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A Novel Algorithm for a Quasiperiodic Plane Lattice with Fivefold Symmetry

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Abstract

Conventionally, Penrose tilings with fivefold symmetry are constructed with the aid of two characteristic rhombic tiles and sets of rules based on either matching of markings on the tiles or their subdivision. Both these procedures involve decision making when tiling is to be done extensively. In the present communication, a fool-proof method of producing Penrose tilings using a set of operations that can be repeated *ad infinitum* is described. The steps in the present procedure are akin to conventional crystallographic operations and can be expressed in simple mathematical terms which bring out some interesting aspects of Penrose tilings.

Introduction

The pioneering work of Penrose (1974) on tiling a floor (Gardner, 1977) to generate patterns exhibiting fivefold rotational symmetry, extension of these ideas to three dimensions by Mackay (1981) and the subsequent discovery by Shechtman, Blech, Gratias & Cahn (1984) of quasicrystals with icosahedral symmetry have generated world-wide interest. Several methods are now available for the generation of two-dimensional aperiodic tilings with forbidden rotational symmetry. These range in approach from the empirical matching rules of Penrose, the geometrical approach of Sasisekharan (1986) and dualization of periodic pentagrids to projection from higher-dimensional space (de Bruijn, 1981). The procedure of tiling due to Penrose involves assembling two types of rhombs, *viz* a prolate (or thick) rhomb with acute angle $2\pi/5$ and an oblate (or thin) rhomb with acute angle $\pi/5$, or a set of kites and darts. For example, the process of building an infinitely large tiling with these two types of rhombs consists of marking them and laying them edge to edge such that the markings match according to set rules so that aperiodicity and fivefold symmetry are ensured. The matching rules are an expression of the self-similarity transformation of the Penrose tiling. Hitherto, this transformation has been exploited to generate a large cluster of tiles from a cluster of a smaller number of tiles obeying the matching rules by subdividing each of its rhombs according to a set pattern. The resultant tiling then

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automatically conforms to matching rules and has rhombs of similar shape but smaller size leading to an 'inflation' in the number of tiles and vertices in the aperiodic lattice. In this communication, we demonstrate that a correct Penrose tiling (one without 'mistakes') (Penrose, 1989) can be generated by a new method starting from only the single thick rhomb. This is achieved by repeatedly performing a given set of operations on the rhomb. Each of these operations is akin to normal crystallographic operations and they are easily expressed through simple mathematical formulae. It will also be shown that the present approach brings out certain interesting aspects with respect to the coordinates of vertices in a two-dimensional Penrose tiling.

The procedure

Consider a thick rhomb *OBCD* (Fig. 1*a*). It fixes the domain to be tiled and can be chosen to be as large as desired. The first of these operations (the α operation) on the rhomb consists of several steps: (i) a twofold rotation around the shorter diagonal, *DB*, of the rhomb; (ii) a translation of every point of the rhomb along a line joining the point to the centre of the rhomb by the distance $1/\tau^2$ times the original distance of the point from the centre. Effectively, this step of the α operation reduces the size of the original rhomb by the golden mean, τ; (iii) a further downward translation of every point obtained by step (ii) through a distance $1/\tau^2$ times the major diagonal of the rhomb.

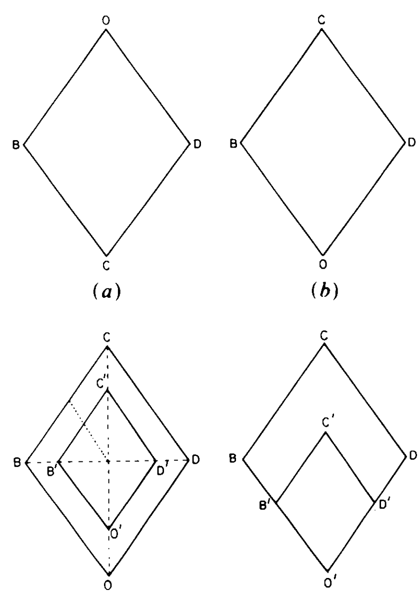


Fig. 1. The sequence of steps involved in the α operation. (*a*) The starting rhomb. (*b*)–(*d*). The steps of rotation and translation. It may be noted that the regions *CBC'DC* and *BO'DC'B* are the conventional kite and dart regions, respectively.

The second operation, the β operation, consists of rotating every point of the half-rhomb *C'D'O'* clockwise through $\pi/5$ around *C'* and translating them parallel to *CO'* such that *C'D'O'* coincides with *CC'B'*. A similar operation on the other half-rhomb *C'B'O'* with an anticlockwise rotation of $\pi/5$ about *C'* results in the domain *CC'D* (Fig. 2*a*).

