Classification of Space Groups for Quasicrystals with (2+1)-Reducible Point Group

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Abstract: Quasicrystalline structures can be viewed as a cut through a periodic structure in a higherdimensional space. In this paper, the crystallography of 5-dimensional periodic structures which can give rise to a quasicrystal in this way is developed. For the five 5d Bravais classes giving rise to quasicrystals periodic in one direction and with symmetry of order 5, 8, 10 or 12 in the plane perpendicular to that direction, a complete classification of point groups and space groups is given. We find a total of 150 distinct space groups, which can be attributed to 44 point groups. For each of these space groups, a set of generators of its point group and the associated non-primitive translations are tabulated, and for the non-symmorphic space groups the indices of the systematic extinctions are given. All the results are expressed in terms of a geometrically natural lattice basis.

1. Introduction

Quasicrystals are materials which show diffraction patterns consisting of sharp Bragg peaks whose positions and intensities can be indexed with finitely many basis vectors, whereby the positions and intensities of these Bragg peaks are arranged with point symmetries which are incompatible with a 3d periodic structure. The fact that finitely many basis vectors are sufficient to index the diffraction pattern implies that it is possible to view such a structure as a cut through a higherdimensional periodic structure. In order to understand the symmetry of quasicrystals it is therefore essential to understand the symmetries of these higherdimensional periodic structures. The symmetries of periodic structures are classified in terms of space groups. We report here on a classification of space groups for 5d periodic structures based on 5 different 5d lattices. Structures based on these lattices lead to quasicrystals which are periodic in z-direction and show rotational symmetries of order 5, 8, 10 or 12. In this paper we present only the results [1], while details of the calculation will appear elsewhere. A similar classification has been obtained earlier for icosahedrally symmetric quasicrystals [2-4], as well as for 2d quasiperiodic structures with rotational symmetry of order 5, 8, 10 or 12 [5]. Moreover, the space groups presented here have also been obtained independently by Janssen [4]. An independent calculation is presented here for mainly two reasons. On the one hand, the calculations involved in such classifications are rather complicated, so that that some of the space groups might "get lost" during the calculation. It is therefore important to have a second, independent source as a check. Since our list of space groups agrees with that of Janssen, we can be confident that it is correct. The second reason is that Janssen's results are expressed mostly in a basis which is not very evident from the geometrical viewpoint. It is, however, computationally convenient for the first step in his algorithm, which has been performed by a computer program. The results presented here have totally been obtained by hand, and we have tried to express the results with respect to a geometrically convenient basis. This should facilitate the use of the tables given below. Moreover, we present here for the first time tables of the extinction patterns for the non-symmorphic space groups, which should prove useful for the determination of the space groups for experimentally observed quasicrystals.

2. Bravais Lattices

We consider here only lattices of minimal dimension compatible with the point symmetry to be studied. It is well known that for 2d quasiperiodic structures with n-fold symmetry a lattice of dimension $\phi(n)$ is required, where ϕ is Euler's function, which takes the value 4 for the symmetries which are of interest here. The 4d lattices are completely known [6], and it turns out that for each of the symmetries (except 5-fold symmetry, which has the same lattice as 10-fold symmetry however), there is a unique 4d lattice (see also [7]). Since the quasicrystals considered here are periodic in one direction, these 4d lattices can be stacked periodically to obtain the 5d lattices we are interested in. These three lattices are generated by the five basis vectors

$$\begin{aligned} e_i^{\parallel} &= (a_{\parallel}\cos(2\pi i/p), a_{\parallel}\sin(2\pi i/p), 0), \quad e_4^{\parallel} = (0,0,a_z), \\ e_i^{\perp} &= (a_{\perp}\cos(2q\pi i/p), a_{\perp}\sin(2q\pi i/p)), \quad e_4^{\perp} = (0,0) \end{aligned} \tag{1}$$

