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Pentagon–hexagon-patches with short boundaries

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Abstract

Pentagon–hexagon-patches are connected bridgeless plane graphs with all bounded faces pentagons or hexagons, all interior vertices of degree 3 and all boundary vertices of degree 2 or 3. In this paper we determine the minimum and maximum possible boundary lengths $\min(h, p)$ and $\max(h, p)$ of pentagon–hexagon-patches with h hexagons and $p \leq 6$ pentagons and determine which intermediate values can occur. We show that the minimal boundary length is obtained by arranging faces in a *spiral* fashion starting with the pentagons, while the maximum boundary length is obtained in cases where the *inner dual* is a tree.

Keywords: Plane graph; Spiral; Boundary

Introduction

Harary and Harborth [9] have given explicit formulae for possible boundary lengths of patches with $p = 0$ that are isomorphic to a subgraph of the hexagonal lattice (these structures are called *hexagonal animals*). Their result found various applications in theoretical chemistry, especially the theory of *benzenoids*, where it was e.g. used to determine *constant isomer series*, that is series of chemical formulae of the type $C_{x_1}H_{y_1}, C_{x_2}H_{y_2}, \ldots$ with a constant number of benzenoids for every formula in the series (see e.g. [4] or [5]).

After the discovery of the fullerenes [10], that is carbon molecules with the bonding structure of a cubic plane graph with all faces hexagons and pentagons, the interest in planar polycyclic hydrocarbons with a limited number of pentagons besides the usual hexagons increased. The result proven in this paper allows us to determine constant isomer series of hydrocarbons with up to six pentagons and is the basis of an efficient

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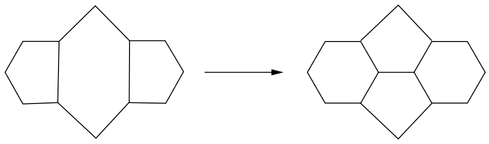

Fig. 1. Two small patches with the same boundary and different number of faces.

construction algorithm for the enumeration of planar polycyclic hydrocarbons with at most six pentagons (see [2]).

Another important application of this result is for a special class of fullerenes themselves: *tubetype fullerenes* or *nanotubes* are fullerenes that are—although topologically spherical—geometrically of the shape of a long tube. They consist of a long tubular body made up of only hexagons and are capped on each side with a patch containing hexagons and exactly six pentagons. These nanotubes are the by far most promising class of fullerenes for possible applications, (see e.g. [11, 12]). The nanotube caps can be chosen in a way that they contain a pentagon in their boundary and the vertices have, alternately, degrees 2 and 3 (only counting edges belonging to the cap) except at possibly two places where two vertices with the same degree—once both of degree 2 and once both of degree 3—follow each other. Except for its length, the structure of the tubular body is completely determined by the boundary structure of the caps. The length of the boundary in the case of an alternating boundary, respectively the two lengths between the special places are invariants of the nanotube called the *tube parameters*. The tube parameters have an effect on some chemical and physical properties of the nanotube (see e.g. [6]). In order to classify all possible nanotubes with given tube parameters up to different tube lengths, it is important to know all possible caps for these tubes (see [3, 6]). In fact the statement above assumes that for given parameters there is just a finite number of such caps. Without the requirement of a pentagon in the boundary, this is obviously false: we can add arbitrarily many hexagon rings without changing the boundary structure of the cap. But even with the requirement of a pentagon in the boundary the number of faces inside a cap is not determined by its boundary structure, as can be seen at the operation described in Fig. 1 which is known as the *Endo-Kroto* C_2 *insertion*. If we could e.g. repeatedly apply this or another operation (see [1]) with the same effect to a cap without touching the pentagon in the boundary of the cap, the number of faces inside a cap for given parameters would not be bounded and therefore we would also have an infinite number of caps.

The result proven in this paper can be used to determine an upper bound on the number of faces inside a cap with given parameters in the following way: for $p < 6$ pentagons we prove an upper bound for the number of faces inside any patch with given boundary length. Inserting a vertex into a boundary edge of a pentagon in the boundary of a cap, we get a patch with a boundary length that is one larger than the boundary length given by the parameters of the cap, and that contains exactly five pentagons and the same number of faces as the cap. So the upper bound for the number of faces for this new boundary length and $p = 5$ is also an upper bound for the number of faces inside a cap with the given parameters.

Due to lack of space we have to omit some proofs or details of proofs, which are not difficult, but must be carefully worked out. The nontrivial ones can be found in [8].

