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Discrete quasiperiodic sets with predefined covering cluster

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Some of the most remarkable tilings and discrete quasiperiodic sets used in quasicrystal physics can be obtained by using strip projection method in a superspace of dimension four, five or six, and the projection of a unit hypercube as a window of selection. We present some mathematical results which allow one to use this very elegant method in superspaces of dimension much higher, and to generate discrete quasiperiodic sets with a more complicated local structure by starting from the corresponding covering cluster. Hundreds of points of these sets can be obtained in only a few minutes by using our computer programs.

Keywords: Strip projection method; quasiperiodic point set; covering cluster.

1. Introduction

Quasicrystals are materials with perfect long-range order, but with no threedimensional translational periodicity. The discovery of these solids in the early 1980's and the challenge to describe their structure led to a great interest in discrete quasiperiodic sets and their coverings ([9] and references therein).

The diffraction image of a quasicrystal often contains a set of sharp Bragg peaks invariant under a finite non-crystallographic group of symmetries G, called the symmetry group of quasicrystal (in reciprocal space). 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). Real structure information obtained by high resolution transmission electron microscopy suggests us that a quasicrystal with symmetry group G can be regarded as a quasiperiodic packing of copies of a well-defined G-invariant cluster C.

In the literature on quasicrystals the term 'cluster' has several meanings [9]. In the present paper, by *G*-cluster we mean a finite union of orbits of a finite group *G* in a fixed representation. A mathematical algorithm for generating quasiperiodic point sets by starting from *G*-clusters was proposed by author in collaboration with Jean-Louis Verger-Gaugry several years ago [2]. It is based on strip projection method ([9] and references therein) and is a direct generalization of the algorithm used by Katz and Duneau in [8]. The model obtained in [8] for the icosahedral quasicrystals starts from the one-shell *Y*-cluster *C* formed by the vertices of a regular icosahedron. The physical space is embedded into the superspace \mathbb{R}^6 such that the orthogonal projections on the physical space of the points

 $(\pm 1, 0, 0, 0, 0, 0), (0, \pm 1, 0, 0, 0, 0), \dots, (0, 0, 0, 0, \pm 1, 0), (0, 0, 0, 0, 0, \pm 1)$

are the vertices of a regular icosahedron.

In our direct generalization, we consider only *G*-clusters invariant under inversion. If our starting *G*-cluster C has 2k points then we embed the physical space into the superspace \mathbb{R}^k in such a way that C is the orthogonal projection on the physical space of the subset

{ $(\pm 1, 0, 0, ..., 0), (0, \pm 1, 0, 0, ..., 0), ..., (0, 0, ..., 0, \pm 1, 0), (0, 0, ..., 0, \pm 1)$ }

of \mathbb{R}^k containing 2k points. One can remark that, in the case of a two-shell or three-shell cluster, the dimension of the involved superspace is rather high.

Our aim is to present some mathematical results which allow one to use our algorithm in the case of multi-shell clusters. We show that in the case of a two-dimensional (resp. three-dimensional) cluster we have to compute only determinants of order three (resp. four), independently of the dimension of the superspace we use. This remark and a simple description of the window (which, generally, is a polyhedron with hundreds or thousands faces) have allowed us to obtain some very efficient computer programs for our algorithm [7].

In the case of a three-shell Y-cluster formed by the vertices of a regular icosahedron, a regular dodecahedron and an icosidodecahedron we use a 31dimensional superspace, the window is a polyhedron lying in a 28-dimensional subspace bounded by 31465 pairs of parallel faces, but we obtain 400-500 points in less than 10 minutes [6]. In the case of a two-shell D_{10} -cluster we use a 10dimensional superspace, the window is bounded by 120 pairs of parallel faces, and we obtain 700-800 points in only one minute [5].

