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ORIGINAL PAPER

Numbers of faces in disordered patches

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Abstract It has been shown that the boundary structure of patches with all faces of the same size k, all interior vertices of the same degree m and all boundary vertices of degree at most m determines the number of faces of the patch (Brinkmann et al., Graphs and discovery, 2005; Guo et al., Discrete Appl Math 118(3):209–222, 2002). In case of at least two defective faces, that is faces with degree $k' \neq k$, it is well known that this is not the case. The most famous example for this is the Endo–Kroto C_2-insertion (Endo and Kroto, J Phys Chem 96:6941–6944, 1992). Patches with a limited amount of *disorder* are especially interesting for the case $k = 6$, $m = 3$ and $k' = 5$. This case corresponds to polycyclic hydrocarbons with a limited number of pentagons and to subgraphs of fullerenes. The last open question was the case of exactly one defective face or vertex. In this paper we generalize the results of Brinkmann et al. (2005) and Guo et al. (2002) and in some cases corresponding to Euclidean lattices also deal with patches that have vertices of degree larger than m on the boundary, have sequences of degrees on the boundary that are identical only modulo m and have vertex and face degrees in the interior that are multiples of m, resp. k. Furthermore we prove that in case of at most one defective face with a degree that is not a multiple of k the number of faces of a patch is determined by the boundary. This result implies that fullerenes cannot grow by replacing patches of a restricted size.

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1 Introduction

It is easy to prove that the cyclic sequence of vertex degrees in the boundary uniquely describes the interior of a *hexagonal patch*, that is a 2-connected planar graph with all faces hexagons, all non-boundary vertices of degree 3 and all boundary vertices of degree at most 3—as long as it is a subgraph of the hexagonal (graphite) lattice. Interpreting the vertices as carbon atoms and attaching a hydrogen to all boundary vertices with degree 2, these structures correspond to the well studied class of *benzenoids* in chemistry.

It has long been believed that this is also the case if the graph is not necessarily a subgraph of the hexagonal lattice (in this case the corresponding molecules are called *fusenes* or *planar polycyclic hydrocarbons* with all faces hexagons), until in [1] a counterexample was given (see Fig. 2) and at the same time it was shown that nevertheless the number of vertices, edges, and faces is well determined. Later this result was proven in a more general context [2].

Patches with the same boundary and different interior also play an important role as *local rearrangements* in *fullerenes*. A fullerene is a molecule of pure carbon on the surface of a *topological* sphere so that the corresponding graph is cubic and all faces have degree 5 or 6. The Euler formula implies that there are exactly 12 pentagons. The first fullerene was discovered in 1985 (see [3]). Since scientists believe that fullerenes may play an important role in future applications (see e.g. [4,5]) a large number of articles has been published on the topic since 1985 and in 1996 the Nobel prize in chemistry was awarded to Curl, Kroto, and Smalley for their discovery.

In [6] Endo and Kroto proposed a mechanism for fullerene growth (see Fig. 1) that is based on the idea of a finite region of the fullerene—that is: a patch in the sense above—being replaced by another patch with more vertices (atoms) and the same boundary structure. In [7] a computer was used to list pairs of patches that can be used for this purpose. All pairs of patches found in this approach had at least two pentagons and though this might have been the case because the list was restricted to relatively small examples, it raised the question whether the number of vertices (or equivalently faces) of patches with only one pentagon is determined by its boundary alone. In this paper we will answer this question in a more general context and prove that this is indeed the case. A chemical consequence is that large fullerenes with long distances between any two pentagons (e.g. large fullerenes with icosahedral symmetry) cannot be formed in this way unless very large patches are involved. Another proposal for the formation of fullerenes would be that some similar process of patch replacement [8,9] occurs with pairs of patches of the same size. While various pairs of patches are known that both contain one or no pentagon and have the same boundary but different interior (see Fig. 2), none of the patches in these known pairs can occur as a subgraph of a fullerene. As mentioned before, such hexagonal patches cannot be subgraphs of the hexagonal (graphite) lattice and Graver even showed that there must be some 3-fold overlap if they are embedded into the graphite lattice [10], but it is still unknown whether they can occur as subgraphs of fullerenes.

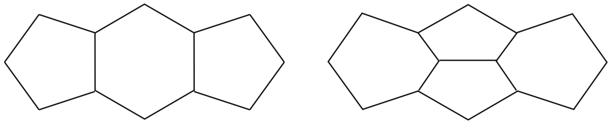


Fig. 1 The Endo–Kroto growth patches

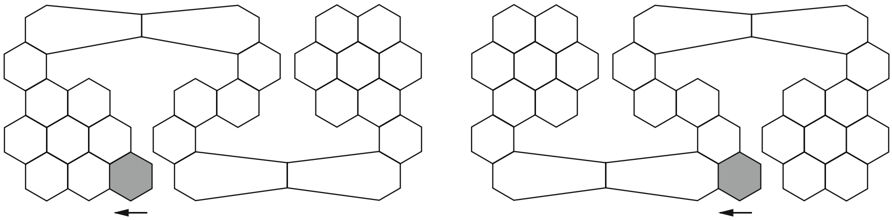


Fig. 2 Two different patches with the same boundary

Though fullerenes and planar polycyclic hydrocarbons are the most important applications, we will prove the results in a more general context with fullerene patches and hydrocarbons being just a special case.

2 Basic definitions and first results

We will always assume plane graphs to come with a combinatorial embedding in the plane (see [11,12]). Undirected edges are identified with a set of two opposite directed edges and for every vertex v we have a rotational order of the directed edges starting at v, which we will interpret as clockwise. For sets D of directed edges and U of undirected edges we will also write $D \cap U$ to denote the set of directed edges in D that have underlying undirected edges in U. The inverse of a directed edge e will be denoted by e^- and for a directed path or cycle P the inverse path or cycle is denoted P^-.

