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Atomistic octagonal random-tiling model

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Abstract. A random-tiling model with octagonal symmetry is presented. The tiles are the square and various hexagons. When each vertex of the tiling is decorated by a disc, a valid disc packing is formed, which is an octagonal disc packing of maximum density under certain constraints. A simple inflation rule is given that produces one member of the random-tiling ensemble. The space group of this tiling is non-symmorphic. The projection description of this tiling involves a fractal acceptance domain with fourfold symmetry for the even nodes of a four-dimensional cubic lattice and the same acceptance domain rotated by $\pi/4$ in perpendicular space for the odd nodes. Other tilings can be generated by an inflation rule with constrained randomness. Additional members of the random-tiling ensemble can be created from inflation-generated tilings by a set of update moves that rearrange the positions of the discs along closed loops. An update move does not always conserve the number of each kind of tile.

1. Introduction

Tiling models have long been studied in the field of statistical mechanics. Renewed interest was generated by the discovery of tilings with quasicrystalline symmetry and the later observation of such symmetries in real materials. The origin of the quasicrystalline phase remains unclear. One hypothesis is that such phases are stabilized by entropy [1, 2]. In a random-tiling model of a quasicrystal, the positions of the atoms are described as the decoration of a set of tiles that fill space in a number of different ways without gaps or overlap. The 'random-tiling hypothesis' states, in part, that the entropy of certain ensembles of tilings is maximized when the proportions of the various tiles in the tiling and their orientations are those associated with quasicrystalline symmetry [2].

Some basic features are common to most quasicrystalline tilings. The edges of the tiles are in a discrete set of directions which is invariant under a non-crystalline point group. These directions, and thus the separation of any two nodes in the tiling, can be represented by an integral linear combination of a set of D vectors, where D is greater then the dimension d of the tiling space. This set of vectors can be associated with basis vectors for a D-dimensional lattice. Each node of the tiling corresponds with a node of the D-dimensional lattice and the tiles themselves are d-dimensional faces of the D lattice. The tiling is a projection of a continuous d-surface in R^D. There is a special mean orientation of the surface associated with quasicrystalline symmetry. Other mean orientations change the proportions of the various tiles in R^d. In the random-tiling hypothesis, the quasicrystal is entropically stable relative to such non-quasicrystalline phases.

In studying random tilings, it is useful to determine a set of rearrangements of the tiles, or 'update moves', that are necessary and sufficient to yield all members of the ensemble†

† A set of update moves which allows one to reach all members of the ensemble except for a subset of zero measure will also be considered an ergodic set.

from any given member; that is, an 'ergodic' set of update moves. The update moves provide both a model for the kinetics of phason fluctuations in the quasicrystal and a tool that can be used in random-tiling calculations. For these reasons, it is useful to find an ergodic set of update moves that involve the minimal number of tiles.

One class of random-tiling models consists of tilings whose tiles are all parallelograms (parallelepipeds, etc). For such tilings, there exists a simple set of 'flip update moves', which is ergodic [2, 3]. In this class of tilings, the random-tiling hypothesis has been verified for the two-dimensional [4, 5] and three-dimensional [3, 6, 7] Penrose tilings, the decagonal binary tiling [4, 8] and the octagonal tiling consisting of squares and rhombi [9].

To obtain a simple random-tiling model for a system of real atoms, however, some additional features are desired, as follows: (i) each kind of tile should have a unique atomic decoration; (ii) each member of the random-tiling ensemble should be a good packing, (i.e. there should be no unphysically close pairs of atoms); (iii) each arrangement of atoms that forms a good packing should belong to the ensemble [10]. A random-tiling model that satisfies these constraints will be termed a 'physical' or 'atomistic' random-tiling model. Of the above models, only the decagonal binary tiling model has a known decoration that yield a physical model. It is somewhat complicated, however, in that it has two atomic components. The discovery of the dodecagonal square–triangle tiling was thus of great interest, since, when each node is decorated by an atom, it provides a physical quasicrystalline random-tiling model that has only one component.

The square–triangle tiling has been studied by many authors [11–16]. There is no flip update move for such tilings; on the other hand, a set of update moves has been found which rearrange the nodes, and thus the tiles, along closed chains of various lengths [11]. It has been proven that the complete set of such update moves is ergodic and that a finite subset of the moves is insufficient for ergodicity [16]. The random-tiling hypothesis has been proven for the square–triangle random-tiling system [10, 13, 14].

