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1993 J. Phys. A: Math. Gen. 26 2153

(http://iopscience.iop.org/0305-4470/26/9/012)

J. Phys. A: Math. Gen. 26 (1993) 2153–2167. Printed in the UK

Symmorphic space groups of finite crystal lattices

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Received 9 June 1992, in final form 22 February 1993

Abstract. The symmorphic space group of a finite n-dimensional crystal lattice is studied and its factorization is presented. This lattice is determined by a direct product of cyclic groups and then its translation, point and space groups are defined as modular images of corresponding ones for a lattice of infinite extent. A factorization of holohedries (of an infinite lattice) is used in order to present a symmorphic finite space group as a direct product. As an example, and as a very special case, a space group in the case of the hypercubic lattice is studied and its irreducible representations are investigated. The results obtained suggest that for vectors lying on a surface of the first Brillouin zone (i.e. for which at least one coordinate is equal to 0 or $\frac{1}{2}$) an additional index describing their symmetry properties should be introduced. This enables us to make a more detailed classification of states (energy levels). On the other hand, finite symmorphic space groups can be used within, e.g., the so-called finite-lattice approach.

1. Introduction

Adequate description of the ordering of constituent elements of matter in its different phases is one of the principal questions of condensed matter physics and it has been discussed by physicists, mathematicians and crystallographers for years. Development of a modern crystallography was started by Seitz (1934a,b, 1935a,b, 1936), who applied mathematical methods, in particular group theory, to the description of crystal symmetries. His works were based on results that had been obtained in the 19th century by, e.g., Barlow, Bravais, Fedorov, Gadolin, Haüy, Schönflies and Sohnecke. On the other hand, there were many breakthroughs in algebra in these years owing to such famous mathematicians as Burnside, Frobenius, Pólya, Jordan, Schur, Weyl and Young. The beginning of the 20th century was also a period of rapid progress in condensed matter physics due to experimental and theoretical achievements (Bragg, Brillouin, Einstein, Hermann, von Laue and others). Properties of crystal lattices in the n-dimensional Euclidean space were (and still are) very interesting for mathematicians and they have been frequently investigated for at least 50 years (Wintgen 1941, Dade 1964). At first Seitz's results were applied to symmorphic space groups by Bouckaert *et al* (1936) and they gave the first description of compatibility relations. These pioneering works, a base of the contemporary theory of crystal symmetry, have been cited and reprinted in many books on crystallography, solid state physics and mathematics (cf e.g., Koster 1957, Koster *et al* 1963, Bradley and Cracknell 1972, Meijer 1964).

On the other hand, Born and von Kármán (1913) had introduced the periodic boundary conditions to determine specific heat and normal modes in crystals and this approach was

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0305-4470/93/092153+15$07.50

soon found to be fruitful in the description of irreducible representations of space groups. Nowadays, these conditions are used in computer calculations within the so-called *finite-lattice method* (see, e.g., Bonner and Fisher 1964, Duxbury and Oitmaa 1983).

Though the most important case in question is the three-dimensional infinite crystal lattice, mathematicians and crystallographers have investigated lattices in spaces of any dimension and over any field (or ring) of numbers (including finite ones). Moreover, it has been discovered that, on the one hand, there are a lot of systems with quasi-linear or quasi-two-dimensional periodicity (see, e.g., Walsted *et al* 1970, Bonner 1978, Botet *et al* 1983, Sólyom and Ziman 1984) and, on the other hand, some structures can be described using point groups of n-dimensional crystal lattices with $n > 3$ (for incommensurate crystals like modulated crystals, intergrowth structures, quasi-crystals, see, e.g., Janner 1991 and references therein, Kramer and Neri 1984, de Wolff 1984). Recently, there has been a big interest in the (quasi-)two-dimensional lattices since the discovery of high-T_c superconductors, due to their antiferromagnetic properties, which can be described introducing a 2D crystal lattice (see, e.g., Huse 1988, van Himbergen and Silbey 1988, Gross *et al* 1989, Bernu*et al* 1992). One-dimensional (linear) models are also applied in investigations of superconductivity in organic crystals (Allender *et al* 1974) or in modelling of biological processes (Tsetlin 1969). Symmetries of finite lattices seem to be good candidates for the description of fractal symmetries (e.g. in-line polymers, see Kuźma 1991, 1993 and references therein) and 'floppy' (non-rigid) crystals, in an analogy with 'feasible' symmetry operations for floppy molecules (see, e.g., Altmann 1977, Bunker 1979). The latter problem was briefly discussed in our previous work (Florek *et al* 1988; see also Mucha 1991). However, in this work we limit ourselves to 'rigid' crystals, thus only the so-called *modular images* of crystal lattice and its symmetry groups will be discussed.

Summarizing, this work has been motivated by three questions: (i) application of the finite-lattice method in solid state physics, (ii) very interesting physical phenomena, which can be described by introducing a crystal lattice in n-dimensional space with $n \neq 3$, and (iii) better understanding of consequences of the Born–von Kármán periodic boundary conditions. A 'cross section' of these questions is an n-dimensional finite crystal lattice with its translational, point and space groups. In the first problem it is important to decompose a space of states into invariant subspaces labelled by irreps of symmetry groups and, therefore, to decrease an eigenproblem dimension. The above-cited examples suggest that it is necessary to consider n-dimensional lattices (and their symmetries with irreducible representations) for any n. However, the case $n = 3$ is still the most important one. Some symmetry operations of the finite lattice can be interpreted as 'feasible' or fractal symmetries (this problem will not be discussed here) and, on the other hand, factorization of (finite) symmorphic space groups (presented below) gives us a new labelling scheme for symmetry points and lines in the (discrete) Brillouin zone.

This aritcle starts with a brief presentation of finite lattices (section 2) and factorization of holohedries (section 3). In the next two sections we consider (modular) images of point and (symmorphic) space groups (sections 4 and 5). The obtained results are discussed in section 6, whereas an overall summary and a comparison with other approaches are presented in section 7.

