# Derivation of multidimensional superperiodic symmetry groups by using Mackay groups

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#### Abstract

The geometrical application of multiple antisymmetry groups and Mackay groups for the derivation of multidimensional subperiodic groups is considered and illustrated by the direct derivation of 4-dimensional groups of the category  $G_{4321}$  from the category  $G_{21}$  by using Mackay 2-multiple antisymmetry groups. In general, symmetry groups of the category  $G_{(r+2)(r+1)r...}$  treated as a subcategory of the category  $G_{(r+2)r...}$  can be derived directly by using Mackay 2-multiple antisymmetry groups.<sup>1</sup>

## 1 Introduction

The concept of antisymmetry was introduced by H.Heesch [2]. The development of the theory of antisymmetry can be followed through the works of A.V. Shubnikov and V.A. Koptsik [7], A.V. Shubnikov and N.V. Belov et all. [6], A.M. Zamorzaev [8], A.M. Zamorzaev and A.F. Palistrant [10], and Kishinev school [9].

Its natural generalization, the idea of multiple antisymmetry was suggested by A.V. Shubnikov and introduced by A.M. Zamorzaev in 1956 [8]. Few months later, another concept of multiple antisymmetry was proposed by A.L. Mackay [5]. After that, mainly by the contribution of Kishinev school (Zamorzaev, Palistrant, Galyarskii...), the theory of multiple antisymmetry was extended to all categories of isometric symmetry groups of the space  $E^n$  ( $n \leq 3$ ), different kinds of non-isometric symmetry groups (of similarity symmetry, conformal symmetry, etc.) and *P*-symmetry groups [8,9,10]. On the other hand, investigation of the Mackay approach to the multiple antisymmetry [5] was not continued for many years.

In the case of *l*-multiple antisymmetry we have a discrete symmetry group G with a set of generators  $\{S_1, \ldots, S_r\}$ , given by the presentation

$$g_n(S_1, \dots, S_r) = E, \quad n = 1, \dots, s$$

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and the set of anti-identities  $e_1, \ldots, e_l$  of the first,...,  $l^{th}$  kind, that generate the group  $C_2^l = \{e_1\} \times \ldots \times \{e_l\}$  and satisfy the relations

$$e_i e_j = e_j e_i$$
  $e_i^2 = E$   $e_i S_q = S_q e_i$ ,  $i, j = 1, ..., l, q = 1, ..., r$ .

The group that consists of transformations S' = e'S, where e' is the identity, anti-identity, or some product of anti-identities, is called *l*-multiple antisymmetry group [8,10,9]. In particular, for l = i = j = 1 we have simple antisymmetry.

All simple and multiple-antisymmetry groups can be divided into the groups of  $S^k$   $(1 \leq k \leq l)$ ,  $S^k M^m$   $(1 \leq k, m; k + m \leq l)$  and  $M^m$   $(1 \leq m \leq l)$ type. Because the groups of  $S^k$  and  $S^k M^m$  type can be derived directly from a generating group G and from the groups of  $M^m$ -type respectively, the only non-trivial problem is a derivation of  $M^m$ -type groups. Hence, in this paper we will consider only the junior multiple-antisymmetry groups of  $M^m$ -type, i.e. the multiple-antisymmetry groups isomorphic with their generating symmetry group G, that possess an independent system of antisymmetries of m different kinds.

Each junior multiple-antisymmetry group G' of  $M^m$ -type can be defined by the extended group/subgroup symbol  $G/(H_1, \ldots, H_m)/H$ , where G is a generating group,  $H_i$  are its subgroups of index 2 satisfying the relationships  $G/H_i \simeq C_2 = \{e_i\}$   $(1 \le i \le m)$ , and H is the subgroup of G of index  $2^m$  – the symmetry subgroup of G'  $(G/H \simeq C_2^m = \{e_1\} \times \ldots \times \{e_m\})$  [8]. According to Zamorzaev approach, two junior multiple antisymmetry groups of  $M^m$ -type are equal *iff* their extended group/subgroup symbols coincide. In this case, the order of the subgroups  $H_i$  in the extended group/subgroup symbol is important, and the anti-identities  $e_i$  (i = 1, 2, ..., l) are treated as non-equivalent.

An efficient method for the derivation of multiple antisymmetry groups – the antisymmetric-characteristic method (AC-method) was introduced in 1984.

