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Discrete quasiperiodic sets with predefined local structure

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Abstract

Model sets play a fundamental role in the structure analysis of quasicrystals. The diffraction diagram of a quasicrystal admits as a symmetry group a finite group G, and there is a G-cluster $\mathcal{C}$ (union of orbits of G) such that the quasicrystal can be regarded as a quasiperiodic packing of interpenetrating copies of $\mathcal{C}$. We present an algorithm which leads from any G-cluster $\mathcal{C}$ directly to a multi-component model set $\mathcal{Q}$ such that the arithmetic neighbours of any point $x \in \mathcal{Q}$ are distributed on the sites of the translated copy $x + \mathcal{C}$ of $\mathcal{C}$. Our mathematical algorithm may be useful in quasicrystal physics.

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1. Introduction

Model sets (also called cut-and-project sets) were introduced by Meyer [29] in his study of harmonious sets and later, in the course of the structure analysis of quasicrystals, rediscovered in a variety of different schemes [18,19,21]. Extensive investigations [11,15,16,19,21,23,24, 28,29,32,33] on the properties of these remarkable sets have been carried out by Y. Meyer, P. Kramer, M. Duneau, A. Katz, V. Elser, M. Baake, R.V. Moody, A. Hof, M. Schlottmann, J.C. Lagarias et al. An extension of the notion of a model set called a *multi-component model set*, very useful in quasicrystal physics, has been introduced by Baake and Moody [3]. Model sets are

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generalizations of lattices, and multi-component model sets are generalizations of lattices with colourings.

Quasicrystals are materials with perfect long-range order, but with no three-dimensional translational periodicity. The structure analysis of quasicrystals on an atomic scale is a highly non-trivial task, and we are still far from a satisfactory solution. The electron microscopy images suggest the existence of some basic structural units which often overlap (interpenetrate) and of some glue atoms. The diffraction spectra contains sharp bright spots, indicative of long range order, called *Bragg reflections*. The reflections with intensity above a certain threshold form a discrete set admitting as a symmetry group a finite non-crystallographic group G. In the case of quasicrystals with no translational periodicity, this group is the icosahedral group Y and, in the case of quasicrystals periodic along one direction (two-dimensional quasicrystals), G is one of the dihedral groups D_8 (octagonal quasicrystals), D_{10} (decagonal quasicrystals) and D_{12} (dodecagonal quasicrystals).

The high resolution microscopy images of a quasicrystal with the symmetry group G show that we can regard the quasicrystal as a quasiperiodic packing of copies of a well-defined G-invariant finite set $\mathcal{C}$ (basic structural unit), most of them only partially occupied. From a mathematical point of view, $\mathcal{C}$ is a finite union of orbits of G, and we call it a *G-cluster*. In the literature on quasicrystals, the term 'cluster' has several meanings [35]. Depending on the context, it may denote a structure motif (purely geometric pattern), a structural building block (perhaps with some physical justification), a quasi-unit cell [36] or a complex coordination polyhedron (with some chemical stability). In our case, $\mathcal{C}$ is a structure motif, perhaps without any physical justification.

The purpose of the present paper is to present a mathematical algorithm that leads from any G-cluster $\mathcal{C}$ directly to a multi-component model set $\mathcal{Q}$ representing a quasiperiodic packing of interpenetrating copies of $\mathcal{C}$, most of them only partially occupied. It shows how to embed the physical space into a superspace $\mathbb{E}_k$ and how to choose a lattice $\mathbb{L} \subset \mathbb{E}_k$ in order to get, by projection, the desired local structure. Our algorithm, based on the strip projection method and group theory, is a generalization of the model proposed by Katz and Duneau [19] and independently by Elser [11] for certain icosahedral quasicrystals. Since the multi-component model sets have several properties desirable from the physical point of view (they are uniformly discrete, relatively dense, have a well-defined density and are pure point diffractive), our algorithm may be useful in quasicrystal physics.

2. Model sets and multi-component model sets

In this section we review some definitions and results concerning the notions of a model set and a multi-component model set.

Let E be a vector subspace of the usual k-dimensional Euclidean space $\mathbb{E}_k = (\mathbb{R}^k, \langle , \rangle)$, where $\langle x, y\rangle = \sum_{i=1}^k x_i y_i$ and $\|x\| = \sqrt{\langle x, x\rangle}$, for any $x = (x_i)_{1\leq i\leq k},\ y = (y_i)_{1\leq i\leq k}$. The subset $B_r(a) = \{x \in E \mid \|x - a\| < r\}$ of E, where $a \in E$, $r \in (0, \infty)$, is the *open ball* of center a and radius r.

Definition 1. Let Λ be a subset of E.

(1) The set Λ is *relatively dense* in E if there is $r \in (0, \infty)$ such that the ball $B_r(x)$ contains at least one point of Λ, for any $x \in E$.
(2) The set Λ is *uniformly discrete* in E if there is $r \in (0, \infty)$ such that the ball $B_r(x)$ contains at most one point of Λ, for any $x \in E$.

(3) The set Λ is a *Delone set* in E if Λ is both relatively dense and uniformly discrete in E.
(4) The set Λ is a *lattice* in E if it is both an additive subgroup of E and a Delone set in E.

Definition 2. A *cut and project scheme* is a collection of spaces and mappings

$$\begin{array}{ccccc} E_1 & \stackrel{\pi_1}{\longleftarrow} & E_1 \oplus E_2 & \stackrel{\pi_2}{\longrightarrow} & E_2 \\ & & \cup & & \\ & & L & & \end{array} \tag{1}$$

formed by two subspaces E_1, E_2 of $\mathbb{E}_k$, the corresponding natural projections π_1, π_2, and a lattice L in $E_1 \oplus E_2$ such that:

(a) π_1 restricted to L is one-to-one;
(b) $\pi_2(L)$ is dense in E_2.

