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On the combinatorial characterization of quasicrystals

Károly J. Böröczky[a,*], Tamás Réti[b], Gergely Wintsche[c]

[a] *Alfréd Rényi Institute of Mathematics, Budapest, PO Box 127, H-1364, Hungary*
[b] *Budapest Polytechnic, Budapest, Népszínház u. 8., H-1081, Hungary*
[c] *Teacher Training Department, Roland Eötvös University, Budapest, Pázmány Péter sétány 1/C, H-1117, Hungary*

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Abstract

In various fields of materials science, many interesting two-dimensional (2D) and three-dimensional (3D) structures (fullerenes, nanotubes, frothes, metal foams, polycrystals and, notably, various quasicrystals) can be considered as finite or infinite cellular systems. For a cell T of a given 2D cellular system, we write $n(T)$ to denote the number of sides of T, and $m(T)$ to denote the average number of sides of the neighbours of T. In the 3D case, we replace sides by faces in the definition. D. Weaire first observed, for trivalent random tilings of the plane, that $\langle n \cdot m \rangle = \langle n^2 \rangle$, where $\langle \cdot \rangle$ stands for the expected value. Following his discovery, the Weaire sum rule has been proved for various tilings of a sphere or a torus, and for periodic tilings of the plane or space. In this paper we extend the Weaire sum rule to quasiperiodic tilings of the plane or space. Actually, the method of this paper yields the Weaire sum rule for tilings of any compact surface or three-manifolds as well.

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1. Tilings and the Weaire sum rule

In various fields of materials science, many interesting two-dimensional (2D) and three-dimensional (3D) structures (fullerenes, nanotubes, frothes, metal foams, polycrystals and, notably, various quasicrystals) can be modeled by a special arrangement of tilings by polygons and polytopes, and thus can be considered as finite or infinite cellular systems. Over the past three decades, many studies have concentrated on random and periodic cellular structures (see [5–7,13,16,17,20,21]). This paper presents a general method, which is designated primarily to detecting certain combinatorial characteristics of quasiperiodic systems composed of d-dimensional cells for $d \geq 2$.

By a *convex polytope* P in the d-dimensional Euclidean space, we mean the intersection of finitely many half-spaces, provided that the intersection is bounded and has non-empty interior. After throwing away the irrelevant

* Corresponding author.
E-mail addresses: carlos@renyi.hu (K.J. Böröczky), reti.tamas@bgk.bmf.hu (T. Réti), wgerg@ludens.elte.hu (G. Wintsche).

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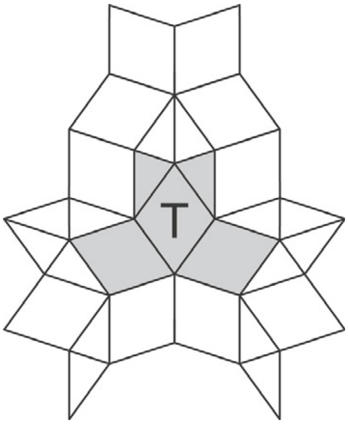

Fig. 1. The corona of a tile.

half-spaces, we may assume that the family of half-spaces is minimal in order to generate P. In this case, the intersections of P with the hyper planes (or, in other words, affine $(d-1)$-planes) bounding the half-spaces are the *facets* of P. In particular, each facet is a convex $(d-1)$-polytope, and the boundary of P is the union of the facets. We note that a facet is a side in the planar case ($d = 2$) and what is traditionally called a face in the $3D$ case ($d = 3$).

Next, we generalize the notion of a polytope. The common examples of spaces that are considered in this area are the d-dimensional Euclidean space $\mathbb{R}^d$, the d-sphere S^d bounding the $(d+1)$-dimensional Euclidean unit ball, and the d-torus that is homeomorphic (topologically equivalent) to the direct product of d circles. We call the homeomorphic image of a d-dimensional convex polytope a d-cell, and the images of the facets the facets of the cell. Here, tiling means that the tiles generate a tessellation without gaps and overlapping, and "facet to facet" stands for the property that any facet of some tile is the facet of some other tile, and any two tiles share at most one common facet. In particular, if a d-manifold (like the Euclidean space, or the sphere, or a torus) is tiled this way, then any facet belongs to exactly two tiles. Given a tile T, the tiles that share a common facet with T are called the neighbours of T, and the family of neighbours together with T form the corona around T (see Fig. 1). Our basic functions of a tile T are $n(T)$, which is the number of facets of T, and the facet coordination number $m(T)$, which is the average number of facets of the neighbours of T. More precisely, if $S_1, \ldots, S_k$, $k = n(T)$, are the neighbours of T, then

$$m(T) = \frac{\sum_i n(S_i)}{n(T)}.$$

We note that $n \cdot m$ is the total number of facets of the neighbours of the tile.

In the case of a finite tiling $\{T_i\}$, let us consider each tile with equal probability. If f is any function of the tiles, then we write $\langle f \rangle$ to denote the expected value of f; namely,

$$\langle f \rangle = \frac{\sum_i f(T_i)}{\#\{T_i\}}$$

where # stands for the cardinality of a set. Then the Weaire sum rule (observed first by Weaire [20] for trivalent random tilings of the plane) states that

$$\langle n \cdot m \rangle = \langle n^2 \rangle. \tag{1}$$

This has been proved for various tilings of a sphere or a torus in [6,7,13,16,17,20,21]. Actually, the method of this paper yields the Weaire sum rule (1) for any finite facet-to-facet tiling of some compact manifold (see Remark 4).

