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Fullerene patches II

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Abstract

In this paper, we show that fullerene patches with nice boundaries containing between 1 and 5 pentagons fall into several equivalence classes; furthermore, any two fullerene patches in the same class can be transformed into the same minimal configuration using combinatorial alterations.

Keywords: Fullerenes, fullerene patches, pseudoconvex patches.

Math. Subj. Class.: 05C10, 05C75, 92E10

1 Introduction

A plane graph with all faces hexagonal except one external face, with all vertices on the boundary of the outside face having valence 2 or 3, and with all other vertices (called *internal vertices*) having valence 3 is called a *graphene patch*. One way to construct a graphene patch is to take a closed simple (non-self-intersecting) curve in Λ, the hexagonal tessellation of the plane, and replace all vertices, edges and faces outside the curve by a single outside face. It is clear that a graphene patch constructed in this way is uniquely determined (up to an isomorphism of plane graphs) by its *boundary code*; that is, the sequence of valences of boundary vertices in cyclic order. A boundary code can be written starting at any vertex and proceeding in either a clockwise or counterclockwise direction. Hence, a given boundary code is actually a representative of the equivalence class of codes under cyclic permutations and inversions.

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However, not every graphene patch may be constructed in this way. Specifically, the boundary of a graphene patch may yield a self-intersecting curve when projected onto Λ. In this case, the patch may not be uniquely determined by its boundary code. In [9], Guo, Hansen, and Zheng described two nonisomorphic graphene patches with the same boundary code. We say that the boundary code of a graphene patch is *ambiguous* if there are two or more nonisomorphic graphene patches with the same boundary code. It is implicit in [4] that ambiguity for graphene patches is topological in the following sense: Consider two nonisomorphic graphene patches with the same boundary code and use the boundary code to trace the boundary as a self-intersecting circuit in Λ. We may think of this self-intersecting circuit as a local homeomorphism f of the unit circle into the plane. Then each patch gives an extension of f to a local homeomorphism into the entire disk. That these graphene patches are nonisomorphic corresponds to the fact that the extensions are not homotopic.

In this paper we investigate patches with ambiguous boundaries that include some pentagonal faces. In particular we will be interested in patches on a *fullerene:* a trivalent plane graph with only hexagonal and pentagonal faces. For the patches we consider, we show that the ambiguities are combinatoral rather than topological.

Definition 1.1. A *fullerene patch* or, in this paper, simply a *patch* is a plane graph with all faces hexagonal or pentagonal except for one external face of a different degree (not 5 or 6), with all vertices on the boundary of the external face having valence 2 or 3, and with all remaining *internal* vertices having valence 3. We again use the term *boundary code* to describe the sequence of valences of 2's and 3's in cyclic order on the boundary.

We will adopt the notation from [7] and let a patch be denoted as $\Pi = (V, E, F, B)$ where V and E are the vertex and edge sets, F is the set of faces *excluding* the external face, and B is the boundary of the external face. One method of constructing a patch is to take a simple closed curve on a fullerene, and consider the subgraph created by deleting all vertices and edges on the "outside" of the curve. However, the uniqueness property of similarly-constructed graphene patches does not hold for fullerene patches constructed in this way. In fact, very frequently nonisomorphic patches will have identical boundary codes. Even graphene patches formed from closed simple curves on fullerenes are not known to have unambiguous boundary.

Definition 1.2. Two patches with the same boundary code are *similar*. For any patch Π the collection of patches similar to Π is called its *similarity class* and is denoted by $\mathcal{S}(\Pi)$; the class is *trivial* when all patches in $\mathcal{S}(\Pi)$ are isomorphic.

In this paper we consider patches containing between 1 and 5 pentagons with "nice boundaries." We show that the similarity classes of these patches are of eight basic types and that for patches in the same similarity class there exists a sequence of combinatorial alterations that transforms one patch to another.

2 Linear patches

Let $\Pi = (V, E, F, B)$ be a patch. For any internal face $f \in F$, let $B(f)$ denote its boundary; so either $B(f) \cap B$ is empty or consists of one or more paths. These paths are the paths on the boundary B joining consecutive degree-3 vertices.

Definition 2.1. The paths of $B(f) \cap B$ over all f are called the *segments* of the boundary. If $B(f) \cap B$ consists of only one segment, then $|B(f) \cap B|$ is the length of the path. A segment of length i will be called an i-*segment*, and the number of i-segments in B will be denoted by s_i.

Definition 2.2. *Linear* patches are patches with $s_1 = 0$ consisting of strings of hexagons capped off at each end with a hexagon or a pentagon – see Figure 1.

In [7] it was shown that the similarity class of a linear patch with at most one pentagonal end is trivial. On the other hand, the similarity class of any linear patch with two pentagonal ends includes some additional nonlinear patches and is nontrivial, as is illustrated in Figure 3.