Definition 1 For a plane graph G we denote the set of vertices, (undirected) edges and faces of G as $V(G)$, $E(G)$, and $F(G)$. The set of directed edges is denoted as $\vec{E}(G)$. In case there is no possibility of misunderstandings, we only write V, E, F, $\vec{E}$.
Two faces are said to be neighbouring if they share an edge.
The degree of a face is given by the number of edges in its boundary with bridges counted twice.
In order to distinguish multisets from sets, we will denote them as $\langle \ldots \rangle$.
An (m, k, V_D, F_D) graph is a connected plane graph with vertex set V, edge set E, face set F, and multisets $V_D = \langle deg(v) | v \in V, \deg(v) \neq m \rangle$ and $F_D = \langle deg(f) | f \in F, \deg(f) \neq k \rangle$.
We call F_D the multiset of *defective face degrees* and V_D the multiset of *defective vertex degrees*. Vertices v with $\deg(v) \neq m$ are called *defective vertices* and faces f with $\deg(f) \neq k$ are called *defective faces*.

In this language, fullerenes are $(3, 6, \langle\rangle, \langle 5, \ldots, 5\rangle)$ graphs with the multiplicity of 5 in F_D being 12. Except for benzene itself for every fusene there exists some number l so that with multiplicity l of 2 in V_D, the fusene is a $(3, 6, \langle 2, \ldots, 2\rangle, \langle 2l-6\rangle)$ graph.

Definition 2 For an (m, k, V_D, F_D) graph with $V_D = \langle d_1, \ldots, d_l\rangle$ and $F_D = \langle f_1, \ldots, f_j\rangle$ we define the *vertex deficiency* as $D_V = \sum_{i=1}^{l}(m - d_i)$ and the *face deficiency* as $D_F = \sum_{i=1}^{j}(k - f_i)$.

Lemma 1 *Given an* (m, k, V_D, F_D) *graph with* $v := |V|$ *the number of vertices,* $e := |E|$ *the number of edges, and* $f := |F|$ *the number of faces. Then the following relations hold*:

$$v = \frac{kf - D_F + D_V}{m} \tag{1}$$

$$e = \frac{kf - D_F}{2} \tag{2}$$

$$(2k - km + 2m)f = 4m + (2 - m)D_F - 2D_V \tag{3}$$

Proof In order to count every edge twice, we can once count vertices and once faces weighted with their degrees to determine the number of edges, i.e. $2e = mv - D_V$ and $2e = kf - D_F$. The second relation directly yields (2) while (1) follows by equating both relations. Inserting (1) and (2) into the Euler formula $v - e + f = 2$, we obtain (3). □

Theorem 1 *Let G be an* (m, k, V_D, F_D) *graph with* $m, k \in \mathbb{N}$, $m, k \geq 3$, *and* $(m, k) \notin \{(3, 6), (4, 4), (6, 3)\}$. *Then the number of faces is uniquely determined by the vertex deficiency and the face deficiency. It is given by*

$$f = \frac{4m + (2 - m)D_F - 2D_V}{2k - km + 2m}. \tag{4}$$

In particular, we can determine the number of faces with degree k by just using m, k and the degrees of the defective faces and vertices.

Proof In case $2k - km + 2m \neq 0$, (4) is immediately obtained by (3). This is not applicable for the pairs of integers (m, k) fulfilling $2k - km + 2m = 0$, or equivalently $k = k(m) = \frac{2m}{m-2}$. $k(m)$ is a monotonically decreasing function with $k(3) = 6$, $k(4) = 4$, $k(5) = 3\frac{1}{3}$, $k(6) = 3$, and $k(7) = 2\frac{4}{5}$. Therefore, the only integers (m, k) with $m, k \geq 3$ that fulfill $2k - km + 2m = 0$ are the pairs $(m, k) = (3, 6)$, $(m, k) = (4, 4)$, and $(m, k) = (6, 3)$. For all other pairs, i.e. $m, k \geq 3$ with $(m, k) \notin \{(3, 6), (4, 4), (6, 3)\}$, we have $2k - km + 2m \neq 0$ and hence formula (4) holds. □

This theorem implies that in case $(m, k) \notin \{(3, 6), (4, 4), (6, 3)\}$, two (m, k, V_D, F_D) graphs contain the same number of faces - and since the number of defective faces is given they also have the same number of non-defective faces. For the other three cases $(m, k) = (3, 6)$, $(m, k) = (4, 4)$, and $(m, k) = (6, 3)$, this is *not* true (see Fig. 3).

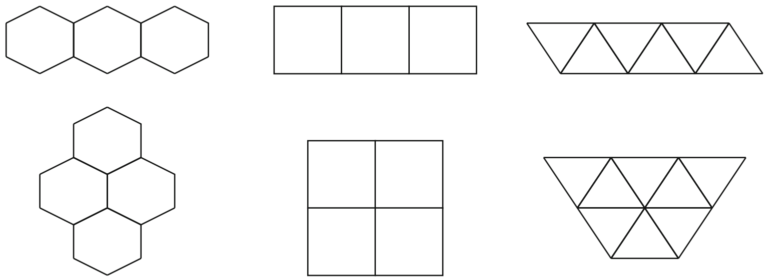


Fig. 3 Two (3, 6, ⟨2, 2, 2, 2, 2, 2, 2, 2, 2, 2⟩, ⟨14⟩) graphs (on the left), two (4, 4, ⟨2, 2, 2, 2, 3, 3, 3, 3⟩, ⟨8⟩) graphs (middle) and two (6, 3, ⟨2, 2, 3, 3, 4, 4, 4, 4⟩, ⟨8⟩) graphs (right) with a different number of faces in each case