The main result of this paper was already announced by the first author at the *Colloquium on Combinatorics* 1995 in Braunschweig. Later it was independently proven by the third author in her diploma thesis [8] supervised by the second author. The present paper is the result of merging the two approaches.

Basic definitions and results

A *pentagon–hexagon-patch* is a 2-connected plane graph with all bounded faces pentagons or hexagons, all vertices not in the boundary of the unbounded face (we will just call this *the boundary*) of degree 3 and all vertices in the boundary of degree 2 or 3. Since there will be no danger of misunderstandings, we will call pentagon–hexagon-patches just patches. A patch with h hexagons and p pentagons is called an (h, p)-patch. An $(h, 0)$-patch that is isomorphic to a subgraph of the hexagonal lattice is called a (hexagonal) *animal*.

Since in 2-connected graphs all face boundaries are cycles, every vertex of degree $k \in \{2, 3\}$ is contained in exactly k pairwise distinct faces, one of them possibly unbounded.

For a patch P we denote the cardinality of the set of vertices of P by $v(P)$, of the set of edges by $e(P)$ and of the set of bounded faces by $f(P)$. For edges e and faces f we write $e \in f$ to denote that e is an edge in the boundary of f. The *inner dual* of a patch is its dual graph with the vertex corresponding to the outer face removed. The distance $d(f, f')$ of two bounded faces f, f' in a patch P is the graph distance of the corresponding vertices in its inner dual.

A *boundary face* is a face that shares an edge with the unbounded face. By *removing a boundary face* f, we mean constructing the graph obtained by removing all those vertices and edges that belong exactly to the bounded face f and the unbounded face. The resulting graph may be disconnected, but all connected components are patches.

The *boundary length* $b(P)$ of an (h, p)-patch P is defined as the number of vertices (or equivalently edges) in the boundary of P.

For a set $\bar{P}$ of patches $P_1, \ldots, P_k$ let $b(\bar{P}) = \sum_{i=1}^{k} b(P_i)$. If for $1 \leq i \leq k$ the patch P_i is an (h_i, p_i)-patch and $h_1 + \cdots + h_k = h$, $p_1 + \cdots + p_k = p$, then $\bar{P}$ is called an (h, p)-patchset.

For $i = 2, 3$ let $v_i(P)$ denote the number of vertices of P with degree i and $v_{i,b}(P)$ denote the number of boundary vertices of P with degree i. By definition we have $v_2(P) = v_{2,b}(P)$ and $b(P) = v_{2,b}(P) + v_{3,b}(P)$.

Lemma 1. *For an (h, p)-patch P we have $v_{2,b}(P) - v_{3,b}(P) = 6 - p$ and $b(P) = 2v_{3,b}(P) + 6 - p$.*

Proof. Summing up the vertices of all bounded faces separately, vertices of degree 2 are counted once, boundary vertices of degree 3 are counted twice and interior vertices are counted 3 times. We get $v(P) = (6h + 5p + v_{3,b}(P) + 2v_{2,b}(P))/3$.

Summing up all edges of all bounded faces, boundary edges are counted once and interior edges are counted twice, so $e(P) = (6h + 5p + v_{3,b}(P) + v_{2,b}(P))/2$.

Finally we have $f(P) = p + h$. Inserting these expressions into the Euler formula for bounded faces, that is $v(P) - e(P) + f(P) = 1$, after some elementary computations we get the result of the lemma.

The second equation now follows from $b(P) = v_{2,b}(P) + v_{3,b}(P)$. □

The boundary sequence $s(P)$ of a patch P is the undirected cyclic sequence given by the degrees of the vertices in cyclic order around the patch.

Corollary 2. *The boundary sequence of every* (h, p)*-patch with* $p < 6$ *contains a subsequence* 22.

Remark 3. Let P be an (h, p)-patch with $f_b > 1$ boundary faces. Then $v_{3,b}(P) \geq f_b$ and $v_{3,b}(P) = f_b$ if and only if every boundary face has a connected intersection with the boundary.

Proof. Fix a rotation direction around the boundary and let ψ denote a mapping from the set of 3-valent boundary vertices to the set of boundary faces with the image of every boundary vertex with valency 3 the boundary face neighbouring it in this rotation direction. This gives a surjective map proving $v_{3,b}(P) \geq f_b$ which is bijective if and only if every boundary face has a connected intersection with the boundary. □

Remark 4. For $p \leq 6$ there are no (h, p)-patches with $b(P) < 5$.

