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Some Generalized Penrose Patterns from Projections of *n*-Dimensional Lattices

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Abstract

Examples of quasi-periodic plane tilings, consisting of rhombi and having n-fold rotational symmetry, are obtained by the projection method from a slice of an n-dimensional cubic lattice (with $n = 5, 7, 8, 9, 10$ and 12). A simplified geometrical description of the method is given. A comparison is made of some of the properties of these tilings with those of the Penrose patterns. The applicability of recursions (composition/decomposition or deflation/inflation) to generalized Penrose patterns with $n = 5$ is discussed.

1. Introduction

There has been much recent interest in reports of phases possessing non-crystallographic fivefold symmetry (Schechtman, Blech, Gratias & Cahn, 1984; Venkataraman, 1985), and more recently also tenfold (Bendersky, 1985; Fung, Yang, Zhou, Zhao, Zhan & Shen, 1986) and 12-fold symmetry (Ishimasa, Nissen & Fukano, 1985). Although doubt still exists as to whether they are based on quasi-periodic patterns rather than on lattices (Pauling, 1987), those with fivefold symmetry have been related to two- or three-dimensional Penrose patterns (Penrose, 1978; Mackay, 1982). Advances in the derivation of quasi-periodic patterns have been based on the work of de Bruijn (1981) who showed that Penrose patterns could be derived by projecting a five-dimensional cubic lattice, and suggested that this process could be generalized. This work has been extended by Kramer & Neri (1984), Duneau & Katz (1985), and Gähler & Rhyner (1986), who have established the mathematical basis of the process. Amongst their specifically illustrated results have been the three-dimensional Penrose pattern of Mackay, a generalized two-dimensional pattern of 72 and 36° rhombi that does not satisfy Penrose's 'forcing rules', and a two-dimensional pattern of 30, 60 and 90° rhombi with a degree of 12-fold symmetry.

More empirical work on quasi-periodic patterns with symmetry other than 5 has been that by Amman [reported by Grünbaum & Shepherd (1987), pp. 554–558] and by Watanabe, Ito & Soama (1987), who have derived two different recursion definitions for the same pattern with eightfold symmetry, along the lines of the original derivation of the Penrose patterns. Amman also defined an aperiodic set of two prototiles with edges decorated in such a way as to force the pattern.

We have followed de Bruijn's method, but have made use of the properties of the symmetry operations that we have discussed previously (Whittaker & Whittaker, 1986) in order to make the derivation as geometrical as possible, and thereby understandable to a wider readership. Following our method we have computed many quasi-periodic patterns having explicit n-fold rotational symmetry with $n = 5$, 7, 8, 9, 10 and 12, and we illustrate some representative examples of these patterns. We derive a general rule for the numbers and proportions of different kinds of rhombus involved in these patterns, and suggest that it is desirable for some purposes to define such 'kinds of rhombus' slightly differently from Gähler & Rhyner (1986), so our rule differs from theirs. We discuss the relevance of the concept of the 'Weiringa roof' (de Bruijn, 1981) to these generalized patterns, and also the applicability to them of the kind of recursion relationships previously discussed for particular fivefold and eightfold patterns by Penrose (1978), Amman (in Grünbaum & Shepherd, 1987) and Watanabe *et al.* (1987).

2. Geometrical derivation of the tilings

There is in n dimensions a symmetry operation of the cubic lattice which permutes all the n axes in order and which is exemplified by the operations represented by

$$\mathbf{M}_3 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \mathbf{M}_4 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\mathbf{M}_5 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \ldots,$$

for $n = 3, 4, 5, \ldots$ dimensions respectively.

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For $n \geq 3$ this has the properties that it leaves the axis $[1\,1\,1\ldots 1]$ invariant and that the set of vectors for which the effect of $\mathbf{M}_n$ is a rotation through $2\pi/n$ forms a two-dimensional plane $\mathbf{\Pi}$. The projection of the positive parts of the n axes on to this plane is a set of equally spaced half-lines emanating from a central point with angles $2\pi/n$ between adjacent pairs.*

In the case $n=5$ de Bruijn (1981) has shown how projecting a certain slice of the five-dimensional cubic lattice on to a plane parallel to this $\mathbf{\Pi}$ can give rise to the Penrose pattern. We here examine and exhibit the results of applying the same process for $n \geq 3$.

For n odd $\mathbf{M}_n$ can be expressed relative to suitable orthogonal axes in the form

$$\begin{pmatrix} \mathbf{R}_1 & & & \\ & \mathbf{R}_2 & & \\ & & \ddots \; \mathbf{R}_m & \\ & & & 1 \end{pmatrix}$$

where $m=(n-1)/2$, each $\mathbf{R}_k$ is the 2×2 block

$$\begin{pmatrix} \cos 2\pi k/n & -\sin 2\pi k/n \\ \sin 2\pi k/n & \cos 2\pi k/n \end{pmatrix},$$

and the rest of the matrix contains only zeros.