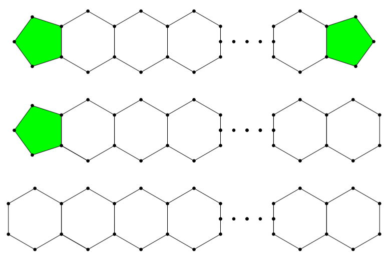


Figure 1: Linear patches.

Lemma 2.3. *Let* $\Pi = (V, E, F, B)$ *be a patch with* $s_1 = 0$.

1. *If* Π *admits a face* f *such that* $B(f) \cap B$ *consists of more than one segment, then* Π *is a linear patch.*
2. *If* Π *admits a pentagonal face* f *such that* $|B(f) \cap B| = 4$*, then* Π *is a linear patch.*
3. *If* Π *admits a hexagonal face* f *such that* $|B(f) \cap B| = 5$*, then* Π *is a linear patch.*

Proof. These results clearly hold for all patches with one or two faces. Let $\Pi = (V, E, F, B)$ be a patch with $s_1 = 0$ and $n > 2$ faces, and assume that these results hold for all such patches with fewer than n faces.

First assume that Π admits a face f such that $B(f) \cap B$ consists of more than one segment. Since $s_1 = 0$, each boundary segment has length at least 2. Thus f is a hexagon, each boundary segment of $B(f) \cap B$ has length 2, and f shares one edge with a face g and the antipodal edge with a face h. Deleting f leaves two subpatches, Π_g and Π_h, where

$|B(g) \cap B(\Pi_g)| \geq 5$ and $|B(h) \cap B(\Pi_h)| \geq 5$. So Π_g and Π_h are both linear by induction, and hence Π is linear.

Assume next that Π admits a pentagonal face f such that $|B(f) \cap B| = 4$ or a hexagonal face f such that $|B(f) \cap B| = 5$. Then f shares an edge with exactly one other face, g. Since Π has more than 2 faces, g has more than one boundary segment and we are back in the first case. □

It is convenient to treat linear patches and non-linear patches separately.

Lemma 2.4. *If* $\Pi = (V, E, F, B)$ *is a non-linear patch with* $s_1 = 0$*, then*

1. *for* $f \in F$*,* $B(f) \cap B$ *is empty or a single segment;*
2. *for* $f \in F$*,* $|B(f) \cap B| = 4$ *implies* f *is a hexagon;*
3. $s_5 = 0$*;*
4. $p(\Pi) = 6 - s_3 - 2s_4$*, where* $p(\Pi)$ *is the number of pentagons contained in the patch* Π.

Proof. The first three conditions follow at once from Lemma 2.3. The fourth condition is a special case of the following direct consequence of Euler's formula, proved in [7]: $p(\Pi) = 6 + s_1 - s_3 - 2s_4 - 3s_5$. □

It is an obvious consequence of this fourth condition that a non-linear patch with $s_1 = 0$ may contain at most six pentagonal faces. If Π is such a patch with six pentagonal faces, $s_3 = s_4 = s_5 = 0$. Hence its boundary consists of m segments of length 2, for some m. Adding a layer of hexagons around this boundary yields another patch with an identical boundary and m more faces; this is the F expansion defined in [10]. Therefore all non-linear patches with $s_1 = 0$ and six pentagonal faces have ambiguous boundary code, and in fact the similarity class of each is infinite. Thus we restrict our attention to non-linear patches with $s_1 = 0$ and with one to five pentagonal faces. Following [3]:

Definition 2.5. A *pseudoconvex patch* is a non-linear patch with $s_1 = 0$ containing one to five pentagonal faces.

3 Pseudoconvex patches

Pesudoconvex patches were discussed in detail in [8], and we use the same terminology here.

Definition 3.1. A *side* of a pseudoconvex patch is the section of the boundary (including the faces) between a consecutive pair of degree 2 vertices. The *length* of a side is one less than the number of faces on the side. Three consecutive degree 2 vertices on the boundary correspond to a side of length zero containing just one face.

For a pseudoconvex patch or a linear patch Π, we introduce several parameters and more notation:

1. $\ell(\Pi)$ denotes the sum of the lengths of every side;

2. $s = s(\Pi)$ denotes the number of sides of Π;
3. The cyclic sequence $[\ell_1, \dots, \ell_s]$ denotes the side lengths of Π listed in cyclic order around the patch and is called the *side parameters* of the patch.
4. The similarity class $\mathcal{S}(\Pi)$ will also be denoted by $\mathcal{S}_{[\ell_1,\dots,\ell_s]}$ when Π has side parameters $[\ell_1, \dots, \ell_s]$.

The following lemma summarizes a few results proven in [8].

