G as generator.

Proof. Let us suppose that both S' and T' are major groups. Any element of S' is of the form $s_i p_l$, where $s_i \in S$ and $p_l \in P$. Similarly any element of T' is of the form $t_j q_m$, where $t_j \in T$ and $q_m \in Q$. Any element of $G' = S' \wedge T'$ is of the form $s_i p_l t_j q_m = s_i t_j p_l q_m$. As $s_i p_l$ vary over S', s_i vary over S and p_l vary over P. Similarly as $t_j q_m$ vary over T', t_j vary over T and q_m over Q. This implies that $s_i t_j$ vary over G and $p_l q_m$ vary over $PQ (\equiv P'$ say). Thus, G' is a full PQ-symmetry group with G as generator. Also by definition (Zamorzaev 1967), Q' is that subgroup of G' with elements of the form $E p_l q_m$ where $p_l q_m \in PQ$. $s_i t_j p_l q_m \in Q' \Rightarrow s_i t_j = E \Rightarrow s_i = E$ and $t_j = E$. Thus $Q' = \{E p_l q_m / p_l q_m \in PQ\}$. In other words $Q' = G' \cap P' = P'$. Therefore G' is a full PQ-symmetry major group with G as generator. If P is invariant with respect to conjugation with every element of Q, then S' and T' satisfy the conditions for semi-direct

† 'Q-symmetry group' means, throughout this paper, that the underlying group of permutations in the corresponding quasisymmetry group is Q. This should not be misunderstood as the non-commutative version of coloured symmetry (Q-symmetry) considered in the resumé of the classic book by Shubnikov and Koptsik (1974).

product since their symmetry parts, namely S and T, already satisfy the conditions for the semi-direct product.

Now suppose that both S' and T' are minor groups. Then from the fundamental quasisymmetry theorem (Zamorzaev 1967), we have

$$S' = \bigcup_i s_i H p_i, \qquad s_i \in S,\, p_i \in P \quad \text{and} \quad s_i H \xrightarrow{f} p_i,$$

where $S/H \overset{f}{\cong} P$. Similarly

$$T' = \bigcup_j t_j \mathscr{K} q_j, \qquad t_j \in T,\, q_j \in Q \quad \text{and} \quad t_j \mathscr{K} \xrightarrow{g} q_j,$$

where $T/\mathscr{K} \overset{g}{\cong} Q$. Any element of G' is of the form

$$s_i h_a p_i t_j k_b q_j = s_i h_a t_j k_b p_i q_j, \qquad \text{where } h_a \in H,\, k_b \in \mathscr{K}.$$

As $s_i h_a p_i$ vary over S', $s_i h_a$ vary over S and p_i vary over P. Similarly as $t_j k_b q_j$ vary over T', $t_j k_b$ vary over T and q_j vary over Q. Hence it follows that G' is a full PQ-symmetry group with G as generator. By definition Q' is that subgroup of G' with elements of the form $Ep_i q_j$, where $p_i q_j \in PQ$. $s_i h_a t_j k_b p_i q_j \in Q' \Rightarrow s_i h_a t_j k_b = E \Rightarrow s_i h_a = E$, $t_j k_b = E \Rightarrow s_i = E$, $h_a = E$, $t_j = E$, $k_b = E \Rightarrow p_i = I$ and $q_j = I$ from the isomorphisms f and g. Thus, $Q' = \{EI\}$. Therefore G' is a full PQ-symmetry minor group with G as generator. Adopting a similar argument all the remaining cases of the theorem can easily be disposed of.

However, when $Q = P \neq \{I\}$, excepting the following modifications, all the other results cited in theorem 1 remain true.

(i) If both S' and T' are intermediate groups and if $G' = S' \wedge T'$, then, G' may be an intermediate group or a major full P-symmetry group with G as generator.

(ii) If one of S' and T' is a major group and the other a minor group, and if $G' = S' \wedge T'$, then G' is a full P-symmetry major group with G as generator.

(iii) If one of S' and T' is a major group and the other an intermediate group, and if $G' = S' \wedge T'$, then G' is a full P-symmetry major group with G as generator.

If S' is a full P-symmetry group with $P = \{I\}$, then S' is a major group as well as a minor group. We shall refer to such a group as a major/minor group. In such case we have the following modifications which can easily be established.