Another physical random-tiling system has been proposed to model quasicrystals with icosahedral symmetry. This 'canonical cells model' is based on decorating the vertices of four distinct tiles with Mackay clusters of atoms [21]. The clusters play the role of atoms in the above list of desired physical conditions. In close similarity to the square–triangle tiling, the tiles are not all parallelepipeds and no flip update move is possible [11]. Studies of large periodic approximants hint that infinite canonical cell tilings exist [18, 19]; however, no deterministic rule for generating an infinite icosahedral canonical-cell tiling is yet known.

Thus, to begin further exploration into the generality of the random-tiling hypothesis and to perhaps shed some light on the nature of the infinite icosahedral canonical-cell tiling, this paper introduces a physical random-tiling model with octagonal symmetry. The tiles involved are squares and various hexagons; a tiling composed of these tiles might thus be termed a 'square–hexagon tiling' in analogy with the terminology 'square–triangle tiling'. In section 2, a square–hexagon tiling that has a particularly simple inflation rule is presented and the corresponding acceptance domains for the projection description of this tiling are found. It is shown that the space group is non-symmorphic. In section 3, the inflation rule found in section 2 is generalized to a inflation rule that is random, subject to geometric constraints. In section 4, a set of update moves that can be used to generate other members of the tiling ensemble is presented. Section 5 discusses several aspects of the tiling, including a proof that these tilings solve a particular octagonal disc-packing problem. Finally, section 6 summarizes the results.

In this work, various tilings and ensembles of tilings of squares and hexagons are described. The generic term 'square–hexagon random-tiling system' refers to the maximally random system of infinite tilings of squares and hexagons with zero average phason strain. The maximally random square–hexagon tiling ensemble will also be referred to as the R (for random) ensemble. All other tilings and ensembles described here are subsets of the R-ensemble or its approximants and will be named when introduced. A single tiling that belongs to an X-ensemble will be called an X-tiling.

2. A deterministic square–hexagon tiling

Consider tilings whose edges are all of unit length in a limited set of directions $\{\pm e_i^{\parallel}\}$ compatible with octagonal symmetry:

$$e_i^{\parallel} = (\cos(2\pi i/8),\ \sin(2\pi i/8)) \tag{1}$$

with $0 \leqslant i \leqslant 3$. Such tilings are conventionally described in four dimensions via a cubic lattice. A continuous surface of 2-parallelograms in R^4 projects to a tiling consisting of squares and 45° rhombi. Subsequently in this work, the word 'rhombus' will refer only to a 45° rhombus. A simple decoration of the nodes of the square–rhombus tiling with discs of radius $\frac{1}{2}$ is not physical, however, since the short diagonal of the rhombus is less than unit length. To obtain a physical random-tiling model (such as might correspond with the packing of atoms in alloys with observed octagonal symmetry [20]), it is necessary to either (i) use a more complicated decoration of the tiles or (ii) choose a different set of tiles that contains no internal diagonals shorter than unit length. Here choice (ii) is followed. The new tiles are shown in figure 1. There is, in fact, an infinite set of tiles. The tiles will be named the 'square', the '1-hexagon', the '2-hexagon', etc. The term 'hexagon', unless otherwise specified, refers to any m-hexagon, $m \geqslant 1$. An m-hexagon is a hexagon with two opposite edges of length m. Each edge of length m, $m > 1$, contains $m - 1$ additional vertices that divide it into segments of length one; thus, strictly speaking, an m-hexagon is a $(2m + 4)$-gon. The second-nearest neighbour distance in a tiling composed of squares and m-hexagons is $\sqrt{2}$.

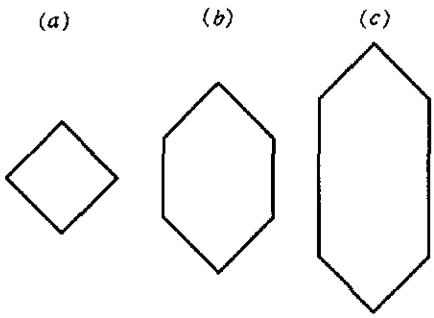

Figure 1. First three tiles of the series of tiles for square–hexagon tilings: (*a*) square, (*b*) 1-hexagon and (*c*) 2-hexagon.

