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A mathematical construction of *n*-dimensional quasicrystals starting from *G*-clusters

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Abstract. We present a mathematical construction of n-dimensional quasicrystals by starting from its symmetry group, an arbitrary finite group, and from its local structure described by using a finite union of orbits of G, called a G-cluster: namely, we construct the periodization space, the G-invariant lattice, the decomposition into the physical and internal space in a canonical way. Using a strip-and-projection method we obtain quasiperiodic patterns corresponding to various generic local structures.

1. Introduction

Many of the actual models of quasicrystals are obtained by using either periodic structures in higher dimensions or packed/interpenetrating atomic clusters in physical space [1]. Here, following some terminology used in the literature, we call a quasicrystal a crystallographic object, a crystal, which is not periodic; see Senechal [2] for more details. In the first case, they are constructed *globally* from a finite group, say G, while, in the second case, the atomic clusters (assumed always finite) are invariant under the action of groups G' linked to G (as subgroups or supergroups), and their centres are arranged in a suitable way to form quasiperiodic patterns (quasiperiodic tilings) [3, 4]. This second approach is *local* and depends upon the (assumed finite) collection of different types of atomic clusters possible. Indeed, the Fourier transform of a quasicrystal is supported by a countable dense set in reciprocal space, it exhibits inflation laws and is invariant under the action of a non-trivial finite group of transformations, generally forbidden for 'periodic' crystals. This latter group of transformations acting in reciprocal space is used in the above *global* construction as 'G', or instead of G, a subgroup, or a supergroup is taken to lower or increase the global symmetry of the corresponding quasicrystal model in real space [5].

By *local*, we mean the following situation in dimension n by analogy with what happens in dimension two and three for the existing quasicrystal models: in 2D and 3D, each cluster—that is the finite collection of points which constitutes the centres of the atoms—can be viewed as a compact cluster of atoms, radially *truncated* to a few shells. This sticks to the approach of crystallographers making models on the computer or by hand from small compact entities, where, by construction, the first central shells of atoms around the centres are the most relevant. The term *truncated* is justified by the fact that the extent of the point symmetry around the centre of the cluster is not necessarily limited to the atoms used in the

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clusters, grouped by orbits, but that other shells of atoms—also constituting orbits—could be considered in the model outside the clusters which could also be used. In this respect, the truncation may appear sometimes arbitrary and several clusters—viewed as subclusters of the others—can provide the same global quasicrystal model. However, the formalism below is entirely general and gets rid of such considerations by keeping the notion of cluster, that is the unions sequences of orbits, at a level of full mathematical generality.

An algebraic theory for modelling quasicrystals in $\mathbb{E}_n = (\mathbb{R}^n, \langle ., . \rangle)$ the usual Euclidean n-dimensional space, controlled *globally* by an arbitrary finite group, say G, was presented at ICQ5 by Pleasants [6]. The method consists in representing G over a real number field K, which always exists, of degree d over $\mathbb{Q}$, and uses the canonical ($r \geqslant 1$) real and ($2s$) complex embeddings of K to send G-invariant $\mathcal{O}_K$-modules onto $\mathbb{Z}$-lattices in $\mathbb{R}^{nd}$, with $d = r + s$. The decomposition $\mathbb{R}^{nd} = \mathbb{E}_n \oplus W$, where $W = \mathbb{R}^{n(r-1)} \oplus \mathbb{C}^{ns}$, the fact that PV-numbers λ exist in K, ensures the possibility of constructing quasicrystals in $\mathbb{E}_n$, exhibiting inflation rules associated with λ, using a suitable window in W. In this procedure, the choice of K is a consequence of the rationality of the characters of the group G [7, 8]. The 'algebraic' dimension of periodization is therefore canonical, and is equal to nd.

In the present paper, we would like to give a different mathematical setting, by considering a generic (finite) G-cluster in $\mathbb{E}_n$, fixed once for all, from which we intend to construct a quasicrystal. Let $G \subset \mathrm{Aut}(\mathbb{E}_n)$ be a non-trivial finite group of orthogonal transformations, such that the representation of G in $\mathbb{E}_n$ is $\mathbb{R}$-irreducible. Let $l \geqslant 1$, and let $v_1, v_2, \ldots, v_l$ be distinct non-zero elements in $\mathbb{E}_n$.