The third operation, the γ operation, consists of rotating every point of the half-rhomb *C'D'O'* clockwise through $2\pi/5$ about *C'* and retaining all points which fall in the domain *C'BB'*. A similar operation is performed anticlockwise with respect to *C'B'O'* to obtain points in the domain *C'DD'* (Fig. 2*b*).

Performance of the α, β and γ operations in that sequence or in the sequence α, γ and β completes one 'generation' of inflation. At the end of the first sequence of operations the pattern generated inside the rhomb is identical to that obtained by using the recursive rule for the subdivision of the rhomb (de Bruijn, 1981). The same set of operations, in the chosen sequence, can be performed repeatedly until

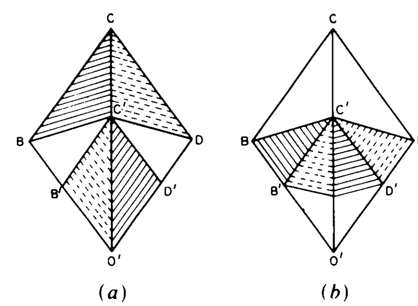


Fig. 2. (*a*) The hatched region *O'C'D'* is shifted to *BCC'* as a result of the β operation and the region *O'C'B'* goes to *DCC'* after the operation. (*b*) Part of *O'C'D'* is rotated clockwise through $2\pi/5$ to superimpose on the domain *BC'B'* as a result of the γ^+ operation. The γ^- operation takes part of *O'C'B'* to *DC'D*.

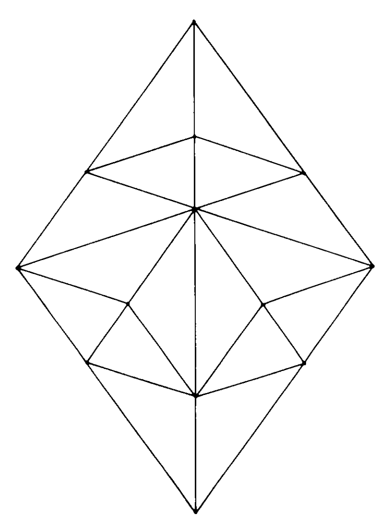
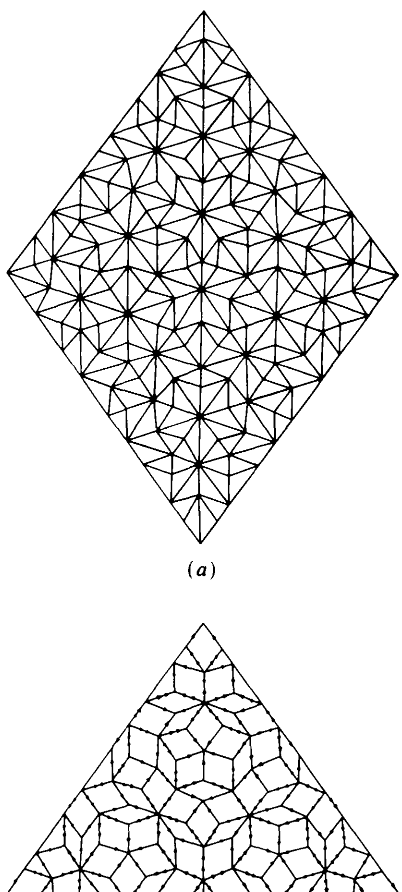


Fig. 3. Appearance of the rhomb in the third generation.

the desired size of individual tiles is reached. Fig. 3 shows the resultant pattern after three generations of inflation. A point to be noted is that, on conducting the β and γ operations, a domain like $C'O'D'$ alternately gets rotated through $\pm\pi/5$ and $\pm2\pi/5$, respectively, during consecutive generations. This is a result of the twofold rotation of the rhomb as the first step in the α operation of every generation. We designate the operations involving the clockwise rotations as β^+ and γ^+ and those associated with anticlockwise rotations as β^- and γ^-. At the level of the third generation, it may be observed from Fig. 3 that not all the eight possible types of configurations of the rhomb at a point (or vertices) that have been described by Henley (1986) are present. Fig. 4 shows the pattern when the operations were repeated for six generations. Note that the resultant pattern has a large number of bonds which are not equal in length to the edge length a of the rhomb. When such bonds are neglected (or erased) we get bond orientational order and the tiling is according to the Penrose matching rules. This is demonstrated by the corresponding arrowed pattern in Fig. 4(b). In this pattern, all of the eight possible types of vertices appear for the first time. During further generations, their numbers increase and tend towards the τ related frequencies reported by Henley. The rhomb depicted in Fig. 4(b) can be rotated through $2\pi/5$ repeatedly to generate a Penrose tiling with a global fivefold centre at the point O of Fig. 1(a).