Definition 3. A subset Λ of $\mathbb{E}_n$ is a *regular model set* if there exist:

- a cut and project scheme (1),
- an isometry $\mathcal{I} : \mathbb{E}_n \longrightarrow E_1$ that allows us to identify $\mathbb{E}_n$ with E_1,
- a set $W \neq \emptyset$ satisfying the conditions:
  (i) $W \subset E_2$ is compact;
  (ii) $W = \overline{\mathrm{int}(W)}$;
  (iii) the boundary ∂W of W has Lebesgue measure 0

such that

$$\Lambda = \{\pi_1 x \mid x \in L,\ \pi_2 x \in W\}. \tag{2}$$

By using the $\star$-mapping

$$\pi_1(L) \longrightarrow E_2 :\ x \mapsto x^\star = \pi_2((\pi_1)|_L)^{-1} x \tag{3}$$

we can re-write the definition of Λ as

$$\Lambda = \{x \mid x \in \pi_1(L),\ x^\star \in W\}. \tag{4}$$

Model sets have strong regularity properties.

Theorem 1 (*[32,33]*). *Any regular model set Λ is a Delone set and has a well-defined density, that is, the following limit exists:*

$$\lim_{r\to\infty} \frac{\#(\Lambda \cap B_r)}{\mathrm{vol}(B_r)} \tag{5}$$

where $\#(\Lambda \cap B_r)$ is the number of points of Λ lying in $B_r = B_r(0)$, and $\mathrm{vol}(B_r)$ is the volume of B_r.

In the structure analysis of quasicrystals, the experimental diffraction image is compared with the diffraction image of the mathematical model Λ, regarded as a set of scatterers. In order to compute the diffraction image of the model set Λ, it is represented as a Borel measure in the form of a weighted Dirac comb:

$$\omega = \sum_{x\in\Lambda} \varphi(x)\delta_x \tag{6}$$

where $\varphi : \Lambda \longrightarrow \mathbb{C}$ is a bounded function and δ_x is the Dirac measure located at x, that is, $\delta_x(f) = f(x)$ for continuous functions f. In this way, atoms of a quasicrystal are modeled by their positions and scattering strengths. In the case (the only one considered in the sequel) when there is a function $\varrho : E_2 \longrightarrow \mathbb{C}$ supported and continuous on W such that $\varphi(x) = \varrho(x^\star)$, that is, in the case $\omega = \sum_{x\in\Lambda} \varrho(x^\star)\delta_x$, one can prove [15,16,4,5,31] the following results:

1. The measure ω is translation bounded, that is, there exist constants C_K so that
$$\sup_{t\in\mathbb{R}^n} \sum_{x\in\Lambda\cap(t+K)} |\varrho(x^\star)| \le C_K < \infty \tag{7}$$
for all compact $K \subset \mathbb{R}^n$.
2. The autocorrelation coefficients
$$\eta(z) = \lim_{n\to\infty} \frac{1}{\mathrm{vol}(B_n)} \sum_{\substack{x,y\in\Lambda\cap B_n\\ x-y=z}} \varrho(x^\star)\overline{\varrho(y^\star)} \tag{8}$$
exist for all $z \in \Delta = \Lambda - \Lambda = \{x - y \mid x, y \in \Lambda\}$.
3. The set $\{z \in \Delta \mid \eta(z) \neq 0\}$ is uniformly discrete.
4. The autocorrelation measure
$$\gamma_\omega = \sum_{z\in\Delta} \eta(z)\delta_z \tag{9}$$
exists.

The diffraction spectrum of Λ (the idealized mathematical interpretation of the diffraction pattern of a physical experiment) is related [15,16] to the Fourier transform $\hat{\gamma}_\omega$ of the autocorrelation measure γ_ω which can be decomposed as

$$\hat{\gamma}_\omega = (\hat{\gamma}_\omega)_{pp} + (\hat{\gamma}_\omega)_{sc} + (\hat{\gamma}_\omega)_{ac} \tag{10}$$

by the Lebesgue decomposition theorem. Here, $\hat{\gamma}_\omega(B)$ is the total intensity scattered into the volume B, $(\hat{\gamma}_\omega)_{pp}$ is a pure point measure, which corresponds to the Bragg part of the diffraction spectrum, $(\hat{\gamma}_\omega)_{ac}$ is absolutely continuous and $(\hat{\gamma}_\omega)_{sc}$ is singular continuous with respect to Lebesgue measure. We say that Λ is *pure point diffractive* if $\hat{\gamma}_\omega = (\hat{\gamma}_\omega)_{pp}$, that is, if $(\hat{\gamma}_\omega)_{sc} = (\hat{\gamma}_\omega)_{ac} = 0$. We have the following result.

Theorem 2 (*[15,33]*). *Regular model sets are pure point diffractive.*

In the case of certain model sets used in quasicrystal physics as a mathematical model, the agreement between theoretical and experimental diffraction images is rather good [11,19].

The notion of a model set admits the following generalization [2,3].

Definition 4. A subset Λ of $\mathbb{E}_n$ is an *m-component model set* (also called a *multi-component model set*) if there exist:

– a cut and project scheme (1),
– an isometry $\mathcal{I} : \mathbb{E}_n \longrightarrow E_1$ that allows us to identify $\mathbb{E}_n$ with E_1,
– a lattice M in $E_1 \oplus E_2$ containing L as a sublattice,
– m cosets $L_j = \theta_j + L$ of L in M, where $j \in \{1, 2, \ldots, m\}$,
– m sets W_j satisfying (i)–(iii), where $j \in \{1, 2, \ldots, m\}$,

such that

$$\Lambda = \bigcup_{j=1}^{m} \{\pi_1 x \mid x \in L_j,\ \pi_2 x \in W_j\}. \tag{11}$$

Theorem 3 (*[3]*). *Any multi-component model set is a Delone set, has a well-defined density, and is pure point diffractive.*

The multi-component model sets have the property of finite local complexity, that is, there are only finitely many translational classes of clusters of Λ with any given size. The orbit of Λ under translation gives rise, via completion in the standard Radin–Wolff type topology, to a compact space X_Λ, and one obtains a dynamical system $(X_\Lambda, \mathbb{R}^n)$. The connection existing between the spectrum of this dynamical system and the diffraction measure allows one to make use of some powerful spectral theorems in the study of multi-component model sets [25,26].

