

WREATH PRODUCT IN FACTORIZATION OF HOLOSMMETRIC GROUP

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The holosymmetric group Q of an n -dimensional crystal lattice determined by a given lattice basis B is considered. This group is contained in the n -dimensional orthogonal group $O(n)$ so its elements preserve the orthogonality of basis vectors and their lengths. These conditions yield the decomposition of lattice basis into orthogonal sublattices and next the factorization of the holosymmetric group, which can be written as a direct product of complete monomial groups of k -dimensional ($k \leq n$) holosymmetric groups. Simple, decomposable and primitive holosymmetric groups are discussed. The results for $n \leq 4$ are presented.

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1. Introduction

Mathematical crystallography plays an important role in condensed matter physics since it is very useful to examine symmetries of a considered system. Algebraic methods, carried over to physics by means of crystallography, allow us to make easier solutions of many problems [1-7]. It is worth noting that results obtained in an n -dimensional space, with $n > 3$, are also valid in physics [8, 9]. On the other hand, dealing with an n -dimensional crystal lattices one can better formulate and understand concepts, definitions, theorems etc., well known in the 3-dimensional crystallography [10-16]. In this paper the holosymmetric group Q of a given n -dimensional crystal lattice A_n is presented as a direct product of wreath products. We assume that the lattice A_n is embedded in the n -dimensional Euclidean space E^n over the field R of real numbers. In the vector space R^n the scalar product is determined and the orthonormal basis \mathcal{E} is chosen. The lattice A_n is an orbit of the regular representation of the translation group

$$T_n = \{t \in R^n \mid t = \sum_{i \in \mathbb{N}} t_i b_i, t_i \in Z, b_i \in \mathcal{B}\}, \quad (1)$$

where Z is the ring of integers, $\tilde{n} \equiv \{1, 2, \dots, n\}$ and $B \subset R^n$ consists of n linearly independent vectors and is called a lattice basis of Λ_n . The factorization of the holosymmetric group Q is connected with a decomposition of the basis B and the lattice Λ_n . As a result one can write the group Q as the direct product of complete monomial groups, i.e. wreath products with a symmetric group [17–19]. There are two special cases of this factorization: (i) the group I_n generated by the n -dimensional inversion i_n , which can be written as a wreath product $wr(I_n, \Sigma_1, \{1\})$ and (ii) the n -dimensional hyperoctahedral group $W_n = wr(I_1, \Sigma_n, \tilde{n})$. The first group is the holohedry of the fully-clinic lattice. The word "fully" means that for each pair b, b' in B we have $b \cdot b' \neq 0$, e.g. for $n = 4$ we obtain the hexaclinic lattice [20]. The group W_n is the holohedry of the hypercubic lattice (i.e. $B \equiv \mathcal{E}$). It has been considered in many papers (see e.g. [21–26]).

The decomposition of lattice basis B into orthogonal subbases is considered in Sec. 2. In the next section we describe the factorization of the holosymmetric group Q into complete monomial groups. A passive subgroup of a wreath product is discussed in Sec. 4. Decomposable and simple groups are considered in Sec. 5. Examples of 2-, 3- and 4-dimensional lattices are presented in the last Section.

2. Decomposition of a lattice basis

The lattice basis B can be decomposed into $m \leq n$ mutually disjoint and orthogonal subsets B^a ($a \in \tilde{m}$) such, that for each pair $b, b' \in B^a$ there exists a series $b_0 = b, b_1, \dots, b_{k-1}, b_k = b'$ with the condition $b_{i-1} \cdot b_i \neq 0$. Let \mathcal{F} be a family of these subsets, n^a be a cardinality of the subset B^a , and let Λ^a be a k -dimensional lattice determined by the basis B^a . The basis vectors $b_i \in B$ will be labelled hereafter as b_i^a and