By definition, a G-cluster [9, 10], denoted by $\mathcal{C} = G\{v_1, v_2, \ldots, v_l\}$, is the finite union of orbits $\cup_{j=1}^{l} G v_j$. This G-cluster can be viewed as an average G-cluster [10] over all possible imperfect G-clusters existing in the quasicrystal, that we will form via this method of modelling. This justifies the terminology used in the present title, and will show how to reach, on an abstract mathematical setting, a compatibility between the *global* and the *local* approaches.

Applications are given in section 3. Some comments about the compactness of the G-clusters with respect to the global symmetry group leaving invariant the Fourier transform of the model are made at the end of section 2.

2. Canonical spaces associated with G-clusters

Let us present the general construction itself. By using the inversion $i : \mathbb{E}_n \longrightarrow \mathbb{E}_n$, $ix = -x$, we obtain the group $\overline{G} = G \cup iG$ and the G-cluster $\overline{\mathcal{C}} = G\{v_1, \ldots, v_l, -v_1, \ldots, -v_l\} = \mathcal{C} \cup i\mathcal{C} = \overline{G}\{v_1, \ldots, v_l\}$. There exists a set $\mathcal{O}_\mathcal{C} = \{v_1, \ldots, v_k\} \subset \overline{\mathcal{C}}$ which does not contain opposite vectors and such that $\overline{\mathcal{C}} = \{v_1, \ldots, v_k, -v_1, \ldots, -v_k\}$. Here the letter $\mathcal{O}$ is used to denote *opposite*, not for any ring of integers associated with $\mathcal{C}$. For any $g \in G$, the following map

$$t_g : \mathcal{O}_\mathcal{C} \longrightarrow \mathcal{O}_\mathcal{C} \qquad t_g(v) = \begin{cases} gv & \text{if } gv \in \mathcal{O}_\mathcal{C} \\ -gv & \text{if } gv \notin \mathcal{O}_\mathcal{C} \end{cases} \tag{1}$$

is one-to-one since $g(-v) = -gv$ for any $v \in \overline{\mathcal{C}}$.

Because of the $\mathbb{R}$-irreducibility of the action of G on $\mathbb{E}_n$, we have $k \geqslant n$, and $\mathcal{O}_\mathcal{C}$ contains a basis of $\mathbb{E}_n$ since the subspace of $\mathbb{E}_n$ generated by $\mathcal{O}_\mathcal{C}$ is G-invariant. For two sets A, B, we denote by B^A the set of all functions $f : A \longrightarrow B$. The relation $(g\varphi)(v) = \varphi(g^{-1}v)$ defines a linear representation of G in the vector space $\mathcal{S} = \{\varphi : \overline{\mathcal{C}} \longrightarrow \mathbb{R} \,|\, \varphi(-v) = -\varphi(v)$ for $v \in \overline{\mathcal{C}}\}$. Since an odd function $\varphi : \overline{\mathcal{C}} \longrightarrow \mathbb{R}$ is well determined by its restriction to $\mathcal{O}_\mathcal{C}$,

the space $\mathcal{S}$ can be identified with the space $\mathcal{E} = \mathbb{R}^{\mathcal{O}_\mathcal{C}}$, and

$$g : \mathcal{E} \longrightarrow \mathcal{E} \qquad (g\varphi)(v) = \begin{cases} \varphi(g^{-1}v) & \text{if } g^{-1}v \in \mathcal{O}_\mathcal{C} \\ -\varphi(-g^{-1}v) & \text{if } g^{-1}v \notin \mathcal{O}_\mathcal{C} \end{cases} \tag{2}$$

is the representation of G in $\mathcal{E}$ corresponding to the representation of G in $\mathcal{S}$.

