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Arithmetic Equivalence of Point Groups for Quasiperiodic Structures

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Abstract

Necessary and sufficient conditions are formulated for an n-dimensional arithmetic point group such that it may be the symmetry group of a d-dimensional quasiperiodic but not periodic, *i.e.* incommensurate, structure with Fourier modulus of rank n. Only point groups leaving invariant a d-dimensional subspace (the physical space) are considered. For an arithmetic point group describing an incommensurate structure, all equivalent choices for the internal space are related by the normalizer in $\mathrm{Gl}(n, \mathbb{Z})$ of the point group. Also, the conditions on arithmetic equivalence of two point groups allowing an incommensurate structure are discussed. These conditions yield a further partition of the arithmetic crystal classes.

1. Introduction

A well known problem in crystallography is the determination of nonisomorphic n-dimensional space groups. According to Ascher & Janner (1965), a space group G can be interpreted as a group extension of $\mathbb{Z}^n$ by a finite subgroup $\Gamma(K) \subset \mathrm{Gl}(n, \mathbb{Z})$, a faithful representation of a point group $K \subset O(n)$. In this formalism, all nonisomorphic extensions of $\mathbb{Z}^n$ can be obtained by taking one representative $\Gamma(K)$ of each arithmetic equivalence class, which consists of conjugate subgroups of $\mathrm{Gl}(n, \mathbb{Z})$. Note that group extensions for arithmetically nonequivalent point groups are not isomorphic. For each representative arithmetic point group $\Gamma(K)$, all nonequivalent extensions can be determined. For this construction,

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knowledge of the presentation of the point group in terms of a set of defining relations satisfied by its generators is needed. Algorithms have been developed to construct a set of defining relations satisfied by the generators of an n-dimensional arithmetic point group (Wijnands & Thiers, 1992).

Among the nonequivalent extensions, some might give isomorphic space groups. Two isomorphic extensions obtained from the same arithmetic point group are related by an element of the n-dimensional normalizer of $\Gamma(K)$ in $\mathrm{Gl}(n, \mathbb{Z})$ (Ascher & Janner, 1965; Janssen, Janner & Ascher, 1969; Fast & Janssen, 1971). An algorithm has been developed to determine a generating set for the normalizer in $\mathrm{Gl}(n, \mathbb{Z})$ of an n-dimensional arithmetic point group (Wijnands, 1991).

For $n=3$, all nonisomorphic space groups have been tabulated (*International Tables for Crystallography*, 1989). For $n=4$, all arithmetic equivalence classes and their normalizers and space groups are known (Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, 1978). All maximal finite subgroups of $\mathrm{Gl}(5, \mathbb{Z})$ have been determined by Ryskov (1972*a*, *b*) and Bülow (1973). For $n=6$, 7, 8, 9, all maximal irreducible subgroups of $\mathrm{Gl}(n, \mathbb{Z})$ have been determined (Plesken & Pohst, 1977, 1980).

Crystallography for dimensions higher than three is important for the description of incommensurate modulated structures (de Wolff, 1974; de Wolff, Janssen & Janner, 1981; Janner & Janssen, 1980*a*), composite incommensurate structures (Janner & Janssen, 1980*b*) and quasicrystals (Bak, 1985; Janssen, 1986). All these structures are quasiperiodic. A quasiperiodic structure in the physical space (called external space, position space or parallel space) can be obtained by intersecting this space with a lattice-periodic structure in a higher-dimensional embedding space. Because of the distinguished physical subspace, the groups describing the symmetry of quasiperiodic structures are n-dimensional space groups satisfying appropriate additional requirements; these groups are called superspace groups.

In this paper, for a given n-dimensional crystallographic point group, we present a method to determine all different distinguished subspaces that can play the role of the physical space. This comes down to determining all different sums of real irreducible representations carried by the orthogonal complement of the physical space (called internal space or perpendicular space) such that the point group allows an incommensurate structure. For each such choice, the formalism is given of how to find all equivalent choices for the internal space. These ideas are based upon two papers. Janssen (1992) gave necessary conditions to be satisfied by a crystallographic point group (these conditions being proved to be sufficient in the case of a cyclic point group) in order to allow an incommensurate structure. [The case of a cyclic point group has also been described by Baake, Joseph & Schlottmann (1991).] The other paper, that of Janssen (1991), gives conditions satisfied by two arithmetic point groups if they are arithmetically equivalent.

In § 2, the conditions satisfied by a crystallographic point group in order to allow an incommensurate structure are formulated. In § 3, the problem of arithmetic equivalence of two arithmetic point groups describing quasiperiodic structures is discussed. The more severe conditions and the problem of arithmetic equivalence for modulated structures (a quasiperiodic structure for which main and satellite reflections in the diffraction pattern can be distinguished) are discussed in § 4. Examples and results are presented in § 5.

2. Conditions on incommensurate structures

Let K be an abstract finite point group generated by a set $\{k_1, \ldots, k_s\}$, denoted as $K=\langle k_1, \ldots, k_s\rangle$. Suppose there exists an integral faithful n-dimensional representation $\Gamma(K)=\langle\Gamma(k_1), \ldots, \Gamma(k_s)\rangle \subset \mathrm{Gl}(n, \mathbb{Z})$ of K. Then $\Gamma(K)$ is called an arithmetic point group. Note that on an appropriate basis there exists a faithful representation of K acting on the space $\mathbb{R}^n$ as a group of orthogonal transformations. Therefore we may also consider K as a subgroup of $O(n)$.

In this section we formulate necessary and sufficient conditions to be satisfied by a given arithmetic point group $\Gamma(K)$ such that it may be the symmetry group of an incommensurate structure. The physical dimension is denoted by d. A point group $\Gamma(K)$ is nonmixing if there is a d-dimensional subspace of $\mathbb{R}^n$ such that $\Gamma(K)$ leaves this subspace invariant. If no such subspace can be found, then the point group is mixing. In this paper only nonmixing point groups are considered, since intensity spots for a d-dimensional diffraction pattern have never been observed to be related by a mixing point group (Janssen, 1992). We assume the character table of K and the irreducible representation matrices $\Gamma^i(k_j)$, for $\Gamma^i(K)$ in the decomposition of $\Gamma(K)$, to be known (throughout the paper, irreducible representations, 'irreps', are considered as complex representations, '$\mathbb{C}$-irreps', unless stated otherwise). To check whether $\Gamma(K)$ is nonmixing, $\Gamma(K)$ has to be decomposed into real irreducible representations, $\mathbb{R}$-irreps. The reduction goes as follows.

