Approximants of quasiperiodic structures generated by the inflation mapping

1989 J. Phys. A: Math. Gen. 22 4549

(http://iopscience.iop.org/0305-4470/22/21/017)

J. Phys. A: Math. Gen. **22** (1989) 4549-4564. Printed in the UK

Approximants of quasiperiodic structures generated by the inflation mapping

Michel Duneau†, Rémy Mosseri‡ and Christophe Oguey†

† Centre de Physique Théorique, Ecole Polytechnique, F-91128 Palaiseau Cedex, France
‡ Laboratoire de Physique des Solides de Bellevue, CNRS, P1 A Briand, F-92195 Meudon Cedex, France

Received 31 May 1989

Abstract. The problem of deriving explicit coordinates for quasicrystal approximants is solved in all the cases where the quasicrystal has an inflation symmetry. In the higher-dimensional space $\boldsymbol{R}^n$, from which the quasiperiodic pattern is obtained by the cut method, the inflation symmetry is represented by a hyperbolic modular matrix (with integer entries) leaving the 'physical' space invariant. But this matrix also generates, by iteration, a sequence of (rational) approximant spaces which converges to the irrational space. A simple algorithm is described, providing the approximant periodic lattice and the set of vertices within a unit cell.

1. Introduction

Since the experimental discovery of quasicrystals in 1985 (Shechtman *et al* 1985) there has been a growing interest in the study of aperiodic tilings. Indeed the main new features of quasicrystals (a point-like diffraction pattern showing an icosahedral symmetry) can be nicely reproduced by the non-periodic space tilings proposed several years before by Penrose (1979). This new kind of order in solids allows previously 'forbidden' symmetries (icosahedral but also octagonal or dodecagonal symmetries) and generalises some features characteristic of incommensurate structures. There are two main methods to generate p-dimensional Penrose patterns: the inflation or decimation techniques (Penrose 1979, Gardner 1977), and the various algorithms based on higher dimensions (multigrid dualisation (de Bruijn 1981), 'cut and project' (CP) (Elser 1985, Kalugin *et al* 1985, Duneau and Katz 1985) or plain sections (Bak 1986, Oguey *et al* 1988)). Many things are known about the geometrical properties of these fascinating structures: local configurations, inflation (self-similar) properties, matching rules, ... However very little is known (except in one dimension) about the expected physical properties of the solid which adopts such a geometry for its atomic order. This may be due to the fact that the vertex positions are not known explicitly but result from an algorithmic procedure: a selection of nodes in an n-dimensional lattice for the CP method, or a pecise indexing of plane intersections for the grid method.

The coordinates can be derived, however, in the case of the so-called 'approximants'; these are periodic structures with larger and larger unit cells where the symmetry locally approaches the quasiperiodic one. When dealing with tilings, the settings can be arranged such that the tiles are the same in the approximant and in the quasiperiodic tilings; the difference relies only in the long-range order of the tiles—periodic in the

0305-4470/89/214549+16$02.50

former case, quasiperiodic in the latter. In many respects these approximants are the n-dimensional analogues of the rational approximants to irrational numbers. The coordinates are obtained very easily for codimension 1 (mapping from n to $n-1$ dimensions) quasicrystal approximants (Mosseri 1988). The generalisation to any codimension was investigated in a subsequent paper (Mosseri *et al* 1988), showing that the calculation is still possible at the price of a (slightly) more complex work.

The purpose of the present paper is to show that this method can be greatly simplified for the class of self-similar tilings. Indeed in the CP method the inflation symmetry is closely related to a hyperbolic modular transformation M of the higher dimensional space $\boldsymbol{R}^n$. The unstable subspace E (associated with the eigenvalue of M larger than one) is identified with the 'physical' space where the quasiperiodic structure X is built. Using this modular transformation M, we can construct a sequence of approximant structures X_k depending on lattice subspaces E_k which converge to E when k goes to infinity. The approximant structures are periodic and we give a simple algorithm to get the translation lattice and the unit cell sites or vertices at any order.

We then study in detail the case of the octagonal tiling approximants. The vertex coordinates are given explicitly for all k. Finally the Fourier transform is calculated. Its relation with the spectrum of the limit quasiperiodic pattern is discussed.

2. Periodic approximants of quasiperiodic tilings

We briefly recall the cut and project method (Elser 1985, Kalugin *et al* 1985, Duneau and Katz 1985) and adapt it to describe the neighbouring periodic patterns.

Let $\boldsymbol{R}^n$ be the n-dimensional real space endowed with its canonical basis $\{\varepsilon_1, \ldots, \varepsilon_n\}$. $\boldsymbol{Z}^n = [\varepsilon_1, \ldots, \varepsilon_n]$ denotes the standard n-dimensional lattice spanned by $\varepsilon_1, \ldots, \varepsilon_n$.

The 'physical' space E is a p-dimensional vector space embedded as a linear subspace in $\boldsymbol{R}^n$; let π and $\pi' = Id - \pi$ be two complementary projectors such that†

$$\begin{aligned} E &= \pi(\boldsymbol{R}^n) \\ E' &= \pi'(\boldsymbol{R}^n) \\ \boldsymbol{R}^n &= E \oplus E'. \end{aligned} \tag{1}$$

If γ is a smooth bounded subset‡ of $\boldsymbol{R}^n$, consider the following 'strip' or cylinder:

$$S = E + \gamma = \{x + x' | x \in E \text{ and } x' \in \gamma\}. \tag{2}$$

Define the 'window' W as the projection $\pi'(\gamma)$ of γ onto E'; W coincides with the intersection of the strip S with E'. Then the definition (2) of S is equivalent to

$$S = E + W = \{x + x' | x \in E \text{ and } x' \in W\}. \tag{2'}$$

The corresponding structure X in E is the projection of the set of lattice points belonging to S:

$$X = \pi(S \cap \boldsymbol{Z}^n) = \pi[(E + \gamma) \cap Z^n]. \tag{3}$$

† Usually these projectors are orthogonal but this is not required by quasiperiodicity.

‡ In most applications, γ is the standard open unit hypercube of $\boldsymbol{R}^n$:

$$\gamma = \{(x_1, \ldots, x_n) | 0 < x_i < 1 \text{ for } i = 1, \ldots, n\}.$$

There are various ways of devising periodic structures close to the above-defined structure X. We consider the one which consists in selecting lattice points in a different strip

$$S_0 = E_0 + \gamma \tag{4}$$

where E_0 is a p-dimensional lattice plane (i.e. E_0 is spanned by p independent vectors of the lattice $\boldsymbol{Z}^n$) close to E (in a sense which we need not specify for the moment) and γ is the same as in (2).