$$B = \{b_i^a | a \in \tilde{m}, i \in \tilde{n}^a\}. \tag{2}$$

The subsets B^a are gathered into families \mathcal{F}_k^p consisting of all subsets B^a with the same cardinality $k \leq n$ and determining identical k -dimensional lattices Λ_k^p (p labels different "types" of k -dimensional lattices). This means that for each $B^a, B^b \in \mathcal{F}_k^p$ a mapping $\psi: E^k \rightarrow E^k$ such, that $\psi(\Lambda^a) \equiv \Lambda^b$ is Euclidean. Let m_k^p denote a cardinality of the family \mathcal{F}_k^p and \tilde{m}_k^p be a set of indices $a \in \tilde{m}$ for which $B^a \in \mathcal{F}_k^p$

$$\tilde{m}_k^p = \{a \in \tilde{m} | B^a \in \mathcal{F}_k^p\}, \quad |\tilde{m}_k^p| = m_k^p. \tag{3}$$

An union

$$B_{k,p} = \bigcup_{a \in \tilde{m}_k^p} B^a \tag{4}$$

is a lattice basis of a $(k \times m_k^p)$ -dimensional sublattice $\Lambda(B_{k,p}^p)$.

The bases $B^a \in \mathcal{F}_k^p$ can be chosen in such a way, that the isomorphism $\psi_*: R^k \rightarrow R^k$, adjacent to the above mentioned mapping ψ , is determined by the following relation:

$$\psi_*(b_i^a) = b_i^b; \quad a, b \in \tilde{m}_k^p. \tag{5}$$

The presented decomposition of the lattice basis \mathcal{B} and the introduced families \mathcal{F} and \mathcal{F}_k^p enable us to factorize the holosymmetric group Q of the lattice Λ_n . We assume that the bases $\mathcal{B}^a \in \mathcal{F}_k^p$ fulfill condition (5) for each pair k, p . It means that each lattice $\Lambda^a, a \in \tilde{m}_k^p$, is a copy of an "abstract" k -dimensional lattice Λ_k^p and each $\mathcal{B}^a \in \mathcal{F}_k^p$ is a copy of the lattice basis of this lattice. Let \mathcal{E}^a be an orthonormal basis in a linear closure $\text{lc}(\mathcal{B}^a) \equiv V^a$. We can assume that the basis \mathcal{E} is the union of these bases, i.e. each vector $b_i^a, i \in \tilde{n}^a$, is a linear combination of only n^a vectors $e_i^a \in \mathcal{E}^a \subseteq \mathcal{E}$.

3. Holosymmetric group factorization

Since each element of the holosymmetric group Q is the orthogonal transformation of the space R^n , then this group can be written as a direct product of holosymmetric groups Q_k^p

$$Q = \bigotimes_{k,p} Q_k^p. \tag{6}$$

Each group Q_k^p is a holosymmetric group of lattice $\Lambda(\mathcal{B}_k^p)$ determined by the union (4).

These factorizations allow us to consider only one group Q_k^p for given k and p . Hence, we assume that the basis \mathcal{B} decomposes into m subsets \mathcal{B}^a with k elements, each of them determines an identical abstract k -dimensional lattice Λ_k . The indices k and $p = 1$ will be omitted and the group Q_k^p will be referred hereafter as Q .

The bases $\mathcal{B}^a, a \in \tilde{m}$, are chosen in such a way that the mapping determined by Eq. (5) is an orthogonal transformation. Therefore, each element of the group Q is a product

$$q = \left(\prod_{a \in \tilde{m}} q_a \right) q_0 = q_0 \left(\prod_{a \in \tilde{m}} q'_a \right), \tag{7}$$

where q_a and $q'_a, a \in \tilde{m}$, are elements of the k -dimensional holosymmetric group Q^a and q_0 is connected with q by the relation

$$q(V^a) = V^b \Rightarrow q_0(b_i^a) = b_i^b \quad \text{for } i \in \tilde{k}. \tag{8}$$

Then, each $q \in Q$ determines a permutation $\sigma_q \in \Sigma_m$

$$\sigma_q(a) = b \Leftrightarrow q(V^a) = V^b \tag{9}$$

and $q_0 \in Q$ can be written as

$$q_0(b_i^a) = b_i^{\sigma_q(a)}. \tag{10}$$

With this permutation one can write the following formulae:

$$q'_a = q_{\sigma_q(a)} \quad \text{or} \quad q_a = q_{\bar{\sigma}_q(a)}, \tag{11}$$

where $\bar{\sigma}_q(a)$ denotes the counter-image of the element $a \in \tilde{m}$.