The space $\mathcal{E}$ has a natural structure of a k-dimensional linear space since $\mathbb{R}^{\mathcal{O}_\mathcal{C}}$ can be identified with $\mathbb{R}^k$. Its Euclidean structure is given by

$$\langle \varphi_1, \varphi_2 \rangle = \sum_{v \in \mathcal{O}_\mathcal{C}} \varphi_1(v)\varphi_2(v) \tag{3}$$

and the representation of G in $\mathcal{E}$ is an orthogonal representation

$$\begin{aligned} \langle g\varphi_1, g\varphi_2 \rangle &= \sum_{v \in \mathcal{O}_\mathcal{C}} (g\varphi_1)(v)(g\varphi_2)(v) = \sum_{v \in \mathcal{O}_\mathcal{C}} \varphi_1(t_g^{-1}(v))\varphi_2(t_g^{-1}(v)) \\ &= \sum_{w \in \mathcal{O}_\mathcal{C}} \varphi_1(w)\varphi_2(w) = \langle \varphi_1, \varphi_2 \rangle. \end{aligned} \tag{4}$$

For all $\varphi \in \mathcal{E}$, the norm of φ is given by $\|\varphi\| = \sqrt{\langle \varphi, \varphi \rangle}$.

Let us now introduce a canonical linear subspace of $\mathcal{E}$, playing the role of the *physical space*. It can be viewed as the dual space of $\mathcal{O}_\mathcal{C}$ parametrized by a quotient space of $\mathbb{E}_n$. For all $r \in \mathbb{E}_n$, let us define $\varphi_r : \mathcal{O}_\mathcal{C} \longrightarrow \mathbb{R} : v \mapsto \langle r, v \rangle$, and

$$\mathcal{E}^\parallel = \{\varphi_r : \mathcal{O}_\mathcal{C} \longrightarrow \mathbb{R}, \varphi_r(v) = \langle r, v \rangle \,|\, r \in \mathbb{E}_n\}. \tag{5}$$

In a complementary way, let us define the subspace

$$\mathcal{E}^\perp = \left\{ \varphi : \mathcal{O}_\mathcal{C} \longrightarrow \mathbb{R} \,\middle|\, \sum_{v \in \mathcal{O}_\mathcal{C}} \varphi(v)v = 0 \right\} \tag{6}$$

in $\mathcal{E}$, which will play the role of internal space. These canonical subspaces have the following properties: $\dim \mathcal{E}^\parallel = n$, $\dim \mathcal{E}^\perp = k - n$ since $\mathcal{O}_\mathcal{C}$ contains a basis of $\mathbb{E}_n$, $\mathcal{E}^\parallel$ and $\mathcal{E}^\perp$ are G-invariant since, with $g \in G$, $v \in \mathcal{O}_\mathcal{C}$, $r \in \mathbb{E}_n$,

$$(g\varphi_r)(v) = \langle r, g^{-1}v \rangle = \langle gr, v \rangle = \varphi_{gr}(v) \tag{7}$$

$$\sum_{v \in \mathcal{O}_\mathcal{C}} (g\varphi)(v)v = \sum_{w \in \mathcal{O}_\mathcal{C}} \varphi(w)gw = g\left(\sum_{w \in \mathcal{O}_\mathcal{C}} \varphi(w)w \right) \tag{8}$$

and orthogonal because of the identity

$$\langle \varphi_r, \varphi \rangle = \sum_{v \in \mathcal{O}_\mathcal{C}} \langle r, v \rangle \varphi(v) = \left\langle r, \sum_{v \in \mathcal{O}_\mathcal{C}} \varphi(v)v \right\rangle. \tag{9}$$

We obtain that $\mathcal{E} = \mathcal{E}^\parallel \oplus \mathcal{E}^\perp$. The corresponding orthogonal projectors $\pi^\parallel : \mathcal{E} \longrightarrow \mathcal{E}$, $\pi^\perp : \mathcal{E} \longrightarrow \mathcal{E}$ satisfy the relations $\pi^\parallel \circ g = g \circ \pi^\parallel$, $\pi^\perp \circ g = g \circ \pi^\perp$, for any $g \in G$. The relation $g\varphi_r = \varphi_{gr}$ shows that the representation of G in $\mathcal{E}^\parallel$ is equivalent to the representation of G in $\mathbb{E}_n$.