For n even the form is

$$\begin{pmatrix} \mathbf{R}_1 & & & & & \\ & \mathbf{R}_2 & & & & \\ & & \ddots & & & \\ & & & \mathbf{R}_{m'} & & \\ & & & & -1 & \\ & & & & & 1 \end{pmatrix}$$

where $m'=(n-2)/2$. When $\mathbf{M}_n$ is expressed in this form the plane $\mathbf{\Pi}$ is that spanned by the axes of the first two coordinates. This plane can be found in the manner we have described in our discussion of four-dimensional fivefold symmetry (Whittaker & Whittaker, 1986).

Following de Bruijn (1981) we project on to $\mathbf{\Pi}$ those points $\mathbf{k}$ of the cubic lattice whose 'open cube' $\{(x_0, x_1, \ldots, x_{n-1})\colon k_i - 1 < x_i < k_i \text{ all } i\}$ intersects the plane $\boldsymbol{\gamma}+\mathbf{\Pi}$, where $\boldsymbol{\gamma}=(\gamma_0, \gamma_1, \ldots, \gamma_{n-1})$. We here exclude any consideration of the cases (involving particular values of $\boldsymbol{\gamma}$ and corresponding to de Bruijn's 'singular cases') in which the process does not lead to a complete and unambiguous tiling of the plane by rhombi.

* Projection of the operations $\mathbf{M}_n$ down $[1\,1\,1\ldots 1]$ leads to the family of symmetry operations described by Whittaker & Whittaker (1986, p. 397). In particular $\mathbf{M}_5$ projects to a V operation in four dimensions, which can be expressed as a double fivefold rotation about absolutely perpendicular planes which are crystallographically irrational.

3. General consideration of the projections

The square faces of the n-dimensional cubes may be distinguished in terms of the relationship between the axes that define their edges, and these distinctions control the kinds of rhombus into which they project. Since the n axes $x_0, x_1, \ldots, x_{n-1}$ are transformed cyclically by the operation $\mathbf{M}_n$ we can distinguish the rhombi as follows:

First kind: projection of a face bounded by two adjacent axes, *e.g.*

$$[1\,0\,0\ldots 0] \quad \text{and} \quad [0\,1\,0\ldots 0].$$

Second kind: projection of a face bounded by axes with one space between, *e.g.*

$$[1\,0\,0\ldots 0] \quad \text{and} \quad [0\,0\,1\ldots 0].$$

rth kind: projection of a face bounded by axes with $r-1$ spaces between.

The number of kinds of cube face distinguished in this way is $(n-1)/2$ for n odd and $n/2$ for n even, but in the latter case one of these faces is perpendicular to the plane of the projection and so does not give rise to a rhombus. There are therefore $(n-1)/2$ kinds of rhombus for n odd and $(n-2)/2$ for n even. A rhombus of the rth kind has angles $2\pi r/n$ and $\pi - 2\pi r/n$. In the diagrams distinctions between the kinds of rhombus are emphasized by shading parallel to the bisector of the angle $2\pi r/n$, except for those in each tiling that have $r=r_{\max}$ which are left unshaded. When n is even the rhombi of kinds r and $n/2-r$ are of the same shape but for reasons that will appear in § 5 we regard them as of different kinds, and they are shaded parallel to opposite diagonals. When $n=4m$ the rhombi of kind $n/4$ are squares and the shading direction is parallel to the positive bisector of the two axes. In Fig. 1(*b*) the squares are shaded even though they correspond to $r=r_{\max}=1$.

4. The tilings

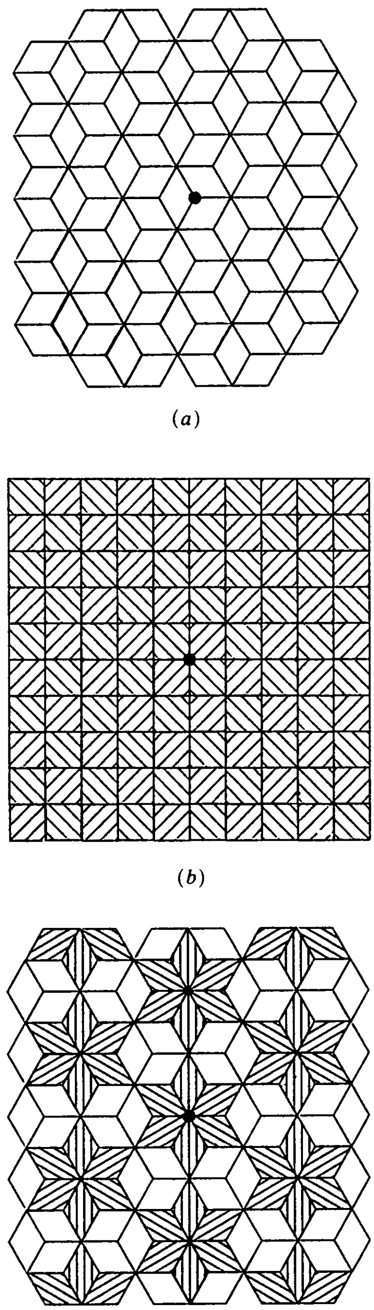
If the vector $\boldsymbol{\gamma}$ is parallel to the axis $[1\,1\,1\ldots 1]$ then the tiling produced by the projection has global n-fold rotational symmetry about the origin, and the examples shown here are confined to this case. If the n equal components of $\boldsymbol{\gamma}$ are denoted γ, then the value of γ serves to identify a given pattern. In the figures the origin of each pattern, about which it has global n-fold symmetry, is shown by a dot.