(i=0,..,3, q(p)=3, 4 and 5 for p=8, 10 and 12 respectively). The superscripts $\parallel$ and $\perp$ refer to physical space and "internal" space, respectively. We will call these lattices the octagonal primitive, decagonal and dodecagonal lattice, respectively. Some of these lattices have centerings, i.e. not all of the layers in z-direction are identical. These centerings are generated by a lattice vector x (and the symmetry-equivalent ones) which has the smallest possible positive z-component x_z, but is not parallel to the z-axis. Suppose now that the point group of the lattice under consideration has a subgroup C_n leaving the z-axis invariant. If we add all vectors in the C_n-orbit through x, we obtain a vector of length $n \cdot x_z$ parallel to the z-axis, which is also a lattice vector. In other words, if a C_n subgroup is present, then every n^{th} layer is identical. If the point group has several such subgroups, we can draw the same conclusion, but with n the smallest common divisor of the orders of the subgroups. Since C_8 has only subgroups of even orders, we conclude that every second layer must be identical so that a centering is possible. The point group of the decagonal lattice has cyclic subgroups of orders 2 and 5 which are relatively prime, so that no centering is possible. If we restrict ourselves to 5-fold symmetry, however, a centering can be present, since C_5 has no proper subgroups. In this centering, every fifth layer is identical. Finally, in the dodecagonal case, there is no centering, since C_{12} has subgroups of orders 2 and 3, which are relatively prime. In conclusion, there are two possible centerings, generated by

$$\begin{aligned} e_i^{\parallel} &= (a_{\parallel}\cos(2\pi i/p), a_{\parallel}\sin(2\pi i/p), a_z), \\ e_i^{\perp} &= (a_{\perp}\cos(2q\pi i/p), a_{\perp}\sin(2q\pi i/p)), \end{aligned} \tag{2}$$

where i runs from 0 to 4. These two centerings will be called the pentagonal lattice and the octagonal centered lattice, respectively. We note here that between the decagonal and the pentagonal lattice there is a similar relation as between the hexagonal and the trigonal or rhombohedral lattice in 3 dimensions, and that the octagonal centering plays a similar rôle as the tetragonal one in 3 dimensions. The five lattices given by the basis (1) or (2) are the only lattices of minimal dimension with the required symmetries [8].

3. Point Groups and Space Groups

For the lattices discussed above, all possible point groups (expressed in the lattice basis (1) or (2)) have been determined. For each of them we give a set of generators, as well as the relations satisfied by these generators. The generator A will denote a rotation by $2\pi/p$ which leaves the z-axis invariant, the generator B is a mirror which leaves the z-axis invariant and exchanges the basis vectors e_0 and e_1, and $C = -1$ is the central inversion. In the decagonal case we also need the generators $A' = A^2$ and $B' = BA$. The latter mirror leaves the basis vector e_0 invariant.

A space group Γ belonging to a point group G is generated by all Euclidean transformations of the form $(A, a+t)x = Ax + a + t$, where A is a generator of G, a is a so-called non-primitive translation belonging to A, and t is any lattice vector. The possible non-primitive translations are determined as follows. For each relation $f(A, B, \ldots) = 1$ of the generators of the point group we have to impose the condition $f((A, a), (B, b), \ldots) = (1, t)$ on the non-primitive translations, where t is any lattice vector. However, many of the sets of non-primitive translations obtained in this way define equivalent space groups. Since a space group should not depend on the choice of the origin or the choice of the lattice basis, we have to build the corresponding equivalence classes. During the calculation, we work with a fixed representative in the conjugation class of the point group in $GL_n(\mathbb{Z})$, and we make use, as much as possible, of the free choice of the origin. In this way most of the ambiguity is already eliminated. However, working with a fixed representative in the conjugation class of the point group in $GL_n(\mathbb{Z})$ does not mean that we have chosen a fixed lattice basis. In general, the point group has a non-trivial normalizer in $GL_n(\mathbb{Z})$. The normalizer consists of those changes of lattice basis which commute with the point group as a whole. Therefore, we have to check whether some of the space groups obtained so far are equivalent under conjugation with an element of the normalizer. Determination of the normalizer is generally the hard part of space group determination. In the present case we can make use of the 4d results [6], and also take advantage of the high symmetry, so that this step is not very difficult. For the cases considered here, conjugation with elements of the normalizer leads to a non-trivial equivalence relation only in the dodecagonal case, but for the 6d icosahedral lattices these relations lead to a considerable reduction of the number of distinct space groups.

