Discrete quasiperiodic sets with predefined local structure

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Abstract

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

Key words: Model set, quasiperiodic set, strip projection method, $G$-cluster, quasicrystal
PACS: 61.44.Br

1 Introduction

Model sets (also called cut-and-project sets) have been introduced by Y. Meyer [28] in his study of harmonious sets and later, in the course of the structure analysis of quasicrystals, rediscovered in a variety of different schemes [17,18,20]. Extensive investigations [10,14,15,18,20,22,23,27,28,30,31] 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 model set called multi-component model set, very useful in quasicrystal physics, has been introduced by Baake and Moody [2]. Model sets are 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 microscopic 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 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 microscopic 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 $C$ (basic structural unit), most of them only partially occupied. From a mathematical point of view, $C$ 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 [33]. 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 [34] or a complex coordination polyhedron (with some chemical stability). In our case, $C$ is a structure motif, perhaps without any physical justification.

The purpose of the present paper is to present a mathematical algorithm which leads from any $G$-cluster $C$ directly to a multi-component model set $Q$ representing a quasiperiodic packing of interpenetrating copies of $C$, most of them only partially occupied. It shows how to embed the physical space into a superspace $E_k$ and how to choose a lattice $L \subset E_k$ 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 [18] and independently by Elser [10] 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 model set and multi-component model set.

Let $E$ be a vector subspace of the usual $k$-dimensional Euclidean space $\mathbb{E}_k = (\mathbb{R}^k, \langle \cdot, \cdot \rangle)$, 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 $\Lambda$ be a subset of $E$.

1. The set $\Lambda$ 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 $\Lambda$, for any $x \in E$.
2. The set $\Lambda$ 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 $\Lambda$, for any $x \in E$.
3. The set $\Lambda$ is a *Delone set in $E$* if $\Lambda$ is both relatively dense and uniformly discrete in $E$.
4. The set $\Lambda$ 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

$$
E_1 \xleftarrow{\pi_1} E_1 \oplus E_2 \xrightarrow{\pi_2} E_2 \cup L \tag{1}
$$

formed by two subspaces $E_1, E_2$ of $\mathbb{E}_k$, the corresponding natural projections $\pi_1, \pi_2$, and a lattice $L$ in $E_1 \oplus E_2$ such that:

(a) $\pi_1$ restricted to $L$ is one-to-one;
(b) $\pi_2(L)$ is dense in $E_2$.

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

- a cut and project scheme (1),
- an isometry $\mathcal{I} : \mathbb{E}_n \longrightarrow E_1$ which allows to identify $\mathbb{E}_n$ with $E_1$,
- a set $W \neq \emptyset$ satisfying the conditions:
  (i) $W \subset E_2$ is compact;
  (ii) $W = \text{int}(W)$;
  (iii) The boundary $\partial W$ of $W$ has Lebesgue measure $0$
such that
\[ \Lambda = \{ \pi_1 x \mid x \in L, \pi_2 x \in W \} \] (2)

By using the \( \star \)-mapping
\[ \pi_1(L) \rightarrow E_2 : x \mapsto x^* = \pi_2((\pi_1)|_L)^{-1} x \] (3)

we can re-write the definition of \( \Lambda \) as
\[ \Lambda = \{ x \mid x \in \pi_1(L), x^* \in W \} \] (4)

Model sets have strong regularity properties.

**Theorem 1.** [30,31] Any regular model set \( \Lambda \) is a Delone set and has a well-defined density, that is, there exists the limit
\[ \lim_{r \to \infty} \frac{\#(\Lambda \cap B_r)}{\text{vol}(B_r)} \] (5)

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

In structure analysis of quasicrystals, the experimental diffraction image is compared with the diffraction image of the mathematical model \( \Lambda \), regarded as a set of scatterers. In order to compute the diffraction image of the model set \( \Lambda \), it is represented as a Borel measure in the form of a weighted Dirac comb
\[ \omega = \sum_{x \in \Lambda} \varphi(x) \delta_x \] (6)

where \( \varphi : \Lambda \rightarrow \mathbb{C} \) is a bounded function and \( \delta_x \) is the Dirac measure located at \( x \), that is, \( \delta_x(f) = f(x) \) for continuous functions \( f \). In this way, atoms of quasicrystal are modeled by their positions and scattering strengths. In the case (the only considered in the sequel) when there is a function \( \varphi : E_2 \rightarrow \mathbb{C} \) supported and continuous on \( W \) such that \( \varphi(x) = \varphi(x^*) \), that is, in the case \( \omega = \sum_{x \in \Lambda} \varphi(x^*) \delta_x \) one can prove [14,15,3,4] the following results:

1. The measure \( \omega \) is translation bounded, that is, there exist constants \( C_K \) so that
\[ \sup_{t \in \mathbb{R}^n} \sum_{x \in \Lambda \cap (t + K)} |\varphi(x)| \leq C_K < \infty \] (7)
for all compact $K \subset \mathbb{R}^n$.

2. The autocorrelation coefficients

$$\eta(z) = \lim_{n \to \infty} \frac{1}{\text{vol}(B_n)} \sum_{x, y \in \Lambda \cap B_n} \varrho(x) \varrho(y)$$

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

$$\gamma_\omega = \sum_{z \in \Delta} \eta(z) \delta_z$$

exists.

The diffraction spectrum of $\Lambda$ (the idealized mathematical interpretation of the diffraction pattern of a physical experiment) is related [14,15] to the Fourier transform $\hat{\gamma}_\omega$ of the autocorrelation measure $\gamma_\omega$ which can be decomposed as

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

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 $(\hat{\gamma}_\omega)^{sc}$ singular continuous with respect to Lebesgue measure. We say that $\Lambda$ 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** [14,31] *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 theoretic and experimental diffraction image is rather good [10,18].

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

**Definition 4.** A subset $\Lambda$ 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 $I : \mathbb{E}_n \rightarrow \mathbb{E}_1$ which allows to identify $\mathbb{E}_n$ with $\mathbb{E}_1$,
- a lattice $M$ in $\mathbb{E}_1 \oplus \mathbb{E}_2$ containing $L$ as a sublattice,
- $m$ cosets $L_j = \theta_j + L$ of $L$ in $M$,
  where $j \in \{1, 2, ..., m\}$,
- $m$ 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.** [2] *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 $\Lambda$ with any given size. The orbit of $\Lambda$ under translation gives rise, via completion in the standard Radin-Wolff type topology, to a compact space $X_\Lambda$, 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 use of some powerful spectral theorems in the study of multi-component model sets [24, 25].

### 3 Model sets with predefined local structure

Let $\{g : \mathbb{E}_n \rightarrow \mathbb{E}_n \mid g \in G\}$ be a faithful orthogonal $\mathbb{R}$-irreducible representation of a finite group $G$, and let
\[
C = \bigcup_{x \in S} Gx \cup \bigcup_{x \in S} G(-x) = \{e_1, \ldots, e_k, -e_1, \ldots, -e_k\} \tag{12}
\]
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
\[
ge_j = s^g_{g(j)}e_{g(j)} \quad \text{for all } j \in \{1, 2, \ldots, k\}. \tag{13}
\]

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

**Lemma 1.** [5, 6] *The formula $g\varepsilon_j = s^g_{g(j)}\varepsilon_{g(j)}$ defines the orthogonal representation*
\[
g(x_i)_{1 \leq i \leq k} = \left(s^g_{1\, x_{g^{-1}(i)}}\right)_{1 \leq i \leq k}. \tag{14}
\]
of \( G \) in \( \mathbb{E}_k \). The subspace

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

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

\[
w_j = \kappa^{-1}(e_{ij})_{1 \leq i \leq k} \quad j \in \{1, 2, ..., n\}
\]