$n=3, 4$ and 6

In these cases the projection plane $\mathbf{\Pi}$ is parallel to a rational crystallographic plane of the n-dimensional lattice, and so its intersections with the (n-dimensional) cubic cells repeat regularly. The resulting tilings are therefore all periodic, as has already been shown by Kramer & Neri (1984). However, we illustrate them in Fig. 1 for comparison with other cases, and because they illuminate the general idea of the projection method, especially in the well known case of $n = 3$. If the distinction between the two kinds of rhombus for $n = 6$ is ignored then this tiling becomes the same as that for $n = 3$ with a shift of origin. The patterns are independent of the value of γ.

$n = 5$

If γ is chosen such that $\sum_i \gamma_i = 0 \pmod 1$ then the projection is a Penrose pattern. Suitable choice of γ can bring either of the two possible global fivefold symmetry points to the origin, as illustrated in Figs. 2(a) and (b). When $\sum_i \gamma_i = 0{\cdot}5 \pmod 1$ the patterns

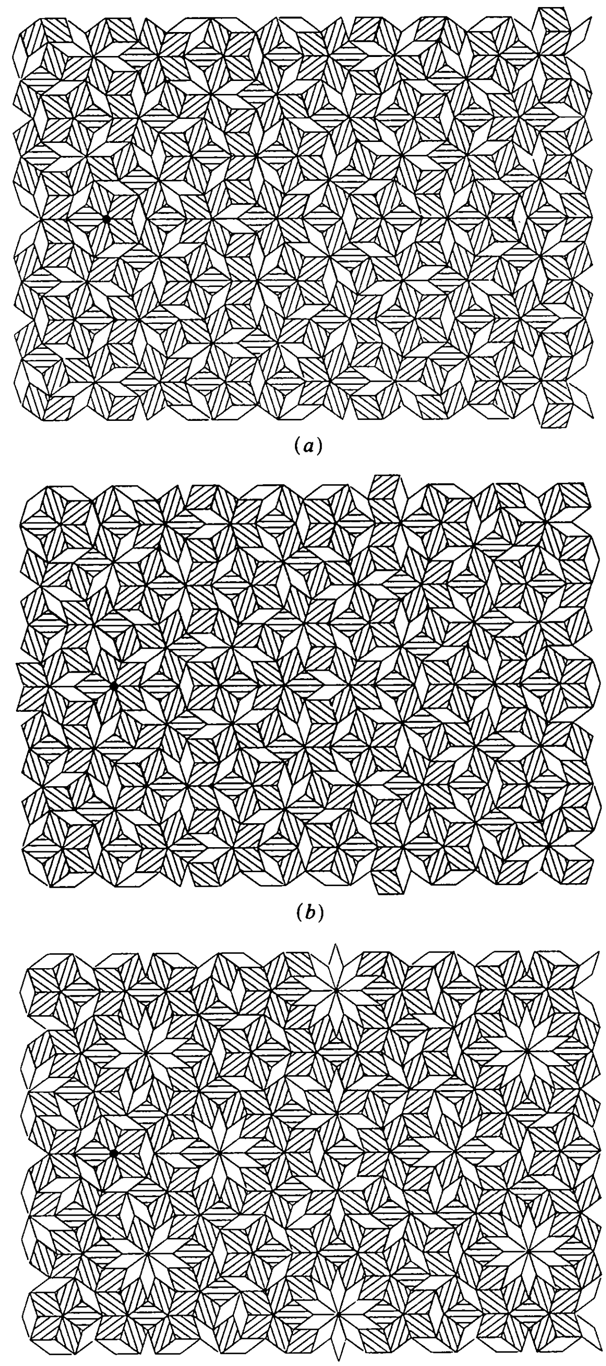


(a)

(b)

(c)

Fig. 1. The projections which give periodic tilings. (a) $n = 3$; (b) $n = 4$; (c) $n = 6$.



(a)

(b)

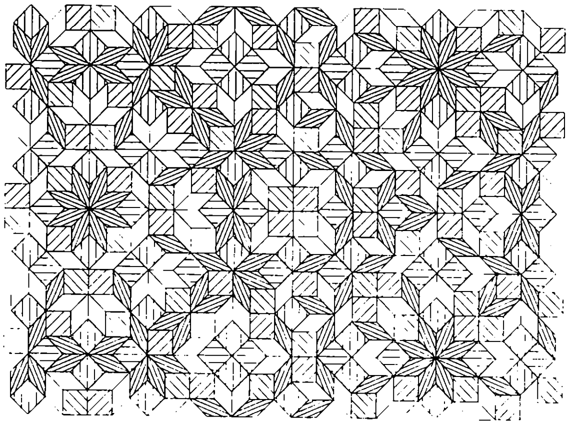
(c)

Fig. 2. Projections with $n = 5$. (a) $\gamma = 0{\cdot}2$; (b) $\gamma = 0{\cdot}4$; (c) $\gamma = 0{\cdot}1$. (a) and (b) are Penrose patterns but (c) is not.