2. Finite crystal lattices

An n-dimensional crystal lattice (from the mathematical point of view) is a set of points in the n-dimensional Euclidean space $\mathbb{E}^n$ given as

$$\Lambda^n = \left\{ a \in \mathbb{E}^n \;\middle|\; a = a_0 + \tau, \tau = \sum_{i=1}^{n} \tau_i \varepsilon_i \in \mathcal{T} \subset \mathbb{R}^n \right\} \tag{1}$$

where a_0 is an arbitrary chosen origin of the lattice and $\mathcal{T} \cong \mathbb{Z}^n$ is its translation group, i.e. a set of vectors with integral coefficients τ_i in a given crystal basis $\mathcal{B}$ consisting of n fundamental translations $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n$—the edges of the unit cell (see, e.g., Bradley and Cracknell 1972). Possible choices of the basis $\mathcal{B}$ (for the same crystal lattice) determines a group Aut $\mathcal{T}$ of all automorphisms of the translation group $\mathcal{T}$. This group is clearly a general linear group over a ring of integers $GL(n, \mathbb{Z})$ (see, e.g., Dade 1964, 1965, Ascher and Janner 1965, Florek *et al* 1988, Michel and Mozrzymas 1985, 1989). However, only a finite number of these transformations belong to the orthogonal group $O(n, \mathbb{R})$, i.e. they leave invariant all distances and angles (with respect to a scalar product assumed in $\mathbb{E}^n$). In the case of a one-dimensional lattice it is easy to find these automorphisms since there are only two of them—$GL(1, \mathbb{Z}) = \{1, -1\} \equiv O(1, \mathbb{R})$. Moreover, all lattices belong to the same crystal system. In higher dimensions the number of crystal systems increases rapidly. Mathematical aspects of n-dimensional crystallography have been studied and presented by many authors in monographs (e.g., Brown *et al* 1978, Schwarzenberger 1980, Mozrzymas 1987) and original papers (see, e.g., Neubüser *et al* 1971, Schwarzenberger 1972, 1974, Mozrzymas and Solecki 1975, Weigel *et al* 1984, Senechal 1985).

By analogy, an n-dimensional finite translation group T can be defined as a direct product of n cyclic groups $\mathbb{Z}_{N_i}$

$$T = \bigotimes_{i=1}^{n} \mathbb{Z}_{N_i} = \{t = (t_1, t_2, \ldots, t_n) \mid t_i \in \mathbb{Z}_{N_i}, N_i > 1, i = 1, 2, \ldots, n\} \tag{2}$$

and a finite crystal lattice is given as a set of 'points' labelled by elements of T. A set of n vectors

$$\begin{aligned} e_1 &= (1, 0, \ldots, 0, 0) \\ e_2 &= (0, 1, \ldots, 0, 0) \\ &\vdots \qquad\qquad \vdots \\ e_{n-1} &= (0, 0, \ldots, 1, 0) \\ e_n &= (0, 0, \ldots, 0, 1) \end{aligned} \tag{3}$$

is in one-to-one correspondence with any (n-dimensional) crystal basis $\mathcal{B}$ and will be hereafter referred to as the set of *canonical generators* of T. This is one possible realizations of the Born–von Kármán periodic boundary conditions. According to an idea proposed by Weyl (1952) in his book, the group of all automorphisms Aut T has to be analysed in order to obtain all essential mathematical features. It means that we are interested in all possible choices of generators of the translation group (2). It turns out that, even in such a simple case as the one-dimensional lattice determined by the cyclic group $\mathbb{Z}_N$, there is a big difference between infinite and finite lattices. For example, the number of automorphisms in this case is given by the arithmetic Euler function $\varphi(N)$—equal to number of integers less than and mutually prime with N—and strongly depends on the arithmetic structure of N (see Lulek 1984, Florek and Lulek 1987 and references therein). This number varies from 1, for $N = 1$ and 2, to $p - 1$ for a prime integer p. On the other hand, for n-dimensional ($n \geqslant 2$) infinite translation groups the group $GL(n, \mathbb{Z})$ always has an infinite number of elements (e.g. for

$n = 2$ it contains, among others, transformations in the form $\varepsilon_1 \to \varepsilon_1$, $\varepsilon_2 \to k\varepsilon_1 + \varepsilon_2$, where k is any integer), whereas a number of automorphisms of a finite translation group is finite for any choice of *identity periods* $N_1, N_2, \ldots, N_n$. For example, when all the identity periods are equal to a prime number p then a direct product $\mathbb{Z}_p^n \equiv \bigotimes_{i=1}^n \mathbb{Z}_p$ has

$$\operatorname{Aut} \mathbb{Z}_p^n = \prod_{l=0}^{n-1} (p^n - p^l)$$

automorphisms. For example, for $p = 5$, $n = 3$ one simply obtains that $\operatorname{Aut} \mathbb{Z}_5^3 = 1\,488\,000$. This number is much greater than an order of the largest three-dimensional point group ($O_h = 48$) but it is divisible by 48, which suggests that $\operatorname{Aut} \mathbb{Z}_5^3$ contains a subgroup isomorphic with O_h (it will be shown below). At this stage a problem of correspondence between infinite lattices and finite ones comes into question. So we are going to introduce *modular images* of translation, point and space groups. They define a modular image of a lattice itself.

A *modular image* of an infinite translation group $\mathcal{T}$ (cf (1)) is determined by a mapping $\phi : \mathcal{T} \to T$ such that

$$\phi(\tau) = (\tau_1 \bmod N_1, \tau_2 \bmod N_2, \ldots, \tau_n \bmod N_n) . \tag{4}$$

According to this definition one can easily obtain

$$\phi(\varepsilon_i) = e_i . \tag{5}$$

Of course, this mapping says nothing about the geometrical properties of a considered (infinite) lattice. For example let us define, in a rather natural way, a notion of *nearest neighbours* in the case of finite lattice as a pair of nodes labelled by $\boldsymbol{t}$ and $\boldsymbol{t}'$ such that $(\boldsymbol{t} - \boldsymbol{t}')$ or $(\boldsymbol{t}' - \boldsymbol{t})$ is one of the canonical generators (3). It is a straightforward matter to show that this definition corresponds to the definition based on a scalar product (i.e. the one used in the case of a infinite lattice) if one considers the simple (hyper)cubic lattice. In other cases the proposed definition is too wide (e.g., for the monoclinic lattice) or too narrow as in the case of the hexagonal lattice. All such properties of an infinite lattice will be 'transformed' to its modular image, i.e. to a finite lattice, by the *modular (homomorphic) image of a point group* Q in the automorphism group $\operatorname{Aut} T$. This problem will be discussed in section 4 after a short presentation of a factorization of holohedries, which then will be applied to (finite) symmorphic space groups (section 5).