3 Patches

Definition 3 An (m, k, V_D, F_D, o) patch is an (m, k, V_D, F_D) graph, together with a distinguished face $o \in F$ called the *outer face*. By definition (m, k, V_D, F_D, o) patches are special (m, k, V_D, F_D) graphs.
Since in patches the outer face—which may have size k or not—is in general not regarded to be a defective face and since defects that are multiples of the regular face or vertex degrees play a special role, it is useful to introduce the notations $F' = F \setminus \{o\}$, $F'_D = F_D \setminus \langle \deg(o) \rangle$, $V'_D = V_D \setminus \langle \deg(v) | v \in o \rangle$, $F''_D = \langle r \in F'_D | r \neq k * n \, \forall n \in \mathbb{N} \rangle$ and $V''_D = \langle r \in V'_D | r \neq m * n \, \forall n \in \mathbb{N} \rangle$.

In case of patches the term *boundary cycle of the patch* always denotes the boundary cycle of the outer face.

For a vertex v we define

$$A(v) := \{(e_1, e_2) | e_2 \text{ follows } e_1 \text{ in the rotational order around } v\}$$

and $A := \bigcup_{v \in V} A(v)$.
where A is called the set of angles. The face $f(e_1, e_2)$ corresponding to an angle (e_1, e_2) is the face between the two edges in the order given.
A labelled plane (m, k, V_D, F_D) graph is a plane graph together with a labelling $l : A \to \{0, \ldots m - 1\}$.
A labelling l of an (m, k, V_D, F_D, o) patch is said to be suitable if $l(e_1, e_2) = 0$ for all (e_1, e_2) with $f(e_1, e_2) \neq o$ and for all $v \in V$ we have $\sum_{a \in A(v)} l(a) + deg(v) = 0(\mathrm{mod} m)$. In the following we will assume all labellings of patches to be suitable.

By this definition, fusenes (except benzene) are not only $(3, 6, \langle 2, \ldots 2, \rangle, \langle 2l - 6 \rangle)$ graphs for some multiplicity l of 2 in V_D, but also $(3, 6, \langle 2, \ldots 2 \rangle, \langle 2l - 6 \rangle, o)$ patches. Benzene is a $(3, 6, \langle 2, 2, 2, 2, 2, 2 \rangle, \langle \rangle, o)$ patch.

Simply connected subgraphs of fullerenes that do not consist of a single hexagon are $(3, 6, \langle 2, \ldots 2 \rangle, \langle n, 5, \ldots, 5 \rangle, o)$ patches with n the size of the boundary and some multiplicity of 5 in F_D that is at most 12.

In our drawings we will always depict the patches embedded into the plane so that the outer face is the unbounded face.

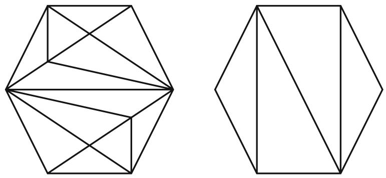


Fig. 4 A $(4, 3, \langle 6, 6, 3, 3\rangle, \langle 6\rangle, o)$ patch and a $(4, 3, \langle 2, 2, 3, 3\rangle, \langle 6\rangle, o)$ patch with similar boundaries but different numbers of faces

Definition 4 The *boundary sequence* of an (m, k, V_D, F_D, o) patch is the cyclic sequence $d_0, d_1, \ldots, d_n$ of vertex degrees in the directed boundary cycle of the outer face o.

For given m, two boundary sequences $d_0, d_1, \ldots, d_n, d'_0, d'_1, \ldots, d'_n$ are said to be *similar* if there is a cyclic reordering or inversion $\bar{d}_0, \bar{d}_1, \ldots, \bar{d}_n$ of one of the sequences (w.l.o.g $d'_0, d'_1, \ldots, d'_n$) so that $d_i = \bar{d}_i (\text{mod } m)$ for $0 \le i \le n$.

Patches with similar boundary sequences are said to have a similar boundary.

One of the things we will prove in this section is that for $(m, k) \in \{(3, 6), (4, 4), (6, 3)\}$ and given m, k, V_D, W_D, F_D, o with $V''_D = W''_D = \emptyset$ and $|F''_D| \le 1$, a 2-connected (m, k, V_D, F_D, o) patch and a 2-connected (m, k, W_D, F_D, o) patch with similar boundary have the same number of faces (and therefore also vertices and edges). For $(m, k) \notin \{(3, 6), (4, 4), (6, 3)\}$ this is not true as can be seen from the example in Fig. 4.

The 3 cases $(m, k) \in \{(3, 6), (4, 4), (6, 3)\}$ correspond to the 3 euclidean lattices and are therefore called the *euclidean cases*. An (m, k, V_D, F_D, o)-patch with $(m, k) \in \{(3, 6), (4, 4), (6, 3)\}$ and $V''_D = F''_D = \emptyset$ is called a euclidean patch.

We will adopt a method similar to that used in [1,2]. It can be used for each of the euclidean cases with some changes and was demonstrated only for the case (3, 6) in [1] and only for (6, 3) in [2]. Here we will demonstrate only the remaining case (4, 4), but comparing the proof to [1,2] it is not difficult to see that for (3, 6) and (6, 3) the proof can be done very similarly. In what follows we will denote $(4, 4, V_D, F_D, o)$ patches as $e4$-patches if $F'_D = V'_D = \emptyset$, as $\bar{e}4$-patches if F'_D and V'_D only contain multiples of 4, as $e4_1$-patches, if $V'_D = \emptyset$ and $|F'_D| = 1$, and as $\bar{e}4_1$-patches, if F'_D contains only one non-multiple of 4 and V'_D none.