Lemma 3.2. *Let* $\Pi = (V, E, F, B)$ *be a pseudoconvex patch with side parameters* $[\ell_1, \dots, \ell_s]$. *Then*

1. $s = s(\Pi) = 6 - p(\Pi)$.
2. There are no consecutive 0's in $[\ell_1, \dots, \ell_s]$.
3. If ℓ_s *and* ℓ_2 *are both nonzero and all faces on the* ℓ_1 *side are hexagons (including both terminal 3-faces when* $\ell_1 > 0$*), deleting all of the faces on the* ℓ_1 *side of* Π *results in* $\Pi' = (V', E', F', B')$ *which is either a linear patch or another pseudoconvex patch. The side parameters of* Π' *are*
   (a) $[\ell_1 + 1, \ell_2 - 1, \ell_3, \dots, \ell_{s-1}, \ell_s - 1]$*, when* $s > 2$*;*
   (b) $[\ell_1 + 1, \ell_2 - 2]$*, when* $s = 2$*;*
   (c) $[\ell_1 - 1]$*, when* $s = 1$

4 Combinatorial ambiguities

Definition 4.1. By a *hexpath* joining two pentagonal faces we mean either a linear patch with pentagonal terminal faces or two linear patches with one pentagonal terminal face and one hexagonal terminal face sharing the hexagonal terminal face and making an angle of 120 degrees. See Figures 3 and 4. The Coxeter coordinates (n) of a straight hexpath is the length of the corresponding straight path in the dual; the Coxeter coordinates (n, k) of a two leg hexpath are the lengths of the corresponding straight paths in the dual. We often refer to them as either (n)-*hexpaths* or (n, k)-*hexpaths*. The notation $(n, 0)$-hexpath, $(0, n)$-hexpath and (n)-hexpath will be used interchangeably.

Lemma 4.2. *Let* Π *be a pseudoconvex patch containing at least two pentagons and let* Π' *be a subpatch of* Π *containing at least one pentagon but not every pentagon. Then there exists a hexpath from a pentagon in* Π' *to a pentagon not in* Π'.

Proof. Let Π and Π' be as stated. Consider the facial distances between every pentagon in Π' to every pentagon not in Π'. Let f be a pentagon in Π' and g be a pentagonal face not in Π' so that the distance between f and g is the minimum over all such pairs. Consider a shortest polygonal path of faces in Π joining f to g. By the choice of f and g, all of the faces on this polygonal path are hexagons; it remains to show that this path is indeed a hexpath. Since all interior faces in the corresponding dual path are triangular, no shortest path can make a sharp, 60° turn (see [1] in Figure 2); otherwise, the hexagon h at the turn may simply be deleted from the path resulting in a shorter path.

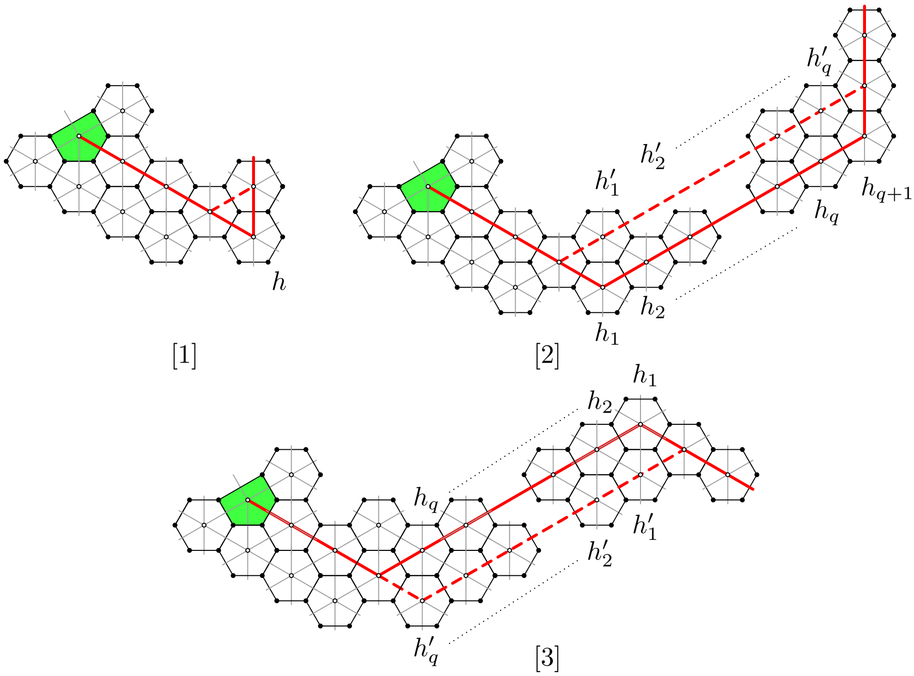


Figure 2: Pictoral proof of existence of hexpath from Lemma 4.2.

Next suppose that the shortest dual path joining f and g makes consecutive left turns (see [2] in Figure 2). Let $h_1, \ldots, h_{q+1}$ denote the faces on the segment between the turns including both faces at the turns. Note that the edge in common with h_1 and face labeled h'_1 would be a boundary segment of length 1 if h'_1 did not belong to the patch. Hence, h'_1 belongs to the patch. Also, h'_1 must be a hexagon, otherwise we contradict the way f and g were chosen. Now the same argument can be applied to h'_2 and so it too belongs to the patch. Inductively, $h'_1, \ldots, h'_q$ are all hexagons belonging to the patch. Replacing $h_1, \ldots, h_{q+1}$ by $h'_1, \ldots, h'_q$ results in a shorter dual path joining f and g and a contradiction. By the same argument there cannot be two consecutive right turns.