Consider the decomposition of $\Gamma(K)$ into $\mathbb{C}$-irreps,

$$\Gamma(K)=C^{-1}\left[\bigoplus_i m_i\Gamma^i(K)\right]C, \quad C \in \mathrm{Gl}(n, \mathbb{C}), \quad (1)$$

where m_i is the multiplicity of the $\mathbb{C}$-irrep $\Gamma^i(K)$ in the decomposition. Each $\mathbb{C}$-irrep $\Gamma^j(K)$ is of one of three types.

Type 1: $\Gamma^j(K)$ is $\mathbb{C}$-equivalent to an $\mathbb{R}$-irrep. We then assume that the irrep is given as an $\mathbb{R}$-irrep.

Type 2: $\Gamma^j(K)$ is not $\mathbb{C}$-equivalent to an $\mathbb{R}$-irrep, but it is $\mathbb{C}$-equivalent to its complex conjugate $\Gamma^{j*}(K)$.

Type 3: $\Gamma^j(K)$ is not $\mathbb{C}$-equivalent to its complex conjugate $\Gamma^{j*}(K)$.

In the latter two cases, the corresponding $\mathbb{R}$-irrep can be constructed using

$$\Gamma^j_r = B^{-1}\begin{bmatrix}\Gamma^j & 0\\ 0 & \Gamma^{j*}\end{bmatrix}B,\quad B=\begin{bmatrix}\mathbf{1}_{d_j} & i\mathbf{1}_{d_j}\\ \mathbf{1}_{d_j} & -i\mathbf{1}_{d_j}\end{bmatrix},\qquad (2)$$

where $\mathbf{1}_{d_j}$ is the identity matrix of dimension d_j, the dimension of $\Gamma^j(K)$. It is easy to prove that Γ^j_r is irreducible over $\mathbb{R}$. The Frobenius–Schur criterion (Frobenius & Schur, 1906; see, for example, Jansen & Boon, 1967) can be used to determine the type of a $\mathbb{C}$-irrep $\Gamma^j(K)$.

Theorem 1. (Frobenius & Schur, 1906.) Let $\Gamma^j(G)$ be a $\mathbb{C}$-irrep of a finite group G of order $|G|$. Denote the character of $\Gamma^j(g)$ by $\chi(g)$, $\forall g\in G$. Then

$$\frac{1}{|G|}\sum_{g\in G}\chi(g^2)=\begin{cases}1 & \text{if } \Gamma^j \text{ is potentially real (type 1);}\\ -1 & \text{if } \Gamma^j \text{ is pseudo-real (type 2);}\\ 0 & \text{if } \Gamma^i \text{ is essentially complex (type 3).}\end{cases}\qquad (3)$$

Next, consider all choices for the d-dimensional external space, denoted by V_E, and its orthogonal complement V_I (recall that the point group is nonmixing),

$$\Gamma(K)=S^{-1}\Gamma_r(K)S$$
$$=S^{-1}\left[\bigoplus_i m_{i,E}\Gamma_r^{i,E}(K)\oplus\bigoplus_j m_{j,I}\Gamma_r^{j,I}(K)\right]S,\qquad (4)$$

where $S\in \mathrm{Gl}\,(n,\mathbb{R})$ and $m_{i,E}$ ($m_{j,I}$) denotes the multiplicity of the $\mathbb{R}$-irrep $\Gamma_r^{i,E}$ ($\Gamma_r^{j,I}$) carried by the external (internal) space. For each such choice, one can check whether the point group allows an incommensurate structure as follows. Two or more $\mathbb{R}$-irreps are called partners if each $\mathbb{Z}$-irrep carrying one of these $\mathbb{R}$-irreps, also carries the other(s).

Condition 1. A nonmixing point group of the form (4) allows an incommensurate structure with Fourier modulus of rank n if and only if

(a) the external space carries a faithful (*i.e.* injective) representation and at least one of the following two conditions is satisfied by each $\mathbb{R}$-irrep $\Gamma_r^{j,I}$ carried by V_I;

(b) V_E carries an $\mathbb{R}$-irrep that is $\mathbb{R}$-equivalent to $\Gamma_r^{j,I}$;

(c) V_E carries a partner of $\Gamma_r^{j,I}$.

Proof of condition 1. The 'if' part. The case of cyclic groups has been proved by Janssen (1992). The arguments for the general case are analogous.

Condition 1(b) is based upon the following argument. Consider the representation $\Gamma(K)=\Gamma^i(K)\oplus\Gamma^i(K)$ on a basis $\{\hat{\mathbf{e}}_1,\ldots,\hat{\mathbf{e}}_{2d_i}\}$, where $\hat{\mathbf{e}}_j$ is defined by $(\hat{\mathbf{e}}_j)_i=\delta_{ij}$, the Kronecker delta, and d_i is the dimension of $\Gamma^i(K)$. Suppose the internal space V_I has basis $\{\hat{\mathbf{e}}_{d_i+1},\ldots,\hat{\mathbf{e}}_{2d_i}\}$. Then V_I carries $\Gamma^i(K)$. Consider as a basis for another V_I' the set $\{\alpha\hat{\mathbf{e}}_1+\beta\hat{\mathbf{e}}_{d_i+1},\ldots,\alpha\hat{\mathbf{e}}_{d_i}+\beta\hat{\mathbf{e}}_{2d_i}\}$, then $\Gamma^i(K)$ is also carried by V_I'. With a suitable choice of α and β, one may obtain a lattice $\mathbb{Z}^n$ that does not have a d-dimensional sublattice in common with the external space. Then the structure described in the external space is incommensurate. Notice that the freedom in choosing α and β is allowed owing to the freedom to choose the coefficients in the transformation matrix S in (4). The matrix S is determined by linear equations satisfied by its n^2 coefficients.

If condition 1(c) is satisfied then there is no basis in the external space V_E such that the matrices are integer valued. Hence there is no d-dimensional lattice in V_E, whereas the n-dimensional space contains a lattice (since the n-dimensional point group is arithmetic).

The 'only if' part. One can bring $\Gamma(K)$ into the form $\Gamma^1(K)\oplus\Gamma^2(K)$ by a matrix $Q\in \mathrm{Gl}\,(n,\mathbb{Q})$, where $\Gamma^1(K)$ contains all $\mathbb{R}$-irreps of $\Gamma(K)$ that are either $\mathbb{R}$-equivalent to an $\mathbb{R}$-irrep carried by V_E or to a partner of an $\mathbb{R}$-irrep carried by V_E. Both $\Gamma^1(K)$ and $\Gamma^2(K)$ can be chosen to be integer representations [if $\Gamma^i(K)$, $i=1,2$, carries an $\mathbb{R}$-irrep, then it also carries its partners; therefore, Q can be chosen to be in $\mathrm{Gl}\,(n,\mathbb{Q})$]. The reciprocal space carries the adjoint representation $\Gamma^*(K)=\Gamma^{1*}(K)\oplus\Gamma^{2*}(K)$. This means that the basis vectors in the space carrying $\Gamma^{2*}(K)$ are projected on the origin in V_E. Therefore, if this space is not empty, the rank of the modulus is smaller than n.