Theorem 2. If one of S' and T' of theorem 1 is a major/minor group, and the other a major or a minor or an intermediate group, and if $G' = S' \wedge T'$, then G' is a major or minor or intermediate group respectively with G as generator. If both S' and T' are major/minor groups and if $G' = S' \wedge T'$, then G' is also a major/minor group with G as generator.

3. Association of the minor quasisymmetry groups with the IR of the generator groups

Niggli and Wondratschek (1960) constructed 58 alternating, 18 cyclic, 23 two-dimensional and 7 three-dimensional simple cryptosymmetries against the one-dimensional alternating, one-dimensional complex, two- and three-dimensional IR respectively of the 32 crystallographic point groups, using the concept of kernel. In this section, a new method of construction of minor quasisymmetry groups and associating them with the IR of the generator groups is developed, using the concept of semi-direct product and the idea of little groups and their one-dimensional AIR. Two concrete examples, by means of diagrammatic representations, of objects possessing the symmetry of minor quasisymmetry groups, when viewed as coloured groups, are given.

It is well known (Altmann 1963a, b) that $D_3 = C_3 \wedge C_2$, where the point group C_3 consists of elements E, C_3^+ and C_3^- and the point group C_2 has the elements E, C'_{23}. The group C'_3: EI, C_3^+ (123), C_3^- (132), is a full P-symmetry minor group with C_3 as generator and the permutations I, (123) and (132) as P. The group C'_2: EI, C'_{23} (13), is a full Q-symmetry minor group with C_2 as generator and the permutations I, (13) as Q. These groups C'_3 and C'_2 satisfy the conditions for semi-direct product and hence we can write $D'_3 = C'_3 \wedge C'_2$, which consists of elements EI, C_3^+ (123), C_3^- (132), C'_{23} (13), C'_{22} (23), C'_{21} (12). By virtue of theorem 1 of § 2, D'_3 is a full PQ-symmetry minor group with D_3 as the generator. We know that the group C'_3 is associated with the one-dimensional complex representation ${}^1E$ of C_3 (Indenbom *et al* 1960, Krishnamurty and Appalanarasimham 1972, Niggli and Wondratschek 1960). C_3 is a little group of D_3 and the one-dimensional complex representation ${}^1E$ of C_3, which is an AIR, induces the two-dimensional IR E of D_3 (Altmann 1963a). As $D'_3 = C'_3 \wedge C'_2$ and since C'_3 is associated with the one-dimensional complex representation ${}^1E$ of C_3 which in turn induces the two-dimensional IR E of D_3, we associate D'_3 with this two-dimensional IR E of D_3. This method of association of the quasisymmetry minor group obtained with the IR of the generator group differs from that of Niggli and Wondratschek (1960), for their method of association was based on the kernel (which is the identity element E alone in this cited example) whereas ours is based on the little group (which is the point group C_3 in the same example).

As an example of an object possessing the symmetry of this minor quasisymmetry group D'_3, we consider the equilateral triangle (figure 1), where the indices 1, 2 and 3 denote the three different colours. COA, AOB and BOC are three triangular plates, forming the equilateral triangle ABC, coloured on both sides with colours 1, 2 and 3 respectively. With the twofold axes as shown in figure 1, one can easily see that D'_3 is a symmetry group of the coloured equilateral triangle.

As our second example, we choose the point group T. $T = D_2 \wedge C_3$, where the group D_2 has the elements $E, C_{2x}, C_{2y}, C_{2z}$ and the group C_3 has E, C_{31}^+, C_{31}^-. D'_2: EI, C_{2x} (13)(24), C_{2y} (12)(34), C_{2z} (14)(23), is a full P-symmetry minor group with D_2 as the generator and with P consisting of permutations I, (13) (24), (12) (34) and (14) (23). C'_3: EI, C_{31}^+ (134), C_{31}^- (143), is a full Q-symmetry minor group with C_3 as the generator and with Q consisting of permutations I, (134) and (143). Since D'_2 and C'_3 satisfy the conditions of the semi-direct product, $T' = D'_2 \wedge C'_3$ has

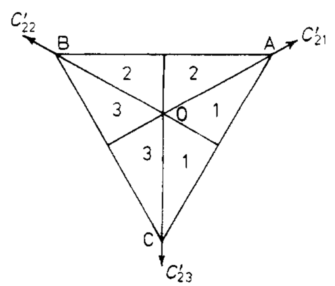

Figure 1.