2. *G*-clusters

Consider a finite group G and a fixed \mathbb{R} -irreducible representation of G in \mathbb{R}^n . In the case of dihedral groups $D_{2m} = \langle a, b \mid a^{2m} = b^2 = (ab)^2 = e \rangle$ we can use the two-dimensional representation defined by $a, b : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$

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

$$b(\alpha,\beta) = (\alpha,-\beta)$$
 (1)

and in the case of the icosahedral group $Y = \langle a, b \mid a^5 = b^2 = (ab)^3 = e \rangle$ the three-dimensional representation generated by the rotations $a, b : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$

$$a(\alpha,\beta,\gamma) = \left(\frac{\tau-1}{2}\alpha - \frac{\tau}{2}\beta + \frac{1}{2}\gamma, \ \frac{\tau}{2}\alpha + \frac{1}{2}\beta + \frac{\tau-1}{2}\gamma, \ -\frac{1}{2}\alpha + \frac{\tau-1}{2}\beta + \frac{\tau}{2}\gamma\right)$$
$$b(\alpha,\beta,\gamma) = (-\alpha,-\beta,\gamma).$$
(2)

where $\tau = (1 + \sqrt{5})/2$. The set $G(\alpha_1, \alpha_2, ..., \alpha_n) = \{ g(\alpha_1, \alpha_2, ..., \alpha_n) \mid g \in G \}$ is called the *orbit* of G generated by $(\alpha_1, \alpha_2, ..., \alpha_n)$. If $\alpha \in (0, \infty)$ then the orbit

 $Y(\alpha, \alpha \tau, 0)$ is formed by the vertices of a regular icosahedron, $Y(\alpha, \alpha, \alpha)$ is formed by the vertices of a regular dodecahedron, $Y(\alpha, 0, 0)$ is formed by the vertices of an icosidodecahedron.

For each $(\alpha, \beta) \neq (0, 0)$, the orbit $D_{2m}(\alpha, \beta)$ is formed by the vertices of a regular polygon with 2m sides. A *G*-cluster is a finite union of orbits of *G*. For example, $\mathcal{C} = D_{2m}(\alpha_1, \beta_1) \cup D_{2m}(\alpha_2, \beta_2)$ is two-shell D_{2m} -cluster, and

$$\mathcal{C} = Y(\alpha, \alpha\tau, 0) \cup Y(\beta, \beta, \beta) \cup Y(\gamma, 0, 0) \}$$

is a three-shell icosahedral cluster.

3. Discrete quasiperiodic sets defined by G-clusters

Let $C = \{v_1, v_2, ..., v_k, -v_1, -v_2, ..., -v_k\}$, where $v_j = (v_{1j}, v_{2j}, ..., v_{nj})$, be a fixed *G*-cluster symmetric with respect to the origin. One can prove [2, 3] that the vectors $w_1, w_2, ..., w_n$, where $w_i = (v_{i1}, v_{i2}, ..., v_{ik})$, are orthogonal and have the same norm (which we denote by κ)

$$\langle w_i, w_j \rangle = v_{i1} v_{j1} + v_{i2} v_{j2} + \dots + v_{ik} v_{jk} = \begin{cases} \kappa^2 & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases}$$
(3)

We identify the space \mathbb{R}^n containing \mathcal{C} ('physical space') with the subspace

$$\mathbf{E} = \{ \alpha_1 w_1 + \alpha_2 w_2 + \dots + \alpha_n w_n \mid \alpha_1, \alpha_2, \dots, \alpha_n \in \mathbb{R} \}.$$
(4)

of the superspace \mathbb{R}^k , and consider the orthogonal complement of **E**

$$\mathbf{E}^{\perp} = \{ x \in \mathbb{R}^k \mid \langle x, y \rangle = 0 \text{ for all } y \in \mathbf{E} \}.$$
(5)

The orthogonal projectors corresponding to ${\bf E}$ and ${\bf E}^\perp$ are

$$\pi : \mathbb{R}^k \longrightarrow \mathbf{E} \qquad \pi x = \left\langle x, \frac{w_1}{\kappa} \right\rangle \frac{w_1}{\kappa} + \left\langle x, \frac{w_2}{\kappa} \right\rangle \frac{w_2}{\kappa} + \dots + \left\langle x, \frac{w_n}{\kappa} \right\rangle \frac{w_n}{\kappa} \pi^{\perp} : \mathbb{R}^k \longrightarrow \mathbf{E}^{\perp} \qquad \pi^{\perp} x = x - \pi x.$$
(6)