Let $L_0 = E_0 \cap \boldsymbol{Z}^n$ denote the p-dimensional intersection lattice of E_0. Then a classical theorem (see for instance Cohn (1980)) states that there exists a complementary space E_0' of dimension $n-p$, with a $(n-p)$-dimensional intersection lattice $L_0' = E_0' \cap \boldsymbol{Z}^n$, such that

$$\boldsymbol{R}^n = E_0 \oplus E_0' \tag{5}$$

$$\boldsymbol{Z}^n = L_0 \oplus L_0'. \tag{6}$$

Consequently a basis of $\boldsymbol{Z}^n$ can be formed by the union of a basis of L_0 and a basis of L_0' (there exists a matrix of $\mathrm{GL}(n, \boldsymbol{Z})$ which maps the canonical basis onto this new basis).

The periodic approximant structure associated with E_0 is thus given by the projection:

$$X_0 = \pi(S_0 \cap \boldsymbol{Z}^n) = \pi[(E_0 + \gamma) \cap \boldsymbol{Z}^n]. \tag{7}$$

Define the new window W_0 as the intersection $W_0 = S_0 \cap E_0'$ of the strip S_0 with E_0'. Then

$$S_0 = E_0 + W_0. \tag{7'}$$

The set of lattice points $(E_0 + W_0) \cap \boldsymbol{Z}^n$ is obviously invariant with respect to the translations of L_0. In view of the decompositions (5) and (6) it is easily checked that

$$\begin{aligned}(E_0 + W_0) \cap \boldsymbol{Z}^n &= (E_0 \cap \boldsymbol{Z}^n) + (W_0 \cap \boldsymbol{Z}^n) \\ &= L_0 + W_0 \cap L_0'.\end{aligned}$$

Call $B_0 = W_0 \cap L_0' = S_0 \cap L_0'$ the (finite) intersection of the strip S_0 with the lattice L_0'; then we have

$$(E_0 + W_0) \cap \boldsymbol{Z}^n = L_0 + B_0. \tag{8}$$

In other words, the set of lattice nodes selected by the strip S_0 is the orbit of the finite pattern B_0 under the lattice L_0. Finally, to get the pattern in the physical space, project everything down:

$$X_0 = \pi(L_0 + B_0) = \pi(L_0) + \pi(B_0). \tag{9}$$

This approximant is characterised by the translation lattice $\pi(L_0)$ and the structural basis $\pi(B_0)$.

3. Algebraic inflation in the cut and project framework

We give a formal definition of the inflation map. This specifies the extra structure used in our construction of sequences of approximants. It implies that the related quasiperiodic pattern is self-similar being, somehow, a 'fixed point' of the inflation map.

Definition. An algebraic inflation is given by a matrix M with integer entries and determinant ± 1† such that

$$M = \lambda\pi + \lambda'\pi' \tag{10}$$

where π and $\pi' = Id - \pi$ are two complementary projectors both different from 0 and Id and where λ and λ' are two real numbers.

The physical and complementary space E and E' are defined as the ranges of those projectors by (1). In particular, λ and λ' are algebraic numbers since they are roots of the polynomial equation $\det(M - xId) = 0$. They satisfy $\lambda^p \lambda'^{p'} = \pm 1$ where $p = \dim(E)$ and $p' = n - p = \dim(E')$. Moreover, the following relations hold for any integer k:

$$\pi M^k = \lambda^k \pi \tag{11}$$

$$\pi' M^k = \lambda'^k \pi'. \tag{11'}$$

Example. In the case of the octagonal tiling ($n = 4$), M is the following matrix:

$$M = \begin{pmatrix} 1 & 0 & 1 & -1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ -1 & 1 & 0 & 1 \end{pmatrix} \tag{12}$$

with eigenvalues $\lambda = 1 + \sqrt{2}$ and $\lambda' = 1 - \sqrt{2}$; the corresponding eigenspaces E and E' are two-dimensional planes obtained as the ranges of the following irrational projectors (set $x = 1/\sqrt{2}$):

$$\pi = \frac{1}{2}\begin{pmatrix} 1 & 0 & x & -x \\ 0 & 1 & x & x \\ x & x & 1 & 0 \\ -x & x & 0 & 1 \end{pmatrix} \quad \text{and} \quad \pi' = \frac{1}{2}\begin{pmatrix} 1 & 0 & -x & x \\ 0 & 1 & -x & -x \\ -x & -x & 1 & 0 \\ x & -x & 0 & 1 \end{pmatrix}. \tag{13}$$

Thus $M = (1+\sqrt{2})\pi + (1-\sqrt{2})\pi'$.

4. Approximant structures associated with an inflation

Assume M is an algebraic inflation, as defined above, with eigenspaces and eigenvalues (E, λ) and (E', λ'); assume that $|\lambda| > 1$. The hyperbolic nature of M allows us to build sequences of rational p-dimensional planes (p-planes for short) converging to the limit E, as we now describe.

Let E_0 be a rational p-plane of $\boldsymbol{R}^n$ together with its intersection lattice $L_0 = \boldsymbol{Z}^n \cap E_0$, complementary space E_0' and lattice L_0' (as in § 2). This provides the 'initial conditions' in the procedure (for instance E_0 can be a coordinate plane of $\boldsymbol{R}^n$).

Then, a sequence $\{E_k\}_{k \text{ in } \boldsymbol{Z}}$ of rational p-planes and a sequence $\{L_k\}$ of p-dimensional lattices is generated by iteration of the map M (see figure 1):

$$E_k = M^k(E_0) \tag{14}$$

$$L_k = \boldsymbol{Z}^n \cap E_k. \tag{15}$$

Since M is in $\mathrm{GL}(n, \boldsymbol{Z})$, the intersection lattice L_k of E_k is simply given by $L_k = M^k(L_0)$.

† M belongs to $\mathrm{GL}(n, \boldsymbol{Z})$, the group of modular matrices (integer entries and $|\det| = 1$).