Proof. Assume the contrary and let P be a counterexample with minimum number of faces. For $b(P) < 5$ not all vertices of a face can be boundary vertices, so there is an interior vertex and therefore $h + p \geq 3$. Since for $v_{3,b}(P) = 0$ the patch P would be a single face that is smaller than a pentagon and by Lemma 1 we have $v_{2,b}(P) \geq v_{3,b}(P)$, we have $1 \leq v_{3,b}(P) \leq 2$. For $v_{3,b}(P) = 1$ there would be a single face f in the boundary with the face boundary not a cycle, so this can't occur. For $v_{3,b}(P) = 2$ we would have a boundary length of four and two boundary faces f, f' with together at most 12 edges. So at most four edges are neighbouring other faces than f, f'. Removing f, f' would leave a set of nonempty smaller patches with sum of boundary lengths at most four—each of them in contradiction to the minimality of P. □

Corollary 5. *For* $p \leq 6$ *two bounded faces in an* (h, p)*-patch can share at most one edge.*

Proof. If two bounded faces f, f' would share more than one edge, these edges could not share a vertex, since this would be a vertex of degree 2 that is not in the boundary of the patch or the boundary of one of the faces would not be a cycle.

So there are at most eight edges in the boundary of f and f' that they do not share and that form at least two cycles—at least one of them with at most four edges and an (h, p)-patch in the interior. This is in contradiction to Remark 4. □

Remark 6. Given an (h, p)-patch P, in which all faces contain boundary edges and a face f in P. Then there is a face f' in P with maximum distance from f and at most two nonboundary edges.

Proof. The situation where the maximum distance is 0 or 1 can be easily checked by hand, so assume a maximum distance $d \geq 2$.

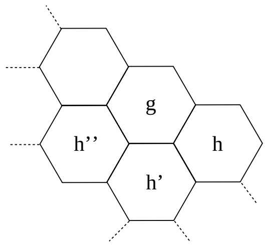

Fig. 2. An example situation for the proof of Remark 6.

Take an arbitrary face g with maximum distance from f. If g has at most two edges not in the boundary we have found the face, so assume g has at least three edges not in the boundary. Let h, h', h'' be three corresponding faces in clockwise direction around g starting after a boundary edge. The fact that h, h', h'' must be pairwise distinct follows immediately from the condition that there are no faces without boundary edges.

An example situation like this is pictured in Fig. 2. In general the edges along which h, h', h'' are adjacent to g do not have to follow each other in the boundary of g. Since h' and g both have boundary edges, removing h' and g disconnects the patch—especially the faces h and h''. Since $d \geq 2$, $f \notin \{h, h', h'', g\}$, so without loss of generality assume that f is not in the same component H as h. Since h' is neighbouring g, $d(f, h') \geq d - 1$, and since all paths to faces in H must pass through g or h', all faces in H must be neighbouring h'. In fact shortest paths must all pass through h' and all faces in H have distance d. In particular, since H is not empty, $d(f, h') = d - 1$. But in this situation one can easily see that one of them (the first one in counterclockwise direction starting at a boundary edge of h') must have at most two edges not in the boundary. □

We define

$$\min(h, p, k) = \min\{l \in \mathbb{N} \mid \exists (h, p)\text{-patchset } \bar{P} \text{ with } k \text{ elements and } b(\bar{P}) = l\}$$
$$\max(h, p, k) = \max\{l \in \mathbb{N} \mid \exists (h, p)\text{-patchset } \bar{P} \text{ with } k \text{ elements and } b(\bar{P}) = l\}.$$

For $\min(h, p, 1)$, $\max(h, p, 1)$ we will also write $\min(h, p)$, $\max(h, p)$.

The fact that patches are 2-connected implies the following remark:

Remark 7. The inner dual of patches is connected.

Remark 7 makes it easy to determine $\max(h, p, k)$:

Lemma 8. *For an (h, p)-patchset $\bar{P}$ with k (nonempty) elements we have $b(\bar{P}) = \max(h, p, k)$ if and only if the inner dual of every patch in $\bar{P}$ is a tree. In this case $b(\bar{P}) = 4h + 3p + 2k$.*

Proof. If for $i = 1, 2$ the number of edges that occur in exactly i bounded faces is denoted by $e_i(\bar{P})$, we have $e_1(\bar{P}) = b(\bar{P})$ and $e(\bar{P}) = e_1(\bar{P}) + e_2(\bar{P})$. On the other hand $e(\bar{P}) = 6h + 5p - e_2(\bar{P})$, since edges that occur in two faces are counted twice in $6h + 5p$. So $e_1(\bar{P}) = 6h + 5p - 2e_2(\bar{P})$. Since the inner dual of every patch in $\bar{P}$ is connected, we have $e_2(\bar{P}) \geq h + p - k$ with equality only if the inner dual of every patch is a tree. So $b(\bar{P}) = e_1(\bar{P}) \leq 6h + 5p - 2(h + p - k) = 4h + 3p + 2k$.