Let $\{e_1, e_2, \ldots, e_n\}$ be an orthonormal basis of $\mathbb{E}_n$, and let $\psi_j = \varphi_{e_j}$. Denoting $ge_j = \sum_{p=1}^n g_{pj}e_p$, we get

$$\begin{aligned} \langle \psi_j, \psi_m \rangle &= \sum_{v \in \mathcal{O}_\mathcal{C}} \langle e_j, v \rangle \langle e_m, v \rangle = \sum_{v \in \mathcal{O}_\mathcal{C}} \langle e_j, t_g^{-1}(v) \rangle \langle e_m, t_g^{-1}(v) \rangle = \sum_{v \in \mathcal{O}_\mathcal{C}} \langle e_j, g^{-1}v \rangle \langle e_m, g^{-1}v \rangle \\ &= \sum_{v \in \mathcal{O}_\mathcal{C}} \langle ge_j, v \rangle \langle ge_m, v \rangle = \sum_{p=1}^n \sum_{q=1}^n g_{pj}g_{qm} \sum_{v \in \mathcal{O}_\mathcal{C}} \langle e_p, v \rangle \langle e_q, v \rangle \\ &= \sum_{p=1}^n \sum_{q=1}^n g_{pj} \langle \psi_p, \psi_q \rangle g_{qm} \end{aligned} \tag{10}$$

and then

$$\sum_{j=1}^{n} g_{sj}\langle\psi_j,\psi_m\rangle = \sum_{p=1}^{n}\sum_{q=1}^{n}\left(\sum_{j=1}^{n} g_{sj}g_{pj}\right)\langle\psi_p,\psi_q\rangle g_{qm} = \sum_{p=1}^{n}\sum_{q=1}^{n}\delta_{sp}\langle\psi_p,\psi_q\rangle g_{qm}$$

$$= \sum_{q=1}^{n}\langle\psi_s,\psi_q\rangle g_{qm}. \tag{11}$$

Denoting by M the symmetrical real matrix $(\langle\psi_j,\psi_m\rangle)_{j,m=1\ldots n}$, and $M_g = (g_{jm})_{j,m=1\ldots n}$ the matrix associated with g, the above computation implies $M_g M = M M_g$, for any $g \in G$. Applying Schur's lemma [7], we obtain $M =$ constant $\times\, Id$, where the constant is real, and the fact that $\{\psi_1,\psi_2,\ldots,\psi_n\}$ is an orthogonal basis with $\|\psi_1\| = \|\psi_2\| = \cdots = \|\psi_n\| \neq 0$. The elements $\phi_1 = \psi_1/\kappa$, $\phi_2 = \psi_2/\kappa$, …, $\phi_n = \psi_n/\kappa$, where $\kappa = \|\psi_1\|$, form an orthonormal basis of $\mathcal{E}^{\parallel}$.

The projector $\pi^{\parallel} : \mathcal{E} \longrightarrow \mathcal{E}^{\parallel}$ is given by the formula

$$(\pi^{\parallel}\varphi)(v) = \frac{1}{\kappa^2}\sum_{w\in\mathcal{O}_\mathcal{C}}\varphi(w)\langle w, v\rangle \tag{12}$$

for all $\varphi \in \mathcal{E}$ and $v \in \mathcal{O}_\mathcal{C}$. Indeed, the relation

$$\sum_{w\in\mathcal{O}_\mathcal{C}}\varphi(w)\langle w, v\rangle = \left\langle \sum_{w\in\mathcal{O}_\mathcal{C}}\varphi(w)w, v\right\rangle = 0 \tag{13}$$

satisfied for all $\varphi \in \mathcal{E}^{\perp}$ and $v \in \mathcal{O}_\mathcal{C}$, shows that all elements of $\mathcal{E}^{\perp}$ go to zero. Now, for any $r = \sum_{j=1}^{n} r_j e_j \in \mathbb{E}_n$, and its corresponding $\varphi_r \in \mathcal{E}^{\parallel}$, and for any $u = \sum_{m=1}^{n} u_m e_m$, we have the following identity

$$\frac{1}{\kappa^2}\sum_{w\in\mathcal{O}_\mathcal{C}}\varphi_r(w)\langle w,u\rangle = \frac{1}{\kappa^2}\sum_{w\in\mathcal{O}_\mathcal{C}}\langle r,w\rangle\langle w,u\rangle = \sum_{j=1}^{n}\sum_{m=1}^{n} r_j u_m \frac{1}{\kappa^2}\langle\psi_j,\psi_m\rangle$$

$$= \sum_{j=1}^{n} r_j u_j = \langle r,u\rangle = \varphi_r(u) \tag{14}$$

that is, $(\pi^{\parallel}\varphi_r)(u) = \varphi_r(u)$.