Some remarks on condition 1. The problem of constructing an integral representation for a given $\mathbb{R}$-irrep is not trivial. If we restrict ourselves to cyclic point groups, then this construction assumes the knowledge of the invariants of the generating matrix (Janssen, 1992). To check condition 1(c), the easier problem has to be solved of whether or not there is an integer representation possible in the external and the internal space. The solution is the knowledge that all one-, two- and three-dimensional arithmetic point groups for $d\le 3$ do not need partners (since their real representations are all $\mathbb{R}$-equivalent to integral representations). We restrict ourselves to $d\le 3$.

Consider an n-dimensional arithmetic point group that is not isomorphic to a one-, two- or three-dimensional arithmetic point group. If this point group satisfies condition 1(a) then it also satisfies condition 1(c). Otherwise, there should be a faithful two- or three-dimensional $\mathbb{R}$-irrep in V_E needing no partner in V_I. This contradicts the fact that the point group is noncrystallographic in V_E.

The construction of a Fourier modulus of rank $\leq n$ follows from the reducing matrix. Let $\Gamma(K) \subset \mathrm{Gl}(n, \mathbb{Z})$ act in the reciprocal space and let d be the physical dimension. There is a reducing matrix U such that $U\Gamma(K)U^{-1} = \Gamma_r(K)$. Suppose for convenience that $\Gamma_r(K)$ acts on the basis $\{\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_n\}$ with V_E having as basis $\{\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_d\}$. Then the n columns of U, projected on V_E and V_I, form a $\mathbb{Z}$-modulus of rank $\leq n$ (consisting of the first d and the last $n-d$ components of the n columns of U) transforming according to the integral representation $\Gamma(K)$ under the action of the representation carried by V_E and V_I, respectively (Kramer, 1987). Only if condition 1 is satisfied is the rank equal to n. In that case there exists an n-dimensional lattice-periodic structure having the constructed Fourier modulus (Bohr, 1924; Janssen, 1988).

3. Arithmetic equivalence of point groups

Two n-dimensional arithmetic point groups $\Gamma(K)$ and $\Gamma'(K)$ are called arithmetically equivalent if there is an intertwining matrix $m \in \mathrm{Gl}(n, \mathbb{Z})$ such that

$$m\Gamma(K)m^{-1} = \Gamma'(K). \quad (5)$$

Then m induces an isomorphism

$$\varphi : \Gamma(K) \to \Gamma'(K): \quad \varphi[\Gamma(k)] = m\Gamma'(k)m^{-1}. \quad (6)$$

To check whether such a matrix m can be found we can use a method that is very similar to a method used to determine the normalizer for an arithmetic point group (Wijnands, 1991). The algorithmic procedure is the following.

1. First, all point-group elements $\Gamma'(k) \in \Gamma'(K)$ are determined that have the same invariants as the point-group generators $\Gamma(k_1), \ldots, \Gamma(k_s)$ of $\Gamma(K)$.

2. Since the isomorphism φ in (6) has the property that the invariants of $\Gamma(k_i)$ and of $\varphi[\Gamma(k_i)]$ have to be the same, we can restrict ourselves to all combinations of images determined in step 1. For each combination we proceed as follows.

3. The task is to find a matrix $m \in \mathrm{Gl}(n, \mathbb{Z})$ satisfying

$$m\Gamma(k_i)m^{-1} = \Gamma'(k_i), \quad 1 \leq i \leq s.$$

The matrix m is determined by $s \times n^2$ linear equations. Of all coefficients, some are independent; all other coefficients depend linearly on them. Now the independent coefficients are varied between two bounds. For each set of values of the coefficients, it is checked whether the resulting matrix is unimodular. If so, we have found an intertwining matrix and the two point groups are arithmetically equivalent; the procedure is then stopped. If not, we turn to the next set of values.

4. If no matrix has been found, there are two possibilities.

(*a*) There does not exist an $m \in \mathrm{Gl}(n, \mathbb{Z})$. By deriving the expression of the determinant of m, denoted by $\det(m)$, in terms of its independent coefficients, one can possibly prove from the factorization of this expression that integer values of the independent coefficients can never yield a value $\det(m) = \pm 1$. In that case it has been proved that there does not exist such an $m \in \mathrm{Gl}(n, \mathbb{Z})$.

(*b*) There does exist a matrix m of the desired form, but the required set of values for the coefficients exceeds the bounds we had put on the coefficients. Only if a matrix m has been found or if nonexistence of $m \in \mathrm{Gl}(n, \mathbb{Z})$ has been proved with help of the determinant expression is the analysis exact.

5. We turn to the next combination in step 3.

If quasiperiodic structures are considered, the problem is how to incorporate the role of the physical space as a distinguished subspace in the problem of arithmetic equivalence of arithmetic point groups.

Condition 2. Two point groups $\Gamma(K)$ and $\Gamma'(K)$, with given choice for the internal space V_I and V'_I, respectively, are arithmetically equivalent if and only if they are arithmetically equivalent as n-dimensional arithmetic point groups by a matrix m [(5)] that maps V_I of $\Gamma(K)$ on V'_I of $\Gamma'(K)$.

This condition is again based on the fact that V_E (and V_I) is a distinguished subspace. Condition 2 can be checked as follows. As described in § 2, the two point groups can be decomposed into $\mathbb{R}$-irreps:

$$S^{-1}\Gamma(K)S = \Gamma_r(K); \quad T^{-1}\Gamma'(K)T = \Gamma'_r(K); \quad S, T \in \mathrm{Gl}(n, \mathbb{R}), \quad (7)$$

where S, T have the property that $\Gamma_r(k) = \Gamma'_r(k)$, $\forall k \in K$. Suppose an intertwining matrix m satisfying (5) has been found. Then,

$$(T^{-1}mS)\Gamma_r(K)(S^{-1}m^{-1}T) = \Gamma_r(K) \quad (8)$$

or, after defining $U \equiv T^{-1}mS$,

$$U\Gamma_r(K)U^{-1} = \Gamma_r(K). \quad (9)$$

Of course, the coordinates of a vector $\mathbf{x} \in V_I$ depend on the choice of the basis or, equivalently, on the form of the representation. For fixed V_I, let $V_I[\Gamma(K)]$ denote the set of coordinates of the internal space V_I on the basis on which the representation has the form $\Gamma(K)$. Analogously, $V'_I[\Gamma'(K)]$ denotes the set of coordinates of another internal space V'_I on a basis on which the representation has the form $\Gamma'(K)$. Then, $V_I[\Gamma(K)] = SV_I[\Gamma_r(K)]$. Given a fixed basis on which the representation has the form $\Gamma_r(K)$, the basis on which the representation takes the form $\Gamma(K)$ is determined up to a basis transformation due to the freedom in the reducing matrix S in (7). If the isomorphism (5) is regarded as a basis transformation then $V_I[\Gamma(K)] = SV_I[\Gamma_r(K)]$ is mapped by m on $V'_I[\Gamma'(K)] = mSV_I[\Gamma_r(K)]$ using (7) and (8). If $\Gamma'(K) = \Gamma(K)$, then the matrix m is in the normalizer of $\Gamma(K)$ in Gl $(n, \mathbb{Z})$, defined by

$$N[\Gamma(K)] = \{m \in \mathrm{Gl}\,(n, \mathbb{Z}) \mid m\Gamma(k)m^{-1} \in \Gamma(K), \quad \forall k \in K\}. \tag{10}$$