Since patches with the inner dual being a tree can easily be constructed, the lemma is proven. □

Lemma 9. *Let P be an (h, p)-patch with at least one internal face and all boundary faces hexagons. Then P^- denotes the set of patches obtained by removing all boundary hexagons and we have $b(P^-) \leq b(P) - 2(6 - p)$.*

We have $b(P^-) = b(P) - 2(6 - p)$ if and only if every boundary hexagon shares exactly two edges with other boundary hexagons.

Proof. The subgraph of the inner dual that is induced by the vertices corresponding to boundary hexagons is a connected graph and since there is an internal face it has at least one cycle. This implies that with h_b the number of hexagons in the boundary it has at least h_b edges. The corresponding edges in the patch have boundary hexagons on both sides.

The set of boundary edges of P^- is the set of edges that belong to a boundary hexagon of P and to a nonboundary face. So we get $b(P^-) \leq 6h_b - 2h_b - b(P)$. By Lemma 1 $b(P) = 2v_{3,b}(P) + 6 - p$, so $b(P^-) \leq 4h_b - (2v_{3,b}(P) + 6 - p)$.

By Remark 3 we have $v_{3,b}(P) \geq h_b$ and therefore $b(P^-) \leq 4v_{3,b}(P) - (2v_{3,b}(P) + 6 - p) = 2v_{3,b}(P) - (6 - p) = b(P) - 2(6 - p)$.

All inequalities become equalities if the requirements of the second part are fulfilled (the boundary hexagons form a cycle, so each boundary hexagon has a connected intersection with the boundary).

On the other hand if all inequalities become equalities, each boundary hexagon has a connected intersection with the boundary and is therefore neighbouring at least two other boundary hexagons: in the case of a hexagon with only one neighbouring boundary hexagon, this is the only neighbouring face and would have a disconnected intersection with the boundary, since there must be more than two faces. But then the first equality can only be fulfilled if all boundary hexagons are neighbouring *exactly* two other boundary hexagons, which completes the proof of the second part. □

Lemma 10. *For all $k > 1$, $p \leq 6$, $h + p \geq k$ we have* $\min(h, p, k) > \min(h, p, k - 1)$.

Proof. Assume a set of patches $P_1, \ldots, P_k$ with a total of h hexagons, p pentagons and $\sum_{i=1}^{k} b(P_i) = \min(h, p, k)$ is given. If two of the patches have a boundary edge with both endpoints of degree 2, then we can identify the patches along these boundary edges and obtain a set of $k - 1$ patches with the same number of pentagons and hexagons but shorter boundary sum. By Corollary 2 such an edge always exists in patches with less than six pentagons.

So the only remaining case is that we have $k = 2$, $p = 6$ and all six pentagons are in the same patch, without loss of generality P_1, which has a boundary with boundary sequence $(2, 3)^n$ for some $n \geq 2$. By Lemma 1 we have $b(P_2) \geq 6$. Arranging $\lfloor \frac{f(P_2)}{n} \rfloor$ rings of n hexagons each around P_1, we get a patch with the same boundary sequence and length as P_1. Adding the remaining $f(P_2) - n\lfloor f(P_2)/n \rfloor$ hexagons in an incomplete (but connected) ring, we have a patch with h hexagons, six pentagons and boundary length at most $b(P_1) + 2 < b(P_1) + 6 \leq b(P_1) + b(P_2)$. □

Spirals

A *spiral* is an (h, p)-patch in which the faces can be numbered from 1 to $h + p$ in a way that for $1 < m \leq h + p$ face m has a connected intersection with the subgraph induced by the faces $1 \ldots m - 1$ which includes an edge of face $m - 1$ and for $m > 2$ an edge of the smallest of the faces sharing a vertex with face $m - 1$ that is in the boundary of the patch induced by the faces 1 to $m - 1$. Such a numbering is called a *spiral numbering*. A special class of spirals has also been studied in the context of fullerenes. Most fullerenes can be described as a spiral with $p = 11$ and the unbounded face a pentagon or $p = 12$ and the unbounded face a hexagon (see [7]).