4. Characteristic Extinctions

Certain non-symmorphic space groups (space groups for which not all non-primitive translations vanish) show systematic extinctions in their Fourier spectrum. If a density $\rho(r)$ is invariant under a space group element (A, a), we have $\rho(r) = \rho(Ar + a)$ and therefore $\hat{\rho}(k) = e^{ik\cdot a}\hat{\rho}(A^{-1}k)$. If for a given k

$$e^{ik\cdot a} \neq 1 \quad \text{and} \quad Ak = k \tag{3}$$

then $\hat{\rho}(k)$ must necessarily vanish, since the latter condition implies that $\hat{\rho}(k) = \hat{\rho}(A^{-1}k)$.

Let us illustrate this with two examples. First, consider a screw axis $(A, \frac{1}{n}e_4)$ for one of the primitive lattices. The k-vectors invariant under A are the vectors $m\hat{e}_4$. Such a peak vanishes unless $k \cdot \frac{1}{n}e_4 \in \mathbb{Z}$, i.e. unless $\frac{m}{n} \in \mathbb{Z}$. In other words: Only every m^{th} peak is present along the z-axis. If k is contained in a glide mirror plane with a non-primitive translation $\frac{1}{2}e_4$, we can conclude with similar arguments that in reciprocal space only every second layer (in z-direction) is present in this plane.

5. Guide to the Tables

The tables presented below give the following information. The first column contains a symbol for the point group in Hermann-Mauguin notation as well as a list of generators. These generators are given with respect to the basis (1) or (2). The second column contains the non-primitive translations of each generator (if present). A non-primitive translation a belongs to the generator A, $\overline{A}$, A' or $\overline{A'}$, whichever is present in the list of generators. Similar rules apply to non-primitive translations b or c. The non-primitive translations contain (integer) parameters, whose range is given in column 3. The total number of distinct space groups for each point group is given in column 4. In column 5, the systematic extinctions are listed for each space group. We give the indices of the extinct peaks with respect to a basis of the reciprocal lattice which is proportional to the basis (1) or (2). Note that this is not always the dual of the real space basis. The expressions for the extinctions contain the same parameters as the non-primitive translations. We list only one representative for symmetry equivalent peaks. To obtain all extinctions, one has to act with the point group on these representatives.

6. Space Groups in the Dodecagonal Bravais Class

In the basis (1) the generators of the dodecagonal Bravais group and its relevant subgroups are

$$A = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{4}$$

Table 1: Space groups in the dodecagonal Bravais class					
Point group	Non-prim. trans.	Parameters	n	Extinctions	
12 A	$a=(0,0,0,0,\frac{p}{12})$	$p=0\dots 6$	7	$(0,0,0,0,i)$	$pi \notin 12\mathbb{Z}$
$\overline{12}$ $\overline{A}$			1		
$12/m$ A, C	$a=(0,0,0,0,\frac{p}{2})$	$p=0,1$	2	$(0,0,0,0,i)$	pi odd
$12\,m\,m$ A, B	$a=(0,0,0,0,\frac{p}{2})$ $b=(0,0,0,0,\frac{m}{2})$	$p,m=0,1*$	3*	(i,j,j,i,ℓ) $(i,j,i,0,\ell)$	$m\ell$ odd $(p+m)\ell$ odd
$12\,2\,2$ $A, \overline{B}$	$a=(0,0,0,0,\frac{p}{12})$	$p=0\dots 6$	7	$(0,0,0,0,i)$	$pi \notin 12\mathbb{Z}$
$\overline{12}\,2\,m^{+}$ $\overline{A}, B$	$b=(0,0,0,0,\frac{m}{2})$	$m=0,1$	2^{+}	(i,j,j,i,ℓ)	$m\ell$ odd
$\overline{12}\,m\,2^{+}$ $\overline{A}, \overline{B}$	$b=(0,0,0,0,\frac{m}{2})$	$m=0,1$	2^{+}	$(i,j,i,0,\ell)$	$m\ell$ odd
$12/m\,m\,m$ A, B, C	$a=(0,0,0,0,\frac{p}{2})$ $b=(0,0,0,0,\frac{m}{2})$	$p,m=0,1*$	3*	(i,j,j,i,ℓ) $(i,j,i,0,\ell)$	$m\ell$ odd $(p+m)\ell$ odd