Now we turn to infinite tilings of $\mathbb{R}^d$. Given such a tiling, a *protoset* is a subcollection of tiles such that any tile in the tiling is the translate of some element of the protoset. Let us consider a facet to facet tiling $\{T_i\}$ of $\mathbb{R}^d$ with finite protoset. We write B^d to denote the unit ball of $\mathbb{R}^d$ centred at the origin, hence rB^d is the ball of radius r. If f is any

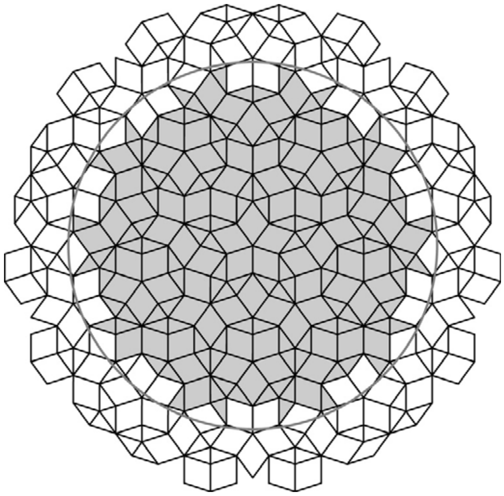

Fig. 2. Tiles in a big circle.

function of the tiles, then the expected value of f is defined by

$$\langle f \rangle = \lim_{r\to\infty} \frac{\sum_{T_i \subset rB^d} f(T_i)}{\#\{T_i : T_i \subset rB^d\}} \tag{2}$$

provided that the limit exists (see Fig. 2, which exhibits this approach on the tiling discussed in Section 6.1).

We briefly recall the argument of [17] concerning periodic tilings. Let us recall that a lattice is a subgroup of the translates of $\mathbb{R}^d$ isomorphic to $\mathbb{Z}^d$. Assume that the tiling $\{T_i\}$ of $\mathbb{R}^d$ is periodic with respect to a lattice Λ, hence both n and m are also periodic with respect to Λ. In this case, $\{T_i\}$ induces a finite tiling $\{\widetilde{T_i}\}$ on the torus $\mathbb{R}^d/\Lambda$ that is the quotient of $\mathbb{R}^d$ by Λ (obtained, say, by identifying opposite facets of a fundamental parallelepiped of Λ). It is easy to see that, if the function f in (2) is periodic with respect to Λ, then the expected value of f coincides with the expected value of the induced function on $\{\widetilde{T_i}\}$. In particular, the Weaire sum rule for the tiling of the torus yields the Weaire sum rule for the periodic tiling of $\mathbb{R}^d$.

Closer inspection of the argument above shows that the proof has two major parts: first to find a finite probability space for the translation types of the coronas occurring in $\{T_i\}$, and secondly to verify the equivalent of the Weaire sum rule on that probability space. In the case of periodic tilings, the first step is easiest to achieve by considering the induced tiling on a corresponding torus. The goal of this paper is to extend the Weaire sum rule (1) to quasiperiodic tilings where certain long-range order still allows us to carry out the first step.

2. Quasiperiodic tilings

The discovery of quasicrystals in 1984 was based on the fact that their structures exhibit some long-range order, while they have symmetries forbidden for crystals (see Janot [9] and Senechal [18] for nice reviews about quasicrystals). Ever since, the so-called quasiperiodic tilings of the plane or the space have been investigated extensively, and the aim of this paper is to verify the Weaire sum rule for such tilings. Now, the Weaire sum rule makes sense for an infinite tiling only if the tiling has the so-called uniform patch frequency (see (3) below for the definition). We note that planar quasiperiodic tilings of five-fold symmetry had already been constructed by Penrose [15] ten years before the discovery of quasicrystals (see Fig. 3). His construction still serves as a fundamental example, and the quasiperiodic tilings with uniform patch frequency discussed below can be considered as generalizations of the Penrose tilings.

We now introduce some fundamental notions. Let us consider a facet-to-facet tiling of $\mathbb{R}^d$ with a finite protoset. A finite collection of the tiles is called a *patch*. We say that the tiling has *uniform patch frequency* if, for any patch Π, there exists a positive number q with the following property (compare [18,19]): given any bounded set S whose

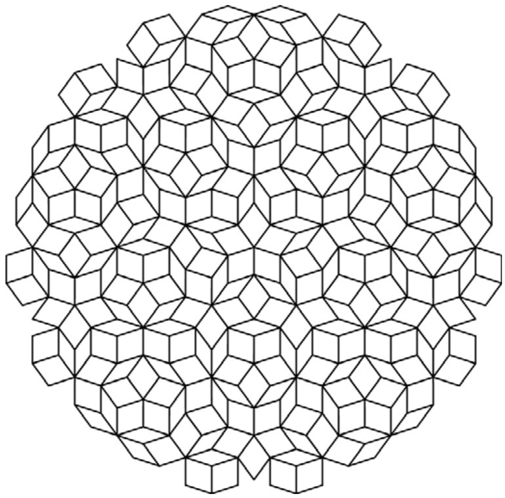

Fig. 3. Penrose tiling with rhombi.

interior is non-empty and whose boundary is of Lebesgue measure zero, we have

$$\lim_{r\to\infty} \frac{\#\{\text{patches that are translates of } \Pi \text{ and contained in } rS\}}{V(rS)} = q \tag{3}$$

where rS is the dilated copy of S by factor r. If, instead of $V(rS)$, we divide by the number of tiles that are contained in rS, then we obtain the *probability* $p(\Pi)$ *of* Π; namely,

$$p(\Pi) = \lim_{r\to\infty} \frac{\#\{\text{patches that are translates of } \Pi \text{ and contained in } rS\}}{\#\{\text{tiles that are contained in } rS\}}. \tag{4}$$

Observe that $p(\Pi)$ is always between zero and one, and is independent of the choice of S.

In this paper we prove the Weaire sum rule for quasiperiodic tilings (see Section 3 for examples of corresponding tilings, and Section 4 for a proof of the theorem):

Theorem 1. *Given a facet-to-facet tiling $\mathcal{T}$ of $\mathbb{R}^d$ with finite protoset and with uniform patch frequency, we have*

$$\langle n \cdot m\rangle = \langle n^2\rangle.$$

Remark 2. While it is essential that any facet of some tile is the facet of some other tile, it is not necessary to assume in Theorem 1 that any two tiles have at most one common facet. The only difference in the notions and in the argument is that, in this case, the definition of $m(T)$ for a tile T should be modified: when calculating the average number of facets of the neighbours of T, each neighbour is counted as many times as the number of common facets it has with T.

Since both $n(T)$ and $m(T)$ depend only on the corona of a tile T, and we have only finitely many translation types of coronas, the quantities occurring in Theorem 1 make sense by uniform patch frequency.