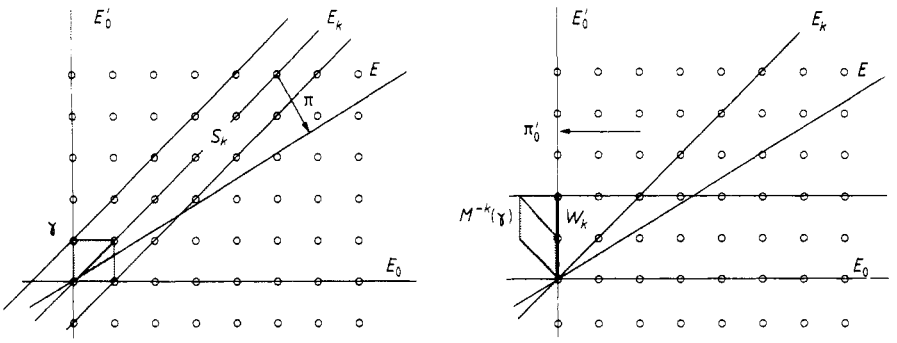

Figure 1. The canonical strip of the approximant E_k is mapped by M^{-k} onto the strip parallel to E_0 with the window $W_k = \pi_0'[M^{-k}(\gamma)]$.

By the cut and project method, a periodic tiling of E can be associated with each p-plane E_k in the way described in § 2 (replacing the index 0 by k).

Consider the strip $S_k = \gamma + E_k = \{x + y | x \in \gamma \text{ and } y \in E_k\}$ and define

$$\Xi_k = S_k \cap \boldsymbol{Z}^n \tag{16}$$

$$X_k = \pi(\Xi_k). \tag{17}$$

Thus Ξ_k is the set of lattice points lying inside S_k; this set is clearly invariant under translations of the lattice L_k. By projection, X_k is invariant with respect to the lattice $\pi(L_k)$. Therefore X_k is the set of vertices of a (periodic) tiling of E. A structural basis can be obtained as the projection of a unit cell of the L_k-periodic set Ξ_k.

In order to easily compare the different structures X_k we will cast the settings in a slightly different manner.

First, it is natural to compare directly the subsets Ξ_k; however, these subsets have different mean orientations (the p-planes E_k); so it is more convenient to consider the subsets $Z_k = M^{-k}(\Xi_k)$ which have the same average orientation E_0. More precisely, by (17), we have $X_k = \pi(\Xi_k) = \pi M^k M^{-k}(\Xi_k)$. Thus, if we set $Z_k = M^{-k}(\Xi_k)$ the structure is simply given by

$$X_k = \pi M^k(Z_k) = \lambda^k \pi(Z_k)$$

where we have applied (11).

Next, since $\boldsymbol{Z}^n$ is invariant by M:

$$Z_k = M^{-k}[(\gamma + E_k) \cap \boldsymbol{Z}^n]$$

$$Z_k = M^{-k}(\gamma + E_k) \cap \boldsymbol{Z}^n = [M^{-k}(\gamma) + M^{-k}(E_k)] \cap \boldsymbol{Z}^n$$

$$Z_k = [M^{-k}(\gamma) + E_0] \cap \boldsymbol{Z}^n.$$

Define γ_k as $\gamma_k = M^{-k}(\gamma)$†:

$$Z_k = (\gamma_k + E_0) \cap \boldsymbol{Z}^n. \tag{18}$$

In other words, Z_k is the subset of nodes of $\boldsymbol{Z}^n$ which belong to the strip $\gamma_k + E_0$. This strip is now oriented along E_0 for all k.

† When γ is the unit n-cube the polyhedron $\gamma_k = M^{-k}(\gamma)$ is a fundamental cell of the lattice $\boldsymbol{Z}^n$ (because M is modular).

We may further introduce the window $W_k = (\gamma_k + E_0) \cap E_0'$ which is simply the profile of the strip in the $(n-p)$-dimensional space E_0'. According to the direct sum (6), the subset Z_k is equal to $L_0 \oplus B_k$, where the pattern B_k is the finite subset of the complementary lattice L_0' selected by the window of W_k.

To summarise, the successive steps of the construction are the following:

$$W_k = (\gamma_k + E_0) \cap E_0' \qquad \text{window of the rational strip in } E_0'. \tag{19}$$

$$B_k = W_k \cap L_0'. \qquad \text{structural basis of the periodic set in the strip.} \tag{20}$$

$$Z_k = L_0 \oplus B_k \qquad \text{decomposition of the lattice points in the strip.} \tag{21}$$

$$X_k = \lambda^k \pi(Z_k) = \lambda^k [\pi(L_0) + \pi(B_k)] \qquad \text{periodic structure in } E. \tag{22}$$

The last formula clearly shows that the structure X_k is periodic. As k increases, the Bravais lattice simply expands by a homothetical factor λ^k. On the other hand, the structural basis B_k is provided by a finite subset of one and the same lattice (L_0'). The only non-trivially varying object is the window W_k. If π_0' denotes the linear projector of $\boldsymbol{R}^n$ onto E_0' with kernel E_0, the window may be built by projecting the polyhedron γ_k: $W_k = \pi_0'(\gamma_k)$.

When γ is the n-dimensional unit cube—the induced quasiperiodic tilings were called 'canonical' in (Oguey *et al* 1988); the Penrose, octagonal and icosahedral tilings are of this type—the successive W_k satisfy simple recursion relations owing to their being zonohedra (see the appendix).

5. The Fibonacci chain revisited

We apply the above described method to a simple case. The Fibonacci chain is a well known tiling of the line by two intervals in the golden ratio. Thus following this example will give familiarity to the different geometrical objects which play an intermediate role in the method. We shall next treat, in § 6, the octagonal tiling approximants and give explicit coordinates for their vertices.