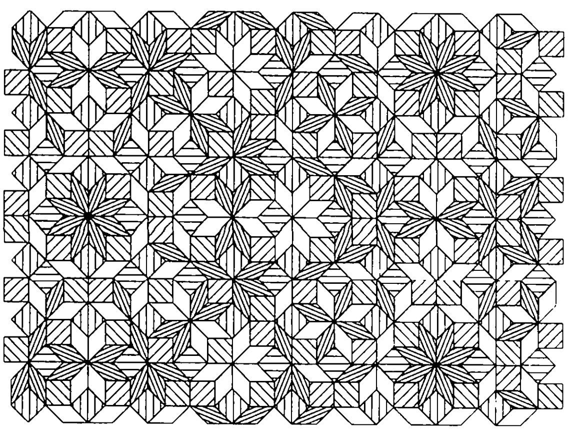
contain many points of local tenfold symmetry, and an example is shown in Fig. 2(c). Other characteristic features occur for different values of γ.

$n = 8$

This case is particularly interesting as it is the only one apart from $n = 5$ (and the periodic one $n = 6$) that is based on rhombi of only two *shapes*, though they are of three kinds, and for which a tiling has been derived by recursion; it has in fact been defined by two different recursions by Amman (Grünbaum & Shepherd, 1987) and by Watanabe *et al.* (1987). Their tiling can be obtained with $\gamma = 0{\cdot}25$ and is shown in Fig. 3(b). However with $n = 8$ the condition $\sum_i \gamma_i = 0 \pmod 1$ is not sufficient to ensure that the tiling conforms to the known recursion, and another with a different value of γ is shown in Fig. 3(a).



(a)

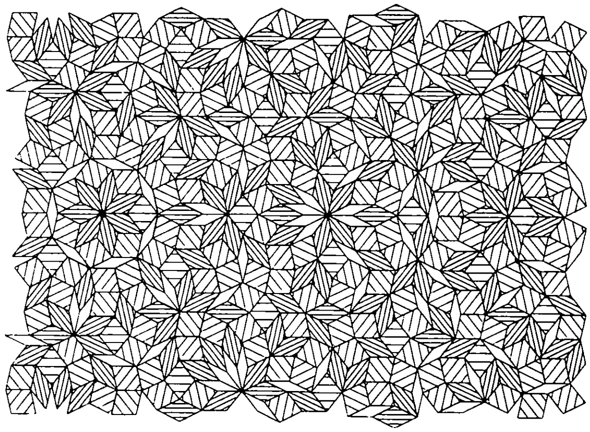


(b)

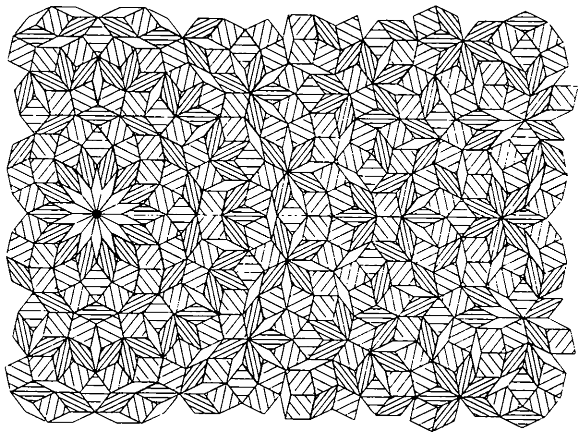
Fig. 3. Projections with $n = 8$. (a) $\gamma = 0{\cdot}125$; (b) $\gamma = 0{\cdot}25$: the tiling devised by Amman (Grünbaum & Shepherd, 1987) and Watanabe *et al.* (1987).

$n = 7$, 9, 10 *and* 12

Examples chosen from the many possibilities that arise with these values of n are shown in Figs. 4–7.



(a)



(b)

Fig. 4. Projections with $n = 7$. (a) $\gamma = 0{\cdot}142857$; (b) $\gamma = 0{\cdot}5$.

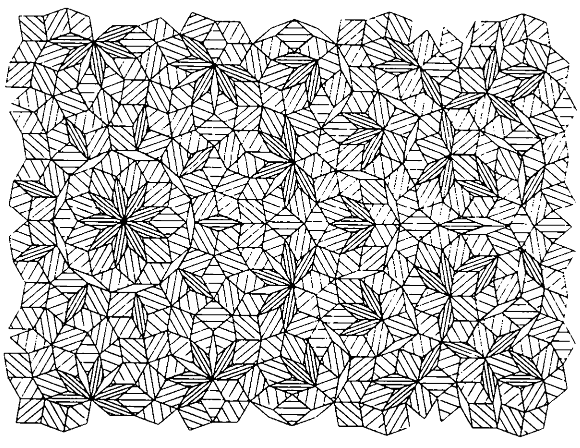


Fig. 5. A projection with $n = 9$; $\gamma = 0{\cdot}111111$.