We note that various examples lead us to believe that the expected value of the facet coordination number is always at least the expected value of the number of facets (see say (27)).

Conjecture 3. *For any facet-to-facet tiling, we have*

$$\langle m\rangle \ge \langle n\rangle,$$

with equality if and only if each tile has the same number of neighbours.

3. Examples for quasiperiodic tilings with uniform patch frequency

We present various classes of quasiperiodic tilings having uniform patch frequency. Our examples can be considered as generalizations of the classical Penrose tilings (see Fig. 3 for the version with two types of rhombi).

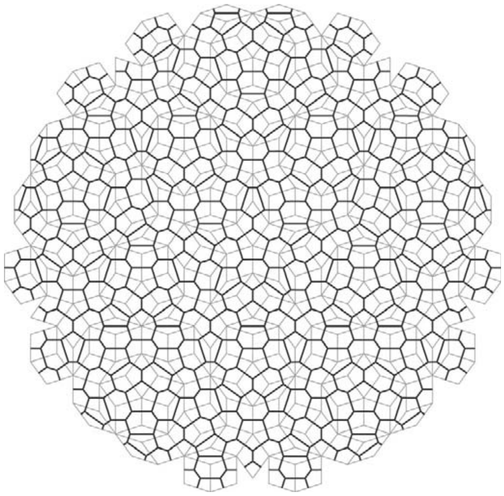

Fig. 4. The Dirichlet–Voronoi tiling w.r.t. the vertices of the Penrose tiling.

We note that the so-called linearly repetitive sets are candidates for being “perfect quasicrystals”, but it is rather hard to determine the actual probability of a given patch. From the practical point of view, self-affine tilings (see Section 3.4) and tilings related to cut and project sets (see Section 3.2) are more interesting.

For all our tilings, it will be easy to see that they have a finite protoset, and the only requirement is to have uniform patch frequency. Many tilings result from a discrete set. All suitable discrete sets are Delone sets of finite type, discussed in Section 3.1. Two examples that always have uniform patch frequency are cut and project sets (see Section 3.2) and linearly repetitive sets (see Section 3.3). Two direct approaches to obtain tilings with uniform patch frequency are linearly repetitive tilings (see Section 3.3) and tilings “resulting from inflation”.

3.1. *Tilings related to Delone sets of finite type*

First we introduce some fundamental notions related to discrete sets. We say that a discrete set $\Gamma \subset \mathbb{R}^d$ is a *Delone set* if there exist positive r and R such that the distance between any two points is at least r, and any ball of radius R contains a point of Γ. We call a finite subset of Γ a *discrete patch*, where subsets have a similar role to patches in the case of tilings. In addition, Γ has *finite type* if balls of radius $2R$ contain only finitely many different discrete patches up to translation. In this case, for any fixed $\omega > 0$, balls of radius ω contain only finitely many different discrete patches up to translation according to Lagarias [10]. We define uniform patch frequency of Γ by (3) analogously to tilings (only Π is naturally a discrete patch in the case of Γ).

Two ways are known to relate a tiling to a Delone set of finite type. First, let us consider a tiling with finite protoset. We say that the vertices of the tiling determine the tiling if the vertex sets of two tiles are translates of each other, then the tiles are translates of each other (see, say, the Penrose tiling on Fig. 3). In this case, the tiling has uniform patch frequency if the vertex set has uniform patch frequency.

Another method for relating a tiling to a discrete set Γ is to assign the Dirichlet–Voronoi cell D_x corresponding to each $x \in \Gamma$. We recall that D_x is the family of points whose distance from x is no larger than the distance from any other point of Γ. If any half-space intersects Γ, then each D_x is a convex polytope, and the Dirichlet–Voronoi cells form a facet-to-facet tiling of the space (see Fig. 4 in the case of the vertex set of the Penrose tiling). Since Γ is of finite type, we have only finitely many Dirichlet–Voronoi cells up to translation. We observe that, if Γ has uniform patch frequency, then the same holds for the tiling by the Dirichlet–Voronoi cells as well.

3.2. *Tilings based on cut and project sets*

Cut and project sets (or model sets) in $\mathbb{R}^d$ arise from projecting suitable chosen points of a higher-dimensional lattice into $\mathbb{R}^d$. A precise definition runs as follows. We consider $L = \mathbb{R}^d$ as a linear subspace in $\mathbb{R}^d$ for $N > d$, and write $L^{\perp}$ to denote the orthogonal complement of L in $\mathbb{R}^N$. Now let Λ be a lattice in $\mathbb{R}^N$ such that the origin is the only lattice point in L. We fix a bounded set W, the so-called window in $L^{\perp}$, and define the cut and project set Γ to be the projections of the points Λ into L whose projection into $L^{\perp}$ lands in W. It is always assumed that the window W has positive measure $|W|$ in $L^{\perp}$, and its boundary is measure zero in $L^{\perp}$. In addition, Γ is called a primitive cut and project set if the origin is the only lattice point in $L^{\perp}$ as well. In this case

$$\lim_{r\to\infty} \frac{\#(\Gamma \cap rB^d)}{V(rB^d)} = \frac{|W|}{\det \Lambda}. \tag{5}$$

This observation is due to De Bruijn [4] (see also Senechal [18]). Now, for any discrete patch Π, we fix a vertex v, and one can define a part W_{Π} of the window satisfying the following property. For $x \in \Lambda$, we write x' to denote its projection into L. Then $\Pi + (x' - v)$ is a discrete patch if and only if the projection of x into $L^{\perp}$ lands into W_{Π}. Therefore, the frequency of Π with respect to the volume is $\frac{|W_{\Pi}|}{\det \Lambda}$.

Since any cut and project set is the union of finitely many primitive ones, we deduce that cut and project sets have uniform patch frequency. In addition, the associated tiling by the Dirichlet–Voronoi cells also have uniform patch frequency. We note that the vertices of the Penrose tiling (see Fig. 3) form a cut and project set. More precisely, let L be a two-dimensional invariant subspace of the action of the cyclic group of order five on the basis vectors, and let us project $\mathbb{Z}^5$ into L. In this case, the window is the projection of the unit cube $[0, 1]^5$ into $L^{\perp}$, and the resulting cut and project set is the union of five primitive ones.