* $p=1, m=0$ and $p=1, m=1$ are equivalent, see text
+ The point groups $\overline{12}\,2\,m$ and $\overline{12}\,m\,2$ are equivalent, differing only in the choice of basis. For the reader's convenience we have listed both forms. For these two point groups we therefore have a total of only two distinct space groups.

as well as $C=-1$, $\overline{A}=CA$, $\overline{B}=CB$. The defining relations are

$$A^{12}=B^2=C^2=BABA=1, \quad [A,C]=[B,C]=0. \tag{5}$$

The dodecagonal case is the only one in which conjugation with an element of the normalizer of the point group in $GL_n(\mathbb{Z})$ leads to a non-trivial equivalence relation (see also [5]). This element of the normalizer is

$$M=\begin{pmatrix} 1 & 0 & 0 & -1 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{6}$$

This matrix is the generator of a free Abelian subgroup of the normalizer. It stretches physical space by a factor $\sqrt{2+\sqrt{3}}$, followed by a rotation, and shrinks internal space by a factor $\sqrt{2-\sqrt{3}}$, also followed by a rotation. This matrix is also known as a selfsimilarity operation for dodecagonal quasiperiodic tilings. This situation is quite typical: for all lattices and point groups relevant for quasicrystals which have been studied so far, the normalizer contains selfsimilarity operations. Conjugation with M exchanges two sets of mirror planes. If one set consists of

Table 2: Space groups in the octagonal primitive Bravais class				
Point gr.	Non-prim. trans.	Parameters	n	Extinctions
8 A	$a=(0,0,0,0,\frac{p}{8})$	$p=0\ldots 4$	5	$(0,0,0,0,i)\quad pi\notin 8\mathbb{Z}$
$\overline{8}$ $\overline{A}$			1	
$8/\mathrm{m}$ A,C	$a=(0,0,0,0,\frac{p}{2})$ $c=(\frac{q}{2},\frac{q}{2},\frac{q}{2},\frac{q}{2},0)$	$p=0,1$ $q=0,1$	4	$(0,0,0,0,i)\quad pi$ odd $(i,j,k,\ell,0)\quad q(i+j+k+\ell)$ odd
$8\,\mathrm{m}\,\mathrm{m}$ A,B	$a=(0,0,0,0,\frac{p}{2})$ $b=(\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{m}{2})$	$p=0,1$ $n,m=0,1$	8 4	$(i,j,j,i,\ell)\quad m\ell$ odd $(i,j,i,o,\ell)\quad nj+(m+p)\ell$ odd
$8\,2\,2$ $A,\overline{B}$	$a=(0,0,0,0,\frac{p}{8})$ $b=(\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{n}{2},0)$	$p=0\ldots 4$ $n=0,1$	10	$(0,0,0,0,i)\quad pi\notin 8\mathbb{Z}$ $(i,j,i,0,0)\quad nj$ odd
$\overline{8}\,2\,\mathrm{m}$ $\overline{A},B$	$b=(\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{m}{2})$	$n,m=0,1$	4	$(i,j,j,i,\ell)\quad m\ell$ odd $(i,j,i,0,0)\quad nj$ odd
$\overline{8}\,\mathrm{m}\,2$ $\overline{A},\overline{B}$	$b=(\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{m}{2})$	$n,m=0,1$	4	$(i,j,i,0,\ell)\quad nj+m\ell$ odd
$8/\mathrm{m}\,\mathrm{m}\,\mathrm{m}$ A,B,C	$a=(0,0,0,0,\frac{p}{2})$ $b=(\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{n}{2},\frac{m}{2})$ $c=(\frac{q}{2},\frac{q}{2},\frac{q}{2},\frac{q}{2},0)$	$p=0,1$ $n,m=0,1$ $q=0,1$	16	$(i,j,j,i,\ell)\quad m\ell$ odd $(i,j,i,0,\ell)\quad nj+(m+p)\ell$ odd $(i,j,k,l,0)\quad q(i+j+k+\ell)$ odd