5. Properties of the tilings

The tilings share the following properties with the Penrose patterns.

(i) For every n there exists a tiling in which the rhombi are arranged radially in order of their kind r_i, from r_1 to r_{max}, around the origin. Those of the kind with r_{max} border a regular $2n$-gon (n odd) or a regular n-gon (n even). Such tilings are given when $\gamma = 1/n$, and their central feature bears a close analogy to that of the fivefold Penrose pattern of Fig. 2(a). When $\gamma = (n-1)/2n$, for n odd, the central feature has a star-like nature, though it is less directly analogous to the corresponding pattern of Fig. 2(b).

(ii) Rhombi of the same kind that share an edge are never in parallel orientations; if they are squares they differ in inherent orientation as shown by the shading. Adjacent rhombi of different kind but the same shape may have their edges in parallel orientation.

For all $n \neq 3$, 4 or 6 the tilings share the following further properties with the Penrose patterns.

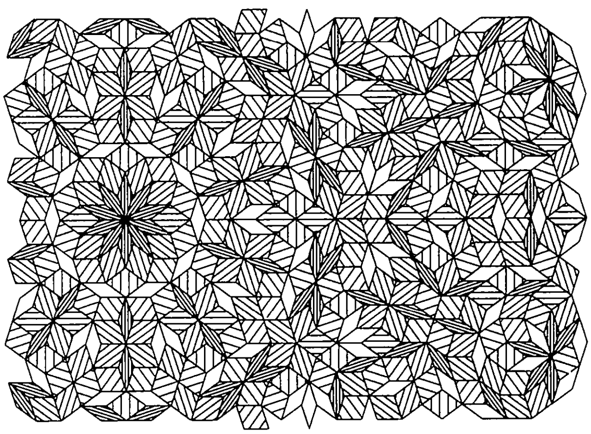


Fig. 6. A projection with $n = 10$; $\gamma = 0{\cdot}1$.

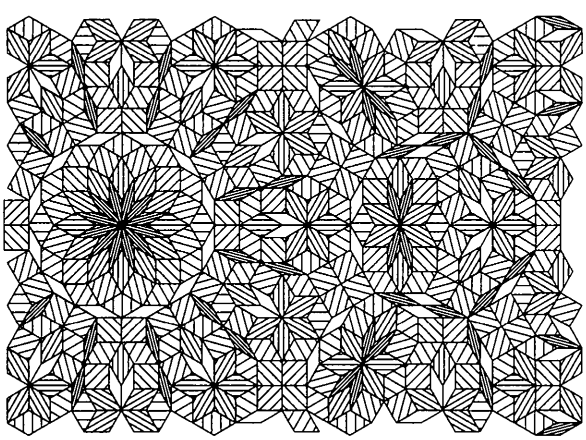


Fig. 7. A projection with $n = 12$; $\gamma = 0{\cdot}083333$.

(iii) The numbers of the different kinds of rhombus per unit area are in the ratio of their areas, as shown in the Appendix. If the distinction were not made between different kinds of rhombus with the same shape this simple relationship would break down for n even.

(iv) Although a finite area of tiling contains at most one point of global n-fold rotational symmetry it may contain many points with local n-fold rotational symmetry and local mirror lines.

(v) Since the plane $\boldsymbol{\gamma} + \boldsymbol{\Pi}$ is irrational any point $\mathbf{k}$ of the n-dimensional cubic lattice is situated differently in relation to it from any other (except those to which it may be symmetrically related *via* the operation $\mathbf{M}_n$). However, a point $\mathbf{k}'$ of the lattice can be found such that $\mathbf{k} - \mathbf{k}'$ can be made as nearly parallel to the plane as desired. Provided that no point of the lattice lies on the plane $\boldsymbol{\gamma} + \boldsymbol{\Pi}$ (and not more than one point can lie on it), it can be shown that any patch of the pattern containing finitely many rhombi appears infinitely many times, and the distance between such similar patches increases with their size. The latter property has been verified empirically on some of the drawings, though in other cases the similarity distance seems to be too large to be visible within the area of the tiling that it is convenient to generate.

6. Weiringa roofs of order *n*

Weiringa (reported by de Bruijn, 1981) has pointed out that the vertices of a tiling by Penrose rhombi [as in Figs. 2(a) and (b)] may be indexed with integers that differ by 1 along any edge and which are restricted to four values which may be regarded as running from 1 to 4. In the present derivation these indices are equivalent to the value of

$$h = \sum_{i=0}^{n-1} x_i$$

where x_i is the ith coordinate of the corresponding point of the n-dimensional lattice. In general h may take a number N of consecutive integral values where

$$N = (n+5)/2 \quad \text{for } n \text{ odd}$$

and

$$N = (n+4)/2 \quad \text{for } n \text{ even,}$$

but in special cases [like the Penrose tilings of Figs. 2(a) and (b)] it is restricted to $N-1$ such values. If each vertex of the tiling is raised to a distance above the plane proportional to h then an undulating 'roof' is obtained. With $n = 5$ and heights of $h\sin 18°$ the roof is composed of only one shape of rhombus. This is true for tilings like Fig. 2(c) as well as for Penrose tilings.