Let L denote the 4-regular square lattice in the euclidean plane equipped with a standard coordinate system, so that the vertices are all pairs (x, y) with $x, y \in \mathbb{Z}$ and the (directed) edges are all pairs $((x, y), (x', y'))$ of vertices with $|x - x'| + |y - y'| = 1$ (see Fig. 5).

For a vertex $v = (a, b) \in L$ we set $x(v) = a$ and $y(v) = b$. The set $\vec{E}_L = \vec{E}(L)$ is partitioned into 4 disjoint sets $\vec{E}_0, \ldots, \vec{E}_3$:

$$\begin{aligned}
\vec{E}_0 &:= \{(v, w) \in \vec{E}_L | x(v) + 1 = x(w)\} \\
\vec{E}_1 &:= \{(v, w) \in \vec{E}_L | y(v) - 1 = y(w)\} \\
\vec{E}_2 &:= \{(v, w) \in \vec{E}_L | x(v) - 1 = x(w)\} \\
\vec{E}_3 &:= \{(v, w) \in \vec{E}_L | y(v) + 1 = y(w)\}
\end{aligned}$$

The set $\vec{E}_h$ of *horizontal* edges is defined by $\vec{E}_h = \vec{E}_0 \cup \vec{E}_2$.

Note that any automorphism of L that is a (counterclockwise) rotation by an angle of $n * 90$ degrees maps an edge in $\vec{E}_i$ onto an edge in $\vec{E}_{i-n \mod 4}$.

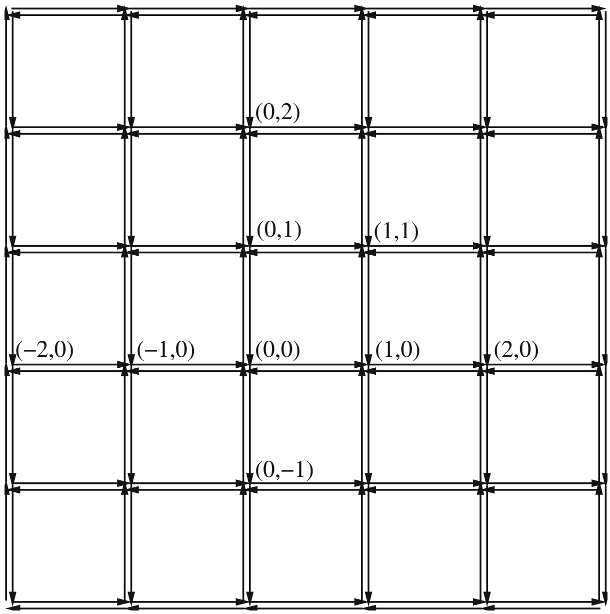


Fig. 5 The lattice L

Now let M be a finite multiset of edges of $\vec{E}_L$ (short $\vec{E}_L$-multiset). For horizontal edges e the y-coordinate of both vertices is the same, so we can define $y(e)$ as the y-coordinate of any of its vertices.

We define

$$S_{lr}(M) := \sum_{e \in M \cap \vec{E}_0} y(e) - \sum_{e \in M \cap \vec{E}_2} y(e)$$

(the index lr stands for *left, right*). If we denote the (disjoint) union of multisets by '+', it is immediate that for two $\vec{E}_L$-multisets M, M' we have $S_{lr}(M + M') = S_{lr}(M) + S_{lr}(M')$.

An *enclosing cycle* of some patch G is a directed cycle with the same underlying set of undirected edges as the directed boundary cycle and the same multiplicity with which an undirected edge occurs as a directed edge (see Fig. 6).

Lemma 2 *Given a euclidean patch P and an enclosing cycle C of P. If B is a simple cycle in the graph Z of undirected boundary edges of P, then $B' = C \cap B$ is a directed subcycle of C.*

Proof Assign a flow of value one to all directed edges of C. Since it is a directed cycle, the Kirchhoff law is fulfilled at every vertex. If B' is not a directed cycle, there is a vertex $v \in B'$ that is the endpoint of two directed edges (a, v) and (b, v) both in B'.

Removing v from Z, a and b are in the same component K, but all other vertices neighbouring v in Z must be in other components (due to the Jordan Curve Theorem).

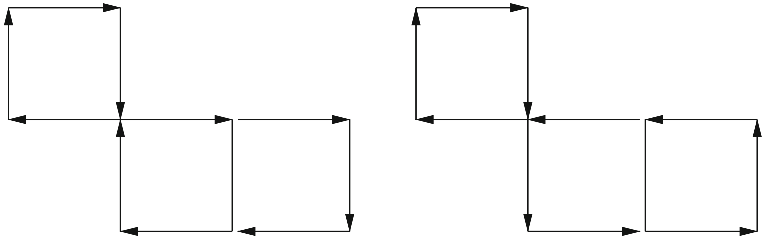


Fig. 6 A directed boundary cycle of an $e4$-patch and an enclosing cycle that is not the boundary cycle of the same patch

So summing up the flows for all vertices in K we get a total outflow of two—violating the Kirchhoff law. So v cannot exist. □

Given a euclidean patch and an enclosing cycle C, it follows easily from the Jordan curve theorem that for each bounded face there is a unique simple cycle B like above surrounding it and due to this lemma, this induces a directed subcycle B'. So every bounded face is either on the right or left hand side of all edges of its surrounding cycle B'. We call these faces *right*, resp. *left* and denote the set of right faces of an enclosing cycle C as $F_r(C)$ and the set of left faces as $F_l(C)$.