An inflation rule that yields a square–hexagon tiling is given in figure 2. The linear expansion in the inflation is $1 + \sqrt{2} \equiv \phi$. The nodes of a tiling before inflation, $\{r^{\parallel}\}$, correspond to what is termed here the 'principal nodes' of the inflated tiling, $\{\phi r^{\parallel}\}$. By applying the inflation rule to an original tiling that is a centred square, a series of square periodic approximants are generated. In the limit of the infinite approximant, the tiling

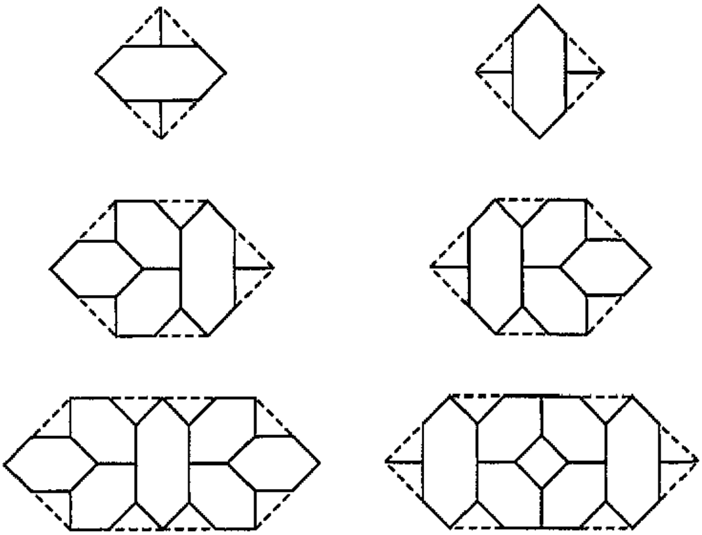

Figure 2. Inflation rule for the tiles that leads to the square–hexagon B-tiling.

will be octagonal and will be indistinguishable from itself under inflation symmetry. The octagonal tiling that is self-similar under this inflation rule is termed here the B (for bipartite) tiling.

In effecting the inflation, the nodes of the tiling, $\{r^{\parallel}\}$, are divided into sets of even and odd parity, $\{r^{\parallel}_{\mathrm{even}}\}$ and $\{r^{\parallel}_{\mathrm{odd}}\}$, according to whether $\sum n_i$ in the projection method as described below is even or odd. The nearest-neighbour vectors are divided into an even subset $\{e^{\parallel}_{\mathrm{even}}\} \equiv (\pm e^{\parallel}_0) \cup (\pm e^{\parallel}_2)$ and an odd subset $\{e^{\parallel}_{\mathrm{odd}}\} \equiv (\pm e^{\parallel}_1) \cup (\pm e^{\parallel}_3)$. For nodes of even parity, the corresponding node in the inflated tiling, $\phi r^{\parallel}$, has four nearest neighbours in the directions $\{e^{\parallel}_{\mathrm{even}}\}$; for nodes of odd parity, the corresponding node in the inflated tiling has four nearest neighbours in the directions $\{e^{\parallel}_{\mathrm{odd}}\}$. When this rule is applied to all the nodes of a tile, there is always a unique way to fill out the rest of the interior of the tile in a way that produces only squares and hexagons. The two possible inflations for each tile are shown in figure 2 and correspond to the two possible sets of parities for the vertices.

The B-tiling contains only squares, 1-hexagons and 2-hexagons. When parity and orientation are considered, there are 20 distinct tiles. The inflation matrix can be written by inspection. The dominant eigenvalue of this matrix is ϕ^2, as expected, and the corresponding eigenvector gives the ratio of squares, 1-hexagons and 2-hexagons in the B-tiling. This ratio is

$$n_S : n_{(1H)} : n_{(2H)} = 2 + \sqrt{2}/2 : 3\sqrt{2}/2 : 1 . \qquad (2)$$

Each orientation of the tiles is equally likely, proving that the symmetry is octagonal. One finds additionally that the 90° vertices of 2-hexagons in the B-tiling are always of even parity if the adjacent edges are among the directions $\{e^{\parallel}_{\mathrm{even}}\}$ and of odd parity otherwise. A square periodic approximant of the B-tiling with edge length $\sqrt{2}\phi^3$ is shown in figure 3. Defining 'local environment' to signify the bonds around a given node (and not the tiles), there are only three different local environments in the B-tiling. The statistics of these environments are given in table 1. The notation used to describe local environments is similar to that

Table 1. Local environments in the square–hexagon tiling.