Finally, we choose from among all shortest dual paths joining f and g the one with the longest straight segment before a first left turn. (If the first turn is a right turn, we will interpret this as starting off with a segment of length 0 followed by a left turn.) We wish to prove that this particular shortest dual path has just two straight segments. Suppose there is a right turn after the first left turn. Starting with the face at the right turn, we label the faces back to but not including the face at the left turn $h_1, \ldots, h_q$ (see [3] in Figure 2). Employing the argument just used above, we see that the faces labeled $h'_1, \ldots, h'_q$ must be hexagons belonging to the patch. Replacing $h_1, \ldots, h_q$ by $h'_1, \ldots, h'_q$ then results in an f, g-path of the same length but with a longer initial straight segment contradicting our choice of this path. $\square$

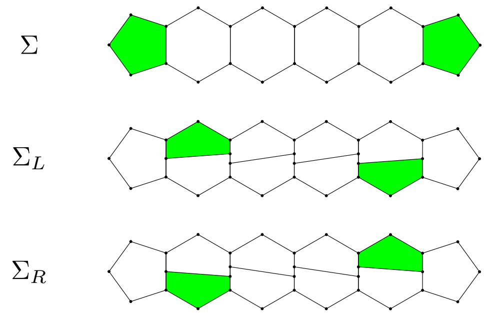


Figure 3: A (5)-hexpath, Σ, and the similar patchs Σ_L and Σ_R, each representing an α step.

Endo and Kroto [5] provided a method of constructing a patch similar to a linear patch. Let Σ be an (n)-hexpath joining a pair of pentagonal faces, where $n > 1$. Then the similar patch is formed by inserting one new vertex on each edge of Σ separating a pentagon from its adjacent hexagon, and two new vertices on each edge of Σ separating two adjacent hexagons. Edges may then be added in two different ways, as demonstrated in Figure 3, resulting in the similar patch Σ'_L containing a $(1, n-2)$- hexpath or the similar patch Σ'_R containing a $(n-2, 1)$-hexpath. If Π is a pseudoconvex patch containing such a hexpath Σ, replacing Σ by Σ_L or Σ_R results in a pseudoconvex patch Π' that is similar to Π and contains $n-1$ more faces. Replacing Π by Π' is called an α *step*; if this replacement is made in a larger patch, then the choice of Σ_L versus Σ_R may result in non-isomorphic patches.

The Endo-Kroto construction can be generalized to any (n, k)-hexpath joining a pair of pentagonal faces with $nk > 1$. Let Σ be such a hexpath. Then a similar patch is formed by inserting one new vertex on each edge of Σ separating a pentagon from its adjacent hexagon, and two new vertices on each edge of Σ separating two adjacent hexagons and adding edges, as demonstrated in Figure 4, is a similar patch containing an $(n-1, k-1)$-hexpath joining a pair of pentagonal faces. We denote this new patch by Σ'. Note that in this case, the edges may be added in just one way. If Π is a pseudoconvex patch containing such a hexpath Σ, replacing Σ by Σ' results in a pseudoconvex patch Π' that is similar to Π and contains $n+k-1$ more faces. Replacing Π by Π' is called an β *step*.

It is clear that any patch obtained from Π by a sequence of α and β steps will be similar to Π. We also note that when a $(1, n-2)$-hexpath, an $(n-2, 1)$-hexpath or an $(n-1, k-1)$-hexpath is bordered by a sufficient set of hexagons, we may reverse these constructions. We call this reverse constructions α^{-1} and β^{-1} steps.

Since each α or β step produces another patch in the same similarity class with more faces, the sequence of similar patches constructed by a sequence of α and β steps must all be distinct. As we will soon verify, the number of patches in the similarity class of a pseudoconvex patch is finite. Therefore starting with any pseudoconvex patch, any sequence of α and β steps must terminate in a similar pseudoconvex patch for which no α or β step is possible.

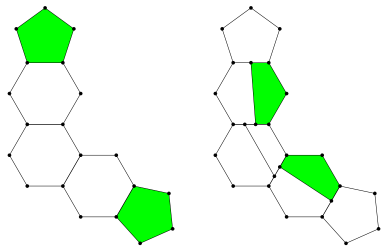


Figure 4: A $(2,2)$-hexpath Σ, and the similar patch Σ' containing a $(1,1)$-hexpath.

Cone	Tip
Λ_1	a pentagonal face
$\Lambda_{2(a)}$	a quadrilateral face
$\Lambda_{3(a)}$	a triangular face
$\Lambda_{3(b)}$	a “half-edge”
$\Lambda_{4(a)}$	a valence 2 face
$\Lambda_{4(b)}$	a pendant vertex
Λ_5	a loop

Table 1: Geometric Cone Tips.