Therefore for any euclidean patch P and enclosing cycle C we can define

Definition 5

$$F_{lr}(P) := \sum_{f \in F_r(C)} (deg(f)/4) - \sum_{f \in F_l(C)} (deg(f)/4)$$

and

$$F_w(P) := \sum_{f \in F, f \neq o} (deg(f)/4)$$

We call $F_w(P)$ the *weighted number of faces* of P.

In case the enclosing cycle is the boundary cycle, we have $F_{lr}(P) = F_w(P)$, since they are all right faces.

Definition 6 Given a labelled patch P. The labelled boundary graph $B = B(P)$ is the graph of all boundary edges and vertices labelled in the following way:

Let $a = (e, e') \in A(B)$. If $a \in A(P)$ we define $l_B(a) = l(a)$. Otherwise let $e = e_0, e_1, \ldots, e_k = e'$ be the rotational order around the vertex $e \cap e'$. Then we define $l_B(a) = (\sum_{i=0}^{k-1} l(e_i, e_{i+1}) + (k-1)) \mod 4$. This is the number of edges and the sum of labels between e and e'.

An embedding of a labelled graph G into L is a graph homomorphism $\psi : G \to L$ so that if $(e, e') \in A(P)$, there are $l(e, e')$ edges in the rotational order around $\psi(v)$ between $\psi(e)$ and $\psi(e')$—or equivalently: if $\psi(e) \in \vec{E}_i$ then $\psi(e') \in \vec{E}_{i+l(e,e')+1 \mod 4}$.

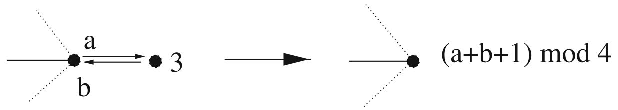
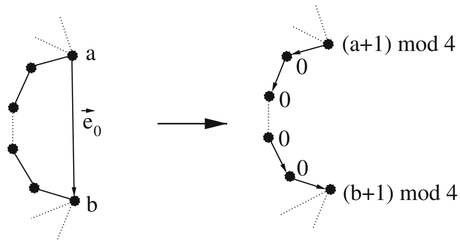


Fig. 7 Reducing a labelled tree

Fig. 8 Reducing a face



Lemma 3 *Given a labelled $\bar{e}4$-patch P with an enclosing cycle C and its labelled boundary graph $B = B(P)$. Then $B(P)$ can be embedded into L by a homomorphism ψ and for each such ψ we have*:

$$F_{lr}(P) = S_{lr}(\langle \psi(\vec{e}) \in \vec{E_L} | \vec{e} \in C \rangle)$$

Proof We will prove this by induction in the number b of bounded faces.

If $b = 0$ the patch is a tree. We will prove this case by induction in the number of edges. In case there is just one edge (with both angles necessarily labelled 3), the result is obvious. So let T be a labelled tree with $n + 1$ edges. Perform the reduction depicted in Fig. 7 to the smaller labelled tree T'. The smaller tree can easily be seen to be a $\bar{e}4$-patch too, so by induction the lemma holds.

The values of the labels given in the construction ensure that every embedding of the smaller patch can be extended to one of the larger patch—ensuring the existence of an embedding ψ. The fact that the two inverse directed edges are embedded on inverse edges in L ensures that S_{lr} stays 0—just like the number of unbounded faces.

On the other hand restricting a given embedding ϕ of T to T' gives an embedding of T' proving that every embedding of T has the requested property.

This gives us the lemma for $\bar{e}4$-patches with 0 bounded faces. So assume it is true for $\bar{e}4$-patches with i bounded faces and given a $\bar{e}4$-patch P with $i + 1$ bounded faces and enclosing cycle C.

W.l.o.g. there is a right face of size $4 * n$. For a boundary edge $\vec{e_0}$ in the enclosing cycle that has a bounded face on the right, perform the reduction to a $\bar{e}4$-patch P' with one bounded face less and a new enclosing cycle as depicted in Fig. 8.

By induction the boundary graph of P' can be embedded and the fact that we have label 0 for the $4n - 2$ angles at those vertices of the new face that are not connected by the new edge e_0 ensures that the images of the endpoints of the path of length $4n - 1$ are the endpoints of an edge in L. So we can extend the homomorphism of $B(P')$ to one of $B(P)$ (and again deduce that any embedding of $B(P)$ can be interpreted as coming from one of $B(P')$). By summing up the labels at the endpoints this homomorphism can easily be shown to be an embedding.

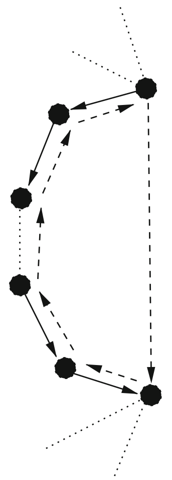


Fig. 9 Splitting the sum

$F_{lr}(P) = F_{lr}(P') + n$, since the new face f of degree $4n$ is on the right hand side of the enclosing cycle and for all other faces the situation does not change.