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

**Lemma 2.** [5,6] a) The subduced representation of \( G \) in \( \mathbf{E} \) is equivalent with the representation of \( G \) in \( \mathbb{E}_n \), and the isomorphism of representations

\[
\mathcal{I} : \mathbb{E}_n \rightarrow \mathbf{E} \quad \mathcal{I} u = \left( \kappa^{-1}\langle u, e_i \rangle \right)_{1 \leq i \leq k}
\]

with the property \( \mathcal{I}(\alpha_1, \alpha_2, ..., \alpha_n) = \alpha_1 w_1 + ... + \alpha_n w_n \) 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 \( \pi : \mathbb{E}_k \rightarrow \mathbb{E}_k \) corresponding to \( \mathbf{E} \) in the basis \( \{\varepsilon_1, \varepsilon_2, ..., \varepsilon_k\} \) is

\[
\pi = \left( \kappa^{-2}\langle e_i, e_j \rangle \right)_{1 \leq i, j \leq k}
\]

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

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 \( \Pi, \Pi^\perp : \mathbb{E}_k \rightarrow \mathbb{E}_k \) corresponding to \( \mathcal{V} \) and \( \mathcal{V}^\perp \) satisfy the relations

\[
\Pi \circ \Pi = \Pi \quad \Pi \circ \Pi^\perp = 0 \quad \Pi \circ g = g \circ \Pi
\]

\[
\Pi^\perp \circ \Pi^\perp = \Pi^\perp \quad \Pi^\perp \circ \Pi = 0 \quad \Pi^\perp \circ g = g \circ \Pi^\perp
\]

for any \( g \in G \).
Theorem 4.

a) If $\Pi(L)$ is dense in $V$ then $L \cap V = \{0\}$.

b) If $\Pi(L)$ is discrete in $V$ then $L \cap V$ contains a basis of $V$.

c) If $\Pi(L)$ is discrete in $V$ then $\Pi^\perp(L)$ is a lattice in $V^\perp$.

Proof. 

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

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

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 $\{H_y \mid y \in L\}$ containing $\Pi(L)$ is $\kappa^2/||z||$. The set $\Pi(L)$ which is contained in union $H = \bigcup_{y \in L} H_y$ can not be dense in $V$. Each point of $\mathbb{R}z - H$ belongs to $V$ but can not be the limit of a sequence of points from $\Pi(L)$.

b) In view of a well-known result [9] concerning lattices in subspaces of $\mathbb{E}_k$, there exist $\lambda_1, \lambda_2, ..., \lambda_s$ in $L$ such that $\{\Pi\lambda_1, \Pi\lambda_2, ..., \Pi\lambda_s\}$ is a basis in $V$ and $\Pi(L) = Z\Pi\lambda_1 + Z\Pi\lambda_2 + ... Z\Pi\lambda_s$. We extend $\{\lambda_1, \lambda_2, ..., \lambda_s\}$ up to a basis $\{\lambda_1, \lambda_2, ..., \lambda_k\}$ of $\mathbb{E}_k$ by adding new vectors $\lambda_{s+1}, ..., \lambda_k$ from $L$. For each $i \in \{s + 1, s + 2, ..., k\}$ there are $\alpha_{i1}, ..., \alpha_{is} \in \mathbb{Z}$ such that

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

that is,

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

The linearly independent vectors

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

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

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

contains $s$ linearly independent vectors $v_1, v_2, ..., v_s$ from $L$. They form a basis of $V$. 

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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 \( \{\kappa_1, \kappa_2, \ldots, \kappa_k\} \) to \( \{v_1, v_2, \ldots, v_k\} \) has rational entries it follows that the entries of \( \Pi \) in the basis \( \{\kappa_1, \ldots, \kappa_k\} \) 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.** [9,32] Let \( \phi : \mathbb{R}^k \rightarrow \mathbb{R}^l \) 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 \( \Pi \) 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 \( x = \lim_{j \rightarrow \infty} \xi_j \) and \( \xi_j \neq x \) for all \( j \). The transformation \( g : \mathbb{E}_k \rightarrow \mathbb{E}_k \) corresponding to each \( g \in G \) is an isometry and \( g(\mathbb{L}) = \mathbb{L} \). Therefore

\[
gx = \lim_{j \rightarrow \infty} g\xi_j \quad g\xi_j \neq gx
\]

\[
g(\Pi(\mathbb{L})) = \Pi(g(\mathbb{L})) = \Pi(\mathbb{L})
\]
Let $\tilde{\pi} = \pi + \pi'$, $\xi = \tilde{\pi}(E_k) = E \oplus E'$, and let $p : \xi \to E$, $p' : \xi \to E'$ be the restrictions of $\pi$ and $\pi'$ to $\xi$.