the following elements: EI, C_{2x} (13)(24), C_{2y} (12)(34), C_{2z} (14)(23), C_{31}^+ (134), C_{32}^+ (142), C_{33}^+ (123), C_{34}^+ (243), C_{31}^- (143), C_{32}^- (124), C_{33}^- (132), C_{34}^- (234). T' is a full PQ-symmetry minor group with T as generator. As D_2' is equivalent (in the sense of Niggli and Wondratschek 1960) to the double coloured group 2′2′2 of D_2, associated with the alternating representation B_1 of D_2 (Indenbom 1959, Niggli and Wondratschek 1960, Bertaut 1968, Krishnamurty and Gopala Krishna Murty 1969), we associate D_2' with the IR B_1 of D_2. We also note that D_2 is a little group of T and the one-dimensional AIR B_1 of D_2 induces the three-dimensional IR T of the point group T. As $T' = D_2' \wedge C_3'$ and D_2' is associated with the one-dimensional AIR B_1 of D_2, which induces the three-dimensional IR T of the point group T, we associate T' with the three-dimensional IR of the group T. Here Niggli and Wondratschek (1960) made use of the kernel consisting of the identity element alone whereas our association is based on the little group D_2.

As an example of an object possessing the symmetry of T', we consider the regular tetrahedron (figure 2).

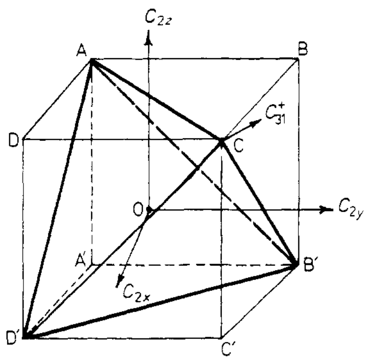

Figure 2.

In the regular tetrahedron CAB′D′, the faces ACD′, B′D′A, B′D′C and ACB′ are coloured with four different colours numbered as 1, 2, 3 and 4 respectively. With the rotation axes as shown in figure 2, it can be seen that T' is a symmetry group of this coloured regular tetrahedron. In this way we are able to construct the minor quasisymmetry groups (simple cryptosymmetries) against all the 23 two-dimensional IR of the crystallographic point groups and the 3 three-dimensional IR of the cubic point groups T and T_h, using the concepts of semi-direct products and little groups.

As we wanted our AIR to be always one dimensional for all the degenerate IR of the crystallographic point groups (Krishnamurty *et al* 1977), both ways of expressing the point group O as the semi-direct product, i.e. $O = T \wedge C_2''$ and $O = D_2 \wedge D_3'$ (where primes denote non-standard settings), are not useful for our purpose because none of the one-dimensional IR of T or D_2 induce the three-dimensional IR of O. On the other hand it may be noted (Bradley and Cracknell 1972, Krishnamurty *et al* 1977) that D_4' (non-standard setting of the point group D_4) is a little group of O and the 2 one-dimensional AIR A_2 and B_2 of D_4' induce respectively the 2 three-dimensional IR T_1 and T_2 of O. The group $(D_4')'$:E, $C_{2x}R_2'$, $C_{2y}R_2$, $C_{2z}R_2R_2'$, $C_{2d}R_2''$, $C_{4x}^+R_2''R_2$, $C_{4x}^-R_2''R_2'R_2$, $C_{2f}R_2''R_2'$, where $R_2 = (12)(34)$, $R_2' = (13)(24)$ and $R_2'' = (24)$, is a quasisymmetry minor group equivalent (in the sense of Niggli and Wondratschek 1960) to the ordinary double coloured group 4′2′2 of D_4', associated with the IR