But $S_{lr}(\langle\psi(\vec{e}) \in \vec{E}_L | \vec{e} \in C\rangle) = S_{lr}(\langle\psi(\vec{e}) \in \vec{E}_L | \vec{e} \in C'\rangle) + S_{lr}(\langle\psi'(\vec{e}) \in \vec{E}_L | \vec{e} \in F'\rangle)$ with C' the enclosing cycle of P', F' the boundary cycle of the face f on the right hand side of $\vec{e}_0$, and ψ' mapping $\vec{e}_0$ onto the same edge as ψ does. This holds since for each edge $\vec{e}$ in $C' \setminus C$ there is an edge in F' being mapped exactly on the oppositely directed edge in L, so contributing the same value with opposite sign. The only edge of $C \setminus C'$ is provided by F' and mapped onto the same directed edge as by ψ. This splitting of the sum is depicted in Fig. 9.

But since it is easy to see that $S_{lr}(\langle\psi'(\vec{e}) \in \vec{E}_L | \vec{e} \in F'\rangle) = n$ we get $S_{lr}(\langle\psi(\vec{e}) \in \vec{E}_L | \vec{e} \in C\rangle) = F_{lr}(P)$ proving the lemma. □

Lemma 4 *Given a closed directed cycle C_L in L. Then there is a $\bar{e}4$-patch P and a labelled enclosing cycle C of P, so that C_L is the image of an embedding of C.*

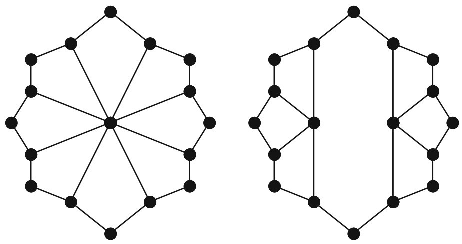
Proof In fact it is even easy to prove this lemma for $e4$-patches instead of $\bar{e}4$-patches by decomposing C_L into simple cycles and taking the interior of these simple cycles to form the patch. A detailed proof can be found in [13]. □

Corollary 1 *For a given labelled cycle C embeddable in L by an embedding ψ, the value of $S_{lr}(\psi(C))$ does not depend on ψ, so we can define $S_{lr}(C) = S_{lr}(\psi(C))$.*

Proof There are a $\bar{e}4$-patch P and enclosing cycle C as in Lemma 4 so that due to Lemma 3 for any ψ the value of $S_{lr}(\psi(C))$ must equal the value of $F_{lr}(P)$. But this value does only depend on the patch and the enclosing cycle and not on the embedding.

Theorem 2 *The weighted number of faces $F_w(P)$ of a labelled $\bar{e}4$-patch P is uniquely determined by its labelled boundary cycle. In case F_D is given, the number of faces is uniquely determined.*

Fig. 10 Two 2-connected $\bar{e}4$-patches with the same boundary, but different F_D and also different number of faces



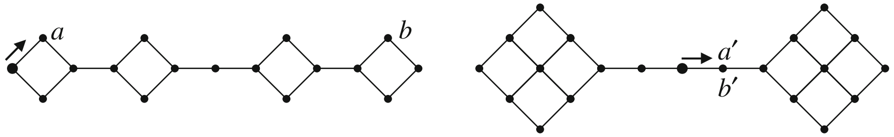


Fig. 11 Two $e4$-patches with the same boundary sequence and different numbers of faces, but equal weighted number of faces

Proof This is a direct consequence of Lemma 3: for any two $\bar{e}4$-patches, the same labelled boundary cycle C implies the same value of $S_{lr}(C)$, so also the same value of $F_{lr}(P)$. Since all faces are right faces, this implies the same weighted sum F_w of faces. In case F_D is given, the number of faces can be deduced from the number of weighted faces.

Figure 10 gives an example where different values of F_D lead to different numbers of faces.

Since in a patch where the boundary is a simple cycle the labels are uniquely determined by the vertex degrees and since 2-connected patches have simple boundary cycles, we get:

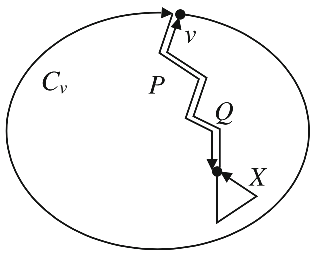
Corollary 2 *Two 2-connected $\bar{e}4$-patches with similar boundaries have the same weighted number of faces. In case they have the same F_D, they also have the same number of faces.*

If the patches are not 2-connected, it is possible that they cannot be labelled in a way that produces identically labelled boundary cycles. In Fig. 11 angle a must have label 2, so if the patches were identically labelled, the corresponding angle a' had label 2 too and therefore angle B' label 0 and also the corresponding angle b, which on the other hand must have label 2—a contradiction. These patches are also an example of two $e4$-patches with the same boundary sequence and a different number of faces.

Definition 7 Two labelled directed paths or cycles P, P' with labellings w, w' are called *inverse isomorphic* if there is an orientation reversing isomorphism $\phi : P \to P'$ so that for every $a \in A(P)$ we have $w(a) + w'(\phi(a)) \equiv 2 \mod 4$. In this case we write $P' = P^-$. Note that a given labelled path P is in fact inverse isomorphic to its inverse, so this notation extends the previous one.

Remark 1 For a labelled cycle C that can be embedded into L we have that C^- is also embeddable and $S_{lr}(C) = -S_{lr}(C^-)$.

Fig. 12 A directed boundary cycle of a $\bar{e}4_1$-patch and a path around the defective face



Proof Choose two edges $e \in C$, $e' \in C^-$ that are mapped onto each other by the isomorphism $\phi : C \to C^-$ and an embedding ψ of C. Then define $\psi'(e') = (\psi(e))^-$. Now we can recursively embed the next edges of C' showing on one hand that we get an embedding and on the other that for every edge $e' \in C'$ we have $\psi'(e') = (\psi(\phi^{-1}(e')))^-$. Now the result follows directly from the additivity of S_{lr}. □

Let us now switch to $\bar{e}4_1$-patches, i.e. F'_D contains exactly one non-multiple of 4 and V'_D none.