A spiral with h hexagons and p pentagons together with a spiral numbering in which the pentagons get numbers $1, \ldots, p$ is called *a spiral* $S_{h,p}$. The reader can easily convince himself that for arbitrary $h \in \mathbb{N}$ and $p \leq 6$ spirals $S_{h,p}$ exist and are uniquely determined up to isomorphisms. This justifies the notation *the spiral* $S_{h,p}$ as long as properties are discussed that are invariant under isomorphisms. For $p > 6$ this result does not hold. A detailed proof can be found in [8]. By definition a spiral $S_{h,p}$ contains spirals $S_{0,1}, \ldots, S_{0,p-1}$ and $S_{0,p}, S_{1,p}, \ldots, S_{h-1,p}$ as subspirals.

In the following lemma we list some useful properties of spirals:

Lemma 11. *Given a spiral* $S_{h,p}$, $p \leq 6$. *Then*

(a) *If* $h + p > 2$ *every face has at least two nonboundary edges.*

(b) *There is* n, $0 \leq n < h + p$ *so that the faces numbered* $1, \ldots, n$ *are interior faces and there is a cyclic order around the boundary so that the boundary faces are numbered* $n + 1, \ldots, h + p$.

(c) *For every* n *there is* h *so that for all* $h' \geq h$ *the face numbered* n *is an interior face of* $S_{h',p}$.

(d) *If face* 1 *is interior and there is a face* f *with exactly two nonboundary edges, then* f *is numbered* $h + p$.

(e) *If face* 1 *is interior and there is no face with exactly two nonboundary edges, every boundary face is neighbouring exactly two other boundary faces.*

Proof. (a) This is a direct consequence of the definition for $h + p > 2$.

(b) This can be proven by induction on the number of faces using the requirements for the position of the last face and the boundary structure of spirals in the induction step. This result is closely related to the existence of spirals. We leave the proof to the reader.

(c) Assume the contrary and let n be a minimal number so that this is not true. Furthermore let $S_{h,p}$ be a spiral so that all faces numbered $1, \ldots, n - 1$ are interior faces. By (b) for all $h' \geq h$ in $S_{h',p}$ face h' shares a boundary vertex with face n and therefore face $h' + 1$ shares an edge with face n in $S_{h'+1,p}$. But this would require an infinite number of edges of face n.

(d) Checking for every p the smallest case with face 1 interior by hand, we can proceed by induction: given a spiral $S_{h+1,p}$. All faces with number smaller than $h + p - 1$ have at least three nonboundary edges by the induction hypotheses. Face $h + p$ has at least two nonboundary edges in $S_{h,p}$ (part (a)) and must share at least one additional edge with face $h+p+1$—so face $h+p+1$ is the only candidate for only two nonboundary edges.

(e) Assume there is a boundary face g neighbouring three other boundary faces h, h', h'' in clockwise direction around g starting at a boundary edge of g. Removing g and h' disconnects the spiral and without loss of generality assume face number 1 is in another component than the component H containing h. Note that face 1 is neither g nor h', since face 1 is an interior face. For every interior face n, face 1 can be connected to face n by a path through the (interior) faces $1, 2, \ldots, n$ (part (b)), so all faces in $H \cup \{g, h'\}$ must be boundary faces. By Remark 6 there is a face f' at maximum distance from g in $H \cup \{g, h'\}$ with at most two nonboundary edges. If $f' \neq h'$, f' also has at most two nonboundary edges in $S_{h,p}$, so $f' = h'$ and all other faces in $H \cup \{g, h'\}$ are neighbouring g. But similar to the last step in the proof of Remark 6 one can see that one of them must have at most two nonboundary edges—again a contradiction. □

Theorem 12.

$$
\begin{aligned}
b(S_{h,0}) &= 2\lceil\sqrt{12h-3}\rceil\\
b(S_{h,1}) &= 2\lceil\sqrt{10h+\tfrac{25}{4}}+\tfrac{1}{2}\rceil-1\\
b(S_{h,2}) &= 2\lceil\sqrt{8h+16}\rceil\\
b(S_{h,3}) &= 2\lceil\sqrt{6h+\tfrac{81}{4}}+\tfrac{1}{2}\rceil-1\\
b(S_{h,4}) &= 2\lceil\sqrt{4h+25}\rceil\\
b(S_{h,5}) &= 2\lceil\sqrt{2h+\tfrac{113}{4}}+\tfrac{1}{2}\rceil-1\\
b(S_{h,6}) &= \begin{cases} 10 & if\ \frac{h}{5}\in\mathbb{N}\\ 12 & else. \end{cases}
\end{aligned}
$$

Proof. We will give the proof only for $b(S_{h,1})$. For the other cases the proofs are very similar, though some of them are a bit more technical in detail. They can be looked up in [8].