Let $\tau = (1+\sqrt{5})/2$ be the golden ratio and consider the modular matrix $M = \left(\begin{smallmatrix} 1 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ with two eigenvalues τ and $-\tau^{-1}$. Let π and π' be the projectors onto the associated eigendirections:

$$\pi = \frac{1}{1+\tau^2}\begin{pmatrix} \tau^2 & \tau \\ \tau & 1 \end{pmatrix} \qquad \text{and} \qquad \pi' = \frac{1}{1+\tau^2}\begin{pmatrix} 1 & -\tau \\ -\tau & \tau^2 \end{pmatrix}. \tag{23}$$

It is easily checked that

$$M = \tau\pi + (-\tau^{-1})\pi'. \tag{24}$$

In terms of the Fibonacci sequence $F = \{F_k\} = \{1, 1, 2, 3, 5, 8, \ldots\}$, one gets

$$M^k = \begin{pmatrix} F_{k+1} & F_k \\ F_k & F_{k-1} \end{pmatrix} \qquad \text{and} \qquad \det(M^k) = (-1)^k. \tag{25}$$

Similarly

$$M^{-k} = (-1)^k \begin{pmatrix} F_{k-1} & -F_k \\ -F_k & F_{k+1} \end{pmatrix}. \tag{26}$$

We take, for γ, the unit square of $\boldsymbol{Z}^2$ defined by its four vertices

$$\gamma = \begin{Bmatrix} (0,0) & (0,1) \\ (-1,0) & (-1,1) \end{Bmatrix}. \tag{27}$$

In the plane, we set E_0 along the x direction and E_0' along the y direction. This means that L_0 and L_0' are the lattices generated by $(1,0)$ and $(0,1)$ respectively.

Now $\gamma_k = M^{-k}(\gamma)$ is a parallelogram defined by its four vertices

$$\gamma_k = \begin{Bmatrix} (0,0) & (-1)^k(-F_k, F_{k+1}) \\ (-1)^k(-F_{k-1}, F_k) & (-1)^k(-F_{k+1}, F_{k+2}) \end{Bmatrix}. \tag{28}$$

It is a fundamental cell of $\boldsymbol{Z}^2$ since M is modular. The window W_k is the projection of γ_k into E_0'. Then $B_k = W_k \cap L_0'$ is simply the set of points

$$B_k = \{p \times (-1)^k \times (0,1) \mid p = 0, \ldots, F_{k+2} - 1\}. \tag{29}$$

Therefore the set of vertices of the approximant structure is

$$X_k = \tau^k[\pi(B_k) + \pi(L_0)].$$

The vertices are explicitly given by

$$X_k^{p,q} = \tau^k\left[(-1)^k p\pi\begin{pmatrix}0\\1\end{pmatrix} + q\pi\begin{pmatrix}1\\0\end{pmatrix}\right] \qquad \text{for } p = 0, \ldots, F_{k+2} - 1 \text{ and } q \in \boldsymbol{Z}. \tag{30}$$

Therefore they have the following coordinates along E:

$$x_k^{p,q} = \tau^k\left((-1)^k \frac{p}{\sqrt{1+\tau^2}} + \frac{q\tau}{\sqrt{1+\tau^2}}\right).$$

The vertices inside the first unit cell approximant are

$$x_k^p = \frac{(-1)^k \tau^k}{\sqrt{1+\tau^2}}[p \bmod \tau] \qquad p = 0, \ldots, F_{k+2} - 1. \tag{31}$$

Note that the index 'p' is not the natural order along the chain. The vertices are ordered according to their distance to the space E; this is always the case in the treatment of codimension 1 approximants (Mosseri 1988).

6. Approximants of the octagonal tiling

The octagonal tiling and its approximants has been invoked to account for the symmetries observed in phases of alloys such as CrNiSi and AlMnSi (Wang and Kuo 1988). On the theoretical side see for example (Benker 1982, Gratias 1988, Socolar 1989).

The modular matrix M and the related projectors are given in (12) and (13). Let $\mathcal{O} = \{\mathcal{O}_k\} = \{1, 2, 5, 12, 29, \ldots\}$ be the 'Octonacci' sequence defined by

$$\mathcal{O}_{k+1} = 2\mathcal{O}_k + \mathcal{O}_{k-1} \qquad \mathcal{O}_1 = 1 \qquad \mathcal{O}_2 = 2. \tag{32}$$

The successive ratios $\mathcal{O}_{k+1}/\mathcal{O}_k$ tend to $\lambda = 1+\sqrt{2}$. Then it is easy to see that the matrix M satisfies the relation

$$M^{-k} = (-1)^{k+1}(\mathcal{O}_k M - \mathcal{O}_{k+1} I)$$

$$M^{-k} = (-1)^k \begin{pmatrix} \mathcal{O}_k + \mathcal{O}_{k-1} & 0 & -\mathcal{O}_k & \mathcal{O}_k \\ 0 & \mathcal{O}_k + \mathcal{O}_{k-1} & -\mathcal{O}_k & -\mathcal{O}_k \\ -\mathcal{O}_k & -\mathcal{O}_k & \mathcal{O}_k + \mathcal{O}_{k-1} & 0 \\ \mathcal{O}_k & -\mathcal{O}_k & 0 & \mathcal{O}_k + \mathcal{O}_{k-1} \end{pmatrix}. \tag{33}$$

In the following we shall use α, β, δ such that

$$\alpha = (-1)^{k+1}\mathcal{O}_k \qquad \delta = (-1)^k \mathcal{O}_{k+1} \qquad \beta = \alpha + \delta = (-1)^k(\mathcal{O}_k + \mathcal{O}_{k-1}).$$

We take as γ the 4D unit cube whose 16 vertices are given in table 1. We choose as E_0 the 2-plane spanned by the first two vectors $\{\varepsilon_1, \varepsilon_2\}$ of the standard orthonormal basis, and as E_0' the 2-plane spanned by $\{\varepsilon_3, \varepsilon_4\}$.

The window W_k is obtained by mapping $\gamma_k = M^{-k}(\gamma)$ onto E_0' which amounts to keeping only the last two coordinates of the γ_k vertices. The vertices of W_k are given in table 2 and W_k is drawn in figure 2.

For the sake of simplicity we shall only illustrate the approximants indexed by even values of k. In these cases, α is a negative integer whereas β and δ are positive. The shape of the cases corresponding to odd values of k differ by a global inversion (change of sign).

W_k is an octagon with two edge lengths, $|\beta|$ and $|\alpha|\sqrt{2}$ which tends, up to an increasing factor λ^k, to a regular octagon as k increases. For any k the W_k vertices have integral coordinates.

Table 1. Coordinates of the vertices of the 4D unit cube γ.

Vertex	Coordinates	Vertex	Coordinates
1	0 0 0 0	9	0 1 1 0
2	1 0 0 0	10	0 1 0 1
3	0 1 0 0	11	0 0 1 1
4	0 0 1 0	12	1 1 1 0
5	0 0 0 1	13	1 0 1 1
6	1 1 0 0	14	1 1 0 1
7	1 0 1 0	15	0 1 1 1
8	1 0 0 1	16	1 1 1 1

Table 2. Coordinates (in the basis $\{\varepsilon_3, \varepsilon_4\}$ of E_0') of the 16 vertices of W_k.