The following techniques come from the theory of disordered tilings (see [14–17]) and correspond to the observation that in a disordered tiling any path around the disorder corresponds to the same automorphism of the underlying periodic tiling. In our case we will see that the boundary of a $\bar{e}4_1$-patch with $F''_D = \langle n \rangle$ corresponds to a rotation by $90 * n$ degrees around the center of a face in L. We will present the proof in a way that does not assume the reader to know the aforementioned articles, nevertheless they do of course help to understand the basic principles.

Definition 8 Given a $\bar{e}4_1$-patch G with $F''_D = \langle n \rangle$. Let d be the defective face with $\deg(d) = n$ and v a vertex in the boundary. Then a directed path PXQ in G with subpaths P, X and Q starting and ending at v is called a *cutpath* (relative to v) iff the endpoint w of P is in the boundary of d, $Q = P^-$ and X is the path from w to w around the boundary of d with d on the left. That is: X has n edges $e_1, \ldots, e_n$ and for $1 \le i < n$ the edge e_{i+1} follows e_i^- in the rotational order around the endpoint of e_i (see Figs. 12 and 13).

A $\bar{e}4_1$-patch G with cutpath PXQ relative to a boundary vertex v and boundary cycle C can be cut along PXQ to get a $\bar{e}4$-patch G' with boundary cycle $C_v PXQ$ if C_v denotes the closed path along C starting and ending at v and with the patch on the right. Defining this patch cutting operation in a formal way is an easy exercise, but details can also be found in [13]. Since $C_v PXQ$ is the boundary of a $\bar{e}4$-patch, it can be embedded into L and forms a closed cycle.

By construction we know the following about the labels of $C_v PXQ$.

Let $p_1, \ldots, p_k$ be the directed edges forming P, $X = x_1, \ldots, x_n$, and $Q = P'_k, \ldots, P'_1$. Then $Q = P^-$, i.e. $l(p_j^-, p_{j+1}) + l(P'_{j+1}, (P'_j)^-) = 2$ for $1 \le j \le k-1$. Furthermore we have $l(p_k^-, x_1) + l(x_n^-, P'_k) = 3$, since w is split into two new vertices w', w'' with $\deg(w') + \deg(w'') = \deg(w) + 1$, and $l(x_i^-, x_{i+1}) = 0$ for $1 \le i \le n-1$.

Lemma 5 *Let $\bar{P} = P, x_1, \ldots, x_n, P^-$ with $P = p_1, \ldots, p_k$, $P^- = P'_k, \ldots, P'_1$ be a labelled path with all labels $l(x_i^-, x_{i+1}) = 0$ for $1 \leq i \leq n-1$ and $l(p_k^-, x_1) + l(x_n^-, P'_k) = 3$.*
If $\bar{P}$ is embedded in L by ψ then

(i) *$\psi(x_1), \ldots, \psi(x_n)$ are in the boundary of the same face f of L and*
(ii) *for $1 \leq j \leq k$ we have that if $\psi(p_j) \in \vec{E}_m$ then $\psi(P'_j) \in \vec{E}_{m+2-n \mod 4}$*

Proof Item (i) is obvious due to $l(x_i, x_{i+1}) = 0$ for $1 \leq i < n$, so we will concentrate on (ii):
By the definition of embedding we have that $\psi(P'_j) \in \vec{E}_{m+l \mod 4}$ with

$$l \equiv \sum_{i=j}^{k-1}(l(p_i^-, p_{i+1}) - 1) + (l(p_k^-, x_1) - 1) + \sum_{i=1}^{n-1}(l(x_i^-, x_{i+1}) - 1) + \left(l(x_n^-, P'_k) - 1) + \sum_{i=j}^{k-1}(l(P'_{i+1}, (P'_i)^-) - 1\right) \mod 4$$

Note that since we use p_k^- instead of p_k, the "+1" in the index of $\vec{E}$ from Definition 6 becomes a "−1".

Using the definition of "inverse path" for $l(p_i^-, p_{i+1}) + l(P'_{i+1}, (P'_i)^-)$ and the values of $l()$ given in the lemma, we get

$$l \equiv 2(k-j) - 2(k-j) + 3 - 2 - (n-1) \mod 4 \equiv 2 - n \mod 4 \quad \square$$

Lemma 6 *Let $\bar{P} = P, x_1, \ldots, x_n, P^-$ with $P = p_1, \ldots, p_k$, $P^- = P'_k, \ldots, P'_1$ be a labelled path with all labels $l(x_i^-, x_{i+1}) = 0$ for $1 \leq i < n$ and $l(p_k^-, x_1) + l(x_k^-, P'_1) = 3$.*

Consider an embedding ψ of $\bar{P}$ into L and for $i \in \{1, \ldots, k\}$ let s_i be the starting point of $\psi(p_i)$ and e'_i the endpoint of $\psi(P'_i)$. Furthermore let s_{k+1} be the endpoint of $\psi(p_k)$ and e'_{k+1} the starting point of $\psi(P'_k)$.

Then for $i \in \{1, \ldots, k+1\}$ we have $\alpha(s_i) = e'_i$ for α the counterclockwise rotation around the center of the face f containing $x_1, \ldots, x_n$ in its boundary by $n*90$ degrees.

Proof We prove this by induction in i starting with $i = k+1$ and going from $i+1$ to i. The case $i = k+1$ can be easily checked since e'_{k+1} and s_{k+1} are both in the boundary of f, so assume the lemma is proven for $i+1$.