Throughout this paper, the normalizer refers to the normalizer in Gl $(n, \mathbb{Z})$. From the analysis about the arithmetic equivalence of two arithmetic point groups, an arithmetic point group $\Gamma(K)$ with internal space V_I is arithmetically equivalent to $\Gamma(K)$ with internal space V'_I if and only if condition 2 is satisfied. If condition 2 is satisfied, then V_I and V'_I are called equivalent choices for the internal space. (In fact, equivalent choices for the internal space refer to a permutation of the conjugacy classes due to an automorphism.)

With respect to the partition in arithmetic conjugacy classes, condition 2 gives rise to a further partition: each arithmetic conjugacy-class representative gives a number of arithmetically nonequivalent point groups in the sense of condition 2. Now the normalizer can be decomposed into cosets with respect to the centralizer in Gl $(n, \mathbb{Z})$, defined by

$$C[\Gamma(K)] = \{m \in \mathrm{Gl}\,(n, \mathbb{Z}) \mid m\Gamma(k)m^{-1} = \Gamma(k), \quad \forall k \in K\}. \tag{11}$$

Denote this decomposition by

$$N[\Gamma(K)] = \bigcup_{i=1}^{p} m_i C[\Gamma(K)]. \tag{12}$$

Each coset $m_i C[\Gamma(K)]$ corresponds to an automorphism $\varphi_i: \varphi_i[\Gamma(k)] = m_i \Gamma(k) m_i^{-1}$, $\forall k \in K$. A further decomposition can be made. The set of automorphisms $\{\varphi_1, \ldots, \varphi_p\}$ forms a group $A(K)$. A subgroup of $A(K)$ is formed by all inner automorphisms $\varphi_1, \ldots, \varphi_q$ defined by $\varphi_i[\Gamma(k)] = m_i \Gamma(k) m_i^{-1}$, $\forall k \in K$, $m_i \in \Gamma(K)$. This further decomposition can be written as

$$N[\Gamma(K)] = \bigcup_{i=1}^{p/q} m_i \Gamma(K) C[\Gamma(K)]. \tag{13}$$

Now the representation of $\Gamma(K)$ carried by the internal space V_I is the same as the representation of $m\Gamma(K)m^{-1}$ on mV_I for each $m \in N[\Gamma(K)]$. If $m \in C[\Gamma(K)]$ or if $m \in \Gamma(K)$, then mV_I can be replaced by V_I [up to the freedom to vary V_I by the freedom in the matrix S in (7)]. For $m \in C[\Gamma(K)]$ this is obvious from (11). For $m \in \Gamma(K)$ we can use the fact that on the reduced basis the matrix $S^{-1}mS$ has the same block form as any other $\Gamma_r(k) \in \Gamma_r(K)$. Hence the internal space is left unchanged (up to the changes due to the freedom of the reducing matrix S). Therefore, if we want to determine all nonequivalent choices for the internal space, only the p/q coset representatives of the normalizer with respect to the subgroup $\Gamma(K)C[\Gamma(K)]$ have to be considered.

4. Modulated structures

If a modulated structure of dimension d is defined as a quasiperiodic structure for which main and satellite reflections can be distinguished in the diffraction pattern, then there has to be a standard basis on which the point-group matrices are of the form

$$\Gamma(K) = \begin{bmatrix} \Gamma^E(K) & 0 \\ \Gamma^M(K) & \Gamma^I(K) \end{bmatrix} \subset \mathrm{Gl}\,(n, \mathbb{Z}) \tag{14}$$

in direct space and of the form

$$\Gamma^*(K) = \begin{bmatrix} \Gamma^{E^*}(K) & \Gamma^{M^*}(K) \\ 0 & \Gamma^{I^*}(K) \end{bmatrix} \subset \mathrm{Gl}\,(n, \mathbb{Z}) \tag{15}$$

in reciprocal space. The representations $\Gamma(K)$ and $\Gamma^*(K)$ are related (Janssen & Janner, 1987),

$$\Gamma(k) = [\Gamma^*(k^{-1})]^T, \quad \forall k \in K, \tag{16}$$

where T means the transpose. Hence the point groups $\Gamma^E(K)$ and $\Gamma^I(K)$ are crystallographic point groups in a d- and an $(n-d)$-dimensional space, respectively.

Condition 3. An arithmetic point group $\Gamma(K)$ allows a modulated structure with Fourier modulus of rank n if and only if

(a) there is an $S \in \mathrm{Gl}\,(n, \mathbb{Z})$ such that $S\Gamma(K)S^{-1}$ is of the form (14) in direct space or (15) in reciprocal space;

(b) $\Gamma^E(K)$ is a faithful d-dimensional representation of K;

(c) for each $\mathbb{R}$-irrep carried by the internal space there is an $\mathbb{R}$-equivalent $\mathbb{R}$-irrep carried by the external space.

Note that it follows from condition 3(a) that no $\mathbb{R}$-irrep carried by V_E should need a partner in V_I. Hence only arithmetic point groups that are crystallographic in a d-dimensional space have to be considered. If we restrict ourselves to physical dimensions $d \leq 3$, then all $\mathbb{R}$-irreps are $\mathbb{R}$-equivalent to $\mathbb{Z}$-irreps. We assume these $\mathbb{Z}$-irreps to be known. So we have $\Gamma_r^{i,E}(K), \Gamma_r^{j,I}(K) \subset \mathrm{Gl}\,(n, \mathbb{Z})$ in (4).