3. Model sets with predefined local structure

Let $\{g : \mathbb{E}_n \longrightarrow \mathbb{E}_n \mid g \in G\}$ be a faithful orthogonal $\mathbb{R}$-irreducible representation of a finite group G, and let

$$\mathcal{C} = \bigcup_{x\in S} Gx \cup \bigcup_{x\in S} G(-x) = \{e_1, \ldots, e_k, -e_1, \ldots, -e_k\} \tag{12}$$

be the G-cluster symmetric with respect to the origin generated by a finite set $S \subset \mathbb{E}_n$. For each $g \in G$, there exist the numbers $s_1^g, s_2^g, \ldots, s_k^g \in \{-1; 1\}$ and a permutation of the set $\{1, 2, \ldots, k\}$, denoted also by g, such that

$$ge_j = s_{g(j)}^g e_{g(j)} \quad \text{for all } j \in \{1, 2, \ldots, k\}. \tag{13}$$

Let $e_i = (e_{ij})_{1\le j\le n}$, and let $\varepsilon_i = (\delta_{ij})_{1\le j\le k}$, where $\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq j$.

Lemma 1 (*[6,7]*). *The formula $g\varepsilon_j = s_{g(j)}^g \varepsilon_{g(j)}$ defines the orthogonal representation*

$$g(x_i)_{1\le i\le k} = (s_i^g x_{g^{-1}(i)})_{1\le i\le k} \tag{14}$$

of G in $\mathbb{E}_k$. The subspace

$$\mathbf{E} = \{(\langle u, e_i\rangle)_{1\le i\le k} \mid u \in \mathbb{E}_n\} \tag{15}$$

of $\mathbb{E}_k$ is G-invariant and the vectors

$$w_j = \kappa^{-1}(e_{ij})_{1\le i\le k} \quad j \in \{1, 2, \ldots, n\}$$

where $\kappa = \sqrt{(e_{11})^2 + (e_{21})^2 + \cdots + (e_{k1})^2}$, form an orthonormal basis of $\mathbf{E}$.

Lemma 2 (*[6,7]*). (a) *The subduced representation of G in $\mathbf{E}$ is equivalent to the representation of G in $\mathbb{E}_n$, and the isomorphism of representations*

$$\mathcal{I} : \mathbb{E}_n \longrightarrow \mathbf{E} \qquad \mathcal{I}u = (\kappa^{-1}\langle u, e_i\rangle)_{1\le i\le k} \tag{16}$$

with the property $\mathcal{I}(\alpha_1, \alpha_2, \ldots, \alpha_n) = \alpha_1 w_1 + \cdots + \alpha_n w_n$ allows us to identify the 'physical' space $\mathbb{E}_n$ with the subspace $\mathbf{E}$ of $\mathbb{E}_k$.

(b) *The matrix of the orthogonal projector* $\pi : \mathbb{E}_k \longrightarrow \mathbb{E}_k$ *corresponding to* $\mathbf{E}$ *in the basis* $\{\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_k\}$ *is*

$$\pi = (\kappa^{-2}\langle e_i, e_j\rangle)_{1\le i,j\le k}. \tag{17}$$

(c) *The lattice* $\mathbb{L} = \kappa\mathbb{Z}^k \subset \mathbb{E}_k$ *is* G*-invariant,* $\pi(\kappa\varepsilon_i) = \mathcal{I}e_i$*, that is,* $\pi(\kappa\varepsilon_i) = e_i$ *if we take into consideration the identification* $\mathcal{I} : \mathbb{E}_n \longrightarrow \mathbf{E}$*, and*

$$\pi(\mathbb{L}) = \mathbb{Z}e_1 + \mathbb{Z}e_2 + \cdots + \mathbb{Z}e_k. \tag{18}$$

Let $\mathcal{V}$ be a G-invariant subspace of $\mathbb{E}_k$. Since the representation of G in $\mathbb{E}_k$ is orthogonal and $\langle gx, y\rangle = \langle gx, g(g^{-1})y\rangle = \langle x, g^{-1}y\rangle$, the orthogonal complement

$$\mathcal{V}^\perp = \{x \in \mathbb{E}_k \mid \langle x, y\rangle = 0 \text{ for all } y \in \mathcal{V}\} \tag{19}$$

of $\mathcal{V}$ is also a G-invariant subspace. The orthogonal projectors $\Pi, \Pi^\perp : \mathbb{E}_k \longrightarrow \mathbb{E}_k$ corresponding to $\mathcal{V}$ and $\mathcal{V}^\perp$ satisfy the relations

$$\begin{array}{lll} \Pi \circ \Pi = \Pi & \Pi \circ \Pi^\perp = 0 & \Pi \circ g = g \circ \Pi \\ \Pi^\perp \circ \Pi^\perp = \Pi^\perp & \Pi^\perp \circ \Pi = 0 & \Pi^\perp \circ g = g \circ \Pi^\perp \end{array}$$

for any $g \in G$.

Theorem 4. (a) *If* $\Pi(\mathbb{L})$ *is dense in* $\mathcal{V}$*, then* $\mathbb{L} \cap \mathcal{V} = \{0\}$.
(b) *If* $\Pi(\mathbb{L})$ *is discrete in* $\mathcal{V}$*, then* $\mathbb{L} \cap \mathcal{V}$ *contains a basis of* $\mathcal{V}$.
(c) *If* $\Pi(\mathbb{L})$ *is discrete in* $\mathcal{V}$*, then* $\Pi^\perp(\mathbb{L})$ *is a lattice in* $\mathcal{V}^\perp$.

Proof. (a) Let us assume that there is $z \in \mathbb{L} \cap \mathcal{V}$, $z \neq 0$. For each $y \in \mathbb{L}$, the solutions $x = (x_1, x_2, \ldots, x_k)$ of the equation

$$z_1(x_1 - y_1) + z_2(x_2 - y_2) + \cdots + z_k(x_k - y_k) = 0$$

form the hyperplane H_y orthogonal to z passing through y. The hyperplane H_y intersect the one-dimensional subspace $\mathbb{R}z = \{\alpha z \mid \alpha \in \mathbb{R}\}$ at a point corresponding to $\alpha = \langle y, z\rangle/\|z\|^2$. Since $\langle y, z\rangle \in \kappa^2\mathbb{Z}$, the minimal distance between two distinct hyperplanes of the family of parallel hyperplanes $\{H_y \mid y \in \mathbb{L}\}$ containing $\Pi(\mathbb{L})$ is $\kappa^2/\|z\|$. The set $\Pi(\mathbb{L})$ which is contained in union $H = \bigcup_{y\in\mathbb{L}} H_y$ cannot be dense in $\mathcal{V}$. Each point of $\mathbb{R}z - H$ belongs to $\mathcal{V}$, but cannot be the limit of a sequence of points from $\Pi(\mathbb{L})$.