3.3. Linearly repetitive tilings

Following Lagarias and Pleasant [12], we call a tiling *linearly repetitive* if, for any given discrete patch of circumradius ω, each ball of radius $c\omega$ contains a discrete patch that is a translate of the given patch where c is a constant. We note that the tiling is an ideal crystal (namely, it is periodic) if and only if the $c\omega$ above can be replaced by $\omega + c$. In addition, if the tiling is not an ideal crystal, then the linear growth rate is the smallest possible growth rate for the difference of the "radius of repetitivity" and of the radius of the discrete patch (see Lagarias and Pleasant [11]). Many of the tilings known in the literature are linearly repetitive, for example the Penrose tilings (see Grünbaum and Shephard [14], p. 563). The fact that linearly repetitive tilings have uniform patch frequency is verified in Lagarias and Pleasant [12].

Analogously, we say that a discrete set Γ is *linearly repetitive* if

- there exists a positive r such that the distance of any two elements is at least r;
- there exists a $c > 1$ such that, for any given discrete patch of circumradius $R \geq r$, each ball of radius cR contains a discrete patch that is a translate of the given discrete patch.

Then Γ has uniform patch frequency as well (see Lagarias and Pleasant [12]). Again, the vertex set of the Penrose tiling on Fig. 3 is linearly repetitive.

3.4. Self-affine tilings and relatives

We say that a linear map φ is *expansive* if it is diagonalizable over $\mathbb{C}$, and each eigenvalue is of absolute value larger than one. We call a tiling *self-affine* if the following conditions are satisfied:

- *Repetitive:* for any given patch, there exists an $\omega > 0$ such that each ball of radius ω contains a patch that is a translate of the given patch;
- *Inflation:* there exists an expansive linear map φ such that the φ image of any tile is the union of a patch;
- *Deflation:* if the tiles T_1 and T_2 are translates, then the patches corresponding to $\varphi(T_1)$ and $\varphi(T_2)$ are translates as well.

It is well known that self-affine tilings have uniform patch frequency (see, say, Solomyak [19]). Since there exist only finitely many tiles up to translation, we deduce that some power of φ acts by multiplication by an $\eta > 1$. The dilatation by η is an inflation, but it may not be a deflation. We note that the term repetitive is used, say, in Senechal [18] or in Lagarias and Pleasant [12], and the same property is called local isomorphism, say, in Solomyak [19].

The most famous example is the Penrose tiling by congruent copies of two rhombi (see Figs. 3 and 5 where $\omega = \frac{\pi}{5}$): The rhombi are built from triangles: one is of side lengths 1, 1 and τ, and the other is of side lengths 1, 1

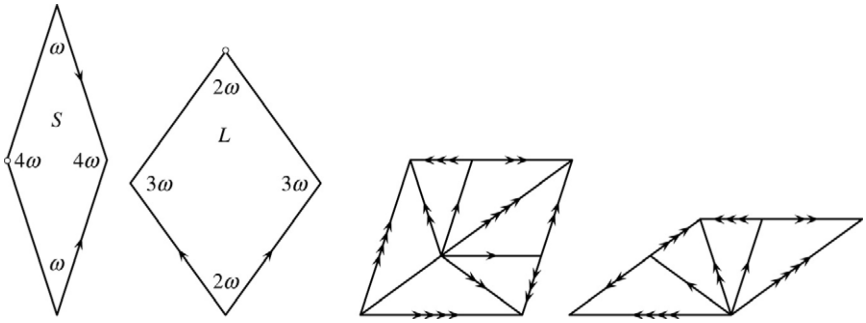

Fig. 5. Deflation for the Penrose tiling.

and $1/\tau$ where τ is the golden ratio $\frac{\sqrt{5}+1}{2}$. Here, the expansive map φ is the multiplication by the complex number $\tau\, e^{\frac{3\pi}{5}\,i}$. In this case, as usual the φ image of a tile is not the union of a patch, but one can still assign a patch to it in a natural way. Numerous self-affine tilings with various symmetry groups have been constructed since the discovery of the Penrose tilings, both in the plane and in the three space (see the papers Baake, Hermisson and Pleasants [2] and Baake, Hermisson and Richard [3] for such examples).

4. The Weaire sum rule for quasiperiodic tilings

In this section we prove Theorem 1. Let $\mathcal{T}$ be a facet-to-facet tiling of $\mathbb{R}^d$ with finite protoset and with uniform patch frequency. A simple-minded approach is to consider the (finitely many) translation types $C_1, \ldots, C_k$ of coronas, and to define the probability space on them where a C_i occurs with probability $p(C_i)$ (compare (4)). Since we are only interested in the combinatorics of the coronas, this approach is not too economic. Say, in the case of Penrose tiling on Fig. 3, a protoset requires 20 rhombi, while we only need two rhombi up to congruence. Therefore we apply a more economic approach.

We may define the probability p_n that the number of facets of a tile is n; namely, p_n is the sum of the probabilities of the tiles that have n facets (see (4)). In particular

$$\sum_n p_n = 1; \tag{6}$$

$$\langle n^z \rangle = \sum_n n^z p_n \quad \text{for any } z \in \mathbb{R} \tag{7}$$

where naturally p_n is non-zero only for finitely many n.