For $b(S_{h,0})$ see also [9].

Let a spiral $S_{h,1}$ be given. For $d \geq 0$ the set of faces at distance d from the pentagon is called the dth layer of the spiral. A dth layer is called complete, if the unbounded face has distance more than d from the central pentagon. In a complete dth layer there are $5d$ hexagons.

A (complete) side of $S_{h,1}$ in layer d is a set of d consecutively numbered faces in layer d so that the last one can be reached from the central pentagon by a straight path in the dual, that is a path that uses every third edge in the cyclic ordering around the vertices with valency 6.

The existence of such layers and sides as well as the result about the number of faces contained in them can be formally proven by discussing the boundary sequences that occur for such spirals and how they change when faces are added. We leave the details to the reader.

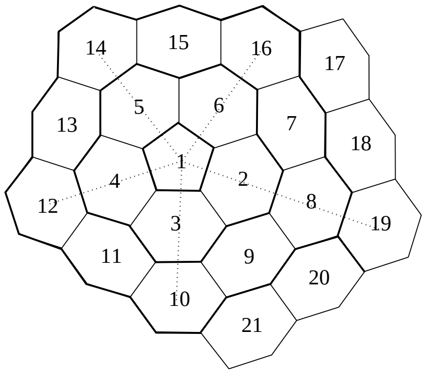

Fig. 3. The spiral $S_{20,1}$. It has two complete layers of hexagons, one complete side that does not belong to a complete layer and two additional faces that do not belong to a complete side.

So the number h of hexagons in a spiral with l complete layers, s complete sides that do not belong to a complete layer and a additional faces that do not belong to a complete side is

$$h = \sum_{i=1}^{l}(5i) + s(l+1) + a = \tfrac{5}{2}l^2 + \tfrac{5}{2}l + sl + s + a.$$

On the other hand the length of the boundary is given by

$$b(S_{h,1}) = \begin{cases} 10l + 5 & \text{if} \quad s = a = 0 \\ 10l + 2s + 7 & \text{else.} \end{cases}$$

The case $s = a = 0$ follows directly from Lemma 9. The other case has to be deduced from details of the boundary sequence.

In the case $s = a = 0$ we have

$$\begin{aligned} &2\lceil\sqrt{10h + \tfrac{25}{4}} + \tfrac{1}{2}\rceil - 1 = 2\lceil\sqrt{25l^2 + 25l + \tfrac{25}{4}} + \tfrac{1}{2}\rceil - 1 \\ &\quad = 2\lceil\sqrt{(5l + \tfrac{5}{2})^2} + \tfrac{1}{2}\rceil - 1 = 2\lceil 5l + \tfrac{5}{2} + \tfrac{1}{2}\rceil - 1 = 10l + 5 = b(S_{h,1}). \end{aligned}$$

In the case $(s, a) \neq (0, 0)$ we have $0 \leq s \leq 4$ and $0 \leq a \leq l$, so

$$s^2 < 5s + 10a < s^2 + 2s + 10l + 6.$$

Adding $25l^2 + 10ls + 25l + 5s + \frac{25}{4}$ and taking roots we get

$$5l + s + \tfrac{5}{2} < \sqrt{10h + \tfrac{25}{4}} < 5l + s + \tfrac{7}{2}$$

and therefore

$$\begin{aligned} &2\lceil\sqrt{10h + \tfrac{25}{4}} + \tfrac{1}{2}\rceil - 1 = 2((5l + s + \tfrac{7}{2}) + \tfrac{1}{2}) - 1 \\ &\quad = 10l + 2s + 7 = b(S_{h,1}). \quad \square \end{aligned}$$

Lemma 13. *Given a spiral $S_{h,p}$, $p \leq 6$. Let $S^+_{h,p} = S_{h',p}$ be the spiral with h' minimal so that all $h + p$ faces of the subspiral $S_{h,p}$ are interior.*

Then $S^+_{h,p}$ *has no boundary face with exactly two nonboundary edges and every boundary hexagon shares exactly two edges with other boundary hexagons.*

In case $p < 6$ *we have* $(S^+_{h,p})^- = S_{h,p}$.

Proof. In $S_{h',p}$ face 1 is interior, so by Lemma 11 only the last hexagon can have exactly two nonboundary edges. Removing such a hexagon does not alter the set of interior faces since all neighbouring faces still have a boundary edge. So removing this last face gives a smaller spiral with the same set of interior faces—contradicting the minimality of h'.