Definition 4.3. A patch Π in the similarity class $\mathcal{S}$ is called a *terminal patch* if no α or β step is possible in Π. The smallest linear or pseudoconvex subpatch of a terminal patch containing all of the pentagonal faces is a *minimal configuration.*

Terminal patches and minimal configurations are closely related to nanocones and the tips of nanocones. We will need several results that were proven in the context of nanocones.

Definition 4.4. A nanocone or *cone* is an infinite trivalent plane graph with hexagonal faces and one to five pentagonal faces. Adopting the terminology from [3], two cones are *equivalent* if each has a finite subgraph so that when the subgraphs are deleted the remaining graphs are isomorphic.

This is an equivalence relation among cones forming eight equivalence classes. These classes are described by Klein and Balaban in [11]. A proof that these are indeed the only possibilities is given in [3]. That paper, in turn, relies in part on a result of Balke in [1]. Using the terminology from [3], we summarize this classification and consolidate the results from these three papers that are relevant to this paper. The classification of cones is based on the classification of the nontrivial rotations in the symmetry group of Λ, the regular hexagonal tessellation; the list of these rotations is given below.

Proposition 4.5. *The nontrivial rotations in the symmetry group of* Λ *are:*

1. *rotations by* 60° *about the centers of faces;*

2. *rotations by* 120°
   (a) *about the centers of faces or*
   (b) *about vertices;*
3. *rotations by* 180°
   (a) *about centers of faces or*
   (b) *about centers of edges;*
4. *rotations by* 240°
   (a) *about the centers of faces or*
   (b) *about vertices;*
5. *rotation by* 300° *about centers of faces.*

If x is the center of one of the above rotations by $k \times 60^\circ$, we may excise a $k \times 60^\circ$ wedge at x and identify the edges to get a *geometric cone,* which we will denote by Λ_k or $\Lambda_{k(a)}$ or $\Lambda_{k(b)}$. A geometric cone is an infinite graph that has, with exactly one exception at the cone tip, only hexagonal faces and only vertices of degree 3. The exceptions at the tip of these geometric cones are pictured in Figure 5 and listed in Table 1.

Now each of these geometric cone tips can be replaced by a tight configuration of pentagonal faces resulting in a unique cone, called the *representative cone*, for each of the eight equivalence classes; the smallest pseudoconvex patch containing the configuration of pentagonal faces is called the *cone tip*. These eight cone tips are also pictured in Figure 5 and are denoted by Ω_i as shown in the figure.

Given a pseudoconvex patch Π with side parameters $(\ell_1, \ldots, \ell_s)$ we may reverse the process discussed in Lemma 3.2: instead of deleting all of the faces of a side we may add a row of hexagons to a side. Adding a row of hexagons to each side in turn results in a patch with all side parameters increased by 1; call this patch Π_1. Repeatedly adding rings of hexagons produces an infinite sequence of nested graphs $\Pi_0 = \Pi$, Π_1, $\Pi_2, \ldots$, and the union of these patches is a trivalent graph with all hexagonal faces except exactly s ($1 \leq s \leq 5$) pentagonal faces - that is, a cone. Hence each linear or pseudoconvex patch may also be thought of as a patch in a uniquely determined cone.

The focus of [3] is the collection of pseudoconvex patches in which all side lengths are equal, *symmetric patches*, or in which $\ell_1 = \ell_2 - 1 = \cdots = \ell_s - 1$, *near-symmetric patches*. These patches are called *cone patches* in [3] when they include a pentagon as a bounding face and correspond to our cone tips. Also, in [3], the appropriate cone tip for a given cone patch is determined by whether the patch is symmetric or near-symmetric.

By repeatedly adding hexagons to the sides of a pseudoconvex patch, we may embed each pseudoconvex patch in a symmetric or near-symmetric patch. To see this we consider the pseudoconvex patches based on the value of s.

Lemma 4.6. *Every pseudoconvex patch* Π *is a subpatch of a symmetric or near-symmetric patch, and there is a unique cone containing* Π.