(b) In view of a well-known result [10] concerning lattices in subspaces of $\mathbb{E}_k$, there exist $\lambda_1, \lambda_2, \ldots, \lambda_s$ in $\mathbb{L}$ such that $\{\Pi\lambda_1, \Pi\lambda_2, \ldots, \Pi\lambda_s\}$ is a basis in $\mathcal{V}$ and $\Pi(\mathbb{L}) = \mathbb{Z}\Pi\lambda_1 + \mathbb{Z}\Pi\lambda_2 + \cdots \mathbb{Z}\Pi\lambda_s$. We extend $\{\lambda_1, \lambda_2, \ldots, \lambda_s\}$ up to a basis $\{\lambda_1, \lambda_2, \ldots, \lambda_k\}$ of $\mathbb{E}_k$ by adding new vectors $\lambda_{s+1}, \ldots, \lambda_k$ from $\mathbb{L}$. For each $i \in \{s+1, s+2, \ldots, k\}$ there are $\alpha_{i1}, \ldots, \alpha_{is} \in \mathbb{Z}$ such that

$$\Pi\lambda_i = \alpha_{i1}\Pi\lambda_1 + \alpha_{i2}\Pi\lambda_2 + \cdots + \alpha_{is}\Pi\lambda_s$$

that is,

$$\Pi(\lambda_i - \alpha_{i1}\lambda_1 - \alpha_{i2}\lambda_2 - \cdots - \alpha_{is}\lambda_s) = 0.$$

The linearly independent vectors

$$v_i = \lambda_i - \alpha_{i1}\lambda_1 - \cdots - \alpha_{is}\lambda_s \qquad i \in \{s+1, s+2, \ldots, k\}$$

belonging to $\mathbb{L}$ form a basis in $\mathcal{V}^{\perp}$. Since the coordinates $v_{i1}, v_{i2}, \ldots, v_{ik}$ of each vector v_i belong to $\kappa\mathbb{Z}$, the space $\mathcal{V}$ that coincides with the space of all the solutions $x = (x_1, x_2, \ldots, x_k)$ of the system of linear equations

$$v_{i1}x_1 + v_{i2}x_2 + \cdots + v_{ik}x_k = 0 \quad i \in \{s+1, s+2, \ldots, k\}$$

contains s linearly independent vectors $v_1, v_2, \ldots, v_s$ from $\mathbb{L}$. They form a basis of $\mathcal{V}$.

(c) The vectors $v_1, v_2, \ldots, v_k$ from $\mathbb{L}$ form a basis of $\mathbb{E}_k$. Since

$$\Pi^{\perp} v_i = \begin{cases} 0 & \text{for } i \in \{1, 2, \ldots, s\} \\ v_i & \text{for } i \in \{s+1, s+2, \ldots, k\} \end{cases}$$

and the change of basis matrix from $\{\kappa\varepsilon_1, \kappa\varepsilon_2, \ldots, \kappa\varepsilon_k\}$ to $\{v_1, v_2, \ldots, v_k\}$ has rational entries, it follows that the entries of Π in the basis $\{\kappa\varepsilon_1, \ldots, \kappa\varepsilon_k\}$ are rational. If q is the least common multiple of the denominators of the entries of $\Pi^{\perp}$, then $\Pi^{\perp}(\mathbb{L})$ is contained in the discrete set $(\kappa/q)\mathbb{Z}^k$. □

In order to obtain a description of the structure of $\mathbb{Z}$-module $\Pi(\mathbb{L})$, we use the following result.

Theorem 5 ([10,34]). *Let $\phi : \mathbb{R}^k \longrightarrow \mathbb{R}^l$ be a surjective linear mapping, where $l < k$. Then there are subspaces V_1, V_2 of $\mathbb{R}^l$ such that:*

(a) $\mathbb{R}^l = V_1 \oplus V_2$;
(b) $\phi(\mathbb{Z}^k) = \phi(\mathbb{Z}^k) \cap V_1 + \phi(\mathbb{Z}^k) \cap V_2$;
(c) $\phi(\mathbb{Z}^k) \cap V_2$ *is a lattice in* V_2;
(d) $\phi(\mathbb{Z}^k) \cap V_1$ *is a dense subgroup of* V_1.

The subspace V_1 in this decomposition is uniquely determined.

Theorem 6. *If $\mathcal{V}$ is a G-invariant subspace of $\mathbb{E}_k$ and if Π is the corresponding orthogonal projector, then there exist two subspaces $\mathcal{V}_1$, $\mathcal{V}_2$ such that:*

(a) $\mathcal{V} = \mathcal{V}_1 \oplus \mathcal{V}_2$;
(b) $\Pi(\mathbb{L}) = \Pi(\mathbb{L}) \cap \mathcal{V}_1 + \Pi(\mathbb{L}) \cap \mathcal{V}_2$;
(c) $\Pi(\mathbb{L}) \cap \mathcal{V}_2$ *is a lattice in* $\mathcal{V}_2$;
(d) $\Pi(\mathbb{L}) \cap \mathcal{V}_1$ *is a $\mathbb{Z}$-module dense in* $\mathcal{V}_1$.

The subspace $\mathcal{V}_1$ is uniquely determined and G-invariant.