**Definition 1** Let all products of the generators of G, within which every generator participates once at the most, be formed and then subsets of transformations that are equivalent in the sense of symmetry with regard to the symmetry group G, be separated. The resulting system is called the antisymmetric characteristic of group G (AC(G)).

As the basic references we will use the list of non-isomorphic ACs with  $1 \le m \le 4$  generators and other results about Z-groups published in the paper [3] and the analogous results for Mackay groups from the paper [4].

### 2 Mackay groups

In the case of Zamorzaev *l*-multiple antisymmetry groups (Z-groups) the antiidentities  $e_i$  (i = 1, 2, ...l) are treated as mutually different. If we accept the equality of those anti-identities – their equal physical or geometrical role, as the result we obtain Mackay *l*-multiple antisymmetry groups (*M*-groups). The Derivation of multidimensional superperiodic symmetry ...

only difference between M- and Z-groups follows from that equality criterion. Because only junior multiple antisymmetry groups of  $M^m$ -type are nontrivial in the sense of derivation, we will restrict our consideration to the multiple antisymmetry M-groups of  $M^m$ -type. In this case,  $G/(H_1, H_2, ..., H_m)/H =$  $G/(H_{i_1}, H_{i_2}, ..., H_{i_m})/H)$ , where  $(i_1, i_2, ..., i_m)$  is some permutation of (1, 2, ..., m). According to that, two M-groups of G' and G'' that belong to the same family (i.e., that have the same generating symmetry group G) are equal *iff* there exist a permutation of the anti-identities  $e_1, e_2, ..., e_m$  transforming AC(G') into AC(G'').

Each AC completely defines a series  $N_m$ , where by  $N_m$  is denoted number of Z-groups of  $M^m$ -type. The same holds for series  $M_m$ , where  $M_m$  denotes the number of the corresponding M-groups derived from a symmetry group G for m fixed. Naturally,  $N_1(G) = M_1(G)$ .

In the paper [3] it is given complete list of the non-isomorphic ACs with  $1 \leq m \leq 4$  generators and a comparative list of the numbers  $N_m$  and  $M_m$  corresponding to that ACs.

The results from the paper [3] can be used for the calculation of the numbers of Z- and M-groups for some well known categories of symmetry groups. For example, in the case of plane symmetry groups  $G_2$ , with regard to the ACisomorphism classes, ACs of symmetry groups cm, p4g and p6m belong to the equivalence class 2.1, ACs of the groups pg, pgg, p4 to the class 2.2, AC of the group p1 to the class 2.3, ACs of the groups pm, pmg, cmm, p4m to the class 3.2, AC of the group p2 to the class 3.9, and AC of the group pmm to the class 4.16. From the remaining plane symmetry groups p3, p31m, p3m1, and p6 we cannot derive M- and Z-groups of  $M^2$ -type. For l = 1 we obtain 46 well known black-white antisymmetry groups,  $M_2(G_2) = 94$ ,  $M_3(G_2) = 137$ ,  $M_4(G_2) = 122$ .

By permuting anti-identities in M-groups we obtain the combinatorial connections between the numbers of M- and Z-groups, representing a double check of the results obtained:

 $N_2(G_2) = 73 \times 2 + 21 \times 1 = 167$   $N_3(G_2) = 97 \times 6 + 39 \times 3 + 1 \times 1 = 700$  $N_4(G_2) = 90 \times 24 + 29 \times 12 + 1 \times 6 + 2 \times 3 = 2520.$ 

# 3 Derivation of multidimensional subperiodic groups by using Mackay groups

From its beginning, in the works of H. Heesch [2] and A.V. Shubnikov [6,7], antisymmetry is used for a dimensional transition from the symmetry groups of friezes  $G_{21}$  to the symmetry groups of bands  $G_{321}$ , or from plane symmetry groups  $G_2$  to the layer symmetry groups  $G_{32}$ . In the similar way, A.V. Shubnikov used antisymmetry groups derived from the plane point symmetry groups  $G_{20}$  in order to obtain 3-dimensional point groups  $G_{320}$  by identifying the antiidentity transformation  $e_1$  with a point inversion. Trying to generalize the idea of antisymmetry and apply it to the derivation of multi-dimensional symmetry groups, H. Heesch proposed the derivation of hyper-layer symmetry groups  $G_{43}$ from 230 space symmetry groups  $G_3$  by identifying anti-identity transformation  $e_1$  with a hyper-plane reflection and introducing this way the additional  $4^{th}$ dimension.