If we describe **E** by using the orthogonal basis $\{\kappa^{-2}w_1, \kappa^{-2}w_2, ..., \kappa^{-2}w_n\}$ then the orthogonal projector corresponding to **E** becomes

$$\mathcal{P}: \mathbb{R}^k \longrightarrow \mathbb{R}^n \qquad \mathcal{P}x = (\langle x, w_1 \rangle, \langle x, w_2 \rangle, ..., \langle x, w_n \rangle). \tag{7}$$

The projection $\mathbf{W} = \pi^{\perp}(\Omega)$ of the unit hypercube

$$\Omega = \left[-\frac{1}{2}, \frac{1}{2} \right]^k = \left\{ (x_1, x_2, ..., x_k) \ \left| \ -\frac{1}{2} \le x_i \le \frac{1}{2} \text{ for all } i \in \{1, 2, ..., k\} \right. \right\}$$

is a polyhedron (called a window) in the (k-n)-subspace \mathbf{E}^{\perp} . Each (k-n-1)dimensional face of \mathbf{W} is the projection of a (k-n-1)-face of the unit hypercube Ω . Each (k-n-1)-face of Ω is parallel to k-n-1 vectors of the canonical basis $\{e_1, e_2, ..., e_k\}$ of \mathbb{R}^k , and orthogonal to n+1 of them. For each n+1distinct vectors $e_{i_1}, e_{i_2}, ..., e_{i_{n+1}}$ the number of (k-n-1)-faces of Ω orthogonal to them is 2^{n+1} , and the set

$$\left\{ \begin{array}{ccc} x = (x_1, x_2, \dots, x_k) \\ x_i = 0 \end{array} \middle| \begin{array}{ccc} x_i \in \{-1/2, 1/2\} & \text{if} & i \in \{i_1, i_2, \dots, i_{n+1}\} \\ x_i = 0 & \text{if} & i \notin \{i_1, i_2, \dots, i_{n+1}\} \end{array} \right\}$$



Figure 1: Left: The strip **S** and the window **W** in the case of a 1D physical space **E** embedded into a 3D superspace. Centre: A one-shell D_8 -cluster \mathcal{C} . Right: A fragment of the set \mathcal{Q} defined by \mathcal{C} . The nearest neighbours of any point q of \mathcal{Q} belong to $q + \mathcal{C}$, which is a copy of \mathcal{C} with the center at point q. Therefore, \mathcal{C} is a covering cluster for \mathcal{Q} .

contains one and only one point from each of them.

There are k!/[(n+1)!(k-n-1)!] sets of 2^{n+1} parallel (k-n-1)-faces of Ω . In the case n = 2 these sets can be labelled by using the elements of

$$\mathcal{I} = \{ (i_1, i_2, i_3) \in \mathbb{Z}^3 \mid 1 \le i_1 \le k - 2, \ i_1 + 1 \le i_2 \le k - 1, \ i_2 + 1 \le i_3 \le k \}$$

and in the case n = 3 the elements of

$$\mathcal{I} = \left\{ (i_1, i_2, i_3, i_4) \in \mathbb{Z}^4 \ \middle| \begin{array}{cc} 1 \leq i_1 \leq k-3, & i_1+1 \leq i_2 \leq k-2, \\ i_2+1 \leq i_3 \leq k-1, & i_3+1 \leq i_4 \leq k \end{array} \right\}.$$

In the case n = 2, the vector defined by the formal determinant

$$y = \begin{vmatrix} e_1 & e_2 & e_3 & e_4 & e_5 & \dots & e_k \\ 0 & 0 & 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & \dots & 1 \\ v_{11} & v_{12} & v_{13} & v_{14} & v_{15} & \dots & v_{1k} \\ v_{21} & v_{22} & v_{23} & v_{24} & v_{25} & \dots & v_{2k} \end{vmatrix} = \begin{vmatrix} e_1 & e_2 & e_3 \\ v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \end{vmatrix}$$
(8)

is a vector orthogonal to the vectors $e_4, e_5, ..., e_k, w_1, w_2$, and

$$\langle x, y \rangle = \begin{vmatrix} x_1 & x_2 & x_3 \\ v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \end{vmatrix}$$
(9)

for any $x \in \mathbb{R}^k$. The vector y belongs to \mathbf{E}^{\perp} , and since $e_i - \pi^{\perp} e_i$ is a linear combination of w_1 and w_2 , it is also orthogonal to $\pi^{\perp} e_4, \pi^{\perp} e_5, ..., \pi^{\perp} e_k$. Therefore, y is orthogonal to the (k-3)-faces of \mathbf{W} labelled by (1,2,3). Similar results can be obtained for any $(i_1, i_2, i_3) \in \mathcal{I}$.



superspace. The starting cluster is a covering cluster, but for most of the points the occupation is extremely low.