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

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

whence $gx \in V_1$. 

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

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

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

$$\pi' : E_k \longrightarrow E_k : x \mapsto \pi' x = x'$$

$$\pi'' : E_k \longrightarrow E_k : x \mapsto \pi'' x = x'' \quad (21)$$

are the orthogonal projectors corresponding to $E'$ and $E''$. 

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

**Proof.** In view of theorem 6, there is a $G$-invariant subspace $V_1$ and a subspace $V_2$ such that $E = V_1 \oplus V_2$, $\pi(L) \cap V_1$ is dense in $V_1$, and $\pi(L) \cap V_2$ is a lattice in $V_2$. Since the representation of $G$ in $E$ is irreducible we must have either $V_1 = \{0\}$ or $V_1 = E$. 

Let $\tilde{\pi} = \pi + \pi'$, $\xi = \tilde{\pi}(E_k) = E \oplus E'$, and let $p : \xi \to E$, $p' : \xi \to E'$ be the restrictions of $\pi$ and $\pi'$ to $\xi$. 

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

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

If $\pi^\perp(\mathbb{L})$ is not discrete in $\mathbb{E}^\perp$ then for any $\rho \in (0, \infty)$ the dimension of the subspace $V_\rho$ 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, $\rho \leq \rho' \implies V_\rho \subset V_{\rho'}$, and there is $\rho_0 \in (0, \infty)$ such that $V_{\rho} = V_{\rho_0}$ for any $\rho \leq \rho_0$. We have $\mathbb{E}' = V_{\rho_0}$. Since

$$x \in \mathbb{L} \quad \pi^\perp x \not\in \mathbb{E}' \quad \implies \quad ||\pi'' x|| > \rho_0$$

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

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

$$\mathbb{E} \xleftarrow{p} \mathcal{E} \xrightarrow{p'} \mathbb{E}' \cup \mathcal{L} \quad \text{(22)}$$

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 $\mathbb{E}'$ it follows that $p'(\mathcal{L})$ is dense in $\mathbb{E}'$.

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

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

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

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

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

$$\mathcal{Q} = \{ \pi x \mid x \in \mathbb{L}, \pi^\perp x \in \mathbb{W} \} \quad \text{(24)}$$
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 $\mathbb{L} = \mathbb{L} \cap \mathcal{E}$ is a sublattice of $\mathcal{L}$. Since $\mathbb{L} \cap \mathcal{E}_i = \theta_i + \mathcal{L}$, the set $\mathcal{L}_i = \tilde{\pi}(\mathbb{L} \cap \mathcal{E}_i) = \pi\theta_i + \mathcal{L}$ is a coset of $\mathcal{L}$ in $\mathcal{L}$ for any $i \in \mathbb{Z}$. Since $\pi''(\mathbb{L})$ is discrete in $\mathbb{E}'$, the intersection (see figure 1)

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

is non-empty only for a finite number of cosets $\mathcal{E}_i$. By changing the indexation of the elements of $\Theta$ if necessary, we can assume that the subset $\mathcal{W}_i = \pi'(\mathbb{W}_i) = \pi'(\mathbb{W} \cap \mathcal{E}_i)$ of $\mathcal{E}'$ 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

$$\mathcal{Q} = \bigcup_{i=1}^{m} \{ \pi x \mid x \in \mathcal{L}_i, \ \pi' x \in \mathcal{W}_i \}.$$  \hspace{1cm} (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 $\pi x$

$$\left\{ \pi y \mid y \in \{ x + \kappa \varepsilon_1, \ldots, x + \kappa \varepsilon_k, x - \kappa \varepsilon_1, \ldots, x - \kappa \varepsilon_k \} \right\}$$

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 [8]. Some examples are presented in figures 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 seem to be very low in the case of a multi-shell cluster.