The further development of that concept we can follow in the works of A.F. Palistrant, A.M. Zamorzaev and Kishinev school, where is given the following general result: every r-dimensional antisymmetry group can be derived as a (r+1)-dimensional symmetry group with the invariant (hyper)plane. By interpreting a color-change "black-white" (this means, the action of the anti-identity transformation  $e_1$ ) as a change of the additional coordinate perpendicular to the invariant hyper-plane, we conclude that to every antisymmetry group of the category  $G_{r...}^1$  corresponds the symmetry group of the category  $G_{(r+1)r...}$ , where to different antisymmetry groups correspond different symmetry groups. The possibility for dimensional transitions holds not only for simple antisymmetry, but also in the general case – in the case of multiple antisymmetry. According to the connections between l- and l+1-multiple antisymmetry and a possibility to reduce the theory of multiple antisymmetry to the series of such recursive transitions, i.e. to the multiple use of simple antisymmetry, according to the relationships  $G_{r...}^m = (G_{r...}^{m-1})^1 = (G_{r...}^1)^{m-1}$ ,  $G_{r...}^1 = G_{(r+1)r...}$ , we conclude that for Z-groups holds:  $G_{r...}^m = G_{(m+r)(m+r-1)...(r+1)r...}$ . This way, it is possible to use multiple antisymmetry Z-groups in order to derive multi-dimensional subperiodic symmetry groups of the higher dimensions, where a dimensional transition goes directly from r-dimensional to (r+m)-dimensional groups.

From that follows the natural question: what will represent Mackay groups in such a dimensional transition? In the case of simple antisymmetry, the result will be the same for Z- and M-groups, because for l = 1 they coincide, but for  $l \ge 2$ , thanks to the different equality criteria holding for Z- and M-groups, the results will be different.

This can be illustrated by the example of symmetry groups of the category  $G_1$  used for the direct derivation of the symmetry groups of the category  $G_{321}$  by applying 2-multiple antisymmetry. For the 2-multiple antisymmetry Z-groups it holds:  $G_1^2 = G_{321}$ ; this means that the extension of the category  $G_1$  by 2-multiple antisymmetry Z-groups results in the symmetry groups of bands  $G_{321}$ . There is the question: what will represent in the 3-dimensional space 2-multiple antisymmetry M-groups derived from the category  $G_1$ ? As it is well known, the category  $G_{321}$  consists of 31 symmetry groups of bands given by the following crystallographic symbols [7]:

$1) \ p1$	2) p121	3) $p2_122$	$4) \ p1m1$

5) p1a1 6) p21ma 7)  $p\frac{2_1}{m}11$  8)  $p11\frac{2}{a}$ 

Derivation of multidimensional superperiodic symmetry ...

$9) \ pm2m$	10) pm2a	11) p211	12) p112
13) $p\overline{1}$	14) $p2mm$	15) p2aa	16) pm11
17) $p11\frac{2}{m}$	$18) \ pma2$	$19) \ pmmm$	20) pmaa
$21) \ pmma$	22) $p2_111$	23) p222	24) $p11m$
25) $p11a$	26) $p2_1 am$	27) $p\frac{2}{m}11$	28) $p1\frac{2}{m}1$
$29) \ pmm2$	30) $p1\frac{2}{a}1$	31) pmam	

In the crystallographic symbols used, p denotes the translation along the invariant line, and the remaining three coordinates indicate different positions of symmetry elements: the first coordinate axis is parallel to the invariant line (to the translation axis), the second belongs to the invariant plane and it is perpendicular to the axis, and the third is perpendicular to the first and second. If two symmetry elements: rotation axis and the perpendicular element of symmetry correspond to the same axis, their symbols appear at the same coordinate, one over another (e.g.,  $\frac{2}{m}$ ).

Some of the bands differ between themselves only by a position of the symmetry elements with regard to the coordinate axes. Without distinguishing different orientations of the invariant plane of a band with regard to the coordinate axes, the number of symmetry groups of bands will be reduced from 31 to 22. Namely, the bands 2 and 12, 4 and 24, 5 and 25, 6 and 26, 10 and 18, 17 and 28, 21 and 31 will coincide, because one of them can be obtained from the other by replacing the symmetry elements corresponding to the second and third coordinate in the coordinate crystallographic symbols of bands. The result obtained – 22 symmetry groups, corresponds to the number of the symmetry groups of bands considered inside the category  $G_{31}$ , this means, if they are treated as the symmetry groups of rods.