The automorphisms $q_0 \in Q$ form the permutational subgroup P of the group Q . Moreover, the family \mathcal{F} is the orbit of this group, i.e. the group P acts transitively on it, and P is isomorphic with the symmetric group Σ_m .

The direct product of the holosymmetric groups Q^a

$$R = \bigotimes_{a \in \tilde{m}} Q^a \quad (12)$$

is the invariant subgroup of Q (it arises from Eq. (7)). This group is called hereafter as rotational subgroup of Q . Since each basis B^a determines the identical lattice, the groups Q^a are isomorphic with an abstract k -dimensional holosymmetric group G and the rotational group R is its m -th power, i.e.

$$R = \underbrace{G \otimes \dots \otimes G}_{m \text{ times}} = G^m, \quad G \approx Q^a \quad \text{for } a \in \tilde{m}. \quad (13)$$

From Eqs. (8) and (11) it follows that the holosymmetric group Q is the semidirect product of the permutational and rotational subgroups

$$Q = R \square P \quad (14)$$

and therefore, Q is the wreath product ([19, 26]):

$$Q = \text{wr}(Q^a, P, \tilde{m}) = \text{wr}(G, \Sigma_m, \tilde{m}). \quad (15)$$

When the group G is a primitive one we obtain that the holosymmetric group $Q \in GL(km, R)$ is the wreath product of primitive subgroup of $GL(k, R)$ and transitive subgroup of the symmetric group Σ_m . It coincides with the results presented by Suprunenko for Sylow subgroups of the general linear group [28]. The case of an imprimitive subgroup G is discussed in the next Section.

Taking into account Eq. (6) and considering the general case of the n -dimensional lattice A_n we obtain that the holosymmetric group Q is the direct product of the wreath products:

$$Q = \bigotimes_{k,p} \text{wr}(G_k^p, P_k^p, \tilde{m}_k^p), \quad (16)$$

where P_k^p is isomorphic with the symmetric group $\Sigma_{m_k^p}$ and G_k^p is the holosymmetric group of an abstract k -dimensional lattice A_k^p . Therefore, each factor in this product is the complete monomial group (of degree m_k^p) of the group G_k^p [17–19].

In the case $k = 1$ the different types of lattices, labelled by p , can differ from each other only in the length of the basis vector b_1^p . It yields that all groups G_1^p are isomorphic with the group $I_1 = \{E, i\}$ generated by the one-dimensional reflection $i: i(b_1) = -b_1$, so one obtains

$$Q_1^p = \text{wr}(I_1, \Sigma_{m_1^p}, \tilde{m}_1^p) = W_{m_1^p}. \quad (17)$$

4. Imprimitve holosymmetric group

The holosymmetric group G is a subgroup of the group $O(n) \subset GL(n, R)$. This group is imprimitive when the space R^n can be decomposed into the direct sum of non-empty subspaces V^a , $a \in \tilde{m}$, $m > 1$, such that [28]

$$\bigwedge_{g \in G} \bigwedge_{a \in \tilde{m}} g(V^a) = V^b, \quad b \in \tilde{m}. \quad (18)$$

In the other case the group is primitive. The simplest (and unique for $n < 4$) example of a primitive group G is the holosymmetric group C_{6v} of the two-dimensional hexagonal lattice. It is impossible to decompose the space R^2 into subspaces which fulfill the condition (18). On the other hand, when G is a subgroup of the n -dimensional hyperoctahedral group W_n , it is the imprimitive group and each subspace V^a is one-dimensional (this case is considered below). In the case of the hexagonal lattice the holosymmetric group is a subgroup of $W_3 \equiv O_h$ not of W_2 .