Proof. The existence of the decomposition follows directly from the previous theorem. It remains only to prove the G-invariance of $\mathcal{V}_1$. For each $x \in \mathcal{V}_1$ there is a sequence $(\xi_j)_{j\geq 0}$ in $\Pi(\mathbb{L})$ such that $x = \lim_{j\to\infty} \xi_j$ and $\xi_j \neq x$ for all j. The transformation $g : \mathbb{E}_k \longrightarrow \mathbb{E}_k$ corresponding to each $g \in G$ is an isometry, and $g(\mathbb{L}) = \mathbb{L}$. Therefore

$$gx = \lim_{j\to\infty} g\xi_j \quad g\xi_j \neq gx$$

$$g(\Pi(\mathbb{L})) = \Pi(g(\mathbb{L})) = \Pi(\mathbb{L})$$

whence $gx \in \mathcal{V}_1$. □

In view of this result, there is a G-invariant subspace $\mathbf{E}'$ and a subspace $\mathbf{V}$ such that $\mathbf{E}^{\perp} = \mathbf{E}' \oplus \mathbf{V}$, $\pi^{\perp}(\mathbb{L}) \cap \mathbf{E}'$ is a $\mathbb{Z}$-module dense in $\mathbf{E}'$, and $\pi^{\perp}(\mathbb{L}) \cap \mathbf{V}$ is a lattice in $\mathbf{V}$. Since $\mathbf{E}^{\perp}$ and $\mathbf{E}'$ are G-invariant, the orthogonal complement (see Fig. 1)

$$\mathbf{E}'' = \{x \in \mathbf{E}^{\perp} \mid \langle x, y\rangle = 0 \text{ for all } y \in \mathbf{E}'\} \tag{20}$$

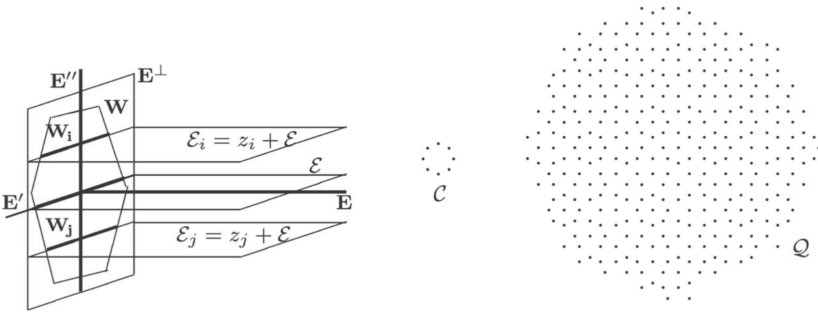

Fig. 1. *Left:* The decompositions $\mathbb{E}_k = \mathbf{E} \oplus \mathbf{E}^\perp = \mathbf{E} \oplus \mathbf{E}' \oplus \mathbf{E}'' = \mathcal{E} \oplus \mathbf{E}''$. *Centre:* A one-shell D_8-cluster $\mathcal{C}$. *Right:* A fragment of the set $\mathcal{Q}$ defined by $\mathcal{C}$.

of $\mathbf{E}'$ in $\mathbf{E}^\perp$ is also a G-invariant space. For each $x \in \mathbb{E}_k$ there exist $\pi x \in \mathbf{E}$, $x' \in \mathbf{E}'$ and $x'' \in \mathbf{E}''$ uniquely determined such that $x = \pi x + x' + x''$. The mappings

$$\begin{aligned} &\pi' : \mathbb{E}_k \longrightarrow \mathbb{E}_k : \ x \mapsto \pi' x = x' \\ &\pi'' : \mathbb{E}_k \longrightarrow \mathbb{E}_k : \ x \mapsto \pi'' x = x'' \end{aligned} \tag{21}$$

are the orthogonal projectors corresponding to $\mathbf{E}'$ and $\mathbf{E}''$.

Theorem 7. *The $\mathbb{Z}$-module $\pi(\mathbb{L})$ is either discrete or dense in* $\mathbf{E}$.

Proof. In view of Theorem 6, there is a G-invariant subspace $\mathcal{V}_1$ and a subspace $\mathcal{V}_2$ such that $\mathbf{E} = \mathcal{V}_1 \oplus \mathcal{V}_2$, $\pi(\mathbb{L}) \cap \mathcal{V}_1$ is dense in $\mathcal{V}_1$, and $\pi(\mathbb{L}) \cap \mathcal{V}_2$ is a lattice in $\mathcal{V}_2$. Since the representation of G in $\mathbf{E}$ is irreducible, we must have either $\mathcal{V}_1 = \{0\}$ or $\mathcal{V}_1 = \mathbf{E}$. □

Let $\tilde{\pi} = \pi + \pi'$, $\mathcal{E} = \tilde{\pi}(\mathbb{E}_k) = \mathbf{E} \oplus \mathbf{E}'$, and let $p : \mathcal{E} \longrightarrow \mathbf{E}$, $p' : \mathcal{E} \longrightarrow \mathbf{E}'$ be the restrictions of π and π' to $\mathcal{E}$.

Theorem 8. *The $\mathbb{Z}$-module $\mathcal{L} = \tilde{\pi}(\mathbb{L})$ is a lattice in $\mathcal{E}$.*

Proof. If $\pi^\perp(\mathbb{L})$ is discrete in $\mathbf{E}^\perp$, then $\mathbf{E}' = \{0\}$ and, in view of Theorem 4, the projection $\mathcal{L} = \pi(\mathbb{L})$ of $\mathbb{L}$ on $\mathcal{E} = \mathbf{E}$ is a lattice in $\mathcal{E}$.

If $\pi^\perp(\mathbb{L})$ is not discrete in $\mathbf{E}^\perp$ then, for any $\rho \in (0, \infty)$, the dimension of the subspace V_ρ generated by the set $\{\pi^\perp x \mid x \in \mathbb{L}, \|\pi^\perp x\| < \rho\}$ is greater than or equal to one. More than that, $\varrho \le \rho' \Longrightarrow V_\rho \subset V_{\rho'}$, and there is $\rho_0 \in (0, \infty)$ such that $V_\rho = V_{\varrho_0}$ for any $\rho \le \rho_0$. We have $\mathbf{E}' = V_{\rho_0}$. Since

$$\left. \begin{array}{l} x \in \mathbb{L} \\ \pi^\perp x \notin \mathbf{E}' \end{array} \right\} \quad \Longrightarrow \quad \|\pi'' x\| > \rho_0$$

$\pi''(\mathbb{L})$ is a lattice in $\mathbf{E}''$. From Theorem 4, it follows that $\mathcal{L}$ is a lattice in $\mathcal{E}$. □

Theorem 9. *If $\pi(\mathbb{L})$ is dense in* $\mathbf{E}$*, then*

$$\begin{array}{ccccc} \mathbf{E} & \xleftarrow{p} & \mathcal{E} & \xrightarrow{p'} & \mathbf{E}' \\ & & \cup & & \\ & & \mathcal{L} & & \end{array} \tag{22}$$

is a cut-and-project scheme.