Vertex	Coordinates		Vertex	Coordinates	
1	0	0	9	$\alpha+\beta$	α
2	α	$-\alpha$	10	α	$\alpha+\beta$
3	α	α	11	β	β
4	β	0	12	$2\alpha+\beta$	0
5	0	β	13	$\alpha+\beta$	δ
6	2α	0	14	2α	β
7	$\alpha+\beta$	$-\alpha$	15	$\alpha+\beta$	$\alpha+\beta$
8	α	δ	16	$2\alpha+\beta$	β

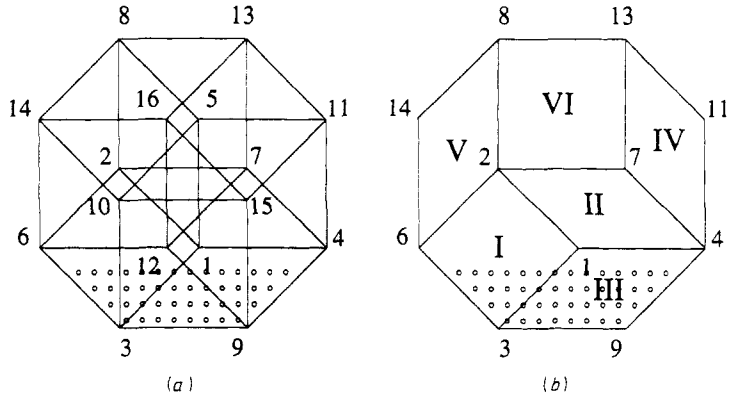

Figure 2. Representation of W_k in E_0': (*a*) with the 16 vertices of γ_k mapped into E_0'; (*b*) a particular partition of W_k with six quadrilaterals (two squares and four parallelograms).

The octagon is used to select the nodes of the lattice $[\varepsilon_3, \varepsilon_4]$ which make, after projection, the structural unit (basis) of the approximant. First of all, to avoid ambiguities on the boundaries of the selection domains, the octagon should be slightly shifted to a generic position (actually the selected set does not depend on the shift but through a global translation). Next, to obtain the selected nodes in a compact form we can partition the octagon into simpler regions as shown in figure 2. These regions are the acceptance domains for the six types of tiles appearing in the tiling (here, tiles of different orientation are considered as distinct: the square appears in two orientations, the rhombus in four (Katz and Duneau 1986)).

For each quadrilateral $i = \mathrm{I}, \mathrm{II}, \ldots, \mathrm{VI}$ of W_k, the coordinates of the integral points in the $\{\varepsilon_3, \varepsilon_4\}$ basis are easily obtained in the following form:

$$\begin{pmatrix} n_3 \\ n_4 \end{pmatrix} = S_i \begin{pmatrix} p \\ q \end{pmatrix} + T_i \tag{34}$$

where (S_i, T_i) is an affine transform (specified by a 2×2 matrix S_i and a translation T_i) and the integers (p, q) run over suitable 'rectangles':

$$\begin{aligned} 0 &\leq p \leq P_i \\ 0 &\leq q \leq Q_i. \end{aligned} \tag{35}$$

For the square region I we describe two subsets of vertices I and I′ which form a centered square lattice parallel to the square edges.

The unit cell contains $N_k = 2(|\alpha|+|\beta|)^2 - |\beta|^2$ sites; table 3 gives the matrices S_i, the vectors T_i and the values P_i, Q_i.

Finally, as for the Fibonacci chain, we can obtain the approximant vertices mapped into E. The coordinates are most conveniently expressed in the basis $\{e_1, e_2\}$, where $e_i = \pi(\varepsilon_i)$ for $i = 1, \ldots, 4$ and the projector is given in (13); the basis $\{e_1, e_2\}$ is orthogonal; the two remaining vectors $\{e_3, e_4\}$ form another basis of the plane related to the former by a 45° rotation J:

$$J = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \tag{36}$$

Table 3. Affine transforms and indexation bounds for the six basic regions.

i	Shape	S_i	T_i	P_i	Q_i
I	square	$\begin{pmatrix} 1 & 1 \\ 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 2\alpha \\ 0 \end{pmatrix}, \begin{pmatrix} 2\alpha+1 \\ 0 \end{pmatrix}$	$\lvert\alpha\rvert-1$	$\lvert\alpha\rvert-1$
II	rhombus	$\begin{pmatrix} 1 & \bar{1} \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \end{pmatrix}$	$\lvert\beta\rvert-1$	$\lvert\alpha\rvert-1$
III	rhombus	$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \alpha \\ \alpha \end{pmatrix}$	$\lvert\beta\rvert-1$	$\lvert\alpha\rvert-1$
IV	rhombus	$\begin{pmatrix} 0 & 1 \\ 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \alpha+\beta \\ -\alpha \end{pmatrix}$	$\lvert\beta\rvert-1$	$\lvert\alpha\rvert-1$
V	rhombus	$\begin{pmatrix} 0 & 1 \\ \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 2\alpha \\ \beta \end{pmatrix}$	$\lvert\beta\rvert-1$	$\lvert\alpha\rvert-1$
VI	square	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \alpha \\ -\alpha \end{pmatrix}$	$\lvert\beta\rvert-1$	$\lvert\beta\rvert-1$

According to § 4, the invariance lattice of the approximant is†

$$\lambda^k \pi(L_0) = \lambda^k [e_1, e_2] = [\lambda^k e_1, \lambda^k e_2] \tag{37}$$

This is a plain dilated square lattice.

Next, we can compute the N_k vertices contained in a square unit cell. The projected pattern is given by the union of the six subsets

$$\lambda^k \pi(B_k) = \lambda^k \bigcup_{i=\mathrm{I},\ldots,\mathrm{VI}} \{n_3 e_3 + n_4 e_4 | n_3, n_4 \text{ given by (34-35)}\}. \tag{38}$$

To express it in the coordinates of the lattice (37), use the transition matrix (36) and divide by the scaling factor λ^k:

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = J \begin{pmatrix} n_3 \\ n_4 \end{pmatrix} \tag{39}$$

then bring the points back into the unit cell. This leads to

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \bmod \pi(L_0) = \mathrm{Frac} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \tag{40}$$

in the $\{\lambda^k e_1, \lambda^k e_2\}$ basis. The coordinates X_1, X_2 are given in table 4: they depend on the index k of the approximant, on the quadrilateral i, and on the variables p, q running within the limits given in table 3 and (35). The unit cell of the approximants for $k=2$ and $k=4$ are shown in figures 3 and 4.