3. Factorization of holohedries

Let Λ be a k-dimensional crystal lattice with the maximal point group in a given crystal system, i.e. its point group Q is the *holosymmetric point group* (or *holohedry*) of a crystal system. From m (identical) lattices Λ one can form a crystal lattice in km dimensions—each copy of Λ is embedded in a k-dimensional subspace and all these subspaces are mutually orthogonal. The holohedry of this new lattice, except for a direct product of m copies of Q, contains elements that permute sublattices. Therefore, this group can be written as a semi-direct product

$$\underbrace{(Q \otimes Q \otimes \cdots \otimes Q)}_{m \text{ times}} \square \Sigma_m \tag{6}$$

where Σ_m is the group of all $m!$ permutations of m elements (sublattices, in the considered case). Semi-direct products of this form are called *wreath products*† (Pólya 1937, Kerber 1971, Kerber and James 1981) and denoted $Q \wr \Sigma_m$. Taking into account different k_s-dimensional lattices Λ_s with the holohedries Q_s and the multiplicities m_s ($1 \leqslant s \leqslant r$) one can construct in the same way a crystal lattice in $n = \sum_s k_s m_s$ dimensions with the holohedry given by a direct product

$$Q = \bigotimes_{s=1}^{r} Q_s \wr \Sigma_{m_s} . \tag{7}$$

Of course some Q_s may be isomorphic (identical), e.g. when lattices Λ_s differ in lengths of vectors only. If $\mathcal{T}_s \equiv \mathbb{Z}^{k_s}$ is a translation group of the lattice Λ_s then the translation group of the whole lattice can be written as

$$\mathcal{T} = \bigotimes_{s=1}^{r} \bigotimes_{j=1}^{m_s} \mathcal{T}_s = \bigotimes_{i=s}^{r} \overline{\mathcal{T}}_s \equiv \mathbb{Z}^n \tag{8}$$

where $\overline{\mathcal{T}}_s \equiv \mathbb{Z}^{k_s m_s}$ is the translation group of lattices in the sth type.

For example, the holohedries of cubic, tetragonal and monoclinic 3D crystal systems can be written, respectively, as (see also table 1)

$$\begin{aligned} O_h &\cong C_s \wr \Sigma_3 \\ D_{4h} &\cong (C_s \wr \Sigma_2) \otimes (C_s \wr \Sigma_1) \cong C_s \wr (\Sigma_2 \otimes \Sigma_1) \\ C_{2h} &\cong (C_2 \wr \Sigma_1) \otimes (C_s \wr \Sigma_1) . \end{aligned}$$

There are two special cases of the factorization (7): (i) the 'fully'-clinic lattice with the holohedry $I_n \wr \Sigma_1$, where the group I_n is generated by the n-dimensional inversion i_n and (ii) the hypercubic lattice constructed from n identical one-dimensional lattices, which holohedry is given as the *hyperoctahedral group* $W_n \cong C_2 \wr \Sigma_n$ (cf Young 1930, de Robinson 1930, Springer 1974, Mayer 1974, 1975, Geissinger and Kinch 1978, Baake 1984, Florek *et al* 1988). A more detailed discussion of this factorization was presented in our previous work (Florek and Lulek 1991). In particular, holohedries Q_i, which cannot be decomposed into a direct product of wreath products, were discussed.

This factorization differs from, e.g., a presentation of point groups as semi-direct products (cf Altmann 1963a,b, Mozrzymas 1977) and corresponds to a decomposition of an n-dimensional lattice into orthogonal sublattices (cf Eichler 1952, Kneser 1954, Dade 1964, 1965). This gives us a very clear interpretation of a point group in the case of lattices with pairwise orthogonal fundamental translations ε_i. In such a case the holohedry can be written as a wreath product $C_s \wr \Sigma_{(n)}$, where $\Sigma_{(n)}$ is a Young subgroup of Σ_n corresponding to the partition $(n) = (n_1, n_2, \ldots, n_r)$. This partition is determined by lengths of the vectors ε_i, i.e. n_i denotes a number of the fundamental translations having length l_i. For example, when $n = 4$ there are 5 such lattices: orthogonal, tetragonal–orthogonal, ditetragonal, cubic and hypercubic determined by partitions (1,1,1,1), (2,1,1), (2,2), (3,1) and (4), respectively

† To be more precise, in general an active group of the semi-direct product (6) can be any subgroup of the symmetric group. If it is equal (or isomorphic) to whole symmetric group, as in our case, a wreath product is sometimes called the *complete monomial group (of degree m) of Q* (Specht 1932) or the *symmetry (of degree m) of Q* (Ore 1942).

Table 1. Factorization of symmorphic finite space groups for 2D and 3D lattices (Σ_1 is omitted everywhere; the asterisk denotes a simple holohedry).

Crystal system	Holohedry	Space group	
Clinic	N_a	C_2 *	$\mathbb{Z}_N^2 \square C_2$
Rectangular	N_r	$C_s \otimes C_s$	$C_{Nv} \otimes C_{Nv}$
Hexagonal	N_h	C_{6v} *	$\mathbb{Z}_N^2 \square C_{6v}$
Square	N_q	$C_s \wr \Sigma_2$	$C_{Nv} \wr \Sigma_2$
Triclinic	Γ_t	C_i *	$\mathbb{Z}_N^3 \square C_i$
Monoclinic	Γ_m	$C_2 \otimes C_s$	$(\mathbb{Z}_N^2 \square C_2) \otimes C_{Nv}$
Orthorhombic	Γ_o	$C_s \otimes C_s \otimes C_s$	$C_{Nv} \otimes C_{Nv} \otimes C_{Nv}$
Tetragonal	Γ_q	$(C_s \wr \Sigma_2) \otimes C_s$	$(C_{Nv} \wr \Sigma_2) \otimes C_{Nv}$
Rhombohedral	Γ_{rh}	$C_{3v} \otimes C_i$ *	$(\mathbb{Z}_N \wr \Sigma_3) \square C_i$
Hexagonal	Γ_h	$C_{6v} \otimes C_s$	$(\mathbb{Z}_N^2 \square C_{6v}) \otimes C_{Nv}$
Cubic	Γ_c	$C_s \wr \Sigma_3$	$C_{Nv} \wr \Sigma_3$