Consider an arithmetic point group $\Gamma(K)$. For each possible choice for the sum of $\mathbb{Z}$-irreps to be carried by V_I, the analysis is as follows. The first problem is to find a matrix $S \in \mathrm{Gl}\,(n, \mathbb{Z})$ that brings the point group onto a standard basis (condition 3a). The matrices $\Gamma(k_i)$, $\Gamma^E(k_i)$, $\Gamma^I(k_i)$ for each point-group generator k_i are known for d, $n-d \leq 4$. Furthermore, the $\Gamma^M(k_i) \in M_{n-d,d}(\mathbb{Z})$ satisfy the following additional conditions. The Fourier spectrum corresponding to the basic structure has basis $\{\mathbf{a}_1^*, \ldots, \mathbf{a}_d^*\}$ and the modulation can be described in terms of modulation vectors $\mathbf{q}_1, \ldots, \mathbf{q}_{n-d}$. The set $\{\mathbf{a}_1^*, \ldots, \mathbf{a}_d^*, \mathbf{q}_1, \ldots, \mathbf{q}_{n-d}\}$ forms a d-dimensional

$\mathbb{Z}$-modulus of rank n. The vectors $\mathbf{q}_j$ can be expressed in terms of the basic structure as

$$\mathbf{q}_j = \sum_{i=1}^{d} \sigma_{ji}\mathbf{a}_i^*, \quad 1 \le j \le n-d. \tag{17}$$

For actual systems, the coefficients $\sigma(p, T)_{ji}$ depend on pressure and temperature. Furthermore, since the modulation vectors $\mathbf{q}_j$ can be chosen inside the basic unit cell, the coefficients of σ satisfy

$$0 \le \sigma_{ji} < 1, \quad 1 \le j \le n-d, 1 \le i \le d. \tag{18}$$

Then $\Gamma^M(k)$ satisfies the relation (Janner & Janssen, 1979)

$$M_{n-d,d}(\mathbb{Z}) \ni \Gamma^M(k) = \sigma\Gamma^E(k) - \Gamma^I(k)\sigma, \quad \forall k \in K, \tag{19}$$

and the matrix σ can be written as

$$\sigma = \sigma^i + \sigma^r; \quad \sigma^i \in M_{n-d,d}(\mathbb{R}), \sigma^r \in M_{n-d,d}(\mathbb{Q}), \tag{20}$$

where σ^i and σ^r satisfy

$$\begin{aligned} \sigma^i\Gamma^E(k) - \Gamma^I(k)\sigma^i &= 0, \\ \sigma^r\Gamma^E(k) - \Gamma^I(k)\sigma^r &= \Gamma^M(k), \quad \forall k \in K. \end{aligned} \tag{21}$$

These relations limit the possibilities of the entries of the block Γ^M. If for each possible choice of $\Gamma^M(K)$ in (19) no S can be found and it can be proved that there does not exist such an S (by use of the technique described by the algorithmic steps in § 3) then condition 3(a) is proved to be violated and $\Gamma(K)$ cannot describe a modulated structure.

Condition 4. Consider two n-dimensional arithmetic point groups $\Gamma(K)$ and $\Gamma'(K)$ with internal (external) space V_I (V_E) and V'_I (V'_E), respectively, with both V_I and V'_I having dimension $n-d$. Denote the internal (external) space $V_{I,\text{st}}$ ($V_{E,\text{st}}$) on which a point group of standard form acts by its basis $\{\hat{\mathbf{e}}_{d+1}, \ldots, \hat{\mathbf{e}}_n\}(\{\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_d\})$. Then $\Gamma(K)$ and $\Gamma'(K)$ are arithmetically equivalent, describing modulated structures, if and only if

(a) there are matrices $S, T \in \mathrm{Gl}(n, \mathbb{Z})$ such that $\Gamma_b(K) = S\Gamma(K)S^{-1}$ and $\Gamma'_b(K) = T\Gamma'(K)T^{-1}$ have the same block form (14) or (15);

(b) in direct space: if $\mathbf{x} \in V_I$, then $S\mathbf{x} \in V_{I,\text{st}}$; if $\mathbf{x} \in V'_I$, then $T\mathbf{x} \in V_{I,\text{st}}$; in reciprocal space: if $\mathbf{x} \in V_E$, then $S\mathbf{x} \in V_{E,\text{st}}$; if $\mathbf{x} \in V'_E$, then $T\mathbf{x} \in V_{E,\text{st}}$;

(c) there is an intertwining matrix m of the same block form as $\Gamma_b(K)$ and $\Gamma'_b(K)$ satisfying $m\Gamma_b(K)m^{-1} = \Gamma'_b(K)$.

Comparison with condition 1 shows that the conditions on arithmetic equivalence are stronger. The reason is the following. Since the Fourier spectrum consists of main and satellite reflections, main reflections have to be mapped onto main reflections by a point-group element (Janner & Janssen, 1979). Therefore, S and T should be such that $\Gamma^E(K)$ and $\Gamma^I(K)$ are $\mathbb{Z}$-equivalent to $\Gamma^{E'}(K)$ and $\Gamma^{I'}(K)$, respectively.

From now on, $\Gamma(K)$ and $\Gamma'(K)$ are assumed to be in standard form. For the case that $\Gamma'(K) = \Gamma(K)$, this means that the normalizer of a point group $\Gamma(K)$ that is already in the standard form must have the same block form as $\Gamma(K)$.

The method to determine the normalizer of an arbitrary arithmetic n-dimensional point group can easily be applied to a modulated structure with the point group in a standard basis. For an n-dimensional point group, each normalizer element m is determined by linear equations satisfied by its n^2 coefficients. For a modulated structure, m has to satisfy the additional condition that $m_{ij} = 0$ for $1 \le i \le d$, $d+1 \le j \le n$ in direct space and $m_{ij} = 0$ for $1 \le j \le d$, $d+1 \le i \le n$ in reciprocal space. The procedure to determine a generating set for (a subset of) the normalizer and the procedure to check whether the set generates the whole normalizer are then completely the same (Wijnands, 1991). Note that for the general case of a quasiperiodic structure there is no such restriction on the normalizer.

5. Examples and results

The first example is a point group isomorphic to $D_2 = \langle k_1, k_2 \rangle$,

$$\Gamma(D_2) = \left\langle \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \right\rangle. \tag{22}$$

The representation $\Gamma(D_2) \sim 2B_1 \oplus 2B_3$, where B_1 and B_3 are irreps of Klein's group, is already in reduced form: $\Gamma_r(D_2) = \Gamma(D_2)$. The matrix S in (4) has the form

$$S = \begin{bmatrix} \alpha & \gamma & 0 & 0 \\ \beta & \delta & 0 & 0 \\ 0 & 0 & \mu & \nu \\ 0 & 0 & \lambda & \eta \end{bmatrix} \in \mathrm{Gl}(4, \mathbb{R}). \tag{23}$$