Table 4. 'Extended' coordinates of a basis of the approximant (in units of $\sqrt{2}$).

i	I	I'	II	III	IV	V	VI
$X_1\sqrt{2}$	$2(q+\alpha)$	$2(q+\alpha)+1$	$p-2q$	p	$-p+2(q+\alpha)+\beta$	$p+2\alpha-\beta$	$p-q+2\alpha$
$X_2\sqrt{2}$	$2(p+\alpha)$	$2(p+\alpha)+1$	p	$p+2(q+\alpha)$	$p+\beta$	$-p+2(q+\alpha)+\beta$	$p+q$

† Remember that $[u, v]$ denotes the lattice spanned by u and v.

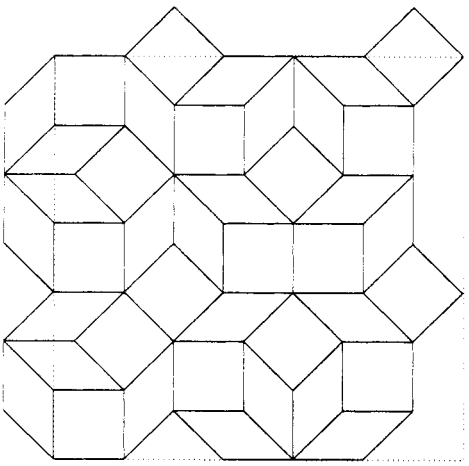

Figure 3. The unit cell of the periodic tiling corresponding to $k = 2$.

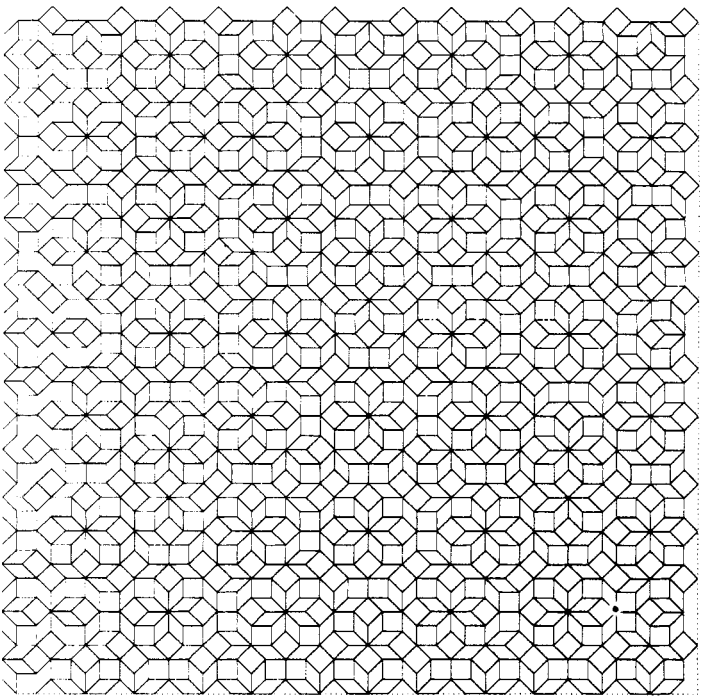

Figure 4. The unit cell of the periodic tiling corresponding to $k = 4$.

To summarise, the successive approximants generated by iterations of the inflation are characterised by

(i) a square lattice of translations (37) scaling as λ^k,

(ii) a set of $N_k = \mathcal{O}_{2k+1} + \mathcal{O}_{2k}$ vertices within a unit cell whose explicit explicit coordinates in the basis of the lattice are given by formula (40) and table 4.

We end this section by a remark about the cases where, as in this one, both the physical E and the complementary space (E' or E'_0) have the same dimension (here

$p = n - p = 2$) or eventually where $\dim(E') \leqslant \dim(E)$. Then the procedure leading to the structural unit contained in a cell—essentially select and project—may be carried out directly in the physical space E after we have mapped, with the projector π, all the required 'tools' into E. In the octagonal example (see the summary at the end of § 4) the finite pattern is

$$\begin{aligned} \lambda^k \pi(B_k) &= \lambda^k \pi(W_k \cap L_0') \\ &= \lambda^k (\Omega_k \cap [e_3, e_4]) \end{aligned} \tag{41}$$

where $\pi(L_0')$ is just the lattice $[e_3, e_4]$ at 45° WRT (e_1, e_2) and the selection window

$$\Omega_k = \pi(W_k) = \pi \pi_0' M^{-k}(\gamma) \tag{42}$$

is an octagon whose coordinates in (e_3, e_4) are precisely those given in table 2.

7. Fourier transform

We give a qualitative account of the intensity spectrum of the approximants. Since the coordinates of the lattice and basis have been explicitly given, the computation is standard. To be specific, we focus on the octagonal case (for icosahedral symmetries, see Verger-Gaugry (1988)).

From § 2, we see that the point measure associated to the approximant X_k

$$m_{X_k} = \sum_{x \in X_k} \delta_x \tag{43}$$

decomposes into a convolution product corresponding to the translation lattice $\lambda^k \pi(L_0)$ and to the basis or unit cell $\lambda^k \pi(B_k)$:

$$m_{X_k} = m_{\lambda^k \pi(L_0)} * m_{\lambda^k \pi(B_k)}. \tag{44}$$

In the octagonal case, the translation lattice is the dilated square lattice (37); the basis is a subset of N_k vertices provided by (41).

The Fourier transforms of the various measures are defined by

$$\tilde{m}(q) = \int \exp(2i\pi q x) m(dx) \qquad q \in \mathbf{R}^2. \tag{45}$$

The convolution (44) implies that

$$\tilde{m}_{X_k} = \tilde{m}_{\lambda^k \pi(L_0)} \tilde{m}_{\lambda^k \pi(B_k)} \tag{46}$$

is a point measure with support in the dual lattice $\lambda^{-k}[e_1^*, e_2^*]$:

$$\tilde{m}_{\lambda^k \pi(L_0)} = \lambda^{-2k} m_{\lambda^{-k}[e_1^*, e_2^*]}. \tag{47}$$

The amplitudes are modulated by a structure factor given by the finite sum of plane waves

$$\tilde{m}_{\lambda^k \pi(B_k)}(q) = \sum_{b \in \pi(B_k)} \exp(2i\pi \lambda^k b q). \tag{48}$$

An evaluation of the Fourier transforms, using (47) and (48), is given in figure 5 for $k = 2$ and 4.