true mirrors and the other one of glide mirrors, one cannot differentiate between them. This leads to the equivalence of two space groups for two point groups. Similarly, if the point group contains only one set of mirror planes, one cannot say which one it is. In other words, conjugation with M exchanges two different point groups (and the corresponding space groups), which thereby become equivalent. Depending on the choice of basis we have one form of the point group or the other, however, the two situations are in fact equivalent. For the reader's convenience, we have listed both forms.

7. Space Groups in the Octagonal Primitive Bravais Class

For point groups in the octagonal primitive Bravais class, we use the generators

$$A=\begin{pmatrix}0&0&0&-1&0\\1&0&0&0&0\\0&1&0&0&0\\0&0&1&0&0\\0&0&0&0&1\end{pmatrix},\quad B=\begin{pmatrix}0&1&0&0&0\\1&0&0&0&0\\0&0&0&-1&0\\0&0&-1&0&0\\0&0&0&0&1\end{pmatrix},\tag{7}$$

and $C=-1$, $\overline{A}=CA$, $\overline{B}=CB$, all expressed with respect to the basis (1). These generators satisfy the relations

$$A^8=B^2=C^2=BABA=1,\quad [A,C]=[B,C]=0.\tag{8}$$

The octagonal primitive lattice is in fact the only case where a non-primitive translation parallel to the quasiperiodic plane occurs (see also [5]). In all other

Table 3: Space groups in the octagonal centered Bravais class				
Point group	Non-prim. trans.	Parameters	n	Extinctions
8 A	$a=(\frac{p}{4},0,0,0,0)$	$p=0,1,2$	3	$(i,0,0,0,i)$ $\quad pi \notin 4\mathbb{Z}$
$\overline{8}$ $\overline{A}$			1	
8/m A,C	$a=(\frac{p}{2},0,0,0,0)$	$p=0,1$	2	$(i,0,0,0,i)$ $\quad pi$ odd
8 m m A,B	$a=(\frac{p}{2},0,0,0,0)$ $b=(\frac{m+p}{2},\frac{p}{2},0,0,\frac{m}{2})$	$p=0,1$ $m=0,1$	4	$(i+\ell,j,i,0,\ell)$ $\quad mj$ odd $(i+\ell,j,j,i,\ell)$ $\quad p\ell$ odd
8 2 2 $A,\overline{B}$	$a=(\frac{p}{4},0,0,0,0)$	$p=0,1,2$	3	$(i,0,0,0,i)$ $\quad pi \notin 4\mathbb{Z}$
$\overline{8}$ 2 m $\overline{A},B$	$b=(\frac{m}{2},0,0,0,\frac{m}{2})$	$m=0,1$	2	$(i+\ell,j,i,0,\ell)$ $\quad mj$ odd
$\overline{8}$ m 2 $\overline{A},\overline{B}$	$b=(\frac{m}{2},0,0,0,\frac{m}{2})$	$m=0,1$	2	
8/m m m A,B,C	$a=(\frac{p}{2},0,0,0,0)$ $b=(\frac{m+p}{2},\frac{p}{2},0,0,\frac{m}{2})$	$p=0,1$ $m=0,1$	4	$(i+\ell,j,i,0,\ell)$ $\quad mj$ odd $(i+\ell,j,j,i,\ell)$ $\quad p\ell$ odd

cases, the non-primitive translations are parallel to the periodic direction or can be transformed into this form by a suitable choice of the origin. Note however that this is not always computationally convenient.