Since D_2 is Abelian, there is only one inner automorphism. The only outer automorphism candidate is: $\varphi[\Gamma(k_1)] = \Gamma(k_2)$, $\varphi[\Gamma(k_2)] = \Gamma(k_1)$. A coset representative is

$$m = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}. \tag{24}$$

The coset representative m in (24) corresponds to the automorphism

$$\Gamma_r=\begin{bmatrix} B_1 & 0 & 0 & 0\\ 0 & B_1 & 0 & 0\\ 0 & 0 & B_3 & 0\\ 0 & 0 & 0 & B_3 \end{bmatrix} \to m\Gamma_r m^{-1}$$

$$=\begin{bmatrix} B_3 & 0 & 0 & 0\\ 0 & B_3 & 0 & 0\\ 0 & 0 & B_1 & 0\\ 0 & 0 & 0 & B_1 \end{bmatrix}. \tag{25}$$

Suppose the external space is three-dimensional. Then V_I can carry either B_1 or B_3. Suppose V_I carries B_1. Take $\{\hat{e}_1\}$ as a basis for $V_I(\Gamma_r)$. Then $V_I(\Gamma)=SV_I(\Gamma_r)$ is transformed by the matrix m to $mSV_I(m\Gamma_r m^{-1})=mSV_I(\Gamma_r)=mV_I(\Gamma)$,

$$V_I(\Gamma)\text{ with basis }\left\{\begin{bmatrix}\alpha\\ \beta\\ 0\\ 0\end{bmatrix}\right\}$$

$$\to mV_I(\Gamma)\text{ with basis }\left\{\begin{bmatrix}0\\ 0\\ \beta\\ \alpha\end{bmatrix}\right\}. \tag{26}$$

With use of (25) we see that $mV_I[m\Gamma(D_2)m^{-1}]$ and $V_I[\Gamma(D_2)]$ carry the same sum of $\mathbb{R}$-irreps. Note that $m\Gamma(D_2)m^{-1}$ and $\Gamma(D_2)$ are the same arithmetic point group. They are ordered differently due to the automorphism induced by m.

It follows from (26) and from the fact that there is only one coset representative to be considered that there are two choices for the internal space carrying B_1 and they are equivalent. The analysis for V_I carrying B_3 is completely analogous, yielding two equivalent choices for V_I, with the same basis vectors as in (26). In the case of a point group $\Gamma(C_2)$, generated by the first matrix in (22), the two choices for the internal space given in (26) are nonequivalent, since then there is no normalizer element relating them.

The second example is the point group denoted by $7mm=\langle\Gamma(k_1),\Gamma(k_2)\rangle\subset \mathrm{Gl}(6,\mathbb{Z})$, which is in the isomorphism class D_7 (Janssen, 1990)

$$7mm=\left\langle\begin{bmatrix} 0&0&0&0&0&-1\\ 1&0&0&0&0&-1\\ 0&1&0&0&0&-1\\ 0&0&1&0&0&-1\\ 0&0&0&1&0&-1\\ 0&0&0&0&1&-1 \end{bmatrix},\begin{bmatrix} 0&0&0&0&0&1\\ 0&0&0&0&1&0\\ 0&0&0&1&0&0\\ 0&0&1&0&0&0\\ 0&1&0&0&0&0\\ 1&0&0&0&0&0 \end{bmatrix}\right\rangle. \tag{27}$$

The character table of D_7 is given below.

D_7	ε	k_1	k_1^2	k_1^3	k_2
Γ^1	1	1	1	1	1
Γ^2	1	1	1	1	−1
Γ^3	2	$2\cos(2\pi/7)$	$2\cos(4\pi/7)$	$2\cos(6\pi/7)$	0
Γ^4	2	$2\cos(4\pi/7)$	$2\cos(8\pi/7)$	$2\cos(12\pi/7)$	0
Γ^5	2	$2\cos(6\pi/7)$	$2\cos(12\pi/7)$	$2\cos(18\pi/7)$	0

(28)

It turns out that $\Gamma\sim\Gamma_r=\Gamma^3\oplus\Gamma^4\oplus\Gamma^5$, all being $\mathbb{C}$-equivalent to $\mathbb{R}$-irreps. The generators $\Gamma^{j+2}(k_1)$ and $\Gamma^{j+2}(k_2)$, $1\le j\le 3$, can be chosen to be

$$\begin{bmatrix} \cos(2\pi j/7)-3\sin(2\pi j/7) & 4\sin(2\pi j/7)\\ -5/2\sin(2\pi j/7) & \cos(2\pi j/7)+3\sin(2\pi j/7) \end{bmatrix},$$

$$\begin{bmatrix} 1 & 0\\ \frac{3}{2} & -1 \end{bmatrix}. \tag{29}$$

The normalizer of $7mm$ has been determined (Wijnands, 1991). There are six (seven) point-group elements having the same invariants as the point-group generator k_1 (k_2). Therefore, there are 42 candidates for automorphisms. Since the inner automorphism group of D_7 has order 14, there are three outer automorphisms to be determined. One coset representative is $\mathbf{1}_6$, the two others are

$$n_2=\begin{bmatrix} -1&0&1&0&0&0\\ -1&0&1&0&-1&0\\ -1&-1&1&1&-1&0\\ 0&-1&1&1&-1&-1\\ 0&-1&0&1&0&-1\\ 0&0&0&1&0&-1 \end{bmatrix},$$

$$n_3=\begin{bmatrix} -1&0&0&1&0&0\\ -1&1&0&1&0&-1\\ -1&1&0&0&0&-1\\ -1&0&0&0&1&-1\\ -1&0&1&0&1&-1\\ 0&0&1&0&0&-1 \end{bmatrix}. \tag{30}$$

To have a nonmixing point group, the external space has to be two-dimensional (since we restrict ourselves to physical dimensions lower than four). Consider a subspace $\mathbb{R}^6\supset V_m=V_E(\Gamma_r)$ with basis $\{\hat{e}_{2m-1},\hat{e}_{2m}\}$, $1\le m\le 3$. Then the coset representative n_2 transforms V_1 to V_3, V_2 to V_1 and V_3 to V_2. Representative n_3 transforms V_1 to V_2, V_2 to V_3 and V_3 to V_1. Hence, all choices for the internal space: $V_I=V_a\cup V_b$, $1\le a<b\le 3$, are equivalent.

The third example is the point group $\Gamma(O\times C_2)=m\bar{3}m\oplus m\bar{3}m$, $K=O\times C_2$, for the incommensurate phase of wüstite, $Fe_{1-x}O$, described by Yamamoto (1982). In the incommensurate phase, wüstite has a three-dimensional cubic fundamental cell with a three-dimensional modulation with arithmetic point group

$$\Gamma(K) = \langle \Gamma(k_1), \Gamma(k_2), \Gamma(k_3) \rangle$$
$$= \left\langle \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}, -\mathbf{1}_6 \right\rangle. \quad (31)$$

There is only one choice for the basis of the internal space $V_I(\Gamma)$: $\{\alpha\hat{\mathbf{e}}_1+\beta\hat{\mathbf{e}}_4, \alpha\hat{\mathbf{e}}_2+\beta\hat{\mathbf{e}}_5, \alpha\hat{\mathbf{e}}_3+\beta\hat{\mathbf{e}}_6\}$. In the incommensurate phase of wüstite, main and satellite reflections can be distinguished. Suppose we have two point groups, one with internal space $V_I(\Gamma)$ having as basis $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$, the other with another internal space $V_I'(\Gamma)$ having as basis $\{\hat{\mathbf{e}}_4, \hat{\mathbf{e}}_5, \hat{\mathbf{e}}_6\}$. First the two point groups have to be transformed to a standard form. In the standard form, the two point groups are identical and therefore the two choices for the internal space are equivalent.