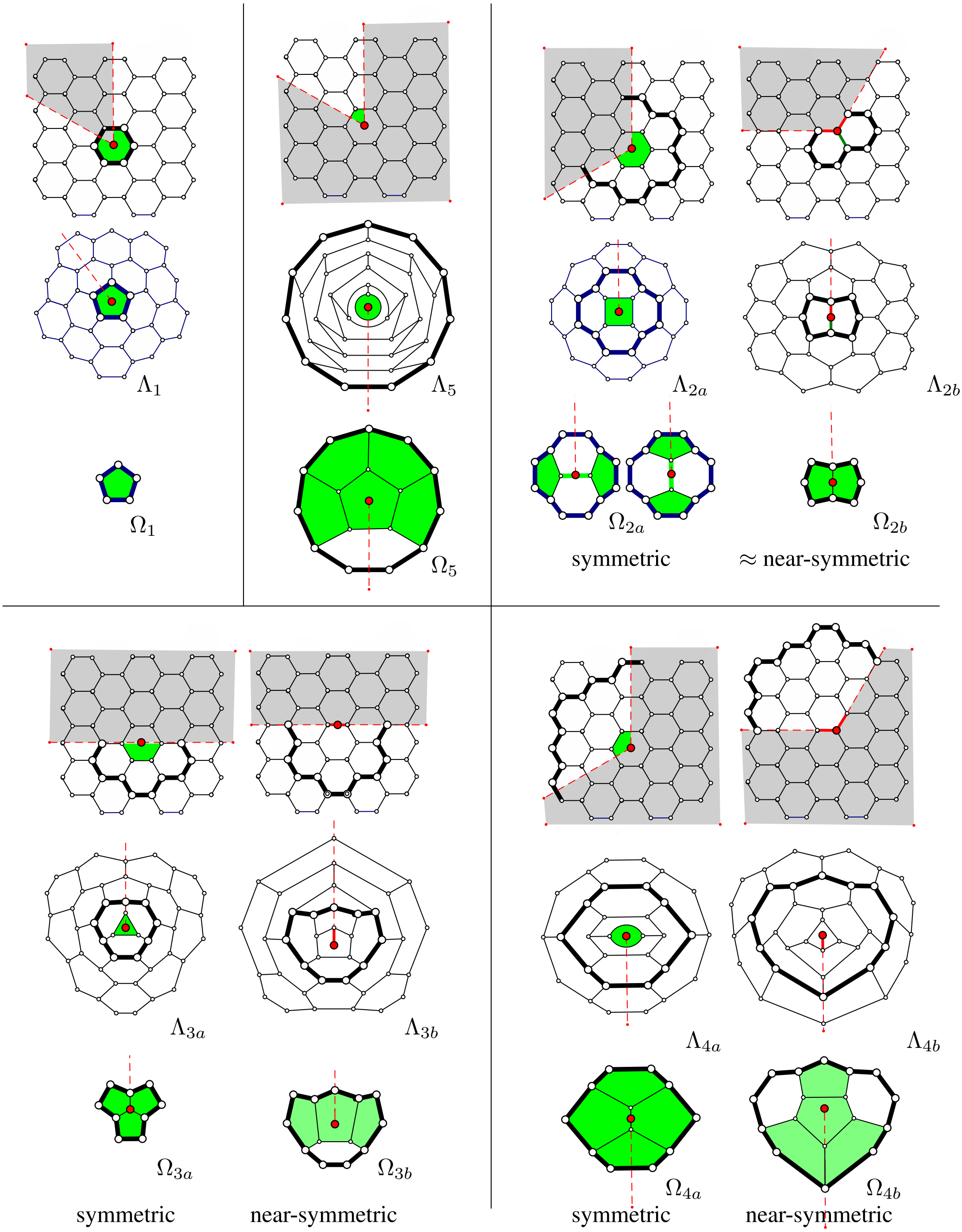


Figure 5: Cone Tips.

Proof. Let Π be a pseudoconvex patch. If $s = 1$, Π is a symmetric patch containing 5 pentagons. It follows from [3] that the unique cone containing Π has the cone tip Ω_5. If $s = 2$, let Π have side lengths $[\ell_1, \ell_2]$ with $\ell_1 \leq \ell_2$. We may add a row of hexagons to the side of length ℓ_2 to get a pseudoconvex patch with side length $\ell_1' = \ell_1 + 2$ and $\ell_2' = \ell_2 - 1$. If $\ell_1' < \ell_2' - 1$, we may repeat the process and we may continue to do so until we reach a cone patch Π^* with side lengths $\ell_1^* = \ell_2^* - 1$, $\ell_1^* = \ell_2^*$ or $\ell_1^* = \ell_2^* + 1$. We also note that $\ell_2' - \ell_1' = \ell_2 - \ell_1 - 3$ and therefore $|\ell_2^* - \ell_1^*| \equiv |\ell_2 - \ell_1| \bmod 3$. We conclude that when $\ell_1 \equiv \ell_2 \bmod 3$ the extension to a cone patch is symmetric and by [3] is the unique cone tip Ω_{4a}; otherwise the extension to a cone patch is near-symmetric and is the unique cone tip Ω_{4b}.

When $s = 3$, let Π have side lengths $[\ell_1, \ell_2, \ell_3]$; we again repeatedly add a row of hexagons to the longest side which will result in a cone patch Π^* with side lengths $\ell_1^* = \ell_2^* - 1 = \ell_3^* - 1$ or $\ell_1^* = \ell_2^* = \ell_3^*$ after suitable reordering. In this case, we note that the process of adding a row of hexagons changes the parity of each length. Hence, if the side lengths of Π are all even or all odd, the resulting cone patch Π^* will have equal side lengths and by [3] the unique cone containing Π has the cone tip Ω_{3a}; if the side lengths of Π do not all have the same parity, the unique cone containing Π has the cone tip Ω_{3b}.