Consider the *strip* \mathbf{S} corresponding to the window \mathbf{W} (see figure 1)

$$\mathbf{S} = \{ x \in \mathbb{R}^k \mid \pi^\perp x \in \mathbf{W} \}$$
(10)

and define for each $(i_1, i_2, ..., i_{n+1}) \in \mathcal{I}$ the number

$$d_{i_{1}i_{2}...i_{n+1}} = \max_{\alpha_{j} \in \{-1/2, 1/2\}} \begin{vmatrix} \alpha_{1} & \alpha_{2} & \dots & \alpha_{n+1} \\ v_{1i_{1}} & v_{1i_{2}} & \dots & v_{1i_{n+1}} \\ v_{2i_{1}} & v_{2i_{2}} & \dots & v_{2i_{n+1}} \\ \dots & \dots & \dots & \dots \\ v_{ni_{1}} & v_{ni_{2}} & \dots & v_{ni_{n+1}} \end{vmatrix} .$$
(11)

A point $x = (x_1, x_2, ..., x_k) \in \mathbb{R}^k$ belongs to the strip **S** if and only if

$$-d_{i_{1}i_{2}...i_{n+1}} \leq \begin{vmatrix} x_{i_{1}} & x_{i_{2}} & \dots & x_{i_{n+1}} \\ v_{1i_{1}} & v_{1i_{2}} & \dots & v_{1i_{n+1}} \\ v_{2i_{1}} & v_{2i_{2}} & \dots & v_{2i_{n+1}} \\ \dots & \dots & \dots & \dots \\ v_{ni_{1}} & v_{ni_{2}} & \dots & v_{ni_{n+1}} \end{vmatrix} \leq d_{i_{1}i_{2}...i_{n+1}}$$
(12)

for any $(i_1, i_2, ..., i_{n+1}) \in \mathcal{I}$.

The set defined in terms of the strip projection method

$$\mathcal{Q} = \mathcal{P}(\mathbf{S} \cap \mathbb{Z}^k) = \{\mathcal{P}x \mid x \in \mathbf{S} \cap \mathbb{Z}^k \}$$
(13)

by using the strip **S** defined above and the hyper-lattice \mathbb{Z}^k is a discrete set. If G is one of the groups occurring in quasicrystal physics then \mathcal{Q} is a quasiperiodic set, and has all the properties of the sets obtained by projection [8, 9]. We have

$$\mathcal{P}e_i = (\langle e_i, w_1 \rangle, \langle e_i, w_2 \rangle, \dots, \langle e_i, w_n \rangle) = (v_{1i}, v_{2i}, \dots, v_{ni}) = v_i \tag{14}$$

for any $i \in \{1, 2, ..., k\}$, whence

$$\mathcal{P}(\{x \pm e_1, x \pm e_2, ..., x \pm e_k\} \cap \mathbf{S}) \\ \subseteq \{\mathcal{P}x \pm v_1, \mathcal{P}x \pm v_2 ..., \mathcal{P}x \pm v_k\} = \mathcal{P}x + \mathcal{C}$$

$$(15)$$

that is, the 'arithmetical' neighbours [8] of any point $\mathcal{P}x \in \mathcal{Q}$ belong to the translated copy $\mathcal{P}x + \mathcal{C}$ of \mathcal{C} . Therefore, the starting cluster \mathcal{C} can be regarded as a *covering cluster* ([9], page 16) of the point set \mathcal{Q} . Some examples are shown in figure 1 and figure 2. A presentation of our algorithm in the particular case of a two-shell D_{10} -cluster can be found in [5].