Vertex type	Frequency	
⟨2222⟩	ϕ^{-2}	(0.1716)
⟨332⟩	$2\phi^{-1} - \phi^{-2} - \phi^{-4}$	(0.6274)
⟨422⟩	$\phi^{-2} + \phi^{-4}$	(0.2010)

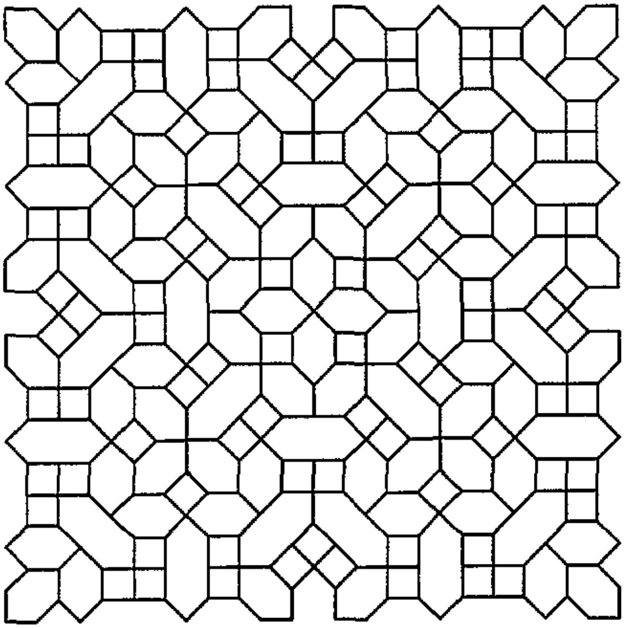

Figure 3. Square periodic approximant of the square–hexagon B-tiling. The edge length of the periodic cell is $\sqrt{2}\phi^3$.

used by Henley [17]. For example, ⟨422⟩ refers to a node that has three nearest neighbours in directions such that the angles between the bonds to successive neighbours are $4\frac{\pi}{4}$, $2\frac{\pi}{4}$, and $2\frac{\pi}{4}$.

This tiling can equally well be described by the projection method [22–24]. Associated with each basis vector e_i of the four-dimensional lattice is its perpendicular-space, or perpendicular-space component $e_i^{\perp}$ which is orthogonal to physical, or parallel, space and which satisfies $e_i^{\perp} = e_i - e_i^{\parallel}$. Here the perpendicular space Cartesian representation

$$e_i^{\perp} = (\cos(10\pi i/8), \sin(10\pi i/8)) \tag{3}$$

is used. Taking the origin of the 4D lattice to be r_0, the node $\sum_i n_i e_i + r_0$ of the lattice is projected as a vertex in the tiling at $\sum_i n_i e_i^{\parallel} + r_0^{\parallel}$ if and only if $\sum_i n_i e_i^{\perp} + r_0^{\perp} \in A$; the region A being termed the acceptance domain for the tiling.

To find the acceptance domain for the B-tiling, it is useful to reformulate the inflation rule for the tiles as an inflation rule for the nodes. Perhaps the simplest such rule is to (i) place around each principal node 12 neighbours as follows: four neighbours at distance 1 in directions consistent with the parity of the node and eight neighbours at distance ϕ in the directions $\pm\{e_i^{\parallel}\}$, and (ii) to then eliminate all nodes that are at unit distance from some principal node but in a direction that violates the parity rule for the nearest neighbours of that node. The node inflation rule is thus

$$\begin{aligned}\{r^{\|}_{\mathrm{even}} \cup r^{\|}_{\mathrm{odd}}\} \to & \Big[\big(\{\phi r^{\|}_{\mathrm{even}}\} \cup \{\phi r^{\|}_{\mathrm{odd}} + e^{\|}_{\mathrm{odd}}\} \cup \{\phi r^{\|}_{\mathrm{odd}} \pm \phi e^{\|}_{i}\}\big) \\ & \cap \overline{\{\phi r^{\|}_{\mathrm{odd}} + e^{\|}_{\mathrm{even}}\}}\Big] \\ & \cup \Big[\big(\{\phi r^{\|}_{\mathrm{odd}}\} \cup \{\phi r^{\|}_{\mathrm{even}} + e^{\|}_{\mathrm{even}}\} \cup \{\phi r^{\|}_{\mathrm{even}} \pm \phi e^{\|}_{i}\}\big) \\ & \cap \overline{\{\phi r^{\|}_{\mathrm{even}} + e^{\|}_{\mathrm{odd}}\}}\Big] . \end{aligned} \tag{4}$$

The nodes in the inflated tiling are grouped into even and odd nodes in (4). The action of inflation on even and odd nodes is different; thus, in translating the inflation rule into perpendicular space, separate acceptance domains, A_{even} and A_{odd} are generated for even and odd nodes. Using the definitions $\{e^{\perp}_{\mathrm{even}}\} \equiv (\pm e^{\perp}_{0}) \cup (\pm e^{\perp}_{2})$ and $\{e^{\perp}_{\mathrm{odd}}\} \equiv (\pm e^{\perp}_{1}) \cup (\pm e^{\perp}_{3})$, and noting that the inflation process multiples distances in perpendicular space by $-1/\phi$, the perpendicular-space action of the inflation rule can be immediately written from (4),