Finally, consider $s = 4$, with Π having side lengths $[\ell_1, \ell_2, \ell_3, \ell_4]$. If $\ell_2 \neq \ell_4$, we may repeatedly add hexagons to the larger of these two sides side until $\ell_2' = \ell_4'$. Then, we may add hexagons to the side corresponding to larger of ℓ_1' and ℓ_3' and repeat this until we have a pseudoconvex patch Π'' with $\ell_1'' = \ell_3''$ and $\ell_2'' = \ell_4''$. If the lengths are not all equal, (without loss of generality) we assume that $\ell_1'' > \ell_2''$. Now alternately adding hexagons to the ℓ_1'' and ℓ_3'' sides will result in a cone patch Π^* with side lengths $\ell_1^* = \ell_2^* = \ell_3^* = \ell_4^*$ or (reordering if needed, $\ell_1^* = \ell_2^* - 1 = \ell_3^* - 1 = \ell_4^* - 1$. Noting that $(\ell_1^* + \ell_3^*) \equiv (\ell_2^* + \ell_4^*) \bmod 3$ if and only if $(\ell_1 + \ell_3) \equiv (\ell_2 + \ell_4) \bmod 3$, we conclude from [3] that the unique cone containing Π has the cone tip Ω_{2a} when $(\ell_1 + \ell_3) \equiv (\ell_2 + \ell_4) \bmod 3$ and the cone tip Ω_{2b} otherwise. □

Two observations: first, the cone tip Ω_{2a} is the Stone-Wales patch from [12]. A 90° rotation of the Stone-Wales patch is boundary preserving; that is, in a larger patch the Stone-Wales patch can be replaced by its rotation. However, this rotation may result in a non-isomorphic larger patch. Secondly, each pseudoconvex patch in a similarity class can be embedded in a fixed cone patch. Since the number of faces in a cone patch is bounded by a function of its side lengths, the number of faces in a patch in a given similarity class is bounded. In the next lemma, we summarize our results along with some of those from [1],[2], [3] and [11].

Definition 4.7. A pseudoconvex patch containing one of the cone tips Ω_1, Ω_{2a} (in either orientation), Ω_{2b}, Ω_{3a}, Ω_{3b}, Ω_{4a}, Ω_{4b} or Ω_5 is called a *cone tip patch*.

Lemma 4.8. *Let $\mathcal{S}$ be a non-empty similarity class of pseudoconvex patches. Then $\mathcal{S}$ is finite and, with the exception of case (2) below, contains one unique cone tip patch.*

1. *If $\mathcal{S} = \mathcal{S}_{[\ell_1,\ell_2,\ell_3,\ell_4,\ell_5]}$, then $\mathcal{S}$ contains the cone tip patches with configuration Ω_1 at the tip.*

2. *If $\mathcal{S} = \mathcal{S}_{[\ell_1,\ell_2,\ell_3,\ell_4]}$, where $(\ell_1+\ell_3) \equiv (\ell_2+\ell_4)$ mod 3, then $\mathcal{S}$ contains two cone tip patches with configuration Ω_{2a} (one in each orientation) at the tip or one cone tip patch with configuration Ω_{2a} when the patch admits a symmetry agreeing with the Stone-Wales transformation at the tip.*
3. *If $\mathcal{S} = \mathcal{S}_{[\ell_1,\ell_2,\ell_3,\ell_4]}$, where $(\ell_1+\ell_3) \not\equiv (\ell_2+\ell_4)$ mod 3, then the cone tip patch in $\mathcal{S}$ has configuration Ω_{2b} at the tip.*
4. *If $\mathcal{S} = \mathcal{S}_{[\ell_1,\ell_2,\ell_3]}$, where ℓ_1, ℓ_2 and ℓ_3 have the same parity, then the cone tip patch in $\mathcal{S}$ has configuration Ω_{3a} at the tip.*
5. *If $\mathcal{S} = \mathcal{S}_{[\ell_1,\ell_2,\ell_3]}$, where ℓ_1, ℓ_2 and ℓ_3 do not have the same parity, then the cone tip patch in $\mathcal{S}$ has configuration Ω_{3b} at the tip.*
6. *If $\mathcal{S} = \mathcal{S}_{[\ell_1,\ell_2]}$, where $\ell_1 \equiv \ell_2$ mod 3, then the cone tip patch in $\mathcal{S}$ has configuration Ω_{4a} at the tip.*
7. *If $\mathcal{S} = \mathcal{S}_{[\ell_1,\ell_2]}$, where $\ell_1 \not\equiv \ell_2$ mod 3, then the cone tip patch in $\mathcal{S}$ has configuration Ω_{4b} at the tip.*
8. *If $\mathcal{S} = \mathcal{S}_{[\ell_1]}$, then the cone tip patch in $\mathcal{S}$ has configuration Ω_5 at the tip.*

The method by which the cone tip patch in $\mathcal{S}_{[\ell_1,\ldots,\ell_s]}$ is constructed is described in [3]. In Figure 5, we have illustrated this or a similar construction for all of the cone tips except Ω_5; the region of Λ included here is not large enough to include the path. Note that in the cases that s equals 4 or 5, the triangle may actually cross the path and the identification cannot be made. This simply means that no pseudoconvex patch exists with those side lengths. For all other values of s the geometric cone can be constructed; but, in some cases, the singularity may be so close to the boundary that the tip can't be inserted and again $\mathcal{S}_{[\ell_1,\ldots,\ell_s]}$ will be empty.