No corresponding reduction in the number of shapes of rhombus occurs for $n \neq 5$. However, the concept is not without its uses in considering other patterns. For example the 'roof' form of Fig. 6 with $n = 10$ contains decagonal pyramidal peaks, whereas the apparently similar tenfold centres in Fig. 2(c) consist of radially arranged ridges and valleys, with fivefold symmetry in the 'roof' form. A similar distinction applies to the sixfold centres with $n = 6$ and $n = 3$.

7. Recursive relationships

The quasi-periodic tilings by rhombi that have previously been discovered independently of the projection method have been definable by recursive relationships described as composition and decomposition or inflation and deflation. For the Penrose patterns the scale factor in this process is $\varphi = (1+\sqrt{5})/2$, for Amman's set $A5$ it is $1+\sqrt{2}$, and for the same pattern in the terms discussed by Watanabe *et al.* (1987) it is $2+\sqrt{2}$.

In a first approach to extending such relationships to more general cases we confine our attention to $n = 5$ and take as our scale factor $1+\varphi$. Since this equals φ^2 it corresponds to two applications of Penrose's recursion, and leads from Fig. 2(a) or (b) to a self-similar pattern turned through 36° about the origin. In this case the decomposition of all the rhombi is as shown in Fig. 8. A similar procedure can be applied to Fig. 2(c) to produce a self-similar pattern turned through 36°, but it is necessary to accept seven different decomposition types of 72° rhombi and four different decomposition types of 36° rhombi, not counting enantiomorphs of those that do not possess mirror symmetry (Fig. 9). In decomposing any rhombus it is necessary to take account of its polarity, which is shown in Figs. 8 and 9 by a + sign

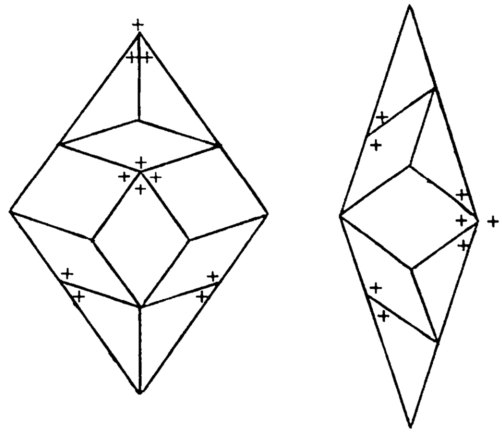


Fig. 8. Decomposition with a scale factor of φ^2 for $n = 5$, $\gamma = 0{\cdot}2$ and $0{\cdot}4$ (Penrose patterns). For $\gamma = 0{\cdot}2$ [Fig. 2(a)] the 72° rhombus has its 'positive' end at the origin; for $\gamma = 0{\cdot}4$ [Fig. 2(b)] it has its 'negative' end at the origin.

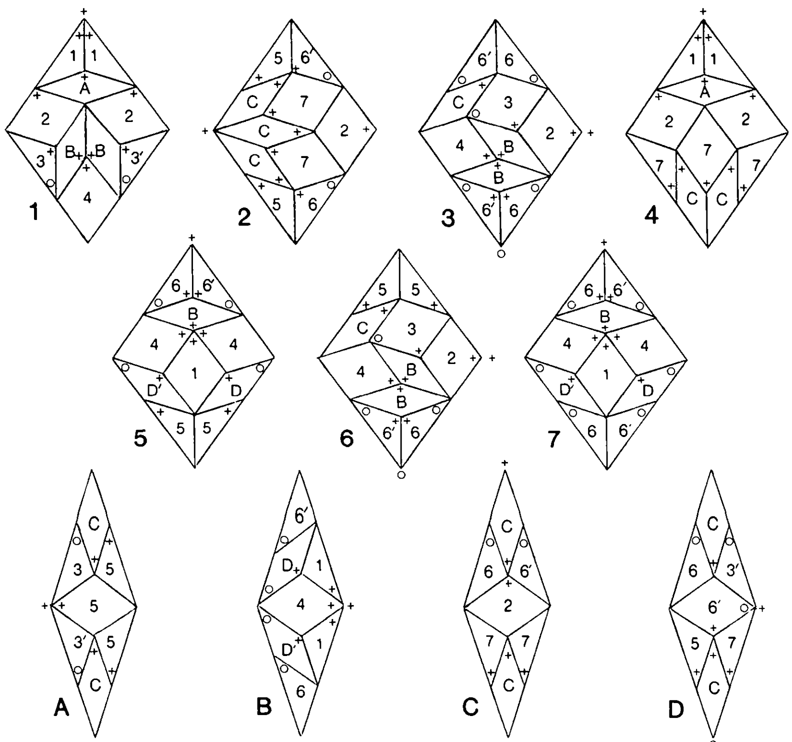


Fig. 9. Decomposition types for $n = 5$, $\gamma = 0{\cdot}1$, $0{\cdot}3$ and $0{\cdot}5$. Types 3′, 6′ and D' are mirror images of 3, 6, and D respectively. For $\gamma = 0{\cdot}1$ [Fig. 2(c)] type 1 has its 'positive' end at the origin; for $\gamma = 0{\cdot}3$ and $0{\cdot}5$ (not illustrated) types 5 and C respectively have their 'negative' ends at the origin.

at one vertex, and where necessary by a small circle at another vertex.