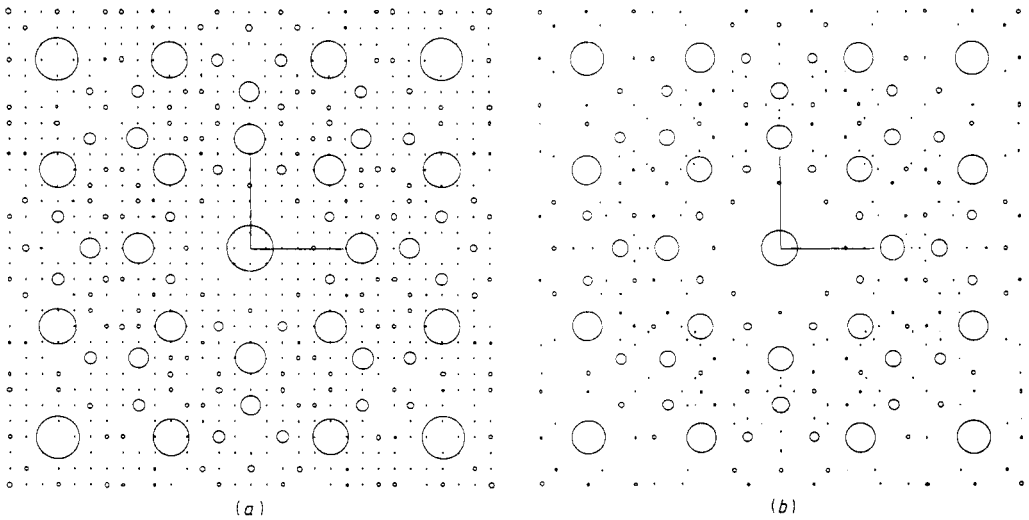

Figure 5. The Fourier transforms of the approximants corresponding to (*a*) $k=2$ and (*b*) $k=4$.

To be complete, we briefly make the connection with the cut and project algorithm (see Duneau 1988). First, notice that the amplitude (48) at the origin is proportional to $\mathrm{card}(B_k)=N_k$. In the large-k limit, this factor compensates the λ^{-2k} factor in (47).

According to (41) and (42), the pattern $\pi(B_k)$ may as well be considered as a product

$$m_{\pi(B_k)}=m_{\Omega_k}m_{[e_3,e_4]} \tag{49}$$

of the $[e_3, e_4]$ lattice by the characteristic function m_{Ω_k} of Ω_k. This means that the Fourier amplitude (48) is equivalent to†

$$\begin{aligned}\tilde{m}_{\lambda^k\pi(B_k)}(q)&=(\tilde{m}_{\Omega_k}*\tilde{m}_{\lambda^{-k}[e_3^*,e_4^*]})(\lambda^k q)\\&=\sum_{z\in[e_3^*,e_4^*]}\tilde{m}_{\Omega_k}(\lambda^k q-z).\end{aligned} \tag{50}$$

To keep track of the orders of magnitude, define

$$\omega_k=\lambda^{-k}\Omega_k \tag{51}$$

which is of order 1. Following §§ 2-4, it should be clear that ω_k is the oblique projection, with rational kernel E'_k, of γ. Then

$$\begin{aligned}m_{\Omega_k}(x)&=m_{\lambda^k\omega_k}(x)=m_{\omega_k}(\lambda^{-k}x)\\\tilde{m}_{\Omega_k}(q)&=\lambda^{2k}\tilde{m}_{\omega_k}(\lambda^k q).\end{aligned} \tag{52}$$

Inserting the above formula into (50) and using (47), we get the following expression for the Fourier transform:

$$\tilde{m}_{\chi_k}=\sum_{n\in Z^4}a(n)\delta_{\lambda^{-k}(n_1e_1^*+n_2e_2^*)} \tag{53}$$

with amplitudes equal to

$$a(n)=\tilde{m}_{\omega_k}[\lambda^k(n_1e_1^*+n_2e_2^*-n_3e_3^*-n_4e_4^*)]. \tag{54}$$

† The sum and convolution should be understood here as limits $N\to\infty$ of sums or integrals over $N\times N$ squares.

Through the linear isometry $e_1^* \to e_1'^*$, $e_2^* \to e_2'^*$, the argument on the RHS of (54) may be identified to the complementary projection†

$$\pi'(\boldsymbol{n}) = \sum n_i e_i'^*. \tag{55}$$

To get rid of the λ^k factors, change the summation variables in (53) to $\boldsymbol{\nu} = M^{-k}(\boldsymbol{n})$ so that (see (11))

$$\pi'(\boldsymbol{\nu}) = \pi' M^{-k}(\boldsymbol{n}) = \lambda^k \pi'(\boldsymbol{n}). \tag{56}$$

On the other hand, if p is the projector onto E^* with kernel $M^{-k}[e_3^*, e_4^*]$, we have

$$\begin{aligned} p(\boldsymbol{\nu}) = pM^{-k}(\boldsymbol{n}) &= n_1 pM^{-k}(\varepsilon_1^*) + n_2 pM^{-k}(\varepsilon_2^*) \\ &= \lambda^{-k}(n_1 e_1^* + n_2 e_2^*). \end{aligned} \tag{57}$$

Substitute (56) and (57) into (53) and (54):

$$\tilde{m}_{X_k} = \sum_{\nu \in \boldsymbol{Z}^4} \tilde{m}_{\omega_k}(\pi'(\boldsymbol{\nu}))\delta_{p(\nu)}. \tag{58}$$

This is the familar expression of the dual cut method. It allows a straightforward comparison of the approximant spectrum with the spectrum of the quasiperiodic octagonal tiling. A spot at $q = \pi(\boldsymbol{n})$ undergoes a shift proportional to $|q'|\lambda^{-2k}$; as to the corresponding intensity $I(q)$, the change is more tedious to evaluate because of the degeneracy in the rational projection. If we neglect such a degeneracy (an approximation which is valid as long as there is a node $\boldsymbol{n}$ which is much closer to q than all the others in $p^{-1}(q)$), the relative change is of the order of

$$\frac{\delta I(q)}{I(q)} = \lambda^{-4k} \begin{cases} O(q'^2) & \text{for } |q'| \ll R^{-1} \\ O(|q'|) & \text{for } |q'| \gg R^{-1} \end{cases}$$

where $2R$ is the diameter of the window approximated by a disc.