The holosymmetric group G is the cross-section of the general linear group over the ring of integers $GL(n, Z) \approx \text{Aut}T_n$ and the n -dimensional orthogonal group $O(n)$ [1, 26]. The form of the holosymmetric group G depends on the relations between the scalar products $M_{ij} = M_{ji} = b_i \cdot b_j$. Each $g \in G \subset W_n$ can be written as a pair (r, σ) , where $\sigma \in \Sigma_n$ is a permutation and r is an element of the n -th power of the group $I_1 = \{E, i\}$:

$$I_1^n \ni r = [r_1, r_2, \dots, r_n]; \quad r_i \in I_1, \quad i \in \tilde{n}. \quad (19)$$

Since for each vector $b_i \in \mathcal{B}$ there is a vector $b_j \in \mathcal{B}$ such that $M_{ij} \neq 0$, then the n -dimensional inversion $i_n = ([i, \dots, i], 1)$ is the unique (except for the identity $E \in I_1^n$) element from the basis group I_1^n in the group G . The inversion commutes with each $g \in G$, so G can be written as a direct product $I_n \otimes G'$, where G' is isomorphic with a quotient group G/I_n .

The special case of an imprimitive group G is obtained when the basis \mathcal{B} can be decomposed into pair-wise disjoint subsets \mathcal{B}^a , $a \in \tilde{m}$, with the following conditions: (i) each subset \mathcal{B}^a contains vectors with the same length λ^a ; (ii) for each pair $b_i^a, b_j^a \in \tilde{m}^a$ the scalar product $b_i^a \cdot b_j^a$ has the same value μ^a ; (iii) the scalar product $b_i^a \cdot b_j^b$ does not depend on the choice of vectors and is equal to ν^{ab} . From these conditions it arises that the quotient group G' is isomorphic with a Young subgroup $\Sigma_{(n)}$ of the symmetric group Σ_n , where the partition (n) is determined by the decomposition of the basis \mathcal{B} into subsets. The group G contains "pure" permutations and their products with the n -dimensional inversion i_n and can be written as a direct product $I_n \otimes \Sigma_{(n)}$. Moreover, in this case the holosymmetric group G is an example of the Coxeter group since a Young subgroup is generated by transpositions [27, 29].

In more general case the group G' is generated by elements which permute and change sign of the basis vectors. It means that for each $a \in \tilde{m}$ only the absolute value of μ^a is fixed. Another possibility is obtained when G' is contained in the Young subgroup $\Sigma_{(n)} = \otimes_{a \in \tilde{m}} \Sigma_{m^a}$ but contains products of permutations

belonging to different factors Σ_m when (at least two of) these factors are not subgroups of G . One can say that in this case a permutation of vectors $b_i^a \in \mathcal{B}$ has to be "connected" with a permutation of vectors belonging to other subsets $\mathcal{B}^b \neq \mathcal{B}^a$.

5. Simple and decomposable holosymmetric groups

An n -dimensional holosymmetric group which cannot be decomposed into a direct product of wreath products will be called a simple holosymmetric group. Let us denote such groups H_p^n , where n is a dimension of considered lattice and $p = 1, 2, \dots, h(n)$ labels different types of simple holosymmetric groups. The number of different types of simple holosymmetric groups are 1, 2, 2 and 16 for $n = 1, 2, 3$ and 4, respectively. We assume that for each dimension n the first (trivial) simple group is generated by the n -dimensional inversion i_n , i.e. $H_1^n \equiv I_n$. The unique nontrivial simple holosymmetric groups in two- and three-dimensional spaces correspond to the hexagonal families (C_{6v} and D_{3d} for hexagonal and rhombohedral lattice, respectively).