8. Space Groups in the Octagonal Centered Bravais Class

The octagonal centered Bravais group is generated by

$$A=\begin{pmatrix}0&0&0&0&1\\1&0&0&0&-1\\0&1&0&0&0\\0&0&1&0&0\\0&0&0&1&1\end{pmatrix},\quad B=\begin{pmatrix}0&1&1&1&1\\1&0&0&0&-1\\0&0&0&-1&0\\0&0&-1&0&0\\0&0&1&1&1\end{pmatrix}. \tag{9}$$

and $C=-1$. For some point groups we again need $\overline{A}=CA$ and $\overline{B}=CB$. The defining relations are

$$A^8=B^2=C^2=BABA=1,\quad [A,C]=[B,C]=0. \tag{10}$$

9. Space Groups in the Decagonal Bravais Class

In the decagonal Bravais class, we require the generators

$$A=\begin{pmatrix}0&0&0&-1&0\\1&0&0&1&0\\0&1&0&-1&0\\0&0&1&1&0\\0&0&0&0&1\end{pmatrix},\quad B=\begin{pmatrix}0&0&0&1&0\\0&0&1&0&0\\0&1&0&0&0\\1&0&0&0&0\\0&0&0&0&1\end{pmatrix} \tag{11}$$

Table 4: Space groups in the decagonal Bravais class

Point group	Non-prim. trans.	Parameters	n	Extinctions	
5 A'	$a=(0,0,0,0,\frac{p}{5})$	$p=0,1,2$	3	$(0,0,0,0,i)$	$pi \notin 5\mathbb{Z}$
5 1 2 $A', \overline{B}$	$a=(0,0,0,0,\frac{p}{5})$	$p=0,1,2$	3	$(0,0,0,0,i)$	$pi \notin 5\mathbb{Z}$
5 2 1 $A', \overline{B'}$	$a=(0,0,0,0,\frac{p}{5})$	$p=0,1,2$	3	$(0,0,0,0,i)$	$pi \notin 5\mathbb{Z}$
5 1 m A', B	$b=(0,0,0,0,\frac{m}{2})$	$m=0,1$	2	(i,j,j,i,ℓ)	$m\ell$ odd
5 m 1 A', B'	$b=(0,0,0,0,\frac{m}{2})$	$m=0,1$	2	$(i,j,i,0,\ell)$	$m\ell$ odd
$\overline{5}$ $\overline{A'}$			1		
$\overline{5}$ 1 m $\overline{A'}, B$	$b=(0,0,0,0,\frac{m}{2})$	$m=0,1$	2	(i,j,j,i,ℓ)	$m\ell$ odd
$\overline{5}$ m 1 $\overline{A'}, B'$	$b=(0,0,0,0,\frac{m}{2})$	$m=0,1$	2	$(i,j,i,0,\ell)$	$m\ell$ odd
10 A	$a=(0,0,0,0,\frac{p}{10})$	$p=0\ldots5$	6	$(0,0,0,0,i)$	$pi \notin 10\mathbb{Z}$
$\overline{10}$ $\overline{A}$			1		
10/m A, C	$a=(0,0,0,0,\frac{p}{2})$	$p=0,1$	2	$(0,0,0,0,i)$	pi odd
10 m m A, B	$a=(0,0,0,0,\frac{p}{2})$ $b=(0,0,0,0,\frac{m}{2})$	$p=0,1$ $m=0,1$	4	$(0,0,0,0,i)$ (i,j,j,i,ℓ) $(i,j,i,0,\ell)$	pi odd $m\ell$ odd $(m+p)\ell$ odd
10 2 2 $A, \overline{B}$	$a=(0,0,0,0,\frac{p}{10})$	$p=0\ldots5$	6	$(0,0,0,0,i)$	$pi \notin 10\mathbb{Z}$
$\overline{10}$ 2 m $\overline{A}, B$	$b=(0,0,0,0,\frac{m}{2})$	$m=0,1$	2	(i,j,j,i,ℓ)	$m\ell$ odd
$\overline{10}$ m 2 $\overline{A}, \overline{B}$	$b=(0,0,0,0,\frac{m}{2})$	$m=0,1$	2	$(i,j,i,0,\ell)$	$m\ell$ odd
10/m m m A, B, C	$a=(0,0,0,0,\frac{p}{2})$ $b=(0,0,0,0,\frac{m}{2})$	$p=0,1$ $m=0,1$	4	$(0,0,0,0,i)$ (i,j,j,i,ℓ) $(i,j,i,0,\ell)$	pi odd $m\ell$ odd $(m+p)\ell$ odd