$$\begin{aligned} A_{\mathrm{even}} &\to \left(-\frac{1}{\phi}A_{\mathrm{even}} \cup \left\{-\frac{1}{\phi}A_{\mathrm{odd}} + e^{\perp}_{\mathrm{odd}}\right\} \cup \left\{-\frac{1}{\phi}A_{\mathrm{odd}} \pm \frac{1}{\phi}e^{\perp}_{i}\right\}\right) \\ &\qquad \cap \overline{\left\{-\frac{1}{\phi}A_{\mathrm{odd}} + e^{\perp}_{\mathrm{even}}\right\}} \\ A_{\mathrm{odd}} &\to \left(-\frac{1}{\phi}A_{\mathrm{odd}} \cup \left\{-\frac{1}{\phi}A_{\mathrm{even}} + e^{\perp}_{\mathrm{even}}\right\} \cup \left\{-\frac{1}{\phi}A_{\mathrm{even}} \pm \frac{1}{\phi}e^{\perp}_{i}\right\}\right) \\ &\qquad \cap \overline{\left\{-\frac{1}{\phi}A_{\mathrm{even}} + e^{\perp}_{\mathrm{odd}}\right\}} . \end{aligned} \tag{5}$$

The B-tiling acceptance domains can be found as the limit of infinite application of (5) to appropriate initial acceptance domains. A starting acceptance domain that is a simple octagon of maximum perpendicular-space radius one is chosen for both A_{even} and A_{odd}. The corresponding tiling contains octagons and flattened octagons in addition to squares and hexagons [25]. These tiles do not belong to the square–hexagon set; thus it is necessary to investigate the behaviour of these tiles under the vertex inflation rule (4). It turns out that for every octagon (concave octagon) in a tiling, there is one octagon (concave octagon) in the inflated tiling. Thus, the density of bad tiles is zero in the final tiling, and the final acceptance domain is that for a self-similar square–hexagon tiling, the B-tiling. The fourth iteration of the inflation rule applied to the starting octagonal acceptance domains is shown in figure 4. It is clear that the B-tiling acceptance domains are fractal. Fractal acceptance domains have been seen for pentagonal [26], square–triangle [27, 28], and octagonal square–rhombus [29] tilings and it has been shown that a generic inflation rule will lead to an acceptance domain which is fractal [30]. The Hausdorff dimension of the boundary of the present acceptance domain is

$$\frac{\ln(2+\sqrt{3})}{\ln(1+\sqrt{2})} \approx 1.49 . \tag{6}$$

This dimension is between the fractal dimensions calculated by Godrèche *et al* for two different octagonal square–rhombus tilings that have fractal acceptance domains [29].

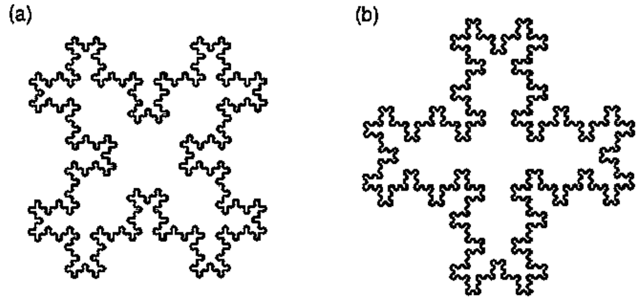

Figure 4. Acceptance domains for (*a*) even nodes and (*b*) odd nodes of the square–hexagon *B*-tiling.

The space group for the *B*-tiling is p8gm [31], the non-symmorphic octagonal space group with point group 8 mm. This space group was described in detail by Janssen [32]. The atomic surfaces corresponding to the acceptance domains A_{even} and A_{odd} occupy the two Wyckoff positions of tetragonal symmetry. The square–rhombus tilings of Godrèche *et al* [29] that have fractal acceptance domains also belong to space group p8gm.

3. Random inflation

The inflation rule presented in section 2 for the square–hexagon tiling is very similar to the inflation rule found by Stampfli for the square–triangle tiling [33]. The set of twelve nearest-neighbour directions in the square–triangle tiling can be divided into two sets, each of hexagonal coordination. The principal nodes in the inflated tiling have their nearest neighbours along one of these sets of six directions. In the maximally random Stampfli inflation, there is complete freedom to choose the orientations of the near-neighbour sets. The rest of the nodes in the inflated tiling are forced, and are independent of the orientations of the near-neighbour sets.