In the present procedure, one is assured of making no mistakes in tiling the originally chosen area with progressively decreasing size of tiles of both types. Also, the thin rhomb is a result of the operations involved and is not postulated *a priori*. Moreover, the deflation scheme followed by the thin rhomb in proceeding from one generation to another also arises as a natural consequence of the operations postulated by us. No predetermined scheme of deflation of the thin rhomb need be established.



(a)

(b)

Fig. 4. The final pattern obtained after six generations of operations on the initial rhomb of Fig. 1. In (a) we depict the pattern as obtained by the α, β and γ operations. If in (a) all bonds which do not form the edges of the rhomb are erased we obtain a correct Penrose tiling as demonstrated by the corresponding arrowed pattern in (b).

The quasilattice

Until now we have used the Penrose rhomb as an aid to an effective description of the translations and rotations involved. We shall now demonstrate that these operations when conducted repeatedly on a single starting point and all resultant points yield the quasilattice formed by the vertices of the tiles. The α, β and γ operations described above can conveniently be represented by the following equations in the reference frame of orthogonal Cartesian coordinates with their origin fixed at point O of Fig. 1(a).

$$X^\alpha = X/\tau; \quad Y^\alpha = |Y|/\tau - 2b;$$
$$X^{\beta\pm} = X^\alpha \cos \pi/5 \pm Y_1^\alpha \sin \pi/5;$$
$$Y^{\beta\pm} = \mp X^\alpha \sin \pi/5 + Y_1^\alpha \cos \pi/5;$$
$$X^{\gamma\pm} = X^\alpha \cos 2\pi/5 \pm Y_1^\alpha \sin 2\pi/5;$$
$$Y^{\gamma\pm} = \mp X^\alpha \sin 2\pi/5 + Y_1^\alpha \cos 2\pi/5 - 2b/\tau^2;$$

where $Y_1^\alpha = (Y^\alpha + 2b/\tau^2)$ with $2b$ being the length of the major diagonal of the rhomb. In the above equations, X and Y refer to the initial points while X^i, Y^i ($i = \alpha, \beta$ and γ) refer to the coordinates of the point resulting from the α, β and γ operations, respectively.

The α operation is performed on all points while the β and γ operations are performed on points resulting from the α operations. Also, if a point is subjected to β^+ and γ^+ operations in a given generation, points from it will be subjected to the β^- and γ^- operations in the immediately next generation and *vice versa*. Keeping these aspects in view, one can generate a tree (Fig. 5) to describe the recursive evolution of the quasilattice points in every generation of inflation. A new generation is associated with every α operation. In the first operation itself, it is sufficient to perform only the β^+ and β^- operations. Performance of the γ operation on the initial point (X_O, Y_O) leads only to superimposition of points and is not shown in the tree. Similar overlaps also occur at several other nodes in the tree. Also, the points generated by the branches of the tree originating at the first β^+ and β^- operations are related through mirror symmetry with respect to the major diagonal of the rhomb. It should be noted that the number of the generation is different from that obtained by the graphical procedure described earlier. It will be one more than in the graphical case.

The following additional properties of the quasilattice are noteworthy and are helpful in arriving at the geometrical structure factor. The coordinates of each lattice point in the nth generation (X_n, Y_n) are expressible in terms of the edge length a_n of that generation by the following relationships:

$$X_n = (m + n\tau)a_n \sin \pi/5;$$
$$Y_n = (p + q\tau)a_n/2;$$

where m, n, p, q are integers. The forms of these expressions are themselves indicative of the quasiperiodicity. Since the global Penrose tiling is obtained by the rotation of the chosen rhomb around its vertex at the top and since all resultant points are expressible by the above equations, there are certain

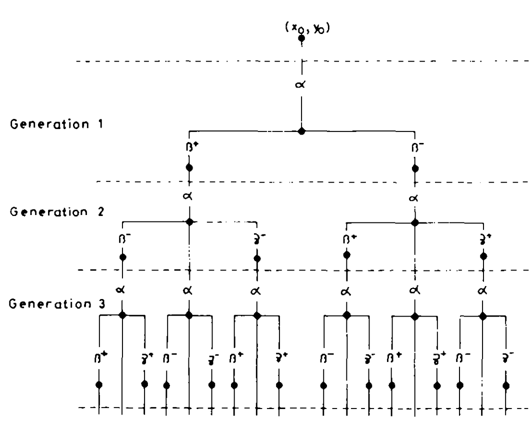


Fig. 5. The recursive occurrence of quasilattice points in each generation, depicted in the form of a tree.

parity conditions that should be laid on the m, n, p, q values. These are

m	n	p	q
even	even	even	even
odd	even	even	odd
even	odd	odd	odd
odd	odd	odd	even.