The isomorphism $\lambda : \mathbb{E}_n \longrightarrow \mathcal{E}^{\parallel} : r \mapsto \varphi_{r/\kappa}$ has the property $\lambda(e_j) = \phi_j$, and allows us to identify the two spaces. The additive G-invariant group $\mathcal{L} = \bigoplus_{j=1}^{k}\mathbb{Z}v_j$, in other terms a G-invariant $\mathbb{Z}$-module of rank k, can be decomposed [11] into a direct sum $\mathcal{L} = \mathcal{L}_\mathrm{s} \oplus \mathcal{L}_\mathrm{d}$ such that $\mathcal{L}_\mathrm{s}$ is a dense $\mathbb{Z}$-module and $\mathcal{L}_\mathrm{d}$ is a discrete $\mathbb{Z}$-module in $\mathbb{E}_n$. The $\mathbb{Z}$-module $\mathcal{L}_\mathrm{s}$ is well determined and defines a linear subspace $V = \overline{\mathcal{L}_\mathrm{s}}$ (adherence of $\mathcal{L}_\mathrm{s}$) in $\mathbb{E}_n$, such that $\mathcal{L}_\mathrm{s} = V \cap \mathcal{L}$. The $\mathbb{Z}$-module $\mathcal{L}_\mathrm{d}$ is non-unique in this decomposition. Since each element $g \in G$ is an isometry in $\mathbb{E}_n$, and each element of V is the limit of a sequence of elements belonging to the G-invariant $\mathbb{Z}$-module $\mathcal{L}$, it follows that each element of $g(V)$ has the same property, whence $g(V) \subset V$, for all $g \in G$. In view of the irreducibility of the representation of G in $\mathbb{E}_n$, we obtain that $V = \{0\}$ or $V = \mathbb{E}_n$, whence $\mathcal{L} = \mathcal{L}_\mathrm{d}$ or $\mathcal{L} = \mathcal{L}_\mathrm{s}$. Obviously, we identify $\mathcal{L}$ with $\lambda(\mathcal{L})$, and one can prove that $\mathcal{L} = \pi^{\parallel}((\kappa\mathbb{Z})^{\mathcal{O}_\mathcal{C}})$.

In the case $\mathcal{L} = \mathcal{L}_\mathrm{s}$, we can consider [12] that the pattern

$$G[v_1, v_2, \ldots, v_l] = \{\pi^{\parallel}\varphi \mid \varphi \in (\kappa\mathbb{Z}^{\mathcal{O}_\mathcal{C}}, \pi^{\perp}\varphi \in \pi^{\perp}([0,1)^{\mathcal{O}_\mathcal{C}})\} \tag{15}$$

is a model of a quasicrystal having the local structure described by the G-cluster $G\{v_1, v_2, \ldots, v_l\}$, viewed as a global average G-cluster [10]. For each point $x \in G[v_1, v_2, \ldots, v_l]$ the 'arithmetic neighbours' of x belong to the translation $x + \overline{\mathcal{C}}$ of the G-cluster $\overline{\mathcal{C}}$. Since each atom belongs to several such translations at the same time, the

quasicrystal having the local structure described by the G-cluster $\overline{\mathcal{C}}$ can be regarded as a set of interpenetrating partially occupied translations of $\overline{\mathcal{C}}$.

If $\mathcal{L} = \mathcal{L}_{\mathrm{d}}$, then $G[v_1, v_2, \ldots, v_l]$ is a model of the crystal.

One can remark that the isomorphism

$$\mathcal{E} \longrightarrow \mathbb{E}_k : \varphi \mapsto (\varphi(v_1), \varphi(v_2), \ldots, \varphi(v_k)) \tag{16}$$

allows us to identify the two spaces, and the method used to define $G[v_1, v_2, \ldots, v_l]$ is equivalent with the well known strip projection method. Indeed, $\mathbb{E} = \mathbb{E}^{\parallel} \oplus \mathbb{E}^{\perp}$ corresponds to the decomposition $\mathbb{E}_k = \mathbb{E}_k^{\parallel} \oplus \mathbb{E}_k^{\perp}$, where

$$\mathbb{E}_k^{\parallel} = \{(\langle r, v_1\rangle, \langle r, v_2\rangle, \ldots, \langle r, v_k\rangle) \mid r \in \mathbb{E}_n\} \tag{17}$$