The rule presented in section 2 for square–hexagon inflation used a strict choice for the directions of the nearest neighbours of principal nodes. However, there is a degree of freedom in the choice of directions of these neighbours. The freedom is not total, as it is for the square–triangle tiling. There is a restriction: two principal nodes separated by distance ϕ in one of the directions $\{e^{\parallel}_{\text{even}}\}$ ($\{e^{\parallel}_{\text{odd}}\}$) cannot both have their nearest neighbours in the directions $\{e^{\parallel}_{\text{even}}\}$ ($\{e^{\parallel}_{\text{odd}}\}$), because, otherwise, there would be a pair of nodes in the inflated tiling separated by $\phi - 2 < 1$. This restriction is illustrated in figure 5. As long as the choice of near-neighbour sets for all the principal nodes leads to no violations of the restriction, it is possible to add additional nodes that create a square–hexagon tiling. At a given inflation step, in fact, the additional nodes needed to form a square–hexagon tiling are forced and are independent of the orientations of the near-neighbour sets, as in random Stampfli inflation.

The entropy due to this random inflation is not known. An upper bound can be determined by the same method that Oxborrow and Henley used to determine the entropy of dodecagonal square–triangle tilings formed by random inflation [10]. In brief, each square–hexagon tiling produced by random inflation or '*I*-tiling' is the result of an infinite sequence of inflation steps. The ancestor tiling j inflation steps before an *I*-tiling contains a fraction ϕ^{-2j} of the nodes of the *I*-tiling, and the inflation rule, as described above, gives

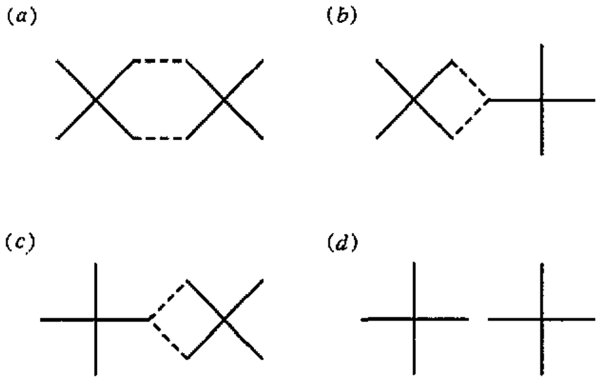

Figure 5. Constraint on random inflation rule for square–hexagon I-tilings. An unrestricted inflation rule leads to four choices (a)–(d) for the near-neighbour sets of two principal nodes separated by ϕ. Choice (d), however, does not lead to a valid square–hexagon tiling.

a maximum of two ways to inflate about each of these nodes. Thus, for N nodes in the end tiling, there are at most

$$\prod_{j=1}^{\infty} 2^{(\phi^{-2j})N} \tag{7}$$

distinct tilings formed by inflation. Taking the log and dividing by N gives an upper bound for the entropy per node, s_v^I, of the ensemble of inflation-generated tilings (I-ensemble):

$$s_v^I \leqslant \frac{\ln(2)}{\phi^2 - 1} \approx 0.1436\,. \tag{8}$$

A crude estimate of the actual entropy can be made by counting all of the distinct tilings generated by random inflation for a finite approximant. For a square periodic approximant of edge length $\sqrt{2}\phi^2$, random inflation generates 181 arrangements of the 58 nodes, yielding

$$s_v^I(\text{approximant}) = \frac{\ln(181)}{58} \approx 0.0896\,. \tag{9}$$

Even if the error due to finite-size effects is 40%, the entropy per node of the square–hexagon I-ensemble is larger than that for the corresponding ensemble of square–triangle tilings [34].

4. The update move

The I-ensemble described in section 3 is only a subset of the full ensemble of octagonal square–hexagon tilings (the R-ensemble). To obtain additional members of the ensemble, one can apply an update move which rearranges the nodes, and thus changes the tiles, along a closed chain. By analogy with the update move for the square–triangle tiling, which similarly rearranges nodes and tiles along a closed chain, an update move of this kind will be termed a 'zipper update move' or 'zipper move'. As in the square–triangle tiling, there is a set of zipper moves of various lengths.

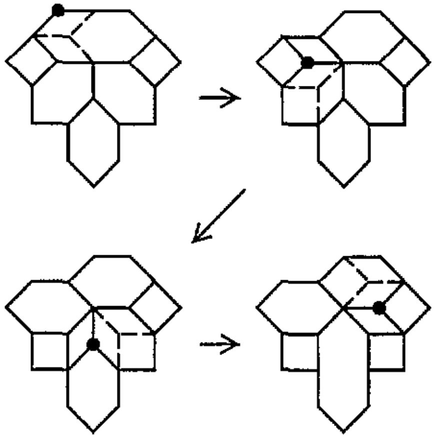

Figure 6. A zipper update move for the square–hexagon tiling. The zipper move shown continues until the zipper returns to the original node.