On the other hand, the possibility to not distinguish the orientation of the plane of the figure with regard to the coordinate axes results in the new approach: we can derive the 22 symmetry groups mentioned as 2-multiple antisymmetry Mackay groups from the symmetry groups of the category  $G_1$ , this means, as M-groups of the category  $G_1^2$ . According to the equality criterion formulated for M-groups, the anti-identities  $e_1$  and  $e_2$  are equivalent among themselves. In the geometrical sense, this simply means that of reflection planes perpendicular to the second and third coordinate in this case play the equal geometrical role, so they can be mutually identified. This can be concluded from the following comparative list of 2-multiple antisymmetry M-groups derived from the symmetry groups of the category  $G_1$ :  $p_1$  generated by translation X and pm generated by two parallel reflections  $R_1$  and  $R_2$ , and the symmetry groups of bands  $G_{321}$ 

corresponding to them:

G	$p1 \ pm$	$ \{X\} \\ \{R_1, R_2\} $	= p1 $= pm11$	(1) (16)	
$S_1$		$ \{X\} \times \{e_1\}  \{R_1, R_2\} \times \{e_1\} $	$= p1m1 \\ = pm2m$	(4) (9)	(24) (29)
$S_{12}$		$ \{X\} \times \{e_1 e_2\} \\ \{R_1, R_2\} \times \{e_1 e_2\} $	$= p211$ $= p\frac{2}{m}11$	(11) (27)	
$S_{1}S_{2}$		$ \{X\} \times \{e_1\} \times \{e_2\} \\ \{R_1, R_2\} \times \{e_1\} \times \{e_2\} $	= p2mm $= pmmm$	(14) (19)	
$M_1$		$ \{ e_1 X \} \\ \{ e_1 R_1, R_2 \} \\ \{ e_1 R_1, e_1 R_2 \} $	= p1a1 $= pm2a$ $= p121$	(5) (10) (2)	(25) (18) (12)
$M_{12}$		$ \{ e_1 e_2 X \} \\ \{ e_1 e_2 R_1, R_2 \} \\ \{ e_1 e_2 R_1, e_1 e_2 R_2 \} $	$ = p 2_1 11 = p \frac{2_1}{m} = p 1 $	(22) (7) (13)	
$M_1 M_2$		$ \{ e_1 R_1, e_2 R_2 \} \\ \{ e_1 e_2 R_1, e_1 R_2 \} $	$= p2_122$ $= p11\frac{2}{a}$	$(3) \\ (8)$	(30)
$M_1S_2$		$ \begin{array}{l} \{e_1 X\} \times \{e_2\} \\ \{e_1 R_1, R_2\} \times \{e_2\} \\ \{e_1 R_1, e_1 R_2\} \times \{e_1 e_2\} \end{array} $	$= p2_1ma$ $= pmma$ $= p11\frac{2}{m}$	$(6) \\ (21) \\ (17)$	(26) (31) (28)
$M_1 S_{12}$		$ \begin{array}{l} \{e_1X\} \times \{e_1e_2\} \\ \{e_1R_1, R_2\} \times \{e_1e_2\} \\ \{e_1R_1, e_1R_2\} \times \{e_1e_2\} \end{array} $	= p2aa $= pmaa$ $= p222$	(15) (20) (23)	

This means that for the direct derivation of  $G_{321} \subset G_{31}$  from the category  $G_1$  by the use of 2-multiple antisymmetry Mackay groups are necessary the following types of groups:  $G, S_1, S_{12}, S_1S_2, M_1, M_{12}, M_1M_2, M_1S_2, M_1S_{12}$ . For the direct derivation of the symmetry groups of the category  $G_{321}$  by the use of 2-multiple antisymmetry Z-groups from the category  $G_1$  are necessary also the additional groups of the types  $S_2, M_2, M_2S_1, M_2M_1$ , where we need to take a care about the intersection of the types  $M_1M_2$  and  $M_2M_1$ .