With the notation of Janner, Janssen & de Wolff (1983), wüstite has symmetry group $Pm\bar{3}m(\alpha, 0, 0)$, meaning that $\Gamma^E(K)$ and $\Gamma^I(K)$ are full cubic point groups without centering and one of the modulation basis vectors can be chosen to be $\mathbf{q}_1 = (\alpha, 0, 0)$ in coordinates with respect to the conventional unit cell. According to Table 1 of Janner, Janssen & de Wolff (1983), there are ten arithmetically nonequivalent (when considered as describing modulated structures) point groups with full cubic symmetry in the external and internal space. The question is: which of these point groups are arithmetically equivalent when considered as describing quasiperiodic structures? Since in all ten cases $\Gamma^E(K)$ and $\Gamma^I(K)$ are $\mathbb{R}$-equivalent, there is only one choice for the internal space and the question comes down to finding all arithmetically equivalent point groups (regarded as n-dimensional point groups). First, the form of $\Gamma^M(k_i)$ for the point-group generators k_i in (31) has to be determined for the ten point groups under consideration.

Suppose $\Gamma^E(K) = \Gamma^I(K) = Pm\bar{3}m$. Starting with an arbitrary matrix σ, we have, with use of (20)

$$\sigma = \begin{bmatrix} \alpha & \beta & \beta \\ \beta & \alpha & \beta \\ \beta & \beta & \alpha \end{bmatrix} \in M_{3\times 3}(\mathbb{R}),$$
$$0 \le \alpha < 1, \beta = 0 \text{ or } \beta = \tfrac{1}{2}. \quad (32)$$

Hence, the two possible arithmetic point groups are $Pm\bar{3}m(\alpha, 0, 0)$, with

$$\sigma^i = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix}, \sigma^r = 0 \Rightarrow \Gamma^M(k) = 0, \quad \forall k \in K \quad (33)$$

and $Pm\bar{3}m(\alpha, \frac{1}{2}, \frac{1}{2})$, with the same σ^i but

$$\sigma^r = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix} \Rightarrow \Gamma^M(k_1) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & -1 & 0 \\ 0 & -1 & 0 \end{bmatrix} \quad (34)$$

and $\Gamma^M(k_2) = \Gamma^M(k_3) = 0$ for the generators k_1, k_2, k_3 of (31). These two point groups are arithmetically nonequivalent when regarded as describing modulated structures. The same analysis shows that the eight other arithmetic point groups have $\Gamma^M(k) = 0, \forall k \in K$. First we try to find an intertwining matrix m for two point groups $\Gamma(K)$ and $\Gamma'(K)$, each having $\Gamma^M(K) = 0$,

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} \Gamma^E(K) & 0 \\ 0 & \Gamma^I(K) \end{bmatrix} = \begin{bmatrix} \Gamma^{E'}(K) & 0 \\ 0 & \Gamma^{I'}(K) \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix}.$$

Suppose $\Gamma^I(K)$ is not $\mathbb{Z}$-equivalent to $\Gamma^{I'}(K)$. Then $D = 0$ because of Schur's lemma. Hence, $B, C = \pm\mathbf{1}_3$, otherwise $\det(m) = 0$. Consequently, Schur's lemma tells us that $\Gamma^I(K) \sim \Gamma^{E'}(K)$ and $\Gamma^E(K) \sim \Gamma^{I'}(K)$. Suppose $\Gamma^I(K)$ is $\mathbb{Z}$-equivalent to $\Gamma^{I'}(K)$. Then $D = \pm\mathbf{1}_3$. We have either (1) $\Gamma^E(K) \sim \Gamma^{E'}(K)$, so $A = \pm\mathbf{1}_3$, or (2) $\Gamma^E(K) \nsim \Gamma^{E'}(K)$, so $A = 0$. Then $B, C = \pm\mathbf{1}_3$ otherwise $\det(m) = 0$. Consequently, $\Gamma^I(K) \sim \Gamma^{E'}(K)$ and $\Gamma^E(K) \sim \Gamma^{I'}(K)$ but then $\Gamma^E(K) \sim \Gamma^{E'}(K)$, which contradicts the assumption that $\Gamma^E(K) \nsim \Gamma^{E'}(K)$. Therefore, $\mathbb{Z}$-equivalence for the nine point groups with $\Gamma^M(K) = 0$ comes down to interchanging $\Gamma^E(K)$ and $\Gamma^I(K)$, *e.g.* by the intertwining matrix

$$m = \begin{bmatrix} 0 & \mathbf{1}_3 \\ \mathbf{1}_3 & 0 \end{bmatrix}: \quad \begin{aligned} &Pm\bar{3}m(\alpha, \alpha, \alpha) \sim Fm\bar{3}m(\alpha, 0, 0); \\ &Im\bar{3}m(\alpha, 0, 0) \sim Pm\bar{3}m(0, \alpha, \alpha); \\ &Im\bar{3}m(\alpha, \alpha, \alpha) \sim Fm\bar{3}m(0, \alpha, \alpha). \end{aligned} \quad (35)$$

The only other possible equivalence is between $\Gamma(K) = Pm\bar{3}m(\alpha, \frac{1}{2}, \frac{1}{2})$ and one of the other nine point groups. It turns out that $\Gamma(K)$ is $\mathbb{Z}$-equivalent to $\Gamma'(K) = Im\bar{3}m(\alpha, \alpha, \alpha)$,

$$m\Gamma(K)m^{-1} = \Gamma'(K),$$
$$m = \begin{bmatrix} 1 & 1 & 1 & 0 & -1 & -1 \\ 1 & 1 & 1 & -1 & 0 & -1 \\ 1 & 1 & 1 & -1 & -1 & 0 \\ 0 & 1 & 1 & 1 & -1 & -1 \\ 1 & 0 & 1 & -1 & 1 & -1 \\ 1 & 1 & 0 & -1 & -1 & 1 \end{bmatrix}. \quad (36)$$

Hence there are six arithmetic equivalence classes splitting into ten arithmetic equivalence classes when the point groups are considered to describe modulated structures.