B_2 of D'_4 (Indenbom 1959, Niggli and Wondratschek 1960, Bertaut 1968, Krishnamurty and Gopala Krishna Murty 1969). We therefore associate $(D'_4)'$ with the one-dimensional AIR B_2 of D'_4. A coset decomposition of the point group O relative to D'_4 is $O = ED'_4 \cup C^+_{31}D'_4 \cup C^-_{31}D'_4$. A quasisymmetry minor group with the group of coset representatives as generator is C'_3: EI, C^+_{31} (134), C^-_{31} (143). The product $(D'_4)'C'_3$, when expanded as the product of two complexes, is a full P-symmetry minor group with O as generator and $P = S_4$, the symmetric group on 4 symbols 1, 2, 3 and 4, as the permutation group. As $(D'_4)'$ is associated with the one-dimensional AIR B_2 of D'_4, which induces the three-dimensional IR T_2 of O, we associate this quasisymmetry minor group $(D'_4)'C'_3$ with the IR T_2 of O. It may be noted that $(D'_4)'C'_3 = T' \wedge (C''_2)'$, where T' is the quasisymmetry minor group already associated with the three-dimensional IR T of the point group T and $(C''_2)'$ with elements EI, C_{2d} (24) is a quasisymmetry minor group with C''_2 as generator. Here C''_2 (non-standard setting of the point group C_2) has the elements E and C_{2d}.

Similarly $(D'_4)''$: E, $C^+_{4x}R_4$, $C_{2x}R^2_4$, $C^-_{4x}R^3_4$, $C_{2z}R_2$, $C_{2y}R^2_4R_2$, $C_{2d}R^3_4R_2$, $C_{2f}R_4R_2$, where $R_2 = (16)(25)(38)(47)$, $R_4 = (1234)(5678)$, is a quasisymmetry minor group associated with the one-dimensional AIR A_2 of D'_4. The product $(D'_4)''C''_3$, where C''_3 has the elements EI, C^+_{31} (168)(274), C^-_{31} (186)(247), when expanded as the product of two complexes, is a quasisymmetry minor group and can be associated with the three-dimensional IR T_1 of O. It can be verified that $(D'_4)'C'_3$ is equivalent to $(D'_4)''C''_3$ and thus we have only one quasisymmetry minor group against the 2 three-dimensional IR T_1 and T_2 of the point group O. Since a similar situation prevails in the case of the three-dimensional IR of the point groups T_d and O_h, we have in total only seven distinct quasisymmetry minor groups against the 11 three-dimensional IR of the cubic point groups. This is in complete agreement with Niggli and Wondratschek (1960). In a similar way using the concepts of semi-direct products and little groups all the 58 double coloured groups and the 18 polychromatic groups can be obtained against the one-dimensional alternating and the one-dimensional complex representations respectively.

4. Discussion

The results of § 2 enable us to obtain all the quasisymmetry groups, with a group G as generator, as semi-direct product of smaller quasisymmetry groups with S and T as generators, whenever $G = S \wedge T$. There are many groups which can be written as semi-direct product of their subgroups. Altmann (1963a, b, 1967) showed that all point groups and all the symmetry groups of non-rigid molecules can be represented as semi-direct products. Shubnikov and Koptsik (1974) have obtained the colour groups $G^{(p)}$, isomorphic with the crystallographic groups G, by finding the normal subgroups H of G and forming the direct, semi-direct or quasiproduct of H with the generating coloured groups $G^{(p)*}$ or with the groups $G^{(p)*}$ (mod G^*_1). In our method both the factors in the semi-direct product are quasisymmetry groups.

The method of associating minor quasisymmetry groups with the IR of the generator groups, using little groups and their one-dimensional AIR, has the following interesting consequences. Firstly, it is easier to deal with a one-dimensional IR than with a degenerate IR directly. Secondly, for any magnetic or physical property, the number of independent constants one gets against a degenerate IR is the same as that occurring against the one-dimensional AIR of the appropriate little group, that induces the degenerate IR (Krishnamurty *et al* 1977). The equality of the above mentioned numbers is a consequence of the well known Frobenius reciprocity theorem.

An example of physical applications of the quasisymmetry groups is that of magnetic symmetry (Naish 1963, Zamorzaev 1967). 'The multiplicative groups' constructed by Naish (1963) are nothing but the quasisymmetry groups. In describing the magnetic symmetry of screw (helicoidal) structures, where the traditional magnetic groups (Shubnikov groups) are not suitable, these quasisymmetry (multiplicative) groups are found to be of much use.

Acknowledgments

The authors take this opportunity to express their sincere thanks to the referees for their constructive suggestions. They are also thankful to Professor T Venkatarayudu, Emeritus Professor, for his helpful discussions on this subject. One of the authors (KRR) is grateful to the UGC of India for the award of a Junior Research Fellowship.

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