The nature of the β and γ operations also leads to identical restrictions even within the chosen rhomb. Further, it can be proved that when the ordinate of a point in the nth generation is expressed in terms of a_n/τ^2 or in terms of the edge length of the $(n+2)$th generation, an additional restriction is placed in that m and n have the same sign and p and q have the same sign. All points that are vertices in the Penrose tiling satisfy these conditions. However, points obeying these conditions need not necessarily be Penrose vertices.

In the light of these restrictions on m, n, p and q and the fact that these can be evaluated along all the branches of the tree of Fig. 5, summation of the contributions to the diffracted intensity from the quasilattice points becomes relatively easy. Further, the coordinates obtained by the β^+ operation in any generation are related to the coordinates of the points obtained from the same node by the α and γ operations through the following equations:

$$X^{\beta\pm} = (X^{\gamma\pm} + X^{\alpha})/\tau;$$
$$Y^{\beta\pm} = (Y^{\gamma\pm} + Y^{\alpha})/\tau + (4b)/\tau^2.$$

These establish relationships between quasilattice points in the kite and dart regions of the main rhomb (see caption to Fig. 1). Three of the length scales used in the present description of the coordinates, *viz* $a_n \sin \pi/5$, $a_n\tau \sin \pi/5$ and $a_n\tau/2$, represent three of the four half-diagonals of the two rhombs used for tiling. The unit vectors associated with these can be identified with the aid of the projection formalism.

In conclusion, it can be said that the present algorithm is a new look at the Penrose tiling and affords a method of deflating a single thick rhomb repeatedly and systematically without the need for any decision making at every stage. The process can be understood in terms of simple operations that are very similar to conventional crystallographic operations and enables the establishment of a tree-related hierarchy of quasilattice points obtained by successive deflation of the rhombs used in a tiling. The procedure described also identifies a new set of diagonally related length scales for the description of the coordinates of the quasilattice points in a Cartesian frame of reference. These are combined in integral multiples to yield the coordinates of the quasilattice points with simple restrictions on the parity of the integers involved.

The present procedure has direct relevance to the structure of decagonal quasicrystalline phases and has the potential for extension to the three-dimensional quasicrystal.

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The Description and Analysis of Composite Crystals

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Abstract

The composition of composite crystals, which contain two often incommensurate sublattices, depends on the ratio of the volumes of the sublattices and is therefore nonstoichiometric if the sublattices are incommensurate. The relation between the two sublattices is described by an interlattice matrix, which has different forms for layer and column composite structures and is restricted by space-fitting requirements. A previously derived formalism for the refinement of incommensurately modulated structures [Petricek, Coppens & Becker (1985). *Acta Cryst.* A**41**, 478-483] has been extended to composite structures and applied in a new computer program. The formalisms have been applied to the composite structures of (BEDO-TTF)$_{2.4}$I$_3$, (BEDT-TTF)Hg$_{0.776}$(SCN)$_2$ and (Bi,Sr,Ca)$_{10}$Cu$_{17}$O$_{29}$.

Introduction

As more complicated solids are being synthesized in the search for new materials, unusual structural phenomena are becoming increasingly common. Prime examples are modulations in crystals and the occurrence of composite (also called misfit) structures which contain at least two components with interpenetrating but distinct lattices.

When the ratio of the volumes of the unit cells of the two sublattices of a composite crystal is irrational, the two components will occur in nonstoichiometric ratios, the stoichiometry being dictated by the ratio of the unit-cell volumes. For ionic or partially ionic compounds, electroneutrality requirements imply that composite solids must contain ions of mixed valency. Since mixed valency is often associated with unusual properties, it is not surprising that the search for synthetic metals and superconductors has led to the discovery of many new composite solids. Some examples of inorganic and organic composite crystals are given in Table 1. Other known examples are minerals and graphite intercalation compounds (Makovicky & Hyde, 1981) and alloys (Jeitschko & Parthé, 1967).

Since the two lattices coexist in the same crystal, there is a mutual interaction which corresponds to a perturbing potential with the periodicity of the other sublattice. The perturbation causes each of the sublattices to be modulated with a repeat of the perturbing potential, which is a translation period of the second sublattice. As a result, the diffraction pattern of a composite crystal is the superposition of the diffraction patterns of the two sublattices, plus satellite reflections representing the modulations (Janner &

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