The fourth example is also an illustration that two arithmetically equivalent point groups describing quasiperiodic structures can be arithmetically nonequivalent when the point groups are to describe modulated structures. Consider the following two realizations of C_2:

$$\Gamma(C_2)=\left\langle\begin{bmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 1 & -1\end{bmatrix}\right\rangle;\qquad \Gamma'(C_2)=\left\langle\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}\right\rangle. \tag{37}$$

Then $\Gamma(C_2), \Gamma'(C_2) \sim A\oplus 2B$. The basis vectors of the internal space $V_I(\Gamma)$ and $V'_I(\Gamma')$ are $(\alpha, 0, \beta)^T$ and $(\gamma, -\gamma, \delta)^T$, respectively. Hence if $\Gamma(C_2)$ and $\Gamma'(C_2)$ are arithmetically equivalent as n-dimensional point groups, they are also arithmetically equivalent as point groups describing a quasiperiodic structure. There is an intertwining matrix

$$m=\begin{bmatrix}0 & 0 & 1\\ 0 & 1 & -1\\ 1 & 0 & 0\end{bmatrix},\quad m\Gamma(C_2)m^{-1}=\Gamma'(C_2) \tag{38}$$

and the point groups describing quasiperiodic structures are arithmetically equivalent.

Next, the problem of equivalence is studied for modulated structures. Suppose that main and satellite reflections can be distinguished. The problem is worked out in direct space. The first problem is to determine all possible choices for the block form (14) with $\Gamma^E(C_2)=A\oplus B$ and $\Gamma^I(C_2)=B$. For $\Gamma^I(C_2)$ there is only one possible representation: $\Gamma^I(C_2)=\langle -1\rangle$. For $\Gamma^E(C_2)$ there are two $\mathbb{Z}$-inequivalent representations,

$$\Gamma^E(C_2)=\left\langle\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\right\rangle \quad\text{and}\quad \Gamma^E(C_2)=\left\langle\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\right\rangle. \tag{39}$$

It follows from (18) and (19) that the only possibilities for the block form (14) are

$$pm(\alpha,0)=\left\langle\begin{bmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}\right\rangle,$$

$$pm(\alpha,\tfrac{1}{2})=\left\langle\begin{bmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 1 & 0 & -1\end{bmatrix}\right\rangle,$$

and

$$cm(\alpha,0)=\left\langle\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}\right\rangle, \tag{40}$$

all with standard basis vector $(0,0,1)^T$. Considered as three-dimensional arithmetic point groups, the first of these three point groups is arithmetically nonequivalent to the latter point groups, which are arithmetically equivalent. Hence there are at most two nonequivalent choices of the internal space for our point groups $\Gamma(C_2)$ and $\Gamma'(C_2)$ [recall that $\Gamma(C_2)$ and $\Gamma'(C_2)$ are arithmetically equivalent three-dimensional arithmetic point groups].

Now $\Gamma(C_2)$, with V_I having basis vector $(0,0,1)^T$ describing a modulated structure, is arithmetically equivalent to $pm(\alpha,\frac{1}{2})$: with

$$S=\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{bmatrix}$$

it holds that

$$S\Gamma(C_2)S^{-1}=\left\langle\begin{bmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 1 & 0 & -1\end{bmatrix}\right\rangle \tag{41}$$

and S maps the basis vector $(0,0,1)^T$ onto $(0,0,1)^T$, the standard basis vector of the internal space for $pm(\alpha,\frac{1}{2})$. Then $\Gamma'(C_2)$ with basis vector $(1,-1,0)^T$ for $V'_I(\Gamma')$ is also arithmetically equivalent to $pm(\alpha,\frac{1}{2})$, since $\Gamma(C_2)$ and $\Gamma'(C_2)$ are arithmetically equivalent as three-dimensional arithmetic point groups, and also $mV_I(\Gamma)=V'_I(\Gamma')$ from (38).

In the same way it can be proved that $V_I(\Gamma)$ with basis vector $(1,0,0)^T$ and $V'_I(\Gamma')$ with basis vector $(0,0,1)^T$ are equivalent choices for the internal space, using (38). With use of (40) we see that both point groups are of type $cm(\alpha,0)$.

On the other hand, $V_I(\Gamma)$ with basis vector $(0,0,1)^T$ and $V'_I(\Gamma')$ with basis vector $(0,0,1)^T$ are nonequivalent choices for the internal space since $mV_I(\Gamma)$ has a nonzero component in the external space $V'_E(\Gamma')$. For the same reason, $V_I(\Gamma)$ with basis vector $(1,0,0)^T$ and $V'_I(\Gamma')$ with basis vector $(1,-1,0)^T$ are nonequivalent choices for the internal space.

Hence, for both point groups $\Gamma(C_2)$ and $\Gamma'(C_2)$ there are two arithmetic equivalence-class representatives. As representatives one can take $\Gamma(C_2)$ and $\Gamma'(C_2)$, both with $(0,0,1)^T$ as basis vector for the internal space. Then $\Gamma(C_2)=pm(\alpha,\frac{1}{2})$ and $\Gamma'(C_2)=cm(\alpha,0)$.

6. Concluding remarks

A procedure has been described to verify whether a given arithmetic point group allows an incommensurate structure. If so, then for a given sum of real irreducible representations to be carried by the internal space, the most general form for this internal space is determined. Equivalent choices for the internal space can be given in the most general form by using the action of the normalizer of the point group. Two point groups, arithmetically equivalent as n-dimensional point groups, can be arithmetically nonequivalent when considered as describing quasi-periodic structures. This gives a further partition of the arithmetic crystal classes.

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On the Sign Ambiguity of Triplet Phases in Nonsystematic Many-Beam Effects in CBED Patterns

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Abstract

The possibility to determine not only the magnitude but also the sign of three-phase structure invariants from nonsystematic many-beam effects in convergent-beam electron diffraction (CBED) patterns is discussed. From the full dynamical many-beam intensity expression it is clear that it is a principal difference between equivalent three-beam cases of opposite sign of the triplet phases. However, the difference and thus the ability to distinguish between the two cases depends strongly both on the relative magnitude of the structure factors involved and the specimen thickness for which the actual CBED discs are obtained. The largest differences are obtained for a weakly coupled three-beam case where the intensity in the line of the primary reflection, which in this case coincides with the kinematical two-beam position, has a distinct maximum or minimum at the three-beam condition depending on the sign of the triplet phase. In a strong coupling case where the intensity in the primary-reflection line near the three-beam condition is split into two individual segments, the differences are generally less and are not so obvious and quantitative measurements are necessary to distinguish the two cases of opposite sign of the triplet phases. Calculated examples with respect to a nonsystematic three-beam example in the noncentrosymmetric InP are given.

Introduction

A general convergent-beam electron diffraction (CBED) method for quantitative determination of structure-factor magnitudes and phases from centrosymmetric as well as noncentrosymmetric crystals

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