8. Conclusion

We may say a word as to the general problem of approximating irrational p-planes by rational ones in $\boldsymbol{R}^n$. First, when the dimension n is larger than 2, there is no natural ordering of the various approximants (the p-planes form a $p(n-p)$-dimensional manifold) so we lack general criteria to single out the best approximants—as the so-called convergents in 1D. Secondly, there is no systematic algorithm, like the continued fraction expansion in 1D, providing exponentially fast converging sequences. Because of the relative 'scarcity' of $\boldsymbol{Z}^n$ in $\boldsymbol{R}^n$, there seem to exist, e.g., p-planes in $\boldsymbol{R}^{2p}$, $p \geqslant 2$, which cannot be reached by iteration of a universal algebraic procedure.

However, nothing prevents us devising such an algorithm—and building the related sequence—for a suitable class of irrational subspaces: this is what we have done for the class of self-similar tilings. Tilings of this class are characterised by suitable algebraic numbers and are therefore far from generic. However, all the quasicrystals observed so far fall in this class.

† Whether we choose π' or $I - p$ does not really matter since both have kernel E^*; the map $(I-p)|_{E'}: E' \to E_k'$ (p defined right before (57)) is a dilation (it commutes with the fourfold rotations).

Besides modelling the large cell structures observed in some ternary alloys, the approximants also underlie theoretical investigations: the exact coincidence of the approximants with the quasiperiodic tiling on larger and larger cells allows studies or simulations of finite samples of the quasicrystal endowed with 'periodic boundary conditions' (for wave equations, statistical mechanical models, relaxations, etc...). Techniques based e.g. on the renormalisation group may then be used to control the limit to the true quasicrystal.

Appendix

This appendix specifies some properties of the windows associated with the n-dimensional unit cube; the notation is the same as in §§ 2-4.

Definition. Let $a_1, \ldots, a_n$ denote n vectors in a vector space. The (open) zonohedron W generated by $a_1, \ldots, a_n$ is the polyhedron

$$W = \left\{ \sum_{i=1}^{n} \lambda_i a_i \middle| 0 < \lambda_i < 1 \text{ for } i = 1, \ldots, n \right\}. \tag{A1}$$

Lemma. The subset $W_k = \pi_0'(\gamma_k)$ is the zonohedron spanned by the following n generators:

$a_i^{(k)} = \pi_0'[M^{-k}(\varepsilon_i)]$ where $\{\varepsilon_1, \ldots, \varepsilon_n\}$ is the standard basis of $\boldsymbol{R}^n$.

The following recursion formula holds:

$$a_i^{(k)} = \sum_{1}^{n} (M^{-1})_{j,i} a_j^{(k-1)}. \tag{A2}$$

Proof. Clearly $\gamma_k = M^{-k}(\gamma)$ is the fundamental cell of $\boldsymbol{Z}^n$ spanned by the n generators $M^{-k}(\varepsilon_i)$; thus

$$M^{-k}(\varepsilon_i) = \sum_{j=1}^{n} (M^{-k})_{j,i} \varepsilon_j$$

and

$$\gamma_k = \left\{ \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i (M^{-k})_{j,i} \varepsilon_j \middle| 0 < \lambda_i < 1 \right\}.$$

By projection on E_0' we obtain

$$a_i^{(k)} = \sum_{j=1}^{n} (M^{-k})_{j,i} a_i^{(0)} \qquad \text{where } a_i^{(0)} = \pi_0'(\varepsilon_i)$$

or

$$a_i^{(k)} = \sum_{j=1}^{n} (M^{-1})_{j,i} a_i^{(k-1)}$$

and

$$W_k = \left\{ \sum_{i=1}^{n} \lambda_i a_i^{(k)} \middle| 0 < \lambda_i < 1 \right\} = \left\{ \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i (M^{-k})_{j,i} a_i^{(0)} \middle| 0 < \lambda_i < 1 \right\}.$$

Remark. Since M belongs to the group $GL(n, \boldsymbol{Z})$, M^{-1} is a matrix with integer entries; the above formula shows that the generators $a_i^{(k)}$ of W_k are integer combinations of those of W_{k-1}. This property ensures a simple relation between the successive W_k.

References

Bak P 1986 *Phys. Rev. Lett.* **56** 861

Benker S E M 1982 *University of Technology, Eindoven TH-Report-WSK*

Cohn H 1980 *Advanced Number Theory* (New York: Dover)

de Bruijn N G 1981 *Nederl. Akad. Wetensch. Proc.* Ser A **43** 33-66

Duneau M 1988 *Du Cristal à l'Amorphe* ed C Godrèche (Paris: Editions de Physique)

Duneau M and Katz A 1985 *Phys. Rev. Lett.* **54** 2688

Elser V 1985 *Phys. Rev. Lett.* **54** 1730; *Phys. Rev.* B **32** 4982

Gardner M 1977 *Sci. Am.* **236** 110

Gratias D 1988 *Du Cristal à l'Amorphe* ed C Godrèche (Paris: Editions de Physique)

Kalugin P A, Kitaev A Yu and Levitov L C 1985a: *JETP Lett.* **41** 145

—— 1985b *J. Physique Lett.* **46** L601

Katz A and Duneau M 1986 *J. Physique* **47** 181

Mosseri R 1988 *Universalities in Condensed Matter* ed R Julien, L Peliti, R Rammal and N Boccara (Proceedings in Physics **32**) (Berlin: Springer)

Mosseri R, Oguey C and Duneau M 1988 *Quasicrystalline Materials.* (Proc. ILL-CODEST workshop) ed G Janot and J M Dubois (Singapore: World Scientific)

Oguey C, Duneau M and Katz A 1988 *Commun. Math. Phys.* **118** 99-108

Penrose R 1979 *Math. Intelligencer* **2** 32-7

Shechtman D, Blech I, Gratias D and Cahn J 1984 *Phys. Rev. Lett.* **53** 1951

Socolar J E S 1989 *Phys. Rev.* B **39** 10519

Verger-Gaugry J L 1988 *J. Physique* **49** 1867

Wang Z M and Kuo K M 1988 *Acta. Crystalogr.* A **44** 857-63