By Lemma 11 this completes the first part of the proof.

By Lemma 11 there is some n so that the faces numbered $n, \ldots, h'$ have been removed, so $(S^+_{h,p})^- \neq S_{h,p}$ implies that there is some $h_a > h$ so that $(S^+_{h,p})^- = S_{h_a,p}$. From the monotonic growth of the boundary length of spirals for $p < 6$ it follows that h_a has at least three boundary edges in $S_{h_a,p}$, since otherwise removing face h_a would increase the boundary length. So there are three pairwise different faces $h_a + 1 < h_b < h_c \leq h'$ in $S^+_{h,p}$ neighbouring h_a along these edges.

In this case $h_a, h_a + 1, \ldots, h_b, h_a$ is a face cycle in $S_{h_b,p}$ with all faces of $S_{h,p}$ in its interior. So these faces are already nonboundary faces in $S_{h_b,p}$ contradicting the minimality of h'. □

The minimality of spirals

For $\min(h, p) = \min\{l \in \mathbb{N} \mid \exists (h, p)\text{-patch } P \text{ with } b(P) = l\}$ we want to prove the following theorem:

Theorem 14. *For* $p \leq 6$ *we have*

$$b(S_{h,p}) = \min(h, p).$$

This theorem follows immediately from the next lemma, which is a bit more technical, but states an even stronger result:

Lemma 15. *For every* (h, p)*-patch* P *and spiral* $S_{h',p'}$ *with* $p \leq p' \leq 6$ *and* $h + p = h' + p'$ *we have* $b(P) + p \geq b(S_{h',p'}) + p'$.

Proof. Assume that P and $S_{h',p'}$ form a counterexample with the 3-tuple (p, p', h) minimal in lexicographical order, so $b(P) + p < b(S_{h',p'}) + p'$.

Let f_b, respectively $(f_S)_b$ denote the number of faces in the boundary of P respectively $S_{h',p'}$. Since the result is obviously true for just one face, assume $h + p \geq 2$.

P cannot have a pentagon in its boundary, because otherwise we could replace this by a hexagon with the result a counterexample with the corresponding (smaller) 3-tuple $(p - 1, p', h + 1)$.

By Lemma 1 and Remark 3 we get

$$b(P) + p = 2v_{3,b}(P) + 6 \geq 2 f_b + 6.$$

Since boundary faces in spirals have a connected intersection with the boundary we also get

$$b(S_{h',p'}) + p' = 2v_{3,b}(S_{h',p'}) + 6 = 2(f_S)_b + 6.$$

From these equations we get $f_b < (f_S)_b$ for our counterexample, so especially $f_b < h + p$, that is P has an interior face.

If $f_b > h'$, we have also $(f_S)_b > h'$, so $S_{h',p'}$ has a pentagon in the boundary and $h \geq f_b > h'$ which gives $p \leq p' - 1$. Since by Lemma 11 especially the pentagon p' is in the boundary, we can make the face p' a hexagon with the result a spiral $S_{h'+1,p'-1}$. But this would give a counterexample with the corresponding (smaller) 3-tuple $(p, p' - 1, h)$—a contradiction. So $f_b \leq h'$ and the spiral $S_{h'-f_b,p'}$ is well defined.

Since the number of interior faces in $S_{h',p'}$ is smaller than in P, where it is $p + h - f_b$, the spiral $S^+_{h'-f_b,p'}$ has more interior faces than $S_{h',p'}$ and therefore also more faces in all.

First assume $p' < 6$:

With P^- the patch-set obtained by removing all f_b boundary hexagons and an $(h - f_b, p)$-patch P' with $b(P') = \min(h - f_b, p)$, using the monotonically increasing boundary length for spirals with $p < 6$ Lemmas 9 and 13 give:

$$\begin{aligned} b(P') + p &\leq b(P^-) + p \leq b(P) + p - 2(6 - p) \\ &< b(S_{h',p'}) + p' - 2(6 - p) \leq b(S_{h',p'}) + p' - 2(6 - p') \\ &\leq b(S^+_{h'-f_b,p'}) - 2(6 - p') + p' = b(S_{h'-f_b,p'}) + p'. \end{aligned}$$

So P' and $S_{h'-f_b,p'}$ would be a counterexample with corresponding 3-tuple $(p, p', h - f_b)$ contradicting minimality.