(cf Wondratschek *et al* 1971, Florek 1988a). It is easy to notice that with each direction the group of one-dimensional reflection (i.e. a reflection in an $(n-1)$-dimensional hyperplane) C_s is connected and these groups are permuted, when this is allowed by the orthogonality conditions. It should be stressed that within this approach holohedries of 'fully'-clinic lattices, consisting of the identity and the inversion, are always non-decomposable (simple). Similarly, the holohedries C_{6v} and D_{3d} (of 2D hexagonal and 3D rhombohedral lattices, respectively) cannot be decomposed. These are all simple holohedries in two- and three-dimensional spaces. In four dimensions there are 15 simple holohedries except for the I_4 group—the holohedry of hexaclinic lattice.

4. Modular images of point groups

It was briefly discussed in the previous sections that the group (2), determining a finite crystal, has the automorphism group $\mathrm{Aut}\,T$, which algebraic structure depends on arithmetic structure of integers N_i. The investigation of this group is a very interesting problem of both group and number theory but it exceeds the scope of our work. We are only interested in these automorphisms, which can be treated as images of elements of a considered holohedry, though it is very interesting to find a physical interpretation of the others. Some predictions can be found in Florek *et al* 1988, Mucha 1991, Kuźma 1991, 1993.

It follows from the factorization (7) that a subspace containing lattices only in the sth type is invariant under any element of the holosymmetric group. Therefore, only one factor $Q \wr \Sigma_m$ will be considered hereafter. Moreover, for the sake of simplicity, we assume that all identity periods N_i, $i = 1, 2, \ldots, km = n$ are equal to N (so $T = (\mathbb{Z}_N^k)^m \equiv \mathbb{Z}_N^n$). In this way none of the 'axes' is distinguished and all restrictions imposed on transformations $\Phi(q)$ have their 'sources' in a point group, which modular image will be investigated. However, it is possible to reduce these requirements (for details see Florek 1988a).

A *modular image* of a given holohedry can be determined basing on the definition (4) of the translation group image. Let $\Phi : Q \to \mathrm{Aut}\,T$ be a group homomorphism. An automorphism $\Phi(q)$ is a modular image of $q \in Q$ if for each $\tau \in \mathcal{T}$ (cf Dirl and Davis 1993)

$$\Phi(q)(\phi(\tau)) = \phi(q(\tau)) \,. \tag{9}$$

If matrix elements of q in the lattice basis $\mathcal{B}$ are given by the relation

$$q(\varepsilon_j) = \sum_{i=1}^{n} q_{ij}\varepsilon_i \qquad q_{ij} \in \mathbb{Z} \tag{10}$$

then for $\Phi(q)$ one obtains

$$\Phi(q)(e_j) = \sum_{i=1}^{n}(q_{ij} \bmod N)e_i\,. \tag{11}$$

It is possible to choose the basis vectors $\varepsilon_j \in \mathcal{T}$ in such a way that each permutation $q \in \Sigma_m \subset Q$ transforms one fundamental translation into another, so $q_{ij} = 1$ if $q(\varepsilon_j) = \varepsilon_i$ and 0 in the other cases. Since $N > 1$, we obtain the same formulae for $\Phi(q)$ and, therefore, $\Phi(\Sigma_m) \equiv \Sigma_m$ (but now its elements permute subgroups $\mathbb{Z}_N^k \subset \mathbb{Z}_N^{km}$). Therefore, it is sufficient to consider only a modular image of non-decomposable k-dimensional holosymmetric group Q—a passive group in the wreath product (6).

First, let us consider the one-dimensional lattice. There is only one crystal system with the holosymmetric point group $Q = \{E, \pi\} \cong C_s \equiv I_1$. On the other hand, $\operatorname{Aut}\mathbb{Z}_N$ consists of mappings

$$\eta_l(t) = lt \bmod N$$

such that l is mutually prime with N (the other homomorphisms η_l are not automorphisms). Since $\pi(\varepsilon) = -\varepsilon$ then, according to (9), $\Phi(\pi)(1) = N - 1$, so $\Phi(\pi) = \eta_{N-1} \equiv \eta_{-1}$. It is clear that this image is non-trivial if $N > 2$ ($N - 1$ is always mutually prime with N, but for $N = 2$ we obtain $\Phi(\pi) = \eta_1 = \Phi(E)$). So in this way we have solved the problem of finding modular images for all holohedries of the form $C_s \wr \Sigma_{(n)}$ (cf the previous section). It is a very important results since, among others cases, they describe (hyper)cubic lattices, which are used in the finite lattice method as a rule.

It follows from the above considerations that, in general, a modular image of Q is faithful if N is greater than $\max(q_{ij}) - \min(q_{ij})$, where maximum and minimum are taken over all pairs $1 \leqslant i, j \leqslant k$ and for all $q \in Q$ (in this way different matrix elements q_{ij} have different 'images' $q_{ij} \bmod N$ so Φ is an isomorphism). It is a straightforward matter to show that in this case $\Phi(q)(e_i)$ is a generator of $\mathbb{Z}_N^k$ (the largest common divisor of integers $q_{1j}, q_{2j}, \ldots, q_{kj}$ is equal to 1, since this column—as a vector in $\mathbb{R}^k$—generates a group isomorphic with $\mathbb{Z}$). In the most important cases ($k = 1, 2, 3$) integers $q_i j$ are always 0 and ± 1 (cf Bradley and Cracknell 1972, table 3.2), so it suffices to assume $N > 2$ (the case $N = 2$ should be considered separately; see, e.g., Mucha 1991). Wondratschek *et al* (1971) presented matrices of generators of 4D holohedries and, again, all entries are equal to ± 1 or 0. It is easy (but tedious) to check that it is true for all elements of point groups.