By induction we know that the endpoint s_{i+1} of $\psi(p_i)$ is mapped onto the starting point e'_{i+1} of $\psi(P'_i)$ by α. Due to Lemma 5 we have that if $\psi(p_i) \in \vec{E}_m$, then $\psi(P'_i) \in \vec{E}_{m+2-n \mod 4}$. But $\alpha(\psi(p_i)) \in \vec{E}_{m-n \mod 4}$ so it must be the unique edge $\vec{e}$ from $\vec{E}_{m-n \mod 4}$ ending at e'_{i+1}. So $\alpha(s_i)$ is the starting point of $\vec{e}$ which is the endpoint of the unique edge $(\vec{e})^- \in \vec{E}_{m+2-n \mod 4}$ starting in e'_{i+1}, which is just $\psi(P'_i)$. So $\alpha(s_i) = e'_i$.

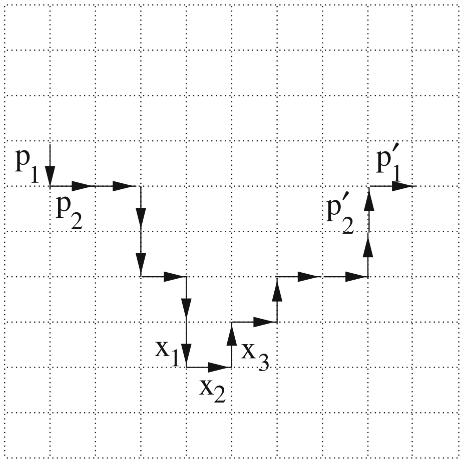


Fig. 13 A cutpath around a triangle (compare Fig. 12) embedded into L

Theorem 3 *Given two $\bar{e}4_1$-patches G, G' with the same labelled boundary cycle and the same face degree n that is not a multiple of 4. Then G and G' have the same weighted number of faces.*

If they also have the same multiset F'_D of defective face degrees then they have the same number of faces.

Proof Choose vertices v resp. v' in the boundary of G resp. G' that correspond to each other in the boundary sequence of the patches, and cutpaths PXQ, $P'X'Q'$ relative to v and v'. Let H and H' be the corresponding $\bar{e}4$-patches with boundary cycles $C_v PXQ$ and $C'_{v'}P'X'Q'$. Since H and H' contain the same faces as G and G' except the one of size n, it is sufficient to show that H and H' have the same weighted number of faces, or equivalently

$$F_{lr}(H) = F_{lr}(H'),$$

because all faces in H and H' are right faces.

The boundary cycles $C_v PXQ$ and $C'_{v'}P'X'Q'$ can be embedded into L such that the embeddings of C_v and $C'_{v'}$ are equal because the labelled boundaries of the patches coincide. Since n is not a multiple of 4, a counterclockwise rotation by $n * 90$ degrees is nontrivial and therefore the center is well determined by one point and its image. Then Lemma 6 applied to the endpoints of the images of C_v and $C'_{v'}$ in L yields that the images of X and X' lie in the boundary of the same face f of L. W.l.o.g. we can assume that the images of X and X' are even equal—otherwise we extend the path P' in H' by an appropriate number of edges of the defective face. For the sake of a simpler notation we denote the images of the paths in the same way as the paths in the patches and obtain the cycles $C_v PXQ$ and $C_v P'XQ'$ in L (see Fig. 14).

Now consider the cycles P^-P' and Q^-Q' as multisets in L. For constructing corresponding labelled cycles, the labels at the meeting points of the two paths can be determined from L and it is easy to see that the label l at the beginning of P' and the label l' at the end of Q' fulfil $l + l' \equiv 2 \mod 4$ (and analogously for the other meeting point). Because of this and $P = Q^-$ and $P' = Q'^-$ we have for the

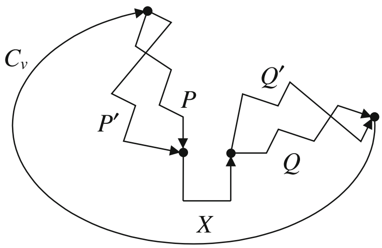


Fig. 14 The two cutpaths embedded into the lattice L

labelled cycles $Q^-Q' = ((Q^-)^-Q'^-)^- = (P^-P')^-$, and therefore by Remark 1 $S_{lr}(Q^-Q') = -S_{lr}(P^-P')$.

So we can add the multisets P^-, P', Q^-, Q' in L to the multiset $C_v PXQ$ without altering the value of S_{lr}. Using again the additivity, Lemma 3, and the observation that S_{lr} only depends on the multiset of the underlying edges and not their numbering in the boundary cycle, we get

$$\begin{aligned} F_{lr}(H) &= S_{lr}(C_v PXQ) \\ &= S_{lr}(C_v PXQ) + S_{lr}(P^-P') + S_{lr}(Q^-Q') \\ &= S_{lr}(C_v PXQ + P^-P' + Q^-Q') \\ &= S_{lr}(C_v P'XQ' + P^-P + Q^-Q) \\ &= S_{lr}(C_v P'XQ') + S_{lr}(P^-P) + S_{lr}(Q^-Q) \\ &= S_{lr}(C_v P'XQ') \\ &= F_{lr}(H') \end{aligned}$$

□

Again we obtain

Corollary 3 *The weighted numbers of faces of a 2-connected $\bar{e}4_1$-patch is uniquely determined by the sequence of vertex degrees in its boundary cycle.*

Fact 1 *Since with r the length of the boundary we have $4 * F_w + r = 2|E|$, in all the cases where we have F_w as an invariant of a labelled or unlabelled boundary cycle, we also have the number of edges as an invariant, while the number of vertices and faces may well vary.*

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