The decomposable (non-simple) groups in the space E^n can be obtained as combinations of the simple groups in spaces E^k , $k < n$. Let $(n) = (n_1, n_2, \dots, n_m)$ be an ordered partition of the number n into m non-zero parts. Considering all simple groups $H_p^{n_i}$, $p \leq h(n_i)$, one obtains the n -dimensional decomposable holosymmetric groups. It is important to underline that in the case $n_i = n_j$, $i, j \in \tilde{m}$, three cases have to be considered: (i) n_i -dimensional groups are different, (ii) these groups are isomorphic but corresponding sublattices differ in vector lengths from each other, (iii) the groups and sublattices are identical. In the last case a wreath product $\text{wr}(H_p^{n_i}, \Sigma_2, \{1, 2\})$ appears in the decomposition of the n -dimensional group. Of course, this procedure has to be applied in the similar way when more than two numbers n_i are equal. The most interesting case is obtained for $m = n$ (i.e. $n_i = 1, i \in \tilde{m}$). In this case the number of non-simple groups is equal to the number of partitions (n) . The decomposable groups for $n = 2, 3$ are gathered in Table. For $n = 4$ there are 4 partitions giving 16 decomposable groups and for $n = 5$ these numbers are 6 and 42, respectively. For $n = 6$ there are 120 groups which can be decomposed into simple groups $H_p^{n_i}$ with $n_i \leq 4$.

It has to be underlined that number of different groups corresponds to number of crystal systems not lattices. Different lattices are obtained after consideration of possible centring in a given crystal system.

6. Examples

The unique one-dimensional holosymmetric group $I_1 = \{E, i\}$ is, of course, primitive and simple and can be written as $I_1 = \text{wr}(I_1, \Sigma_1, \{1\})$. The two- and three-dimensional lattices are described in many books on crystallography or solid state physics (see e.g. [30, 31]). Below we consider holosymmetric groups of crystal systems in accordance with the concepts presented by Neubüser, Wondratschek and Bülow [10].

TABLE

Decomposable holosymmetric groups in two and three dimensions.

n	(n)	decomposition	family	Schoenflies symbol
2	(1,1)	$I_1 \otimes I_1$	orthogonal (rectangular)	C_{2v}
2	(1,1)	$\text{wr}(I_1, \Sigma_2, \{1, 2\})$	square	C_{4v}
3	(1,1,1)	$I_1 \otimes I_1 \otimes I_1$	orthogonal	D_{2h}
3	(1,1,1)	$\text{wr}(I_1, \Sigma_2, \{1, 2\}) \otimes I_1$	tetragonal	D_{4h}
3	(1,1,1)	$\text{wr}(I_1, \Sigma_3, \{1, 2, 3\})$	cubic	O_h
3	(2,1)	$I_2 \otimes I_1$	monoclinic	C_{2h}
3	(2,1)	$C_{6v} \otimes I_1$	hexagonal	D_{6h}

The decomposable groups in two- and three-dimensional Euclidean space are presented in Table. The simple groups are following (there are lattice names in parenthesis): (i) $C_2 \equiv I_2$ (clinic), (ii) C_{6v} (hexagonal — this is the unique primitive group), (iii) $C_i \equiv I_3$ (triclinic) and (iv) D_{3d} (rhombohedral).

For four-dimensional groups we obtain that there are 16 simple groups and 7 of them are primitive. In Sec. 5 we obtain 16 decomposable groups, then we have 32 holosymmetric groups, but it is known that there are 33 crystal systems in the space E^4 (see [20]). The applied procedure has not described the ditetragonal orthogonal D -centred lattice (family XIV and system 18 in [20]). This lattice can be described as a composition of two identical centred orthogonal lattices (i.e. rhombic lattices) and the holosymmetric group is given as $\text{wr}(C_{2v}, \Sigma_2, \{1, 2\})$. This example shows that the number of decomposable groups given in Sec. 5 for $n = 5, 6$ are only the bottom limits.

As examples we consider three four-dimensional lattices: (i) ditetragonal (XII.16), (ii) octagonal (XVIII.26) and (iii) icosahedral (XXII.31). They correspond to decomposable, simple imprimitive and simple primitive groups, respectively. In each case the crystal family and crystal system (F.S) is given according to [20].