4. Concluding remarks

It is known that, generally, the discrete sets Q considered in the previous section can also be defined as multi-component model sets [1, 4] by using superspaces of smaller dimension and root lattices, but generally we have to use a large number of very complicated windows [4].

The starting cluster C is a covering cluster for the set Q, but unfortunately, for most of the points of Q the occupation is extremely low. Therefore, our discrete quasiperiodic sets can not be used directly in the description of atomic positions in quasicrystals.

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References

- M. Baake and R. V. Moody, in *Aperiodic '97* ed. M. de Boissieu, J.-L. Verger-Gaugry, R. Currat (World Scientific, Singapore 1998), pp. 9-20.
- [2] N. Cotfas and J.-L. Verger-Gaugry, J. Phys. A: Math. Gen. 30 4283 (1997).
- [3] N. Cotfas, Lett. Math. Phys. 47 111 (1999).
- [4] N. Cotfas, J. Phys. A: Math. Gen. **37** 3125 (2004).
- [5] N. Cotfas, *Preprint* math-ph/0504036 (2005).
- [6] N. Cotfas, *Preprint* math-ph/0504044 (2005).
- [7] N. Cotfas, http://fpcm5.fizica.unibuc.ro/~ncotfas.
- [8] A. Katz and M. Duneau, J. Phys. (France) 47 181 (1986).
- P. Kramer and Z. Papadopolos (Eds), Coverings of Discrete Quasiperiodic Sets. Theory and Applications to Quasicrystals (Springer-Verlag Berlin Heidelberg 2003).

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 $\{(\pm 1, 0, 0, ..., 0), (0, \pm 1, 0, 0, ..., 0), ..., (0, 0, ..., 0, \pm 1, 0), (0, 0, ..., 0, \pm 1)\}$

of \mathbb{R}^k containing 2k points. One can remark that, in the case of a two-shell or three-shell cluster, the dimension of the involved superspace is rather high.

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- $Y(\alpha, 0, 0)$ is formed by the vertices of an icosidodecahedron.

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The orthogonal projectors corresponding to \mathbf{E} and \mathbf{E}^{\perp} are

$$\pi : \mathbb{R}^k \longrightarrow \mathbf{E} \qquad \pi x = \left\langle x, \frac{w_1}{\kappa} \right\rangle \frac{w_1}{\kappa} + \left\langle x, \frac{w_2}{\kappa} \right\rangle \frac{w_2}{\kappa} + \dots + \left\langle x, \frac{w_n}{\kappa} \right\rangle \frac{w_n}{\kappa} \qquad (6)$$
$$\pi^{\perp} : \mathbb{R}^k \longrightarrow \mathbf{E}^{\perp} \qquad \pi^{\perp} x = x - \pi x.$$

If we describe **E** by using the orthogonal basis $\{\kappa^{-2}w_1, \kappa^{-2}w_2, ..., \kappa^{-2}w_n\}$ then the orthogonal projector corresponding to **E** becomes

$$\mathcal{P}: \mathbb{R}^k \longrightarrow \mathbb{R}^n \qquad \mathcal{P}x = (\langle x, w_1 \rangle, \langle x, w_2 \rangle, ..., \langle x, w_n \rangle). \tag{7}$$

The projection $\mathbf{W} = \pi^{\perp}(\Omega)$ of the unit hypercube

$$\Omega = \left[-\frac{1}{2}, \frac{1}{2}\right]^k = \left\{ (x_1, x_2, ..., x_k) \ \left| \ -\frac{1}{2} \le x_i \le \frac{1}{2} \text{ for all } i \in \{1, 2, ..., k\} \right. \right\}$$

is a polyhedron (called a *window*) in the (k-n)-subspace \mathbf{E}^{\perp} . Each (k-n-1)dimensional face of \mathbf{W} is the projection of a (k-n-1)-face of the unit hypercube Ω . Each (k-n-1)-face of Ω is parallel to k-n-1 vectors of the canonical basis $\{e_1, e_2, ..., e_k\}$ of \mathbb{R}^k , and orthogonal to n+1 of them. For each n+1distinct vectors $e_{i_1}, e_{i_2}, ..., e_{i_{n+1}}$ the number of (k-n-1)-faces of Ω orthogonal to them is 2^{n+1} , and the set

$$\left\{ \begin{array}{c} x = (x_1, x_2, \dots, x_k) \\ x_i \in \{-1/2, 1/2\} & \text{if} \quad i \in \{i_1, i_2, \dots, i_{n+1}\} \\ x_i = 0 & \text{if} \quad i \notin \{i_1, i_2, \dots, i_{n+1}\} \end{array} \right\}$$