The set of decomposition types in Fig. 8 applies to patterns derived with $\gamma = 0{\cdot}2$ and $0{\cdot}4$ and is the simplest case. The set in Fig. 9 applies to patterns with $\gamma = 0{\cdot}1$, $0{\cdot}3$ and $0{\cdot}5$ and is the next simplest case. In considering other values of γ it is necessary to take account of a specific feature of Fig. 9. Types 5 and 7 do not differ in the geometrical arrangement of their parts after one stage of decomposition, but only after two stages; they may be said to differ at a depth of two stages. The same is true of types 3 and 6, and of types *A*, *C* and *D*. When γ departs from one of the simple values ($0{\cdot}1, 0{\cdot}2$ *etc.*) by an arbitrarily small amount the pattern only changes beyond a correspondingly large radius, and therefore the number of decomposition types will be indefinitely large owing to differences at an indefinite depth of decomposition. Only for certain special values of γ can one expect to find practicably definable sets of decomposition types.

When a set of decomposition types can be defined then it appears to be possible to decorate the edges of the rhombi of each type in distinctive ways so as to define an aperiodic set of prototiles corresponding to a set of forcing rules for assemblage into the pattern.

8. Concluding remarks

Non-periodic ('quasi-periodic') tilings exist which possess at most one point of global n-fold rotational symmetry but many points having such symmetry locally, for all values of $n \neq 2, 3, 4$ and 6. They have many properties in common with the fivefold Penrose patterns, although they are generally more complex. However, there seems to be no *prima facie* reason why their differences from these patterns should preclude their occurrence as quasi-lattices of quasi-crystalline phases if such phases exist. More detailed study is in progress of the relationships of the tilings and of their recursive properties to the vector $\boldsymbol{\gamma}$ used in their derivation.

We thank P. M. de Wolff for initially drawing our attention to the possible relationship of Penrose patterns to the fivefold symmetry operation of four-dimensional crystallography, and R. Penrose for encouraging us to pursue the study at an early stage.

APPENDIX
The proportions of rhombi of different kinds

The pattern is defined as the projection on to a plane $\boldsymbol{\Pi}$ of certain squares of the n-dimensional lattice that bound cubes which are intersected internally by $\boldsymbol{\gamma} + \boldsymbol{\Pi}$. Hence the 'average direction' of those squares whose projections constitute the pattern must be the same as the direction of $\boldsymbol{\Pi}$.

The condition that a vector $\mathbf{x}$ lies in $\boldsymbol{\Pi}$ can be expressed in the form

$$(\mathbf{M}^2 - 2\mathbf{M} \,.\, \cos 2\pi/n + \mathbf{I}) \,.\, \mathbf{x} = \mathbf{0}$$

(Whittaker & Whittaker, 1986). Two independent solutions of this are always

$$(0, \sin 2\pi/n, \sin 4\pi/n, \ldots, \sin 2(n-1)\pi/n)$$

and

$$(1, \cos 2\pi/n, \cos 4\pi/n, \ldots, \cos 2(n-1)\pi/n).$$

Thus the plane $\boldsymbol{\Pi}$ is spanned by vectors

$$\sum_{j=0}^{n-1} \mathbf{e}_j \sin 2\pi j/n \quad \text{and} \quad \sum_{j=0}^{n-1} \mathbf{e}_j \cos 2\pi j/n$$

where $\mathbf{e}_j$ is the unit vector along the jth axis.

Let $\boldsymbol{\tau}$ be the projection on to the 3-space S spanned by $\mathbf{e}_0$, $\mathbf{e}_1$, and $\mathbf{e}_r$ $(2 \leq r \leq n-1)$, *i.e.*

$$\boldsymbol{\tau}\left(\sum_{j=0}^{n-1} x_j \mathbf{e}_j\right) = x_0\mathbf{e}_0 + x_1\mathbf{e}_1 + x_r\mathbf{e}_r.$$

Then in S the projection $\boldsymbol{\tau}(\boldsymbol{\Pi})$ is spanned by

$$\mathbf{e}_1 \sin 2\pi/n + \mathbf{e}_r \sin 2\pi r/n$$

and

$$\mathbf{e}_0 + \mathbf{e}_1 \cos 2\pi/n + \mathbf{e}_r \cos 2\pi r/n.$$

A vector normal in S to $\boldsymbol{\tau}(\boldsymbol{\Pi})$ is

$$\mathbf{e}_0 \sin 2(r-1)\pi/n - \mathbf{e}_1 \sin 2\pi r/n + \mathbf{e}_r \sin 2\pi/n.$$