$$\mathbb{E}_k^{\perp} = \left\{ \boldsymbol{x} = (x_1, x_2, \ldots, x_k) \middle| \sum_{j=1}^{k} x_j v_j = 0 \right\} \tag{18}$$

$$\pi^{\parallel} = \frac{1}{\kappa^2} \begin{pmatrix} \langle v_1, v_1\rangle & \langle v_1, v_2\rangle & \ldots & \langle v_1, v_k\rangle \\ \langle v_2, v_1\rangle & \langle v_2, v_2\rangle & \ldots & \langle v_2, v_k\rangle \\ \ldots & \ldots & \ldots & \ldots \\ \langle v_k, v_1\rangle & \langle v_1, v_1\rangle & \ldots & \langle v_k, v_k\rangle \end{pmatrix} \tag{19}$$

and

$$G[v_1, v_2, \ldots, v_l] = \{\pi^{\parallel} x \mid x \in \kappa\mathbb{Z}^k \, \pi^{\perp} x \in \pi^{\perp}([0, 1)^k)\}. \tag{20}$$

All the above results can be obtained directly in terms of $\mathbb{E}_k$, but the mathematical expressions are more complicated.

From the presented construction, it follows that

$$G[v_1, v_2, \ldots, v_l] = \overline{G}[v_1, v_2, \ldots, v_l] \tag{21}$$

with a true global symmetry of the model which could be higher than G.

In a well known way [12], one can prove that the Fourier transform of $G[v_1, v_2, \ldots, v_l]$ is a sum of weighted Dirac delta peaks supported by an everywhere dense G-invariant additive group, for which, in each compact set, there are finitely many points with an absolute value of the amplitude above any given strictly positive threshold.

Actually, the finite symmetry group, say H, leaving invariant the Fourier transform (the origin in reciprocal space is a fixed point) may be different from G and such that the index $(H : G)$ be finite. However, if we apply the present construction to H instead of G, we will work with clusters of atoms composed of H-orbits and not G-orbits, that is much more compact (compact in the sense of sphere packings compactness where atoms are modelled by spheres) clusters of atoms locally. Therefore, if we start from G-clusters that we consider as very compact clusters, it will become impossible to get an index $(H : G)$ different from one. If, on the contrary, we consider the present G-clusters just as a backbone which could be decorated, meaning that we allow space between the points in G-orbits to position more atomic sites, then we could get more elevated $(H : G)$ indices. A bound for $(H : G)$ could be given depending upon the allowed *'remaining space'* for decoration, that is as a function of a *minimal distance*—the small Delaunay constant—viewed as the smallest atom diameter. This provides a link between an intrinsic metric in real space associated with the notion of *size* of the atoms (in dimension n) and the various possibilities of supergroups H leaving invariant the quasicrystal formed. Questions about the density of quasiperiodic sphere packings are evoked in [21]. In the present work, we consider general clusters for the mathematical constructions.

In dimension three, the icosahedral compact clusters of atoms are not arbitrary and have already been classified by Tamura and Verger-Gaugry [13] for simple systems (Al-based,

Ti-based,...) in Mackay or Bergman types. For covalent boron-based systems (Weygand and Verger-Gaugry [14]), other icosahedral clusters composed of different sequences of icosahedral orbits are stable and can be used for the present construction method. Some quasicrystals also exhibit several types of typical generic clusters which coexist—these clusters are currently described from the different cubic lattice types used in the common six-dimensional description [1, 2]. In this contribution we allow only one generic G-cluster as the basic ingredient in dimension n.

3. Applications

Let us show how this general method applies in a certain number of concrete cases which are well known to crystallographers used to periodic and non-periodic tilings. We will consider the icosahedral, dihedral, tetrahedral groups; and continuous deformations of G-clusters allowing, for instance, limits to be taken of crystalline tilings to form quasiperiodic tilings. The control of the continuous deformation of the microstructure of the G-clusters seems reasonable since experimentally clusters in good approximant phases and related quasicrystals are almost the same. The dihedral case will cover the decagonal, dodecagonal and octogonal cases.