Next we define the *neighbourly indicator* $H(n, k)$ that is proportional to the frequency of ordered pairs (T, S) of neighbouring tiles with $n(T) = n$ and $n(S) = k$ among all tiles. More precisely, let $\mathcal{T}_{n,k}$ denote the family of patches that consist of two neighbouring tiles, one of which has n facets and the other has k facets. We have

$$H(n,k) = \lim_{r\to\infty} \frac{\#\{\Pi \in \mathcal{T}_{n,k} : \Pi \subset rB^d\}}{\#\{T \in \mathcal{T} : T \subset rB^d\}} \quad \text{if } n \neq k;$$

$$H(n,n) = \lim_{r\to\infty} \frac{2\cdot\#\{\Pi \in \mathcal{T}_{n,n} : \Pi \subset rB^d\}}{\#\{T \in \mathcal{T} : T \subset rB^d\}}$$

where the limits make sense because of uniform patch frequency. Naturally, $H(n, k)$ is non-zero only for finitely many pairs. The neighbourly indicator is symmetric in its variables, hence for any n, k we have

$$H(k,n) = H(n,k). \tag{8}$$

If, for fixed n, we calculate the total number of neighbours of n-faceted tiles (in a big ball) by classifying the neighbours according to their number of facets, then we obtain

$$n \cdot p_n = \sum_k H(n,k). \tag{9}$$

In addition for any tile T, $n(T) \cdot m(T)$ is the total number of facets of the neighbours of T, hence again classifying the neighbours of a tile according to their number of facets leads to

$$\langle n \cdot m \rangle = \sum_n \sum_k k H(n,k). \tag{10}$$

Using these formulae, we can express $\langle n^z \rangle$ for $z \in \mathbb{R}$ in terms of the neighbourly indicator as follows:

$$\begin{aligned}\langle n^z \rangle &= \sum_n n^z p_n = \sum_n n^{z-1} n p_n \\ &= \sum_n \sum_k n^{z-1} H(n,k) = \sum_n \sum_k k^{z-1} H(n,k).\end{aligned} \tag{11}$$

Comparing (11) for $z = 2$ and (10) completes the proof of the Weaire sum rule Theorem 1.

Remark 4. The Weaire sum rule (1) holds for any finite tiling by d-cells of some topological space if any facet is contained in exactly two cells. In particular, (1) holds for any facet-to-facet tiling of any compact topological d-manifold.

The proof of this statement runs as the proof of Theorem 1, only there is no need to take limits in the definition of p_n and $H(n,k)$.

Remark 5. If, in a tiling, any facet is contained exactly in two tiles, but two tiles may have more than one common facet, then, in the definition of $H(n,k)$, each pair (T, S) of neighbouring tiles is counted as many times as there are common facets S and T. Using this modified notion, the proof of Theorem 1 goes through, hence we have the Weaire sum rule (1) both for quasiperiodic tilings and for finite tilings of compact topological d-manifolds.

Remark 6. Given a tiling $\mathcal{T}$ of either types discussed above, we can associate a natural probability space defined on the space $\mathbb{Z}$ of integers. In this space, any integer n occurs with probability p_n, where p_n is the probability that tile of $\mathcal{T}$ has n facets. If f is any function of integers, then its expected value is

$$\langle f \rangle_{\text{int}} = \sum_n f(n) p_n. \tag{12}$$

For any positive integer n, we define $m(n)$ to be the average of $m(T)$ over all tiles T with n facets. More precisely, let $\mathcal{T}_n$ be the family of tiles with n facets, and let $N(r)$ be the number of tiles of $\mathcal{T}$ that are contained in rB^d. In the case of quasiperiodic tilings, we have

$$m(n) = \lim_{r\to\infty} \frac{\sum_{\{T\in\mathcal{T}_n:\, T\subset rB^d\}} m(T)}{\#\{T \in \mathcal{T}_n : T \subset rB^d\}}, \tag{13}$$

which in turn yields that

$$m(n) = \lim_{r\to\infty} \frac{\left(\sum_{\{T\in\mathcal{T}_n:\, T\subset rB^d\}} n \cdot m(T)\right) \Big/ N(r)}{n \cdot \#\{T \in \mathcal{T}_n : T \subset rB^d\}/N(r)} = \frac{\sum_k k H(n,k)}{n p_n}. \tag{14}$$

Naturally, the same formulae hold for finite tilings, only we do not need the limiting process. We also deduce that

$$\begin{aligned}&\langle n^z \rangle_{\text{int}} = \langle n^z \rangle \quad \text{for any } z \in \mathbb{R};\\ &\langle m(n) \rangle_{\text{int}} = \langle m \rangle;\\ &\langle n \cdot m(n) \rangle_{\text{int}} = \langle n \cdot m \rangle.\end{aligned}$$

Therefore we conclude the Weaire sum rule (1) in the equivalent form

$$\langle n^2 \rangle_{\text{int}} = \langle n \cdot m(n) \rangle_{\text{int}}. \tag{15}$$

This is the traditional form of the Weaire sum rule in the papers [20,21,6,7,16,17].

5. Valences of vertices and dual tilings in the planar case

In this section we introduce some notions related to vertex figures for planar tilings. These notions are important from the point of view of the Weaire sum rule, because they yield corresponding characteristics of the dual tilings.

If $\mathcal{T}$ is an edge-to-edge tiling of $\mathbb{R}^2$ with finite protoset and uniform patch frequency, then the *star of a vertex* v is the union of the edges of the tiling containing v. We say that two stars are of the same type if they are congruent, and observe that there are only finitely many types of stars up to congruence. Given a star Π, its probability $\pi(\Pi)$ is defined with respect to congruence and not translational equivalence; namely,

$$\pi(\Pi) = \lim_{r\to\infty} \frac{\text{number of stars congruent to } \Pi \text{ in } rB^2}{\text{number of vertices in } rB^2}.$$

We write $\mathcal{V}$ to denote the family of vertices of $\mathcal{T}$, and $\varrho(v)$ to denote the valence (or degree) of the vertex v. Therefore, for any positive integer n, we may define π_n to be the probability that a vertex has valence n. We note that, for any $z \in \mathbb{R}$, the expected value of ϱ^z is

$$\langle \varrho^z \rangle_{\text{vert}} = \lim_{r\to\infty} \frac{\sum_{v\in\mathcal{V}\cap rB^2} \varrho^z(v)}{\#(\mathcal{V}\cap rB^2)} = \sum_k k^z \pi_k. \tag{16}$$

An edge-to-edge tiling $\mathcal{T}_{\text{dual}}$ with finite protoset and uniform patch frequency is called the dual of $\mathcal{T}$ if the following holds. There exist bijective correspondences between the tiles of $\mathcal{T}$ and the vertices of $\mathcal{T}_{\text{dual}}$, and between the vertices of $\mathcal{T}$ and the tiles of $\mathcal{T}_{\text{dual}}$ in such a way that, for any tile T of either $\mathcal{T}$ or $\mathcal{T}_{\text{dual}}$ and for any vertex v of T, the image of T is a vertex of the image of v. If f is a function on the tiles of $\mathcal{T}_{\text{dual}}$, then we write $\langle f \rangle_{\text{dual}}$ to denote the expected value provided that it exists. Now the probability p_n that a tile of $\mathcal{T}_{\text{dual}}$ has n sides is π_n, therefore, for any $z \in \mathbb{R}$, we have

$$\langle n^z \rangle_{\text{dual}} = \langle \varrho^z \rangle_{\text{vert}}. \tag{17}$$

For any planar tiling, the expected value of the valences of the vertices and the number of sides of the tiles are related as follows.