Of those squares whose projections on to $\boldsymbol{\Pi}$ appear as rhombi of the pattern only those with sides parallel to $\mathbf{e}_0$ and $\mathbf{e}_1$, $\mathbf{e}_0$ and $\mathbf{e}_r$, or $\mathbf{e}_1$ and $\mathbf{e}_r$ have projections by $\boldsymbol{\tau}$ on to squares in S (all other squares are edge-on to S). These produce rhombi in the pattern of the first, rth and $(r-1)$th kinds respectively, and we denote the relative frequency of rhombi of the rth type in the pattern as p_r. Then in S we have squares as follows:

Sides parallel to	Normal vector	Relative frequency
$\mathbf{e}_0, \mathbf{e}_1$	$\mathbf{e}_r$	p_1
$\mathbf{e}_0, \mathbf{e}_r$	$-\mathbf{e}_1$	p_r
$\mathbf{e}_1, \mathbf{e}_r$	$\mathbf{e}_0$	p_{r-1}.

The sign of $\mathbf{e}_1$ here ensures that all these make an acute angle with the normal vector to $\boldsymbol{\tau}(\boldsymbol{\Pi})$ above.

Hence the average normal vector* of these squares is

$$p_{r-1}\mathbf{e}_0 - p_r\mathbf{e}_1 + p_1\mathbf{e}_r$$

* The distance from the plane $\boldsymbol{\gamma} + \boldsymbol{\Pi}$ of points of the lattice which project to points of the pattern is bounded. The average normal vector of the squares which project to rhombi in any patch R of the pattern will therefore tend to this limit as the size of R increases whatever its shape or position, and so the pattern is metrically balanced in the sense defined by Grünbaum & Shepherd (1987).

and this must be normal to $\boldsymbol{\tau}(\boldsymbol{\Pi})$ in S. Hence

$$(p_{r-1}\mathbf{e}_0 - p_r\mathbf{e}_1 + p_1\mathbf{e}_r).(\mathbf{e}_1 \sin 2\pi/n + \mathbf{e}_r \sin 2\pi r/n) = 0$$

giving

$$p_1/(\sin 2\pi/n) = p_r/(\sin 2\pi r/n).$$

Since the area of a rhombus of the rth kind with unit sides is $\sin 2\pi r/n$, it follows that the frequency with which the different kinds of rhombi occur is in proportion to their areas. For all values of $n \neq 3$, 4 or 6 some ratios of $\sin 2\pi/n : \sin 2\pi r/n$ are irrational, which conforms with an earlier proof of the non-periodicity of Penrose tilings.

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Restrained Refinement of Two Crystalline Forms of Yeast Aspartic Acid and Phenylalanine Transfer RNA Crystals

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Abstract

Four transfer RNA crystals, the monoclinic and orthorhombic forms of yeast $tRNA^{Phe}$ as well as forms *A* and *B* of yeast $tRNA^{Asp}$, have been submitted to the same restrained least-squares refinement program and refined to an *R* factor well below 20% for about 4500 reflections between 10 and 3 Å. In yeast $tRNA^{Asp}$ crystals the molecules exist as dimers with base pairings of the anticodon (AC) triplets and labilization of the tertiary interaction between one invariant guanine of the dihydrouridine (D) loop and the invariant cytosine of the thymine (T) loop (G19-C56). In yeast $tRNA^{Phe}$ crystals, the molecules exist as monomers with only weak intermolecular packing contacts between symmetry-related molecules. Despite this, the tertiary folds of the *L*-shaped tRNA structures are identical when allowance is made for base sequence changes between $tRNA^{Phe}$ and $tRNA^{Asp}$. However, the relative mobilities of two regions are inverse in the two structures with the AC loop more mobile than the D loop in $tRNA^{Phe}$ and the D loop more mobile than the AC loop in $tRNA^{Asp}$. In addition, the T loop becomes mobile in $tRNA^{Asp}$. The present refinements were performed to exclude packing effects or refinement bias as possible sources of such differential dynamic behavior. It is concluded that the transfer of flexibility from the anticodon to the D- and T-loop region in $tRNA^{Asp}$ is not a crystalline artefact. Further, analysis of the four structures supports a mechanism for the flexibility transfer through base stacking in the AC loop and concomitant variations in twist angles between base pairs of the anticodon helix which propagate up to the D- and T-loop region.

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1. Introduction

Biological macromolecules often present crystalline polymorphism and this effect is particularly pronounced with tRNA molecules (Dock, Lorber, Moras, Pixa, Thierry & Giegé, 1984). Such a polymorphism offers the possibility of studying different conformational states of the molecules. The crystal structures of two crystal forms of yeast aspartic acid tRNA ($tRNA^{Asp}$) have recently been refined to an *R* factor below 20% at 3 Å resolution (Westhof, Dumas & Moras, 1985; Dumas, Westhof & Moras, 1988). For these refinements, a restrained least-squares program,