In the first case non-zero elements of a scalar product matrix M are following: $M_{1,1} = M_{3,3} = A$, $M_{2,2} = M_{4,4} = B$ and $M_{1,2} = M_{3,4} = C$. Then the four-dimensional space can be decomposed into two two-dimensional orthogonal subspaces spanned over bases $\{b_1, b_2\}$ and $\{b_3, b_4\}$, respectively. The lattices determined in these subspaces are identical and their basis vectors have the same lengths. Since the holosymmetric group of the clinic lattice is generated by the two-dimensional inversion i_2 (two-fold rotation) then the holosymmetric group Q of the considered lattice can be written as a wreath product

$$Q = \text{wr}(I_2, \Sigma_2, \{1, 2\}). \quad (20)$$

The symmetric group Σ_2 is a permutational subgroup of Q and I_2^2 is a rotational subgroup of Q . This group is isomorphic with the D_4 group and is generated by the transposition $\tau = ([E, E], (12))$ and by the inversion (in the first or the second subspace) $i = ([E, i_2], (1)(2))$.

In the second case the matrix M has the following non-zero elements: $M_{1,1} = M_{2,2} = M_{3,3} = M_{4,4} = A$ and $M_{1,3} = M_{1,4} = M_{2,4} = -M_{2,3} = B$. The lattice

basis cannot be decomposed and the holosymmetric group Q is a subgroup of the hyperoctahedral group W_4 . Moreover, any subgroup of Σ_4 is not contained in Q . It is easy to show that the holosymmetric group is generated by elements which permute the basis vectors and change their signs. For example the generators can be chosen as $g_1 = ([E, E, i, E], (12)(3)(4))$ and $g_2 = ([E, i, E, i], (13)(24))$. This group is isomorphic with the group D_8 , so it is also a Coxeter group.

The third case is very similar to two-dimensional crystal lattice (also to body centered cubic lattice which, however, do not form a new crystal system). There are 10 vectors with the same length and their ends form two regular four-dimensional simplexes. Therefore, it is easy to show that this group can be written as $I_4 \otimes \Sigma_5$ and is a subgroup of the hyperoctahedral group W_5 .

7. Final remarks

In this paper we have examined the holosymmetric group of a given n -dimensional crystal lattice Λ_n . The factorization of this group has been performed in accordance with the geometric properties of the lattice described by a matrix of scalar products M . On the other hand, the proposed method cannot be applied to the holosymmetric groups G_k^p (Eqs. (15, 16)). These groups, in both primitive and imprimitive cases, can be considered to be the simplest parts of the holosymmetric group. Knowing all groups G_k^p with $k < n$ one can construct the holosymmetric groups of the n -dimensional lattices except for the n -dimensional groups G_n^p . Of course, in this way we will not obtain any simple groups. Moreover, in general case we can construct only a part of all decomposable groups.

The proposed method can be useful in the examination of symorphic space groups. The translation group T_n of the lattice Λ_n can be decomposed into a direct product of subgroups T_k^p accordingly with the decomposition of the lattice basis B into subbases B_k^p (Eq. (4)). From Eq. (6) it follows that in this case the space group S can be written as $S = \otimes_{k,p} S_k^p$, where S_k^p is the symorphic space group of the $(k \times m_k^p)$ -dimensional lattice and

$$S_k^p = T_k^p \square Q_k^p. \quad (21)$$

Since T_k^p is a direct product of m_k^p translation groups T_K defined in an abstract space R^k , then Eqs. (15, 16) give us

$$S_k^p = \text{wr}(T_k \square G_k^p, P_k^p, \tilde{m}_k^p). \quad (22)$$

We use the isomorphism

$$H^n \square \text{wr}(G, \Sigma_n, \tilde{n}) \approx (H \square G, \Sigma_n, \tilde{n}) \quad (23)$$

which is proved in one of us Ph.D. Thesis [32]. In the case $k = 1$ (see Eq. (17)) we obtain ($T_1 = T$)

$$S_1^p = \text{wr}(T \square I_1, P_1^p, \tilde{m}_1^p). \quad (24)$$

If we consider a finite lattice with $T \approx C_N$ then the group S_1^p is a complete monomial group (of degree m_1^p) of the group C_{Nv} . The groups $\text{wr}(C_{Nv}, \Sigma_n, \tilde{n})$ for $n = 2, 3$ have also been considered in the above mentioned Ph.D. Thesis [32].

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