(a) The Y-quasicrystal $Y[(1, 0, \tau)]$ obtained by using the representation in $\mathbb{E}_3$ of the icosahedral group $Y = 235 = \langle a_Y, b_Y \,|\, a_Y^5 = b_Y^2 = (a_Y b_Y)^3 = e\rangle$ defined by

$$a_Y(x, y, z) = \tfrac{1}{2}(x - \tau y + (\tau - 1)z, \tau x + (\tau - 1)y - z, (\tau - 1)x + y + \tau z) \tag{22}$$

$$b_Y(x, y, z) = (-x, -y, z) \tag{23}$$

where $\tau = (1 + \sqrt{5})/2$, has as points the vertices of the well known three-dimensional Penrose tiling.

(b) The quasicrystals $D_5[(1, 0)]$ (respectively $D_8[(1, 0)]$, $D_{12}[(1, 0)]$) corresponding to the two-dimensional Penrose tiling (respectively octagonal, and dodecagonal tiling) can be obtained by using the representations in $\mathbb{E}_2$ of the dihedral groups $D_m = \langle a_D, b_D \,|\, a_D^m = b_D^2 = (a_D b_D)^2 = e\rangle$ defined by

$$a_D(x, y) = (x \cos 2\pi/m - y \sin 2\pi/m, x \sin 2\pi/m + y \cos 2\pi/m) \tag{24}$$

$$b_D(x, y) = (x, -y). \tag{25}$$

More sophisticated quasicrystal models can be obtained as follows. In the Y-quasicrystal

$$Y[(\alpha/\sqrt{\tau + 2}, 0, \alpha\tau/\sqrt{\tau + 2}), (\beta/\sqrt{3}, \beta/\sqrt{3}, \beta/\sqrt{3}), (\gamma, 0, 0)]$$

where $0 < \alpha < \beta < \gamma$, each point has neighbours lying on three shells formed by the vertices of a regular icosahedron, a regular dodecahedron, and an icosidodecahedron, respectively.

Similarly, in the Y-quasicrystal $Y[(1, 0, \tau), (1/2, 0, \tau/2)]$ each point has neighbours lying in the vertices of two parallel regular icosahedra.

For $\alpha, \beta \in (0, \infty)$,

$$D_4[(\alpha, \beta)] \text{ is a } \begin{cases} D_4\text{-crystal} & \text{if } \alpha/\beta \in \mathbb{Q} \\ D_4\text{-quasicrystal} & \text{if } \alpha/\beta \notin \mathbb{Q}. \end{cases} \tag{26}$$

The D_4-quasicrystal $D_4[(\alpha, 0), (1/\sqrt{2}, 1/\sqrt{2})]$, where $\alpha \in (0, \infty)$, studied by Duneau [15], is called a skeleton.

By using the representation in $\mathbb{E}_3$ of the complete cubic group $O_h = m\bar{3}m = \langle a_O, b_O \mid a_O^4 = b_O^6 = (a_O b_O)^2 = e\rangle$ defined by

$$a_O(x, y, z) = (y, -x, z) \tag{27}$$

$$b_O(x, y, z) = (-y, -z, -x) \tag{28}$$

we obtain that

$$O_h[(1, 0, 0), (\alpha, 0, 0)] \text{ is a } \begin{cases} O_h\text{-crystal} & \text{if } \alpha \in \mathbb{Q} \\ O_h\text{-quasicrystal} & \text{if } \alpha \notin \mathbb{Q}. \end{cases} \tag{29}$$

This model allowed Wang *et al* [16] to describe the structure of the rapidly solidified $V_6Ni_{16}Si_7$ alloy.

The clusters $G_1\{v_1, v_2, \ldots, v_l\}$ and $G_2\{w_1, w_2, \ldots, w_{l'}\}$, where G_1, G_2 are two finite groups of orthogonal transformations of $\mathbb{E}_n$, are called equal if they contain the same points. In this case, the corresponding quasicrystals (crystals) coincide: $G_1[v_1, v_2, \ldots, v_l] = G_2[w_1, w_2, \ldots, w_{l'}]$. For example,

$$D_8[(1, 0)] = D_4[(1, 0), (1/\sqrt{2}, 1/\sqrt{2})] \tag{30}$$

$$Y[(1, 0, \tau)] = T[(1, 0, \tau)] \tag{31}$$

where the T-quasicrystal $T[(1, 0, \tau)]$ is obtained by using the representation in $\mathbb{E}_3$ of the tetrahedral group $T = 23 = \langle a_T, b_T \mid a_T^2 = b_T^3 = (a_T b_T)^3 = e\rangle$ defined by