It is worthwhile to note that each holohedry contains the k-dimensional inversion $i_k \in I_k \subset Q$, which modular image can be interpreted as a simultaneous action of all $\eta_{N-1}^{(j)}$, $j = 1, 2, \ldots, k$, i.e.

$$\Phi(i_k)(t_1, t_2, \ldots, t_k) = (-t_1, -t_2, \ldots, -t_k)\,.$$

Since i_k commutes with any element of Q then this group can written as a direct product

$$Q = Q' \otimes I_k \tag{12}$$

where Q' is isomorphic to a quotient group Q/I_k. For example, $C_{6v} \cong C_{3v} \otimes C_2$ ($I_2 \equiv C_2$) and $D_{3d} \cong C_{3v} \otimes C_i$. This additional factorization of a holohedry is, of course, transformed to its modular image.

Example. The holohedry of a two-dimensional hexagonal lattice is the group C_{6v} generated by two reflections σ_1 and σ_2. In the lattice basis $B = \{\varepsilon_1 = 1, 0|, \varepsilon_2 = -\frac{1}{2}, \sqrt{3}/2|\}$ we have

$$\sigma_1 = \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix}.$$

Therefore, for the canonical generators of $T = \mathbb{Z}_N^2$, $N > 2$, we obtain

$$\Phi(\sigma_1)(1,0) = (1,0) \qquad \Phi(\sigma_1)(0,1) = (-1,-1)$$
$$\Phi(\sigma_2)(1,0) = (1,1) \qquad \Phi(\sigma_2)(0,1) = (0,-1).$$

One can easily find images of the other elements $q \in C_{6v}$.

5. Symmorphic finite space groups

A modular image of a symmorphic space group is simply a semi-direct product of the translation group $T \equiv \mathbb{Z}_N^{km}$ and the modular image of a point group considered in the previous section (we again take into account only one factor from (7) given as a wreath product $Q \wr \Sigma_m$). It should be stated here that our considerations can be generalized at least in two ways: (i) consideration of non-symmorphic groups and their modular images; (ii) investigation of a whole group $\mathrm{Aut}\, T$ and its extensions by T (including, as the most important case, a holomorph $\mathrm{Hol}\, T := T \,\square\, \mathrm{Aut}\, T$). In the first case we meet a problem of determining all extensions of $\Phi(Q)$ by T for all non-trivial factor systems $\omega : \Phi(Q) \times \Phi(Q) \to T$. Please note that, in general, it is impossible to introduce 'rational' translations in the case of a finite translation group, as is usually done for $\mathcal{T} \equiv \mathbb{Z}^n$. This question has been partially discussed by Dirl and Davis (1993) and Florek *et al* (1993). In the second case, we come back to the problem of investigation and interpretation of non-orthogonal transformations (e.g. fractal symmetries, cf Kuźma 1991, 1993). In this work we are interested only in finite symmorphic space groups corresponding to infinite ones, so only a semi-direct product $T \,\square\, \Phi(Q)$ is considered.

Let us start again from the one-dimensional case (i.e. $km = 1$). The translation group is the cyclic group $\mathbb{Z}_N$ and $\Phi(Q) = \{\eta_1, \eta_{-1}\} \cong C_s$ (for $N > 2$). Therefore, the symmorphic finite space group in this case is simply given as a semi-direct product

$$S = \mathbb{Z}_N \,\square\, C_s \cong C_{Nv} \cong D_N. \tag{13}$$

More detailed discussion of one-dimensional lattices with the Born–von Kármán periodic conditions are presented in the previous works of the authors (Lulek 1984, Florek and Lulek 1987, Florek 1988b), where some applications were presented, too.

In a general case ($n = km$) a symmorphic finite space group can be written as

$$S = (\mathbb{Z}_N^k)^m \,\square\, (\Phi(Q) \wr \Sigma_m). \tag{14}$$

An action of $\Phi(Q) \wr \Sigma_m$ on $\mathbb{Z}_N^{km}$ is described in the previous section. It is a straightforward matter to show that the above semi-direct product is isomorphic to a wreath product (see, e.g., Florek 1988a pp 169–71)

$$S = (\mathbb{Z}_N^k \,\square\, \Phi(Q)) \wr \Sigma_m \,. \tag{15}$$

For $k = 1$, i.e. if we consider m copies of a one-dimensional lattice, what corresponds to the (hyper)cubic lattice, we immediately obtain

$$S = C_{Nv} \wr \Sigma_m \tag{16}$$

so in this case the space group is the symmetry (of order m) of C_{Nv}. Since, according to (12), Q can be written as a direct product $Q' \otimes I_k$, then from (15) it follows that

$$S = (\mathbb{Z}_N^k \,\square\, (\Phi(Q') \otimes I_k)) \wr \Sigma_m \,. \tag{17}$$

In the special case $Q' \cong \Sigma_k$ (it is true, e.g., for the 3D rhombohedral lattice—$C_{3v} \cong \Sigma_3$) we obtain

$$S = ((\mathbb{Z}_N^k \,\square\, \Sigma_k) \,\square\, I_k) \wr \Sigma_m \cong ((\mathbb{Z}_N \wr \Sigma_k) \,\square\, I_k) \wr \Sigma_m \tag{18}$$

since the inversion commutes with each element $q' \in Q'$ and i_k acts only on translations $\boldsymbol{t} \in \mathbb{Z}_N^k$, but not on $\sigma \in \Sigma_k$, i.e.

$$i_k((t_1, \ldots, t_k), \sigma) = ((-t_1, \ldots, -t_k), \sigma) \,.$$

For example, in the case of the rhombohedral lattice one obtains the symmorphic space group as a semi-direct product of a generalized symmetry group and the inversion group, that is to say

$$S = (\mathbb{Z}_N \wr \Sigma_3) \,\square\, C_i \,. \tag{19}$$

A passive group of the semi-direct product $\mathbb{Z}_N \wr \Sigma_k$ is the *generalized symmetry group* (see, e.g., Kerber 1971). These groups were investigated by Osima (1954, 1956), so we do not present them here.