Figure 1: Left: The strip **S** and the window **W** in the case of a 1D physical space **E** embedded into a 3D superspace. Centre: A one-shell D_8 -cluster \mathcal{C} . Right: A fragment of the set \mathcal{Q} defined by \mathcal{C} . The nearest neighbours of any point q of \mathcal{Q} belong to $q + \mathcal{C}$, which is a copy of \mathcal{C} with the center at point q. Therefore, \mathcal{C} is a covering cluster for \mathcal{Q} .

contains one and only one point from each of them.

There are k!/[(n+1)!(k-n-1)!] sets of 2^{n+1} parallel (k-n-1)-faces of Ω . In the case n = 2 these sets can be labelled by using the elements of

$$\mathcal{I} = \{ (i_1, i_2, i_3) \in \mathbb{Z}^3 \mid 1 \le i_1 \le k - 2, \quad i_1 + 1 \le i_2 \le k - 1, \quad i_2 + 1 \le i_3 \le k \}$$

and in the case n = 3 the elements of

$$\mathcal{I} = \left\{ (i_1, i_2, i_3, i_4) \in \mathbb{Z}^4 \ \middle| \begin{array}{cc} 1 \le i_1 \le k - 3, \\ i_2 + 1 \le i_3 \le k - 1, \end{array} \begin{array}{c} i_1 + 1 \le i_2 \le k - 2, \\ i_3 + 1 \le i_4 \le k \end{array} \right\}.$$

In the case n = 2, the vector defined by the formal determinant

$$y = \begin{vmatrix} e_1 & e_2 & e_3 & e_4 & e_5 & \dots & e_k \\ 0 & 0 & 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & \dots & 1 \\ v_{11} & v_{12} & v_{13} & v_{14} & v_{15} & \dots & v_{1k} \\ v_{21} & v_{22} & v_{23} & v_{24} & v_{25} & \dots & v_{2k} \end{vmatrix} = \begin{vmatrix} e_1 & e_2 & e_3 \\ v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \end{vmatrix}$$
(8)

is a vector orthogonal to the vectors $e_4, e_5, ..., e_k, w_1, w_2$, and

$$\langle x, y \rangle = \begin{vmatrix} x_1 & x_2 & x_3 \\ v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \end{vmatrix}$$
(9)

for any $x \in \mathbb{R}^k$. The vector y belongs to \mathbf{E}^{\perp} , and since $e_i - \pi^{\perp} e_i$ is a linear combination of w_1 and w_2 , it is also orthogonal to $\pi^{\perp} e_4, \pi^{\perp} e_5, ..., \pi^{\perp} e_k$. Therefore, y is orthogonal to the (k-3)-faces of \mathbf{W} labelled by (1, 2, 3). Similar results can be obtained for any $(i_1, i_2, i_3) \in \mathcal{I}$.



Figure 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, obtained by using strip projection method in a ten-dimensional superspace. The starting cluster is a covering cluster, but for most of the points the occupation is extremely low.

Consider the *strip* \mathbf{S} corresponding to the window \mathbf{W} (see figure 1)

$$\mathbf{S} = \{ x \in \mathbb{R}^k \mid \pi^\perp x \in \mathbf{W} \}$$
(10)

and define for each $(i_1, i_2, ..., i_{n+1}) \in \mathcal{I}$ the number

$$d_{i_{1}i_{2}\dots i_{n+1}} = \max_{\alpha_{j} \in \{-1/2, 1/2\}} \begin{vmatrix} \alpha_{1} & \alpha_{2} & \dots & \alpha_{n+1} \\ v_{1i_{1}} & v_{1i_{2}} & \dots & v_{1i_{n+1}} \\ v_{2i_{1}} & v_{2i_{2}} & \dots & v_{2i_{n+1}} \\ \dots & \dots & \dots & \dots \\ v_{ni_{1}} & v_{ni_{2}} & \dots & v_{ni_{n+1}} \end{vmatrix} .$$
(11)