as well as $C=-1$, $A'=A^2$, $B'=AB$, $\overline{A}=CA$, $\overline{B}=CB$, $\overline{A'}=CA'$ and $\overline{B'}=CB'$. These generators satisfy the relations

$$\begin{gathered} A^{10}={A'}^5=B^2={B'}^2=C^2=1 \\ BABA=B'AB'A=BA'BA'=B'A'B'A'=1 \\ [A,C]=[A',C]=[B,C]=[B',C]=0. \end{gathered} \tag{12}$$

10. Space Groups in the Pentagonal Bravais Class

In the pentagonal Bravais class, we use the generators

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}, \tag{13}$$

and $C = -1$, $\overline{B} = CB$. The generators (13) satisfy the relations

$$A^5 = B^2 = C^2 = BABA = 1, \quad [A, C] = [B, C] = 0. \tag{14}$$

Table 5: Space groups in the pentagonal Bravais class				
Point group	Non-prim. trans.	Parameters	n	Extinctions
5 A			1	
$\overline{5}$ $\overline{A}$			1	
5 m A, B	$b = (\frac{m}{2}, \ldots, \frac{m}{2})$	$m = 0, 1$	2	(i, j, i, k, k) mj odd
5 2 $A, \overline{B}$			1	
$\overline{5}$ m $\overline{A}, B$	$b = (\frac{m}{2}, \ldots, \frac{m}{2})$	$m = 0, 1$	2	(i, j, i, k, k) mj odd

11. Conclusions

We have presented a complete classification of quasicrystal space groups for 1-periodic quasicrystals with 5-, 8-, 10- and 12-fold symmetry. For the five 5d Bravais lattices relevant for these symmetries, we find a total of 44 point groups and 150 space groups. In contrast to icosahedral quasicrystals, where only symmorphic space groups have been observed so far, non-symmorphic space groups for 1-periodic quasicrystals actually occur in nature: The decagonal phase [9,10] contains a screw axis and a set of glide mirror planes, and there are strong arguments [11] that the same is true also for the dodecagonal phase [12-14], although in this latter case not all forbidden peaks are completely extinct [15], which can be attributed to disorder however. Note that the octagonal phase [16], however, belongs to a symmorphic space group of the octagonal centered lattice – the missing layers in some of the planes are due to the geometry of the lattice, not to extinctions caused by a non-symmorphic space group. In fact, such an extinction pattern can not be produced by any non-symmorhic space group in the octagonal primitive Bravais class. We conclude that non-symmorphic space groups are quite common for 1-periodic quasicrystals, which makes this classification particularly interesting. We have tried to express everything in a geometrically natural basis, in order to facilitate the determination of an experimentally observed space group by means of the extinction pattern, and we hope that the tables given in this paper will prove useful for the determination of experimentally observed space groups.

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12. References

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