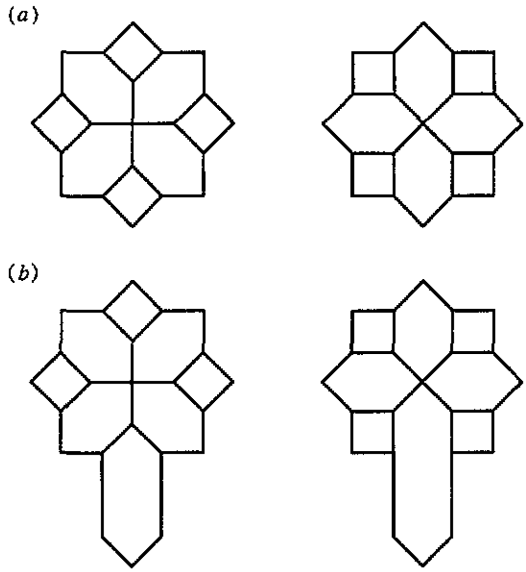

Figure 7. (*a*) Smallest region whose interior can be rearranged by a zipper move. (*b*) A zipper move can change the absolute numbers of each kind of tile.

The details of a zipper update move are shown in figure 6. It is necessary to begin with a 135° vertex of a hexagon. Two rhombi that share the adjacent 90° degree vertex of the hexagon are drawn. The original node is erased from the structure and the new node produced by the rhombus is added. One of the rhombi shares with the origin hexagon the 135° vertex opposite the original vertex. This vertex must be a 135° vertex of a second hexagon. This vertex is deleted from the structure and a new vertex is added inside the second hexagon as before. Then the process is repeated for the 135° vertex of a third hexagon and so forth until the chain returns to the original vertex. Note that the zipper move exactly fits the definition of a zipper move given in [10]—a pair of defect tiles are formed (in this case, two rhombi), the defects propagate, as shown in figure 6, until they meet and annihilate, completing the zipper move.

The shortest zipper moves operate on a closed chain of four nodes. In effect, four nodes are removed and four new nodes added. One example of such a short move is the fundamental 'repackable volume' of the octagonal tiling studied in [25] and is shown in figure 7(*a*). It is equally possible, however, to have a minimum-length zipper move, such as that shown in figure 7(*b*), which changes the tiles inside a region with a different boundary. The zipper move in figure 7(*b*) illustrates two other aspects of the zipper move for the square–hexagon tiling: (i) The number of each kind of tile is not necessarily conserved and (ii) 3-hexagons, etc can be introduced into a tiling where such tiles did not previously exist.

In the square–triangle tiling system, the defects in the zipper move sometimes have choices where they can proceed. In the square–hexagon system, it can be easily proven that the defect tile never has any choices where to proceed. While this lack of freedom makes the square–hexagon zipper moves easy to implement, it raises questions about whether the set of zipper moves is sufficient for ergodicity.

It is unknown whether the set of zipper update moves is sufficient for ergodicity and, if so, whether it is necessary to include zippers of arbitrary length for ergodicity (as is the case for the square–triangle tiling). The question of zipper length has physical implications—as discussed in the introduction and in [10], one might consider a zipper move to correspond to an actual physical rearrangement of atoms. As described above, a zipper move is equivalent to the formation of a defect pair, which propagates until it rejoins itself and annihilates. Although such a defect might have only a small positive energy relative to the tiling ground states, it remains unknown whether the propagation of such defects over arbitrarily long distances is a plausible physical process.

5. Discussion

In [25], the question was asked: for an octagonal disc packing with nearest-neighbour vectors of the form (1), what is the maximum density that can be achieved?

Here, this question is answered, under the additional restriction that the lines connecting near neighbours form tiles which can be subdivided into squares and rhombi without holes or overlap. The area of any such tile is in the form

$$A = jA_S + kA_R \tag{10}$$

where $A_S = 1$ is the area of the square, $A_R = \sqrt{2}/2$ is the area of the rhombus and j and k are both integers. In the octagonal square–rhombus tiling, the number of nodes equals the number of tiles. For a tile that can be subdivided into squares and rhombi, however, the number of nodes for a tile is in general fewer than $j + k$, due to 'internal' vertices of the tile. Each rhombus inside a tile forces at least one 'internal' vertex. The number of internal vertices per rhombus can be minimized if each internal vertex is shared by two rhombi; thus, in principle, the maximum number of nodes per tile, $N_{\max}$, satisfies

$$N_{\max} = j + k/2\,. \tag{11}$$

There exists an infinite number of tiles that meet this maximum density. This set consists of the square, and the series of 'hexagons' described in section 2. With the square considered as a 0-hexagon, the area of the m-hexagon, $A_{(m\mathrm{H})}$ is given by

$$A_{(m\mathrm{H})} = A_S + 2mA_R \tag{12}$$

and the number of nodes contained is

$$V_{(m\mathrm{H})} = m + 1\,. \tag{13}$$

All other tiles whose interiors can be filled with squares and rhombi have fewer nodes than given by (11); thus a tiling consisting of squares and hexagons must have the maximum density for an octagonal tiling of such tiles†.