Proof. From the relation $p'(\mathcal{L}) = \pi'((\pi + \pi')(\mathbb{L})) = \pi'(\mathbb{L})$ and the definition of $\mathbf{E}'$, it follows that $p'(\mathcal{L})$ is dense in $\mathbf{E}'$.

Let $\tilde{x}, \tilde{y} \in \mathcal{L}$ with $p\tilde{x} = p\tilde{y}$, and let $x, y \in \mathbb{L}$ be such that $\tilde{x} = \tilde{\pi}x$ and $\tilde{y} = \tilde{\pi}y$. From $p\tilde{x} = p\tilde{y}$ it follows $\pi x = \pi y$, whence $x - y \in \mathbf{E}^\perp$. Since $\mathbb{L} \cap \mathbf{E}''$ contains a basis of $\mathbf{E}''$ and $\mathbb{L} \cap \mathbf{E}' = \{0\}$, we must have $x - y \in \mathbf{E}''$, whence $\tilde{x} = \tilde{y}$. Therefore, p restricted to $\mathcal{L}$ is one-to-one. $\square$

Let $\mathbf{W} = \pi^\perp(\mathbb{W})$ be the projection of the hypercube

$$\mathbb{W} = v + \{(x_i)_{1\le i\le k} \mid 0 \le x_i \le \kappa\} \tag{23}$$

where the translation $v \in \mathbf{E}'$ is such that no point of $\pi^\perp(\mathbb{L})$ belongs to $\partial\mathbf{W}$.

Theorem 10. *If $\pi(\mathbb{L})$ is dense in $\mathbf{E}$, then the set*

$$\mathcal{Q} = \{\pi x \mid x \in \mathbb{L},\ \pi^\perp x \in \mathbf{W}\} \tag{24}$$

is a multi-component model set.

Proof. Let $\Theta = \{\theta_i \mid i \in \mathbb{Z}\}$ be a subset of $\mathbb{L}$ such that $\pi''(\mathbb{L}) = \pi''(\Theta)$ and $\pi''\theta_i \neq \pi''\theta_j$ for $i \neq j$. The lattice $\mathbb{L}$ is contained in the union $\bigcup_{i\in\mathbb{Z}} \mathcal{E}_i$ of all the cosets $\mathcal{E}_i = \theta_i + \mathcal{E}$ of $\mathcal{E}$ in $\mathbb{E}_k$. The lattice $\mathbf{L} = \mathbb{L} \cap \mathcal{E}$ is a sublattice of $\mathcal{L}$. Since $\mathbb{L} \cap \mathcal{E}_i = \theta_i + \mathbf{L}$, the set $\mathcal{L}_i = \tilde{\pi}(\mathbb{L} \cap \mathcal{E}_i) = \tilde{\pi}\theta_i + \mathbf{L}$ is a coset of $\mathbf{L}$ in $\mathcal{L}$ for any $i \in \mathbb{Z}$. Since $\pi''(\mathbb{L})$ is discrete in $\mathbf{E}''$, the intersection (see Fig. 1)

$$\mathbf{W}_i = \mathbf{W} \cap \mathcal{E}_i = \mathbf{W} \cap \pi^\perp(\mathcal{E}_i) = \pi^\perp(\mathbb{W} \cap \mathcal{E}_i) \subset \pi''\theta_i + \mathbf{E}'$$

is non-empty only for a finite number of cosets $\mathcal{E}_i$. By changing the indexing of the elements of Θ if necessary, we can assume that the subset $\mathcal{W}_i = \pi'(\mathbf{W}_i) = \pi'(\mathbb{W} \cap \mathcal{E}_i)$ of $\mathbf{E}'$ has a non-empty interior only for $i \in \{1, \ldots, m\}$. The 'polyhedral' sets $\mathcal{W}_i$ satisfy the conditions (i)–(iii) from Definition 3, and

$$\mathcal{Q} = \bigcup_{i=1}^{m} \{\pi x \mid x \in \mathcal{L}_i, \pi' x \in \mathcal{W}_i\}. \quad \square \tag{25}$$

The set $\mathcal{Q}$ is a union of interpenetrating copies of the starting cluster $\mathcal{C}$, most of them only partially occupied. For each point $\pi x \in \mathcal{Q}$, the set of all the arithmetic neighbours of πx

$$\left\{ \pi y \;\middle|\; \begin{array}{l} y \in \{x + \kappa\varepsilon_1, \ldots, x + \kappa\varepsilon_k, x - \kappa\varepsilon_1, \ldots, x - \kappa\varepsilon_k\} \\ \pi^\perp y \in \mathbf{W} \end{array} \right\}$$

is contained in the translated copy

$$\{\pi x + e_1, \ldots, \pi x + e_k, \pi x - e_1, \ldots, \pi x - e_k\} = \pi x + \mathcal{C}$$

of the G-cluster $\mathcal{C}$. An algorithm and some software for generating such patterns is available via internet [9]. Some examples are presented in Figs. 1 and 2. In each case, the quasiperiodic pattern is a packing of partially occupied copies of the corresponding cluster. One can remark that the occupation of these copies seems to be very low in the case of a multi-shell cluster.