Remark 7. If $\mathcal{T}$ is an edge-to-edge planar tiling with finite protoset and uniform patch frequency, then

$$\frac{1}{\langle n \rangle} + \frac{1}{\langle \varrho \rangle} = \frac{1}{2}. \tag{18}$$

Moreover, if the valence of each vertex is at least three, then $3 \le \langle n \rangle, \langle \varrho \rangle \le 6$, and for trivalent tilings, we have $\langle n \rangle = 6$.

The statement is well known, but we provide a quick proof for the sake of completeness. We write $\Sigma(r)$ to denote the cell complex that consists of the tiles lying in rB^2, their edges and their vertices, and write $e(r)$ to denote the number of edges of $\Sigma(r)$. In addition, let $\mathcal{V}$ be the family of vertices of $\mathcal{T}$.

Since, for large r, both the union of the two-cells in $\Sigma(r)$ and its complement are connected, we deduce that the Euler characteristics of $\Sigma(r)$ is one (see Armstrong [1]). In particular,

$$\#(\Sigma(r)\cap\mathcal{V}) - e(r) + \#(\Sigma(r)\cap\mathcal{T}) = 1. \tag{19}$$

Since any edge of a tile of $\mathcal{T}$ that has an endpoint in $\Sigma(r)$ has exactly two endpoints in $\Sigma(r)$ unless the edge is close to the boundary of rB^2, we deduce

$$\lim_{r\to\infty} \frac{\sum_{v\in\Sigma(r)\cap\mathcal{V}} \varrho(v)}{2e(r)} = 1. \tag{20}$$

In addition, counting the edges of the tiles in $\Sigma(r)$ leads to

$$\lim_{r\to\infty} \frac{\sum_{T\in\Sigma(r)\cap\mathcal{T}} n(T)}{2e(r)} = 1. \tag{21}$$

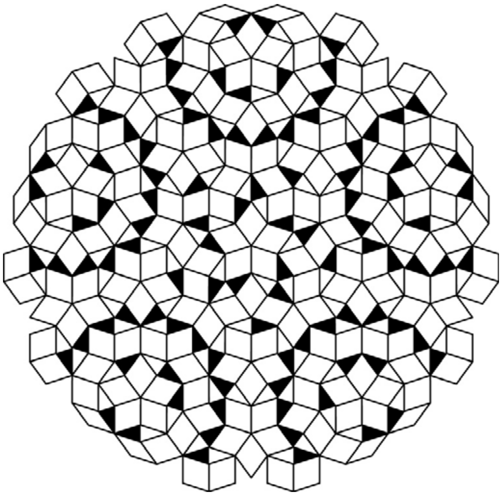

Fig. 6. The modified Penrose tiling.

We deduce by (19)–(21) that

$$\frac{1}{\langle n\rangle}+\frac{1}{\langle \varrho\rangle}=\lim_{r\to\infty}\frac{\#(\Sigma(r)\cap\mathcal{T})}{\sum\limits_{T\in\Sigma(r)\cap\mathcal{T}} n(T)}+\lim_{r\to\infty}\frac{\#(\Sigma(r)\cap\mathcal{V})}{\sum\limits_{v\in\Sigma(r)\cap\mathcal{V}}\varrho(v)}$$
$$=\lim_{r\to\infty}\frac{\#(\Sigma(r)\cap\mathcal{T})}{2e(r)}+\lim_{r\to\infty}\frac{\#(\Sigma(r)\cap\mathcal{V})}{2e(r)}=\lim_{r\to\infty}\frac{e(r)+1}{2e(r)}=\frac{1}{2}.$$

Finally, since any tile has at least three edges, if the valences of the vertices are always at least three, then (18) proves $3\le\langle n\rangle,\langle\varrho\rangle\le 6$.

6. Examples — some simple quasiperiodic tilings generated from the Penrose tiling

If $\mathcal{T}$ is any of the tilings in the examples below, then the dual tiling $\mathcal{T}_{\text{dual}}$ can be defined as follows. For any vertex v of $\mathcal{T}$, we define the associated cell of $\mathcal{T}_{\text{dual}}$ to be a convex hull of the circumcentres of the tiles of $\mathcal{T}$ that contain v. These associated cells form the tiles of $\mathcal{T}_{\text{dual}}$.

6.1. The Weaire sum rule for the modified Penrose tiling

In this section we calculate separately the two sides of the Weaire sum rule Theorem 1 for a modified version of the Penrose tiling, and demonstrate that the two sides coincide. The modified Penrose tiling is constructed as follows. We start with the version with two rhombi as in Fig. 3, and cut each thin rhombus into two triangles by the shorter diagonal (see Fig. 6). Both $\langle n^2\rangle$ and $\langle nm\rangle$ are determined on the basis of formulae at the end of Section 2. In the calculations, we use the golden ratio $\tau=\frac{\sqrt{5}+1}{2}$ satisfying $\tau^2=\tau+1$.