From that follows that the 22 groups mentioned we obtain as 2-multiple antisymmetry M-groups, and their number is  $4G + 4M_1 + M_2$ . The number of the corresponding 2-multiple antisymmetry Z-groups is  $5G + 6M_1 + 2M_2 - (M_1M_2, M_2M_1)$ , where by  $(M_1M_2, M_2M_1)$  is denoted the number of the groups belonging to the intersection of the types  $M_1M_2$  and  $M_2M_1$ , this means, the number of Z-groups that by permuting anti-identities  $e_1$  and  $e_2$  are transformed into themselves, without giving new Z-groups. That will be M-groups remaining invariant when  $e_1$  and  $e_2$  change their places, so they will not give new Zgroups. They can be very easily recognized from the form of the AC. In our case, there is only one such group (3). Its AC is  $\{e_1R_1, e_2R_2\}$  and by the permutation of anti-identities  $e_1$  and  $e_2$  it remains unchanged, so we obtain:  $5 \times 2 + 6 \times 3 + 2 \times 2 - 1 = 31$ . Certainly, this indicates the possibility of a direct derivation of symmetry groups of the category  $G_{(r+m)(r+m-1)...(r+1)r...}$  from the groups of the category  $G_{r...}$  by using m-multiple antisymmetry Mackay groups.

As a next example of we can consider direct derivation of 4-dimensional groups of the category  $G_{4321}$  from the symmetry groups of friezes  $G_{21}$  by using 2-multiple antisymmetry groups. For the category  $G_{21}$  we have: G = 7 and  $M_1 = 17$ . In order to find  $M_2$  we know that two symmetry groups of friezes p2, pm have the AC:  $\{A, B\}$ . From each of them we derive two groups of the type  $M_2$  (this means,  $M_1M_2$ ); two symmetry groups of the friezes p1m, pmghave the AC:  $\{A\}\{B\}$  and each of them generate three groups of the type  $M^2$ ; one symmetry group of friezes pmm has the AC:  $\{A\}\{B, C\}$  and generates 13 Mackay 2-multiple antisymmetry groups of the type  $M^2$ .

Hence,  $M_2 = 2 \times 2 + 2 \times 3 + 13 = 23$ . The intersection  $(M_1M_2, M_2M_1)$  contains four groups: two groups with the AC  $\{e_1, e_2\}$  (derived from p1m and pmg) and two groups with the ACs  $\{E\}\{e_1, e_2\}$  and  $\{e_1, e_2\}\{e_1, e_2\}$  derived from pmm, so  $(M_1M_2, M_2M_1) = 4$ . From that follows:

$$G_{4321} = 5G + 6M_1 + 2M_2 - (M_1M_2, M_2M_1) = 5 \times 7 + 6 \times 17 + 2 \times 23 - 4 = 179.$$

On the other hand, the groups of the category  $G_{4321}$  we obtain from the category  $G_{321}$  by using simple antisymmetry, where G = 31,  $M_1 = 117$ , and  $G_{4321} = 2G + M_1 = 2 \times 31 + 117 = 179$ , that confirms the first result.

Analogously, it is possible to consider direct derivation of the symmetry groups of the category  $G_{432}$  from the category  $G_2^2$ . All the results obtained can be generalized: the number of the groups of the category  $G_{(r+2)(r+1)r...}$  derived directly from the category  $G_{r...}$  by the use of 2-multiple antisymmetry is given by the formula:  $5G + 6N_1 + N_2$ , where we are dealing with Z-groups  $(M_1 = N_1, N_2 = 2M_2 - (M_1M_2, M_2M_1))$ . On the other hand, by the formula  $4G + 4M_1 + M_2$  is given the number of the groups of the category  $G_{(r+2)(r+1)r...}$  derived by the use of 2-multiple antisymmetry Mackay groups and treated inside the category  $G_{(r+2)r...}$ .

In the general case, we can calculate the number of Z-groups of the category  $G_{(r+m)(r+m-1)\dots(r+1)r\dots}$  by the formula:

$$a_1G + a_2N_1 + \dots + a_{m-1}N_{m-1} + N_m$$

where G is the number of generating groups, and the coefficients  $a_i$   $(i = \overline{1, m-1})$  are, respectively:

 $\begin{array}{ll} m=2 & (5,6) & 5G+6N_1+N_2 \\ m=3 & (16,35,14) & 16G+35N_1+14N_2+N_3 \\ m=4 & (67,240,175,30) & \dots \\ m=5 & (374,2077,2480,775,62) & \dots \\ m=6 & (2825,2356,4361,22320,3255,126) & \dots \end{array}$ 

The original results from Section 3 are at the same time a comment to [1].

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