$$a_T(x, y, z) = (-x, -y, z) \tag{32}$$

$$b_T(x, y, z) = (y, z, x). \tag{33}$$

(c) A sequence of G-clusters $(G\{v_{1j}, \ldots, v_{lj}\})_{j=1}^{\infty}$, such that each sequence $(v_{mj})_{j=1}^{\infty}$ is convergent, is called convergent. Its limit is the G-cluster $G\{\lim_{j\to\infty} v_{1j}, \ldots, \lim_{j\to\infty} v_{lj}\}$. A sequence of G-crystals (G-quasicrystals)

$$(G[v_{1j}, \ldots, v_{lj}])_{j=1}^{\infty} \tag{34}$$

is called convergent if the corresponding sequence of G-clusters is convergent. The corresponding limit is the G-crystal (G-quasicrystal)

$$G\left[\lim_{j\to\infty} v_{1j}, \ldots, \lim_{j\to\infty} v_{lj}\right]. \tag{35}$$

In this case, one can prove that

$$\lim_{j\to\infty} \mathcal{F}(G[v_{1j}, \ldots, v_{lj}]) = \mathcal{F}\left(\lim_{j\to\infty} G[v_{1j}, \ldots, v_{lj}]\right). \tag{36}$$

By using (24) and (25) we get

$$\lim_{j\to\infty} D_4[(1 + 1/j, 0), ((1/\sqrt{2}, 1/\sqrt{2})] = D_8[(1, 0)] \tag{37}$$

$$\lim_{j\to\infty} D_4[(1, 0), (j\sqrt{3}/(2j + 1), j/(2j + 1))] = D_{12}[(1, 0)] \tag{38}$$

the dimensions of periodization spaces being four and six, respectively. Denoting

$$u_j = (2\tau_j, 0, 0) \qquad v_j = (1, \tau_j, 1 + \tau_j) \qquad w_j = (-1, \tau_j, 1 + \tau_j)$$

$$u'_j = (1 + \tau_j, 1 + \tau_j, 1 + \tau_j) \qquad v'_j = (-1 - \tau_j, 1 + \tau_j, 1 + \tau_j) \qquad w'_j = (0, \tau_j, 1 + 2\tau_j)$$

where $\tau_j = f_{j+1}/f_j$, $f_0 = f_1 = 1$, $f_{j+1} = f_{j-1} + f_j$, and using (22), (23), (32) and (33) one obtains

$$\lim_{j\to\infty} T[(1, 0, \tau_j)] = Y[(1, 0, \tau)] \tag{39}$$

$$\lim_{j\to\infty} T[u_j, v_j, w_j] = Y[(2\tau, 0, 0)] \tag{40}$$

$$\lim_{j\to\infty} T[u'_j, v'_j, w'_j] = Y[(1+\tau, 1+\tau, 1+\tau)]. \tag{41}$$

The corresponding dimensions k of the spaces $\mathcal{E}$ used in the last three examples are 6, 15 and 10, respectively. In the case of the Y-quasicrystal $Y[(1+\tau, 1+\tau, 1+\tau)]$ the arithmetic neighbours of a point are placed in the vertices of a regular dodecahedron, and it can be used [17] as a model for the AlMnSi quasicrystal.

The continuous family of D_4-quasicrystals

$$D_4[(1, 0), ((1-t)/\sqrt{2} + t\sqrt{3}/2, (1-t)/\sqrt{2} + t/2)] \tag{42}$$

considered for $t \in [0, 1]$, is a continuous deformation of $D_8[(1, 0)]$ into $D_{12}[(1, 0)]$.

4. Concluding remarks

In order to obtain a mathematical model for modelling a quasicrystal, it is necessary to first determine the corresponding symmetry group G by examining its diffraction diagram in reciprocal space [5]. Then it is necessary to choose a G-cluster describing the local structure, for instance, from electron-density maps [18] or from HREM images [19]. If the agreement of the obtained model with experimental data is not acceptable, it is necessary to look for a more suitable G-cluster. The limits of the present method, as well as some of the limits of Pleasants's method, consist in the fairly high dimension of the representations of G which are used. A convenient and efficient algorithm for the strip projection method, applicable to any dimension, recently proposed by Vogg and Ryder [20], allows us to use the present method in the case of quasicrystals having the local structure described by G-clusters having many orbits.

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