The number $\alpha$ is called a scaling factor of $\mathcal{Q}$ if there is $y \in \mathcal{E}$ such that $\mathcal{Q}$ is invariant under the affine similarity [26]

$$A : \mathcal{E} \longrightarrow \mathcal{E} \quad A x = y + \alpha(x - y)$$ \hspace{1cm} (26)
The action of \( D \) is a Delone set, has a well-defined density and is pure point diffractive. In view of the theorem 3, each quasiperiodic set defined by the above algorithm has some facilities \([8,18]\) in the study of the self-similarities of \( D \). 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 \([26]\) that \( y \) is an inflation center corresponding to \( \alpha \), and \( A \) is a self-similarity of \( \mathcal{Q} \). The definition (25) offers some facilities \([8,18]\) in the study of the self-similarities of \( \mathcal{Q} \).

In view of the 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

\[
\begin{align*}
  a(\alpha, \beta) &= \left( \alpha \cos \frac{\pi}{5} - \beta \sin \frac{\pi}{5}, \alpha \sin \frac{\pi}{5} + \beta \cos \frac{\pi}{5} \right) \\
  b(\alpha, \beta) &= (\alpha, -\beta)
\end{align*}
\]

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 \( \mathcal{C} \) generate the orthogonal representation of \( D_{10} \) in \( \mathbb{E}_5 \)

\[
\begin{align*}
  a(x_1, x_2, x_3, x_4, x_5) &= (-x_3, -x_4, -x_5, -x_1, -x_2) \\
  b(x_1, x_2, x_3, x_4, x_5) &= (x_1, x_5, x_4, x_3, x_2).
\end{align*}
\]

Fig. 2. \textit{Left}: A one-shell \( D_{12} \)-cluster and a fragment of the corresponding quasiperiodic set. \textit{Right}: A fragment of the quasiperiodic set defined by a two-shell \( D_{10} \)-cluster.
The matrices of the projectors corresponding to \( E, E', E'' \) are 
\[
\pi = M \left( \frac{2}{5}, -\frac{\tau'}{5}, -\frac{\tau}{5} \right), \quad \pi' = M \left( \frac{2}{5}, -\frac{\tau}{5}, -\frac{\tau'}{5} \right), \quad \pi'' = M \left( \frac{1}{5}, \frac{1}{5}, \frac{1}{5} \right),
\]
where \( \tau = (1 + \sqrt{5})/2, \quad \tau' = (1 - \sqrt{5})/2 \) and 
\[
M(\alpha, \beta, \gamma) = \begin{pmatrix}
\alpha & \beta & \gamma & \gamma \\
\beta & \alpha & \beta & \gamma \\
\gamma & \beta & \alpha & \beta \\
\gamma & \gamma & \beta & \alpha \\
\end{pmatrix}.
\] (28)

In this case \( \kappa = \sqrt{5}/2 \), and the projection of \( \mathbb{L} = \kappa \mathbb{Z}^5 \) on the space 
\[
\mathcal{E} = E \oplus E' = \{ (x_1, x_2, ..., x_5) \mid x_1 + x_2 + ... + x_5 = 0 \}
\]
is the lattice \( \mathcal{L} = \mathbb{Z}_1 + \mathbb{Z}_2 + \mathbb{Z}_3 + \mathbb{Z}_4 \), where \( \chi_j = (\pi + \pi')(\kappa \varepsilon_j) \). If \( \mathbb{W} = \pi^\perp(\mathbb{W}) \) is the projection on \( \mathbb{E}^\perp = E' \oplus E'' \) of a hypercube 
\[
\mathbb{W} = v + \{ (x_1, x_2, x_3, x_4, x_5) \mid 0 \leq x_j \leq \kappa \text{ for any } j \}
\]
with \( v \in E' \) chosen such that no point of \( \pi^\perp(\mathbb{L}) \) belongs to \( \partial \mathbb{W} \) then 
\[
\mathcal{Q} = \{ \pi x \mid x \in \mathbb{L}, \pi^\perp x \in \mathbb{W} \}
\] (29)
is the set of all the vertices of a rhombic Penrose tiling \[18\].