For the original Penrose tiling in Fig. 3, Henley [8] (see p. 799) calculated that the probability p_{thin} of the thin rhombi and the probability p_{fat} of the fat rhombi satisfy $\frac{p_{\text{fat}}}{p_{\text{thin}}}=\tau$. We deduce by $p_{\text{fat}}+p_{\text{thin}}=1$ that

$$p_{\text{thin}}=2-\tau;$$
$$p_{\text{fat}}=\tau-1.$$

It follows that, for the modified Penrose tiling on Fig. 6, we have

$$p_3=\frac{2p_{\text{thin}}}{2p_{\text{thin}}+p_{\text{fat}}}=\frac{6-2\tau}{5};\tag{22}$$

$$p_4=\frac{p_{\text{fat}}}{2p_{\text{thin}}+p_{\text{fat}}}=\frac{2\tau-1}{5}.\tag{23}$$

In particular, (7) yields that

$$\langle n^2 \rangle = 9p_3 + 16p_4 = \frac{38 + 14\tau}{5}. \tag{24}$$

Let us calculate the numbers $H(n, k)$. The fact that makes their calculation simple is that any rhombus in the modified Penrose tiling has two rhombus neighbours and two triangle neighbours. In particular, $H(4, 4) = H(4, 3)$, hence combining $4p_4 = H(4, 4) + H(4, 3)$ (cf. (9)) and (8) leads to

$$H(4, 4) = H(4, 3) = H(3, 4) = 2p_4 = \frac{4\tau - 2}{5}.$$

It follows by (9) that

$$H(3, 3) = 3p_3 - H(3, 4) = 4 - 2\tau.$$

We conclude by (10) that

$$\langle n \cdot m \rangle = 3H(3, 3) + 4H(3, 4) + 3H(4, 3) + 4H(4, 4) = \frac{38 + 14\tau}{5}, \tag{25}$$

which agrees with $\langle n^2 \rangle$ according to (24), as is required by the Weaire sum rule.

6.2. More on the modified Penrose tiling

We discuss some additional characteristics of the modified Penrose tiling defined in Section 6.1 using the values calculated in Section 6.1. The expected number of facets is

$$\langle n \rangle = 3p_3 + 4p_4 = \frac{2\tau + 14}{5} = 3.4472. \tag{26}$$

Next, we calculate the possible values of $m(n)$. Since any rhombus has two triangular and two quadrilateral neighbours, we have

$$m(4) = \frac{2 \cdot 3 + 2 \cdot 4}{4} = 3.5.$$

It follows by (12) applied to $f(n) = n \cdot m(n)$ and by (25) that

$$3m(3)p_3 + 4m(4)p_4 = \langle n \cdot m(n) \rangle_{\text{int}} = \langle n \cdot m \rangle = \frac{38 + 14\tau}{5},$$

therefore

$$m(3) = \frac{\langle n \cdot m(n) \rangle_{\text{int}} - 4m(4)p_4}{3p_3} = \frac{9 + \tau}{3} = 3.5393.$$

It also follows (compare (26)) that the expected value of the facet coordination number is

$$\langle m \rangle = \langle m(n) \rangle_{\text{int}} = m(3)p_3 + m(4)p_4 = \frac{83 + 14\tau}{30} = 3.5217 > \langle n \rangle; \tag{27}$$

namely, the expected value of the facet coordination number is larger than the expected value of the number of facets in accordance with Conjecture 3.

6.3. Vertex types and dual tiling for the Penrose tiling

Let us consider the "marked" version of the Penrose tiling in Fig. 3; namely, the edges are marked to force the deflation rule (see Fig. 5). de Bruin [4] proved that the vertices in the Penrose tiling have eight different types of (marked) stars. Following tradition, the eight vertex types denoted by S, K, Q, D, J, S3, S4 and S5 are shown in Fig. 7. Later, Henley (see [8], Table I) calculated the probability of these vertex types (see Table 1).

Fig. 7 shows that the possible values of the valences of the vertices are 3, 4, 5, 6 and 7, as in Table 2.

Table 1
Probability distribution of the vertex types in the Penrose tiling

$\pi(S) = \frac{18-11\tau}{5}$; $\pi(K) = 5\tau - 8$; $\pi(Q) = 5 - 3\tau$; $\pi(D) = 2 - \tau$
$\pi(J) = 2\tau - 3$; $\pi(S3) = 13 - 8\tau$; $\pi(S4) = 13\tau - 21$; $\pi(S5) = \frac{47-29\tau}{5}$

Table 2
Probability distribution of the valences in the dual Penrose tiling

$\pi_3 = \pi(Q) + \pi(D) = 7 - 4\tau = 0.5278$
$\pi_4 = \pi(K) = 5\tau - 8 = 0.0901$
$\pi_5 = \pi(S) + \pi(J) + \pi(S5) = 10 - 6\tau = 0.2917$
$\pi_6 = \pi(S4) = 13\tau - 21 = 0.0344$
$\pi_7 = \pi(S3) = 13 - 8\tau = 0.0557$

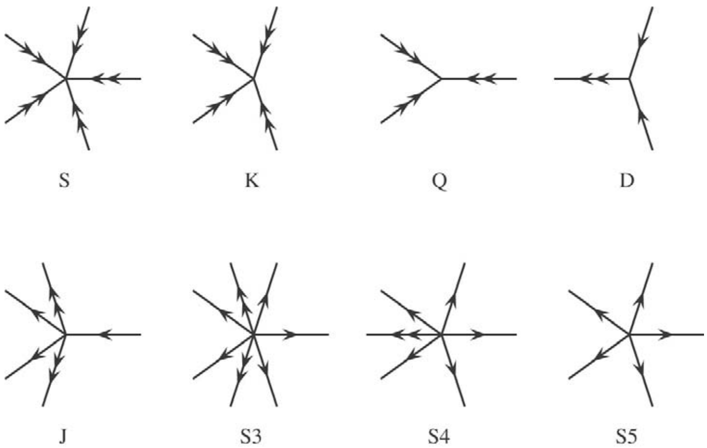

Fig. 7. Vertex figures for the Penrose tiling.