A point $x = (x_1, x_2, ..., x_k) \in \mathbb{R}^k$ belongs to the strip **S** if and only if

$$-d_{i_{1}i_{2}...i_{n+1}} \leq \begin{vmatrix} x_{i_{1}} & x_{i_{2}} & \dots & x_{i_{n+1}} \\ v_{1i_{1}} & v_{1i_{2}} & \dots & v_{1i_{n+1}} \\ v_{2i_{1}} & v_{2i_{2}} & \dots & v_{2i_{n+1}} \\ \dots & \dots & \dots & \dots \\ v_{ni_{1}} & v_{ni_{2}} & \dots & v_{ni_{n+1}} \end{vmatrix} \leq d_{i_{1}i_{2}...i_{n+1}}$$
(12)

for any $(i_1, i_2, ..., i_{n+1}) \in \mathcal{I}$.

The set defined in terms of the strip projection method

$$\mathcal{Q} = \mathcal{P}(\mathbf{S} \cap \mathbb{Z}^k) = \{\mathcal{P}x \mid x \in \mathbf{S} \cap \mathbb{Z}^k\}$$
(13)

by using the strip **S** defined above and the hyper-lattice \mathbb{Z}^k is a discrete set. If G is one of the groups occurring in quasicrystal physics then \mathcal{Q} is a quasiperiodic set, and has all the properties of the sets obtained by projection [8, 9]. We have

$$\mathcal{P}e_i = (\langle e_i, w_1 \rangle, \langle e_i, w_2 \rangle, ..., \langle e_i, w_n \rangle) = (v_{1i}, v_{2i}, ..., v_{ni}) = v_i \tag{14}$$

for any $i \in \{1, 2, ..., k\}$, whence

$$\mathcal{P}(\{x \pm e_1, x \pm e_2, ..., x \pm e_k\} \cap \mathbf{S})$$

$$\subseteq \{\mathcal{P}x \pm v_1, \mathcal{P}x \pm v_2 ..., \mathcal{P}x \pm v_k\} = \mathcal{P}x + \mathcal{C}$$
(15)

that is, the 'arithmetical' neighbours [8] of any point $\mathcal{P}x \in \mathcal{Q}$ belong to the translated copy $\mathcal{P}x + \mathcal{C}$ of \mathcal{C} . Therefore, the starting cluster \mathcal{C} can be regarded as a *covering cluster* ([9], page 16) of the point set \mathcal{Q} . Some examples are shown in figure 1 and figure 2. A presentation of our algorithm in the particular case of a two-shell D_{10} -cluster can be found in [5].

4. Concluding remarks

It is known that, generally, the discrete sets Q considered in the previous section can also be defined as multi-component model sets [1, 4] by using superspaces of smaller dimension and root lattices, but generally we have to use a large number of very complicated windows [4].

The starting cluster C is a covering cluster for the set Q, but unfortunately, for most of the points of Q the occupation is extremely low. Therefore, our discrete quasiperiodic sets can not be used directly in the description of atomic positions in quasicrystals.

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References

- M. Baake and R. V. Moody, in *Aperiodic '97* ed. M. de Boissieu, J.-L. Verger-Gaugry, R. Currat (World Scientific, Singapore 1998), pp. 9-20.
- [2] N. Cotfas and J.-L. Verger-Gaugry, J. Phys. A: Math. Gen. 30 4283 (1997).
- [3] N. Cotfas, Lett. Math. Phys. 47 111 (1999).
- [4] N. Cotfas, J. Phys. A: Math. Gen. **37** 3125 (2004).
- [5] N. Cotfas, *Preprint* math-ph/0504036 (2005).
- [6] N. Cotfas, *Preprint* math-ph/0504044 (2005).
- [7] N. Cotfas, http://fpcm5.fizica.unibuc.ro/~ncotfas.
- [8] A. Katz and M. Duneau, J. Phys. (France) 47 181 (1986).
- P. Kramer and Z. Papadopolos (Eds), Coverings of Discrete Quasiperiodic Sets. Theory and Applications to Quasicrystals (Springer-Verlag Berlin Heidelberg 2003).