The lattice \( \mathbb{L} \) is contained in the union \( \bigcup_{j \in \mathbb{Z}} \mathcal{E}_j \) of subspaces 
\[
\mathcal{E}_j = \{ (x_1, x_2, ..., x_5) \mid x_1 + x_2 + ... + x_5 = j\kappa \} = \theta_j + \mathcal{E}
\]
where \( \theta_j = (j\kappa, 0, 0, 0, 0) \in \mathbb{L} \). Since \( \mathbb{L} \cap \mathcal{E}_j = \theta_j + \mathcal{L} \), the set 
\[
\mathcal{L}_j = \pi(\mathbb{L} \cap \mathcal{E}_j) = \pi \theta_j + \mathcal{L} = j\mathbb{Z}_1 + \mathcal{L}
\] (30)
is a coset of \( \mathcal{L} = \mathbb{L} \cap \mathcal{E} \) 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 \( \mathcal{P} \subset E' \) be the set of all the points lying inside or on the boundary of the regular pentagon with the vertices \( \pi'(\kappa, 0, 0, 0, 0), \pi'(0, \kappa, 0, 0, 0), ..., \pi'(0, 0, 0, 0, \kappa) \). One can remark that
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 $\circ$ in order to distinguish the four components of this model set.

$\mathcal{W}_1 = v + P$, $\mathcal{W}_2 = v - \tau P$, $\mathcal{W}_3 = v + \tau P$, $\mathcal{W}_4 = v - P$, and express the pattern $\mathcal{Q}$ as a multi-component model set (see figure 3)

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

This definition is directly related to de Bruijn’s definition [28].

The particular case of the icosahedral group, very important for quasicrystal physics, has been presented (with direct proofs) in [7].

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 to determine the short-range order, but the description of the long-range order is still a major problem [33]. Only in the case of a few decagonal and icosahedral phases, the electron microscopic and diffraction data have allowed us to have an idea about the structure of the building unit and long-range ordering.

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

- Elser & Henley [11] and Audier & Guyot [1] have obtained models for icosahedral quasicrystals by decorating the Ammann rhombohedra occurring in a tiling of the 3D space defined by projection [10,18].
- In his quasi-unit cell picture Steinhardt [34] has shown (following an idea of Petra Gummelt [13]) that the atomic structure can be described entirely by using a single repeating cluster which overlaps (shares atoms with) neighbour 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 & Hiraga [35,36], Katz & Gratias [19], Gratias, Puyraimond and Quiquandon [12] by using the section method in a 6D superspace decorated with several polyhedra (acceptance domains).
- Janot and de Boissieu [16] have shown that a model of 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 we can observe is too small for an accurate structure description [33]. The experimental devices allow us to obtain diffraction patterns and to have a direct view on some small fragments of the quasicrystal. These data provide easy access to the symmetry group $G$ and allows us to look for an adequate cluster $C$. The pattern $Q$ 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 $C$, but unfortunately, in the case of complex clusters the occupation is extremely low for most of the points of $Q$. Therefore, our discrete quasiperiodic sets can not be used directly in the description of atomic positions in quasicrystals.

The cluster $C$ can be regarded as a covering cluster, and $Q$ as a quasiperiodic set which can be covered by partially occupied copies of a single cluster. This kind of covering is different from the covering of Penrose tiling by a decorated decagon [13] proposed by Gummelt in 1996 or the coverings of discrete quasiperiodic sets presented by Kramer, Gummelt, Gähler et. al. in [21]. In our case the generating cluster $C$ is a finite set of points and the quasiperiodic pattern is obtained by projection. In [13,21] the covering clusters are congruent overlapping polytopes (with an asymmetric decoration) and the structure is generated by imposing certain overlap rules which restrict the possible relative positions and orientations of neighbouring clusters. When the theory from [13,21] 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 on electron microscopic images, and it is believed that larger clusters automatically introduce disorder. The defects occurring in the tilings constructed from electron microscopic images show that a certain amount of disorder either in glue atoms or in the clusters seems to be unavoidable [12]. In the case of Gummelt’s approach, the transition from perfect to random quasicrystalline order is obtained by passing to relaxed overlap rules [29]. The frequency of occurrence of fully occupied clusters in our quasiperiodic patterns can be increased by a certain relaxation in the use of 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.

Acknowledgement. This research was supported by the grant CEEX 582/2005.

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