Complete monomial groups $C_{Nv} \wr \Sigma_m$ for $m = 2, 3$ were studied by Florek (1988a). It is important to underline that: (i) for $N = 2$ there are not any non-trivial automorphisms, so $S = \mathbb{Z}_2 \wr \Sigma_m \equiv W_m$ (see Mucha 1991) and (ii) properties of groups S, written as a wreath product (16), depend on parity of N and the cases (a) N odd, (b) N even, have to be investigated separately. Some results are presented in the next section.

6. Results for two- and three-dimensional lattices. The symmetry of the group C_{Nv}

The considerations presented above enable us to write symmorphic finite space groups as direct products of wreath products, which basis groups are semi-direct products $\mathbb{Z}_N^k \,\square\, Q$. Moreover, it is sufficient to consider such semi-direct products only for non-decomposable (simple) holohedries Q. There are 1, 2, 2 and 16 such holohedries for $k = 1, 2, 3$ and 4, respectively (see Florek 1988a, Florek and Lulek 1991). For each k one of these groups is the group I_k generated by the k-dimensional inversion i_k, which corresponds to the 'fully'-clinic lattice (clinic, triclinic and hexaclinic for $k = 2, 3, 4$). The others, for $k = 2, 3$, are C_{6v} and D_{3d}, respectively. In table 1 factorization of symmorphic finite space groups is presented for $n = 2, 3$ according to the formulae derived in the previous section ($N_1 = N_2 = N_3 > 2$ is assumed in each case). More detailed discussion of these results has been presented elsewhere (Florek 1988a, see also Florek and Lulek 1991). The symmetry groups of C_{Nv} of order $m = 2, 3$ (square and cubic lattices, respectively; $k = 1$, $n = m$) are very interesting due to their possible applications in the finite-lattice method calculations. Therefore, we are going to present their properties below. The results have been obtained applying methods for investigations of wreath products (see, e.g., Kerber 1971).

A number of irreducible representations (and classes of conjugated elements, too) of $C_{Nv} \wr \Sigma_m$ for $m = 2, 3$ is given by the following formulae (for details see Kerber 1971, Florek 1988a):

$$
\begin{array}{lll}
(N+3)(N+9)/8 & m=2 & N \text{odd} \\
(N+6)(N+12)/8 & m=2 & N \text{even} \\
(N+3)(N+5)(N+19)/48 & m=3 & N \text{odd} \\
(N+6)(N+8)(N+22)/48 & m=3 & N \text{even}.
\end{array}
$$

For example, for the square lattice 4×4 the space group $D_{4v} \wr \Sigma_2$ has 128 elements in 20 classes, so there are also 20 irreducible representations (irreps), which may be used as 'quantum' numbers to label eigenspaces of a considered Hamiltonian. These irreps can be obtained by the induction procedure from the irreps of C_{Nv}^m, i.e. from products of m irreps of C_{Nv}. The latter ones will be denoted by Γ_k with $k = 0+, 0-, 1, 2, \ldots, p, N/2+, N/2-$, where $p = (N-1)/2$ for N odd or $p = N/2 - 1$ for N even denotes a number of two-dimensional irreps. The others are one-dimensional, but these labelled by $N/2$ occur only for N even (and this case will be considered hereafter; when N is odd a border of the first Brillouin zone 'disappears'). The $-/+$ symbol says whether or not the basis vector changes its sign under an action of the reflection $\pi \equiv \eta_{-1}$. Of course, the reduction $C_{Nv} \downarrow \mathbb{Z}_N$ gives

$$
\Gamma_{0\pm} = \Delta^0 \qquad \Gamma_{N/2\pm} = \Delta^{N/2} \qquad \Gamma_k = \Delta^k \oplus \Delta^{-k} \qquad \text{for} \quad k = 1, 2, \ldots, p \tag{20}
$$

whereas the reduction $C_{Nv} \downarrow C_s$ yields

$$
\begin{array}{l}
\Gamma_{k+} = \Xi_0 \qquad \Gamma_{k-} = \Xi_1 \qquad \text{for} \quad k = 0, \tfrac{1}{2}N \\
\Gamma_k = \Xi_0 \oplus \Xi_1 \qquad \text{for} \quad k = 1, 2, \ldots, p
\end{array} \tag{21}
$$

where $\Xi_{0(1)}$ denotes the symmetric (antisymmetric, respectively) irrep of C_s. The two possible decompositions of Γ_k for $1 \leqslant k \leqslant p$ correspond to two possible bases in the subspace labelled by Γ_k. In the first case the basis is complex whereas in the second it is real. Of course, in both cases states labelled by Γ_k have the same energy. On the contrary, energy levels labelled by $k = 0, N/2$ can split into symmetric and antisymmetric parts (with different energies, in general).