Table 3
Probability distribution of the valences in the modified Penrose tiling

$\pi_4 = \pi(D) = 2 - \tau = 0.3819$
$\pi_5 = \pi(S) + \pi(S5) + \pi(J) + \pi(K) + \pi(Q) = 7 - 4\tau = 0.5287$
$\pi_6 = \pi(S4) = 13\tau - 21 = 0.0344$
$\pi_7 = \pi(S3) = 13 - 8\tau = 0.0557$

Since $\langle n\rangle = 4$ for the Penrose tiling, we deduce $\langle\varrho\rangle_{\text{vert}} = 4$ by the formula $\frac{1}{\langle n\rangle} + \frac{1}{\langle\varrho\rangle} = \frac{1}{2}$ (see (18)). In addition,

$$\langle\varrho^2\rangle_{\text{vert}} = 9\pi_3 + 16\pi_4 + 25\pi_5 + 36\pi_6 + 49\pi_7 = 66 - 30\tau = 17.4589.$$

Concerning the dual of the Penrose tiling (depicted in Fig. 8), we have $\langle n^2\rangle_{\text{dual}} = \langle\varrho^2\rangle_{\text{vert}}$ according to (17), therefore the Weaire sum rule Theorem 1 yields

$$\langle nm\rangle_{\text{dual}} = \langle n^2\rangle_{\text{dual}} = 66 - 30\tau = 17.4589.$$

6.4. The dual tiling for the modified Penrose tiling

Let us now turn to the modified Penrose tiling in Fig. 6. Based on the values in Table 1, it is not hard to determine the probability distribution of valences of the vertices. In this case, the possible values of the valences of the vertices are 4, 5, 6 and 7, and we have Table 3.

In particular,

$$\langle\varrho\rangle_{\text{vert}} = 4\pi_4 + 5\pi_5 + 6\pi_6 + 7\pi_7 = 8 - 2\tau = 4.7639;$$

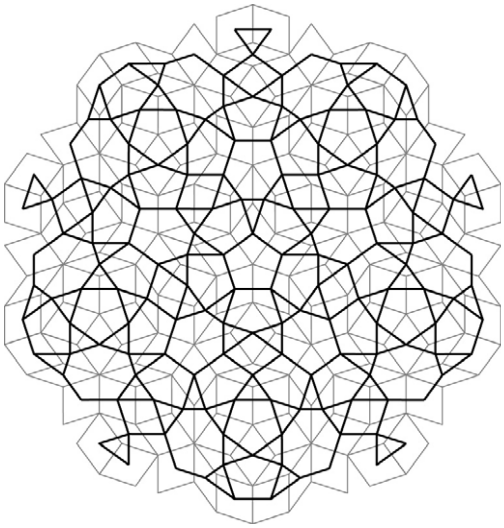

Fig. 8. The dual of the Penrose tiling.

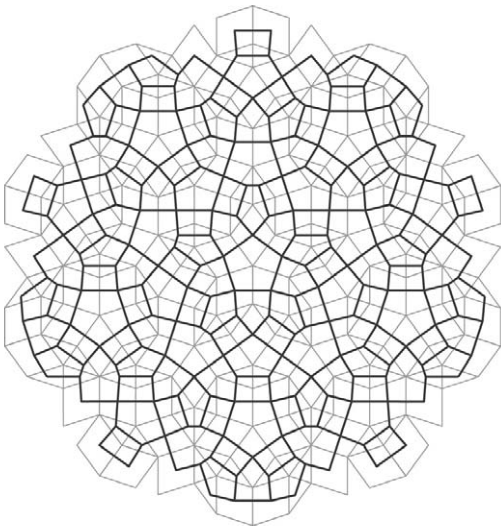

Fig. 9. The dual of the modified Penrose tiling.

$$\langle \varrho^2 \rangle_{\text{vert}} = 16\pi_4 + 25\pi_5 + 36\pi_6 + 49\pi_7 = 88 - 40\tau = 23.2786.$$

Let us turn to the dual of the modified Penrose tiling (see Fig. 9). Since $\langle n^2 \rangle_{\text{dual}} = \langle \varrho^2 \rangle_{\text{vert}}$ according to (17), we conclude by the Weaire sum rule Theorem 1 that

$$\langle nm \rangle_{\text{dual}} = \langle n^2 \rangle_{\text{dual}} = 88 - 40\tau = 23.2786.$$

6.5. The Dirichlet–Voronoi tiling with respect to the vertices of the Penrose tiling

In this section we discuss the Dirichlet–Voronoi tiling $\mathcal{T}_{DV}$ with respect to the vertices of the Penrose tiling (see Fig. 4). Now $\mathcal{T}_{DV}$ is the dual of the triangular tiling, which is obtained from the Penrose tiling in Fig. 3 by cutting each rhombus into two by its shorter diagonal (see Henley [8], p. 799, Fig.4). Checking the eight vertex types in Fig. 7 of the Penrose tiling shows that $\mathcal{T}_{DV}$ consists of tiles with 5, 6 and 7 sides. Writing p_n to denote the probability that a tile of $\mathcal{T}_{DV}$ has n sides, Table 1 yields Table 4.

Table 4
Probability distribution of the side numbers in the Dirichlet–Voronoi tiling

$p_5 = \pi(S) + \pi(K) + \pi(Q) + \pi(S5) = 10 - 6\tau = 0.2917$
$p_6 = \pi(D) + \pi(S4) = 12\tau - 19 = 0.4164$
$p_7 = \pi(J) + \pi(S3) = 10 - 6\tau = 0.2917$

We have

$$\langle n \rangle = 5p_5 + 6p_6 + 7p_7 = 6.$$

In addition, the Weaire sum rule Theorem 1 yields

$$\langle nm \rangle = \langle n^2 \rangle = 25p_5 + 36p_6 + 49p_7 = 56 - 12\tau = 36.5835.$$

7. Conclusion

A general method has been developed to characterize the first neighbour topological structure (i.e. the nearest-neighbour local environment) in quasiperiodic cellular systems composed of d-dimensional generalized polytopes (cells).

By introducing the notion of the facet coordination number and of neighbourly indicators, we have proved that the validity of the Weaire sum rule can be extended to all quasiperiodic systems that are generated as a result of tessellation with uniform patch frequency. It should be emphasized that the neighbourly indicators are simply topological invariant by which the local topological structure of periodic and quasiperiodic cellular systems can be quantitatively evaluated and compared (see [16]).

The application of the method outlined was demonstrated in simple examples based on the analysis of various 2D quasiperiodic systems constructed from the well-known Penrose tiling with two decorated rhombus tiles.

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