In the square rhombus tiling, for octagonal symmetry, the ratio of squares to rhombi must be [35]

$$n_S : n_R = 1 : \sqrt{2}. \tag{14}$$

According to (2), (12) and (13), the density of nodes in the square–hexagon tiling is $(2+\sqrt{2})/4$. The packing fraction with a disc placed on each node is approximately 0.6704. The absolute concentrations of each tile in the square–hexagon tiling are not fixed by symmetry. Equation (14) only leads to the constraint that, for an octagonal tiling of m-hexagons (the square considered as a 0-hexagon),

$$\frac{\sum_{m=0}^{\infty} 2mn_{(m\mathrm{H})}}{\sum_{m=0}^{\infty} n_{(m\mathrm{H})}} = \sqrt{2}. \tag{15}$$

Note that (2) satisfies (15).

In [25], the octagonal disc-packing problem was studied entirely within the context of perpendicular space as the problem of maximizing the area of the acceptance domain subject to certain perpendicular-space constraint vectors. It was shown that by replacing certain regions around the vertices of the unit octagonal acceptance domain by half-filled regions, i.e. performing the 'pinwheel construction' [36], a denser packing of discs of radius $\frac{1}{2}$ could be obtained at the cost of having a non-connected acceptance domain. The tiling in the present work is obtained by relaxing the restriction in the previous work that the acceptance domain be identical for each four-dimensional lattice point. By dividing the 4D lattice into even and odd sublattices, the problem is greatly simplified: it becomes possible to completely fill the 'pinwheel regions' about half of the vertices of the unit octagon and to completely delete these regions about the other half. The steps in obtaining the fractal in figure 4 are akin to the 'iterated pinwheel construction'; the use of difference acceptance domains for even and for odd nodes eliminates the effects of the constraint vector of perpendicular-space length $1+\sqrt{2}$ that is the limiting factor for the pinwheel construction when a single acceptance domain is used [25]. It is possible that, for the related problem of finding the densest icosahedral b–c packing (associated with the problem of finding deterministic canonical-cell tilings), the use of a superstructure of the higher-dimensional lattice might also greatly simplify the problem.

There are a number of unanswered questions concerning the random-tiling ensemble. Perhaps the most interesting unsolved problems concern the symmetry of the R-ensemble presented here and related systems. The B-tiling is bipartite; is the R-ensemble as a whole bipartite, or do the even and odd nodes become indistinguishable?

Additionally, it has been shown [37] that the subset of the R-ensemble consisting of tilings containing only squares and 1-hexagons (the $R1$-ensemble) form a random-tiling system with finite entropy density; however, there is no known $R1$-tiling with symmetry 8 mm. If it is impossible to form an $R1$-tiling at zero phason strain that has full octagonal symmetry, then is there any reason for the entropy density of ensembles of tilings of squares

† There are tiles that cannot be subdivided into squares and rhombi, whose area is of the form (10), and which have a number of nodes that exceeds (11). For example, letting i denote an edge in the direction $e_i^{\parallel}$ and $i+4$ denote an edge in the direction $-e_i^{\parallel}$, the tile formed by successive edges in the directions 013342457706 contains five nodes, but has an area of $2A_S + 5A_R$. Thus the general octagonal disc-packing problem remains unsolved.

and 1-hexagons to be a maximum for zero phason strain, or will the entropy density be a maximum for some finite phason strain? The problems of symmetry posed by this subset of the R-ensemble make it important to determine whether the hypothesis that the entropy is a maximum at zero phason strain actually holds for the R-ensemble and under what circumstances, if any, this hypothesis fails for related systems.

6. Conclusion

A simple octagonal random-tiling model is presented. A decoration of each vertex with an atom leads to a good atomic packing. The tiling model is the octagonal analogue of the dodecagonal square–triangle tiling model. It presents, however, several distinctive characteristics, such as a non-symmorphic space group, a set of zipper update moves that do not always conserve the number of each kind of tile, and a constrained random inflation rule. The octagonal tiling model presented is a good model for testing the generality of and for extending previous results on quasicrystalline random tilings, disc packings, and symmetry.

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