The number α is called a *scaling factor* of $\mathcal{Q}$ if there is $y \in \mathbf{E}$ such that $\mathcal{Q}$ is invariant under the affine similarity [27]

$$A : \mathbf{E} \longrightarrow \mathbf{E} \quad Ax = y + \alpha(x - y) \tag{26}$$

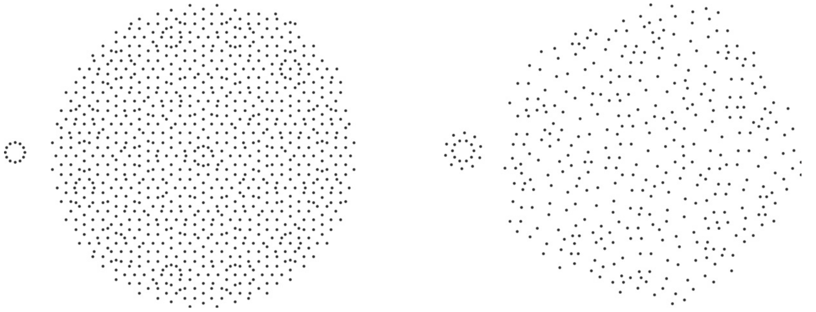

Fig. 2. *Left:* A one-shell D_{12}-cluster and a fragment of the corresponding quasiperiodic set. *Right:* A fragment of the quasiperiodic set defined by a two-shell D_{10}-cluster.

that is, if $A(\mathcal{Q}) \subset \mathcal{Q}$. In this case, we say [27] that y is an *inflation center* corresponding to α, and A is a *self-similarity* of $\mathcal{Q}$. The definition (25) offers some facilities [9,19] in the study of the self-similarities of $\mathcal{Q}$.

In view of Theorem 3, each quasiperiodic set defined by the above algorithm is a Delone set, has a well-defined density, and is pure point diffractive.

4. An example

In order to illustrate the algorithm presented in the previous section, we consider the dihedral group $D_{10} = \langle a, b \mid a^{10} = b^2 = (ab)^2 = e \rangle$, the two-dimensional representation

$$a(\alpha, \beta) = \left(\alpha \cos \frac{\pi}{5} - \beta \sin \frac{\pi}{5}, \alpha \sin \frac{\pi}{5} + \beta \cos \frac{\pi}{5}\right)$$
$$b(\alpha, \beta) = (\alpha, -\beta)$$

and the D_{10}-cluster $\mathcal{C} = D_{10}(1, 0)$ generated by the set $S = \{(1, 0)\}$.

The action of a and b on $\mathcal{C}$ generates the orthogonal representation of D_{10} in $\mathbb{E}_5$:

$$\begin{aligned} &a(x_1, x_2, x_3, x_4, x_5) = (-x_3, -x_4, -x_5, -x_1, -x_2) \\ &b(x_1, x_2, x_3, x_4, x_5) = (x_1, x_5, x_4, x_3, x_2). \end{aligned} \tag{27}$$

The matrices of the projectors corresponding to $\mathbf{E}$, $\mathbf{E}'$, $\mathbf{E}''$ are $\pi = \mathcal{M}(\frac{2}{5}, -\frac{\tau'}{5}, -\frac{\tau}{5})$, $\pi' = \mathcal{M}(\frac{2}{5}, -\frac{\tau}{5}, -\frac{\tau'}{5})$, $\pi'' = \mathcal{M}(\frac{1}{5}, \frac{1}{5}, \frac{1}{5})$, where $\tau = (1 + \sqrt{5})/2$, $\tau' = (1 - \sqrt{5})/2$ and

$$\mathcal{M}(\alpha, \beta, \gamma) = \begin{pmatrix} \alpha & \beta & \gamma & \gamma & \beta \\ \beta & \alpha & \beta & \gamma & \gamma \\ \gamma & \beta & \alpha & \beta & \gamma \\ \gamma & \gamma & \beta & \alpha & \beta \\ \beta & \gamma & \gamma & \beta & \alpha \end{pmatrix}. \tag{28}$$

In this case, $\kappa = \sqrt{5/2}$, and the projection of $\mathbb{L} = \kappa \mathbb{Z}^5$ on the space

$$\mathcal{E} = \mathbf{E} \oplus \mathbf{E}' = \{(x_1, x_2, \ldots, x_5) \mid x_1 + x_2 + \cdots + x_5 = 0\}$$

is the lattice $\mathcal{L} = \mathbb{Z}\chi_1 + \mathbb{Z}\chi_2 + \mathbb{Z}\chi_3 + \mathbb{Z}\chi_4$, where $\chi_j = (\pi + \pi')(\kappa\varepsilon_j)$. If $\mathbf{W} = \pi^\perp(\mathbb{W})$ is the projection on $\mathbf{E}^\perp = \mathbf{E}' \oplus \mathbf{E}''$ of a hypercube

$$\mathbb{W} = v + \{(x_1, x_2, x_3, x_4, x_5) \mid 0 \leq x_j \leq \kappa \text{ for any } j\}$$

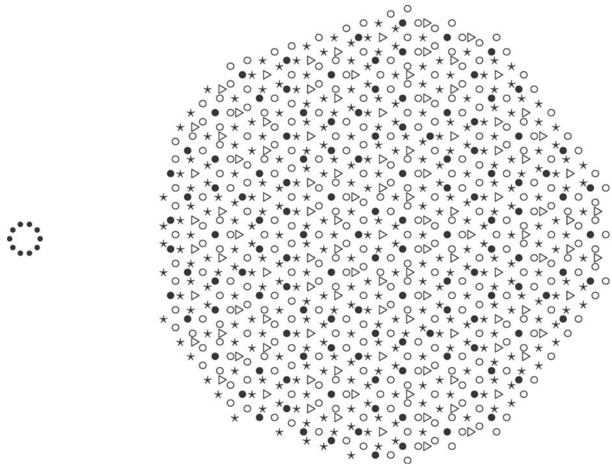

Fig. 3. The cluster $\mathcal{C} = D_{10}(1,0)$ and a fragment of the quasiperiodic pattern defined by this cluster. The positions of the points are indicated by using the symbols $\bullet$, $\circ$, $\star$ and $\triangleright$ in order to distinguish the four components of this model set.

with $v \in \mathbf{E}'$ chosen such that no point of $\pi^{\perp}(\mathbb{L})$ belongs to $\partial\mathbf{W}$, then

$$\mathcal{Q} = \{\pi x \mid x \in \mathbb{L},\ \pi^{\perp} x \in \mathbf{W}\} \tag{29}$$

is the set of all the vertices of a *rhombic Penrose tiling* [19].