The standard induction procedure starts from the irreps of a translation group $\mathbb{Z}_N^m$, where a point group is the hyperoctahedral group $W_m = C_s \wr \Sigma_m$. A representation domain, identical with the basic domain when the isogonal group of a space group is the holosymmetric point group, contains vectors $\boldsymbol{k} = (k_1, k_2, \ldots, k_m)$ from the first Brillouin zone, for which $0 \leqslant k_1 \leqslant k_2 \leqslant \cdots \leqslant k_m \leqslant \frac{1}{2}$ and a representative of each star can be chosen to lie in this area. Within the approach presented in this work labels of the irrep are always non-negative—it is caused by inclusion of reflections $\pi \equiv \eta_{-1}$ into an invariant subgroup C^m_{Nv}—therefore, we consider only a part of the Brillouin zone containing vectors with non-negative coordinates. However, each point (and some lines, planes etc) of symmetry has at least one coordinate equal 0 or $N/2$, so it is split into a number of different (maybe equivalent) irreps of C^m_{Nv} (cf (20)). For example, the centre of the Brillouin zone is labelled by the vector $(0, 0, \ldots, 0)$ and corresponds to the unit irrep of $\mathbb{Z}^m_N$. Considering the group C^m_{Nv} ones obtain 2^m irreps with $k = 0\pm$ (the unit one is, of course, labelled by $(0+, 0+, \ldots, 0+)$). Under an action of Σ_m they can be divided into $m+1$ orbits (stars) O_l; the lth orbit contains irreps, which are products of $m-l$ irreps Γ_{0+} and l irreps Γ_{0-}. It should be stressed that a general point (and some lines, planes etc), i.e. the one labelled by $\boldsymbol{k}$ with different coordinates $0 \neq k_i \neq N/2$, does not change its meaning—it is labelled now by m different two-dimensional irreps Γ_k. Of course, it is possible when $m \geqslant p$. In this way, points (lines etc) of symmetry receive an additional index describing their symmetry properties under an action of reflections π for these directions for which $k_i = 0$ or $N/2$. It is important in many physical applications. For example, we know that the ground state of the Heisenberg antiferromagnet is non-degenerate (Marshall 1955), so it belongs to a subspace labelled by a one-dimensional irrep. Considering only a translation group we do not obtain any hints—all irreps are one-dimensional. On the other hand, introducing the C^m_{Nv} group we find that this ground state has to be labelled by a point of symmetry (all coordinates have to be 0 or $N/2$), which is not so surprising. However, when one stops at this stage—i.e. when one does not take into account a whole space group—then in the first case there are $m+1$ possible labels of one-dimensional invariant subspaces (labelled by a number of coordinates equal to $\frac{1}{2}$), whereas in the second case this number is equal to $\sum_{l=0}^{m}(m-l+1)(l+1) = (m^3 + 6m^2 + 11m + 6)/6$, which corresponds to non-equivalent distributions of numbers 0 and $N/2$ and signs $\pm$. Of course, when we include an active group, i.e. the hyperoctahedral group W_m in the first case and the symmetric group Σ_m in the second one, all results (irreps with character tables) have to be reproduced. For example, the number of one-dimensional irreps is always equal to 8 (4 for $m = 1$), but this result is obtained in two different ways. In the first case we have two points, say $\Gamma = (0, 0, \ldots, 0)$ and $R = (\frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2})$, with little co-groups equal to a point group (cf Bradley and Cracknell 1972, table 3.6) and the hyperoctahedral group, as a wreath product $C_s \wr \Sigma_m$, has 4 (2 for $m = 1$) one-dimensional irreps. Therefore, the induction procedure gives $2 \times 4 = 8$ (2×2 for $m = 1$) one-dimensional irreps. Within the approach discussed here we have 4 irreps with a little co-group Σ_m: $(0+, 0+, \ldots, 0+)$, $(0-, 0-, \ldots, 0-)$, $(\frac{1}{2}N+, \frac{1}{2}N+, \ldots, \frac{1}{2}N+)$, $(\frac{1}{2}N-, \frac{1}{2}N-, \ldots, \frac{1}{2}N-)$ and the symmetric group has two one-dimensional irreps (1 for $m = 1$), so the results of induction is the same as above. In table 2 we present a correspondence between points, lines and planes of symmetry (cf Bradley and Cracknell 1972) with representatives of stars (orbits) of C^m_{Nv} irreps for $m = 3$, i.e. for simple cubic lattice. In table 3 we compare different notions of space group irreps for $k = (0, 0, 0)$—they are equivalent to $W_3 \equiv O_h$ irreps. We will discuss obtained formulae and tables in the next section.

7. Conclusions and final remarks

The factorization of a space group presented and discussed in this work gives us an intermediate step in the construction of space groups irreps. In the standard approach one starts from $\mathbb{Z}^m_N$ and in the next step (by the induction procedure) reaches a space group. This

Table 2. Comparison of vector stars with orbits of C^3_{Nv} irreps ($0 < \alpha < \beta < \gamma < \frac{1}{2}$; only labels (a, b, c) of irreps in a product $\Gamma_a \otimes \Gamma_b \otimes \Gamma_c$ are given, $0 < a < b < c < \frac{1}{2}N$, $s, t = \pm$, $\bar{s} \equiv -s$).

Point of symmetry		Irrep of C^3_{Nv}		Little co-group
Label	Coordinates	Dimension	Label	
Γ	(000)	1	$(0s, 0s, 0s)$	Σ_3
			$(0s, 0s, 0\bar{s})$	$\Sigma_2 \otimes \Sigma_1$
R	$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	1	$(\frac{1}{2}Ns, \frac{1}{2}Ns, \frac{1}{2}Ns)$	Σ_3
			$(\frac{1}{2}Ns, \frac{1}{2}Ns, \frac{1}{2}N\bar{s})$	$\Sigma_2 \otimes \Sigma_1$
X	$(00\frac{1}{2})$	1	$(0s, 0s, \frac{1}{2}Nt)$	$\Sigma_2 \otimes \Sigma_1$
			$(0+, 0-, \frac{1}{2}Ns)$	$\Sigma_1 \otimes \Sigma_1 \otimes \Sigma_1$
M	$(0\frac{1}{2}\frac{1}{2})$	1	$(0s, \frac{1}{2}Nt, \frac{1}{2}Nt)$	$\Sigma_1 \otimes \Sigma_2$
			$(0s, \frac{1}{2}N+, \frac{1}{2}N-)$	$\Sigma_1 \otimes \Sigma_1 \otimes \Sigma_1$
$\Lambda(\Gamma R)$	$(\alpha\alpha\alpha)$	8	(a, a, a)	Σ_3
$\Delta(\Gamma X)$	(00α)	2	$(0s, 0s, a)$	$\Sigma_2 \otimes \Sigma_1$
			$(0+, 0-, a)$	$\Sigma_1 \otimes \Sigma_1 \otimes \Sigma_1$
$\Sigma(\Gamma M)$	$(0\alpha\alpha)$	4	$(0s, a, a)$	$\Sigma_1 \otimes \Sigma_2$
$S(XR)$	$(\alpha\alpha\frac{1}{2})$	4	$(a, a, \frac{1}{2}Ns)$	$\Sigma_2 \otimes \Sigma_1$
$Z(XM)$	$(0\alpha\frac{1}{2})$	2	$(0s, a, \frac{1}{2}Nt)$	$\Sigma_1 \otimes \Sigma_1 \otimes \Sigma_1$
$T(MR)$	$(\alpha\frac{1}{2}\frac{1}{2})$	2	$(a, \frac{1}{2}Ns, \frac{1}{2}Ns)$	$\Sigma_1 \otimes \Sigma_2$
			$(a, \frac{1}{2}N+, \frac{1}{2}N-)$	$\Sigma_1 \otimes \Sigma_1 \otimes \Sigma_1$
$O(\Delta\Sigma Z)$	$(0\alpha\beta)$	4	$(0s, a, b)$	$\Sigma_1 \otimes \Sigma_1 \otimes \Sigma_1$
$J(\Delta\Lambda S)$	$(\alpha\alpha\beta)$	8	(a, a, b)	$\Sigma_2 \otimes \Sigma_1$
$C(\Sigma\Lambda T)$	$(\alpha\beta\beta)$	8	(a, b, b)	$\Sigma_1 \otimes \Sigma_2$
$B(SZT)$	$(\alpha\beta\frac{1}{2})$	4	$(a, b, \frac{1}{2}Ns)$	$\Sigma_1 \otimes \Sigma_1 \otimes \Sigma_1$
General point	$(\alpha\beta\gamma)$	8	(a, b, c)	$\Sigma_1 \otimes \Sigma_1 \otimes \Sigma_1$