In the case $p' = 6$ we have $b(S_{h',6}) + p' \in \{16, 18\}$ for all h', so $b(P) + p \leq 16$. Since $f_b < h + p$ we can apply Lemma 9 and since P has no pentagon in the boundary, with the notation above we have $b(P') + p \leq b(P) + p$. Due to minimality, P' together with $S_{h'-f_b,6}$ forms no counterexample, so $b(P') + p \geq 16$. So $b(P') + p = b(P) + p = 16$ and $b(S_{h',6}) + p' = 18$. Lemma 9 implies $p = 6$ and that each boundary hexagon of P has a connected intersection with the boundary and therefore that $b(P) = 10$ and that $f_b = v_{3,b}(P)$. By Lemma 1 this gives $f_b = 5$. But in this case $h' = h \geq 5$ and $b(S_{h'-f_b,6}) + p' = b(S_{h'-5,6}) + p' = 18$. This again contradicts the minimality of P. □

Related results

Theorem 16. *For $p \leq 6$ there exists an (h, p)-patch P with $b(P) = b$ if and only if* $\min(h, p) \leq b \leq \max(h, p)$ *and* $b \equiv p \mod 2$.

Proof. The *only if* direction follows directly from the definition and Lemma 1.

The cases with $b = \min(h, p)$ are covered by spirals and for $h + p \leq 2$ we have $\min(h, p) = \max(h, p)$, so there is nothing more to prove. Since for $h = 0$ we can check all cases by hand, from now on we assume $h \geq 1$ and $h + p > 2$ and will proceed by induction on h except for some values close to $\min(h, p)$ where we will prove the result directly:

First we will prove that for $p < 6$ patches with $b = \min(h, p) + 2$ with subsequence 22 of the boundary sequence exist:

For $p < 6$ the spiral $S_{h-1,p}$ has 22 as well as 232 as subsequences of the boundary sequence, so gluing an additional hexagon to the spiral $S_{h-1,p}$ at position 22, respectively 232 of the boundary sequence—depending on whether $b(S_{h-1,p}) = b(S_{h,p}) - 2$ or

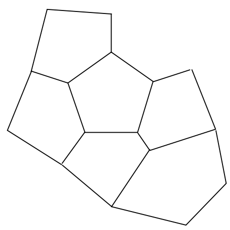

Fig. 4. A $(0, 6)$-patch P_0 and a $(1, 6)$-patch P_1 with $b(P_0) = b(P_1) = 12$.

$b(S_{h-1,p}) = b(S_{h,p})$ we get a patch P' with $b(P') = b = \min(h, p) + 2$ and subsequence 22 of the boundary sequence at the new face.

For $p = 6$ we will prove this result for $b = 12$ and 14:

For the $(1, 6)$-patch P_1 in Fig. 4 we have $b(P_1) = 12$ and a boundarysequence 223323232323. Adding a new hexagon at the position 2332 we have a $(2, 6)$-patch P_2 with the same boundary length and boundarysequence. This process can be repeated to prove that for any h there are $(h, 6)$-patches P_h with $b(P) = 12$ and subsequences 232 and 22 in the boundary sequence. Adding a hexagon at a position 232 of patch P_{h-1} with P_0 from Fig. 4, we obtain the same result for $b = 14$.

Now let $\min(h, p) + 4 \leq b \leq \max(h, p)$, $b \equiv p \mod 2$, and $b \geq 16$ in case $p = 6$. Then $\min(h - 1, p) \leq b - 4 \leq \max(h - 1, p)$ and $b - 4 \equiv p \mod 2$, so by induction an $(h - 1, p)$-patch P with $b(P) = b - 4$ and subsequence 22 exists and by gluing an additional hexagon to an edge with two endpoints of degree 2 we obtain an (h, p)-patch P' with $b(P') = b$ and also a subsequence 22. □

A natural question to ask is how many pentagons and hexagons can be assembled to form a patch P not exceeding some given boundary length b. As soon as six pentagons are allowed and $b \geq 10$ no upper bound exists, so assume $p < 6$ pentagons are allowed. The answer to this question is an easy corollary of the main theorem.

Corollary 17. *For $p < 6$ let $m(b, p) := \max\{h \mid \exists(h, p)\text{-patch } P : b(P) \leq b\}$.*

Then $m(b, p) = \max\{h \mid b(S_{h,p}) \leq b\}$.

Proof. Since for $p < 6$ the value of $b(S_{h,p})$ is monotonically increasing in h and approaching infinity, for every b there is h_b so that $b(S_{h_b,p}) \leq b < b(S_{h,p})$ for all $h > h_b$. A patch P with $h' > h_b$ hexagons and $b(P) \leq b$ would contradict the minimality of the boundary of $S_{h',p}$. □

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