The lattice $\mathbb{L}$ is contained in the union $\bigcup_{j\in\mathbb{Z}} \mathcal{E}_j$ of subspaces

$$\mathcal{E}_j = \{(x_1, x_2, \ldots, x_5) \mid x_1 + x_2 + \cdots + x_5 = j\kappa\} = \theta_j + \mathcal{E}$$

where $\theta_j = (j\kappa, 0, 0, 0, 0) \in \mathbb{L}$. Since $\mathbb{L} \cap \mathcal{E}_j = \theta_j + \mathbf{L}$, the set

$$\mathcal{L}_j = \tilde{\pi}(\mathbb{L} \cap \mathcal{E}_j) = \tilde{\pi}\theta_j + \mathbf{L} = j\chi_1 + \mathbf{L} \tag{30}$$

is a coset of $\mathbf{L} = \mathbb{L} \cap \mathcal{E}$ in $\mathcal{L}$, for any $j \in \mathbb{Z}$.

The set $\mathbb{W} \cap \mathcal{E}_j$ is non-empty only for $j \in \{0, 1, 2, 3, 4, 5\}$, but $\mathcal{W}_j = \pi'(\mathbb{W} \cap \mathcal{E}_j)$ has non-empty interior only for $j \in \{1, 2, 3, 4\}$. Let $\mathcal{P} \subset \mathbf{E}'$ be the set of all the points lying inside or on the boundary of the regular pentagon with the vertices $\pi'(\kappa, 0, 0, 0, 0)$, $\pi'(0, \kappa, 0, 0, 0), \ldots, \pi'(0, 0, 0, 0, \kappa)$. One can remark that $\mathcal{W}_1 = v + \mathcal{P}$, $\mathcal{W}_2 = v - \tau\mathcal{P}$, $\mathcal{W}_3 = v + \tau\mathcal{P}$, $\mathcal{W}_4 = v - \mathcal{P}$, and express the pattern $\mathcal{Q}$ as a multi-component model set (see Fig. 3):

$$\mathcal{Q} = \bigcup_{i=1}^{4} \{px \mid x \in \mathcal{L}_i,\ p'x \in \mathcal{W}_i\}. \tag{31}$$

This definition is directly related to de Bruijn's definition [29].

The particular case of the icosahedral group, very important for quasicrystal physics, has been presented (with direct proofs) in [8].

5. Concluding remarks

Quasicrystal structure analysis comprises the determination on an atomic scale of the short-range order (atomic arrangement inside the structural building unit) as well as the long-range order (the way the structural building units are arranged on the long scale). The rational approximants (periodic crystals with the same building unit as the considered quasicrystal) provide a powerful way of determining the short-range order, but the description of the long-range order is still a major problem [35]. Only in the case of a few decagonal and icosahedral phases, the electron microscopy and diffraction data have allowed us to have an idea about the structure of the building unit and long-range ordering.

The atomic structure cannot be extracted directly from the experimental data. One has to postulate a structure and to compare the forecasts with the electron microscopy and diffraction data. There exist several attempts in this direction:

- Elser and Henley [12] and Audier and Guyot [1] have obtained models for icosahedral quasicrystals by decorating the Ammann rhombohedra occuring in a tiling of the three-dimensional (3D) space defined by projection [11,19].
- In his quasi-unit cell picture, Steinhardt [36] has shown (following an idea of Petra Gummelt [14]) that the atomic structure can be described entirely by using a single repeating cluster that overlaps (shares atoms with) neighbouring clusters. The model is determined by the overlap rules and the atom decoration of the unit cell.
- Some important models have been obtained by Yamamoto and Hiraga [37,38], Katz and Gratias [20], and Gratias et al. [13] by using the section method in a six-dimensional (6D) superspace decorated with several polyhedra (acceptance domains).
- Janot and de Boissieu [17] have shown that a model of an icosahedral quasicrystal can be generated recursively by starting from a pseudo-Mackay cluster and using some inflation rules.

Most information about the type of quasiperiodic long-range order is in the very weak reflections. The number of Bragg reflections that we can observe is too small for an accurate structure description [35]. The experimental devices allow us to obtain diffraction patterns and to have a direct view of some small fragments of the quasicrystal. These data provide easy access to the symmetry group G and allow us to look for an adequate cluster $\mathcal{C}$. The pattern $\mathcal{Q}$ obtained by using our algorithm is exactly defined and has the remarkable mathematical properties of the patterns obtained by projection. Each point of our pattern (without exception) is the center of a more or less occupied copy of $\mathcal{C}$ but, unfortunately, in the case of complex clusters the occupation is extremely low for most of the points of $\mathcal{Q}$. Therefore, our discrete quasiperiodic sets cannot be used directly in the description of atomic positions in quasicrystals.

The cluster $\mathcal{C}$ can be regarded as a covering cluster, and $\mathcal{Q}$ as a quasiperiodic set that can be covered by partially occupied copies of a single cluster. This kind of covering is different to the covering of Penrose tiling by a decorated decagon [14] proposed by Gummelt in 1996 or the coverings of discrete quasiperiodic sets presented by Kramer, Gummelt, and Gähler et al. in [22]. In our case the generating cluster $\mathcal{C}$ is a finite set of points and the quasiperiodic pattern is obtained by projection. In [14,22], the covering clusters are congruent overlapping polytopes (with an asymetric decoration) and the structure is generated by imposing certain overlap rules that restrict the possible relative positions and orientations of neighbouring clusters. When the theory from [14,22] is applied to quasicrystals, atomic positions are assigned to the covering clusters.

There are some indications that stable clusters are smaller than the basic structural units seen in electron microscopy images, and it is believed that larger clusters automatically introduce disorder. The defects occuring in the tilings constructed from electron microscopy images show that a certain amount of disorder, either in glue atoms or in the clusters, seems to be unavoidable [13]. In the case of Gummelt's approach, the transition from perfect to random quasicrystalline order is obtained by passing to relaxed overlap rules [30]. The frequency of occurrence of fully occupied clusters in our quasiperiodic patterns can be increased by a certain relaxation in the use of the strip projection method, but this leads to some defects. In order to correct these defects, one has to eliminate some points from interpenetrating clusters if they become too close.

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