'way' is now divided into four steps: (i) from $\mathbb{Z}_N^k$ to $\mathbb{Z}_N^k \,\square\, Q$ (or, more precisely, $\Phi(Q)$), i.e. to a space group S_k of a k-dimensional lattice with a non-decomposable holohedry Q; (ii) from S_k to its mth power S_k^m, when this type of lattice can be found m times in a decomposition of an n-dimensional crystal lattice; (iii) from S_k^m to a semi-direct product $S_k^m \,\square\, \Sigma_m$—possible permutations of identical lattices are included; (iv) the simplest step—a construction and consideration of a direct product of all groups obtained in the previous steps (sometimes, like for hypercubic lattices, there is only one factor in the decomposition (7). When three-dimensional space groups are in question, then it suffices to consider (in the first step) the following groups: C_{Nv} for $k = 1$, $\mathbb{Z}_N^2 \,\square\, C_2$ and $\mathbb{Z}_N^2 \,\square\, C_{6v}$ for $k = 2$, $\mathbb{Z}_N^3 \,\square\, C_i$ and $\mathbb{Z}_N^3 \,\square\, D_{3d}$ for $k = 3$ (cf table 1 and (19)). In the case of four-dimensional lattices one also has to include 16 non-decomposable 4D holohedries. Considering a direct product of m identical groups S_k (like C_{Nv}) we obtain a base for investigations of all space groups in the form $S_k \wr \Sigma_{(m)}$ (cf section 3; for $k = 1$ one obtains a 'family' of lattices with orthogonal basis vectors) and provides us with additional indices for irreps obtained in the previous step (like the $\pm$ sign in the considered example of hypercubic lattices). The last two steps reproduce in a simple way results obtained within the standard approach. It has be underlined that steps (ii) and (iii) can be performed as a single step when one exploits the structure of wreath products. The above considerations suggest that groups S_k (like C_{Nv}) are the basic constituents of every space group in any dimension.

The modular image of an infinite lattice has been introduced in order to construct a formal connection between infinite lattices (embedded in the Euclidean space with a

Table 3. Different notions of the one-dimensional irreps of $W_3 \equiv O_h$; (3) ((1^3)) denotes the symmetric (antisymmetric, respectively) irrep of Σ_3 (cf Bradley and Cracknell 1972, table 5.8 for G^7_{48}).

Bradley and Cracknell (1972)	R_1	R_2	R_3	R_4
Mulliken (1933)	A_{1g}	A_{2g}	A_{2u}	A_{1u}
Koster *et al* (1963)	Γ_1^+	Γ_2^+	Γ_2^-	Γ_1^-
This work	$\Gamma^3_{0+} \otimes (3)$	$\Gamma^3_{0+} \otimes (1^3)$	$\Gamma^3_{0-} \otimes (3)$	$\Gamma^3_{0-} \otimes (1^3)$

scalar product defined) and finite ones which, in general, cannot be embedded in a vector space. Moreover, it turns out that finite lattices—without restrictions imposed by a scalar product—can describe other structures of condensed matter (e.g. 'non-rigid' crystals or fractal symmetries), but we have not considered these possibilities in this work. It should be also underlined that the Born–von Kármán periodic conditions can be introduced in a different way. In our approach the edges of crystal lattices are identified (so the number of crystal nodes is finite). One can also consider a lattice of infinite extent but constructed from finite lattices containing $N_1 N_2 \ldots N_m$ nodes (i.e. one assumes that all physical properties of a crystal in points τ and $\tau' = N_1\varepsilon + \cdots + N_m\varepsilon_m$ are identical). For example, Dirl and Davis (1993) investigated finite lattices (and their symmetry groups) considering a quotient group $\mathbb{Z}^3/(N_1\mathbb{Z} \otimes N_2\mathbb{Z} \otimes N_3\mathbb{Z})$. Of course, this group is isomorphic with a direct product $\mathbb{Z}_{N_1} \otimes \mathbb{Z}_{N_2} \otimes \mathbb{Z}_{N_3}$, but such an approach allows a generalization of the Born–von Kármán conditions to investigations of all possible finite quotient groups $\mathcal{T}/\mathcal{T}'$, where $\mathcal{T}'$ is an infinite group different from direct products of $N_i\mathbb{Z}$ groups. The difference between these two approaches is similar to the difference between the reduced and repeated zone schemes in the reciprocal lattice considerations.

From table 3 one can easily notice that the standard labelling scheme of irreps (A_{1g} etc) differs from the one obtained when this group is treated as a wreath product $C_s \wr \Sigma_3$. The 'symmetry' index—g or u—is replaced by 0+ and 0−, respectively, but the indices 1 and 2 describe global properties of an irrep rather than properties of its second ('permutational') part. It is clear that 1 corresponds to the symmetric irrep, which can be constructed from two symmetric or two antisymmetric irreps, whereas A_2 is a product of symmetric and antisymmetric irreps. The labelling scheme introduced gives at once results of irreps products, e.g. it is evident that $(\Gamma^3_{0+} \otimes (1^3)) \otimes (\Gamma^3_{0-} \otimes (3)) = \Gamma^3_{0-} \otimes (1^3)$ which is not so clear in the notation $A_{2g} \otimes A_{2u} = A_{1u}$.

Acknowledgment

This work was realized within the project no PB 695/2/91 supported by the Polish State Committee for Scientific Research (KBN).

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