We now turn to minimal configurations. By definition, these linear or pseudoconvex patches contain no pair of pentagons that are joined by an (n)-hexpath for $n > 1$ or an (n, k)-hexpath for $nk > 1$ and they admit no pseudoconvex subpatch containing all of the pentagonal faces. The cone tips Ω_{2a} (in either orientation), Ω_{2b}, Ω_{3a}, Ω_{3b}, Ω_{4a}, Ω_{4b} or Ω_5 are clearly minimal. There is one other configuration that is clearly minimal: three pentagons sharing alternate edges with a central hexagon, the left-hand configuration in Figure 8 which we denote by Ω_3.

Lemma 4.9. *The only minimal configurations are the cone tips and Ω_3.*

Proof. We see at once that Ω_{2b} is the only minimal configuration that is linear. Let Ω be a minimal configuration other than Ω_{2b}. Since Ω is pseudoconvex, any side of length 0 must be a hexagonal face that can be deleted to get a smaller pseudoconvex patch containing all of the pentagonal faces. Hence all of the side lengths are positive and all boundary segments have lengths 2 and 3. It will be convenient to call the faces with boundary segments of length 3 *corner faces*. If all of the faces on a side, including both corners, are hexagons, they may all be deleted resulting in a smaller pseudoconvex patch containing all of the pentagonal faces. Hence, each side of Ω contains a pentagonal face. There are two basic cases to consider: there is just one pentagon on the boundary or there are at least two pentagons on the boundary.

Suppose first that Ω has more than one pentagonal face on its sides and list them in counterclockwise order $f_1, \ldots, f_m$. Since no side is devoid of pentagons, any two consecutive pentagonal faces are joined by an (n)-hexpath or an (n,m)-hexpath on the boundary. Hence f_i is joined to f_{i+1} by a (1)-hexpath or a $(1,1)$-hexpath, for $i = 1, \ldots, m-1$, and f_m is joined to f_1 by a (1)-hexpath or a $(1,1)$-hexpath. We note that, if f_i is joined to f_{i+1} by a $(1,1)$-hexpath, the intervening hexagonal face must be a corner. We also note that the number of corners is equal to the number of sides.

By formula (1) from Lemma 3.2, the number of pentagons on the sides (the number of hexpaths) plus the number of sides (the number of $(1,1)$-hexpaths) is six or less. We conclude that the number of (1)-hexpaths plus twice the number of $(1,1)$-hexpaths on the boundary is six or less while the total number of hexpaths is less than six. Hence the possibilities for the sequences of Coxeter coordinates for the hexpaths joining consecutive pentagons around the boundary are:

1. $\{(1), (1)\}$;
2. $\{(1), (1,1)\}$;
3. $\{(1,1), (1,1)\}$;
4. $\{(1), (1), (1)\}$;
5. $\{(1), (1), (1,1)\}$;
6. $\{(1), (1,1), (1,1)\}$;
7. $\{(1,1), (1,1), (1,1)\}$;
8. $\{(1), (1), (1), (1)\}$;
9. $\{(1),(1), (1), (1,1)\}$;
10. $\{(1), (1), (1,1), (1,1)\}$;
11. $\{(1), (1,1), (1), (1,1)\}$;
12. $\{(1), (1), (1), (1), (1)\}$;
13. $\{(1), (1),(1), (1), (1,1)\}$.

The number of (1) hexpaths plus 2 times the number of $(1,1)$ hexpaths is the number of faces on the boundary. If this number is less than 5 (cases 1 to 5 and 8) then every face is on the boundary. Case (1) with only 2 bounding faces is Ω_{2b}. Case (2) can only be two pentagons and a hexagon sharing a common vertex; this is not a minimal configuration but contains Ω_{2b}. Case (3) with 2 pentagonal faces alternating with two hexagonal corners is Ω_{2a}; Case (4) can only be Ω_{3a} and Case (5) can only be Ω_{3b}. Case (6) has five faces in its boundary hence the interior is a single pentagon and the patch is Ω_{4b}. Case (7) has six faces in its boundary; hence the interior is a single hexagon bounded by pentagons on alternate edges: Ω_3. The boundary in Case (8) consists of 4 pentagons giving Ω_{4a}.

In case Case (9), we have 4 pentagons and 1 hexagon on the boundary; hence, they bound a pentagon giving Ω_5. Cases (10) and (11) have boundaries consisting of 4 pentagons and 2 hexagons all incident with a common interior hexagon. In these cases there is always a pair of pentagons joined by a (2) hexpath through the central hexagon; hence, these are not minimal configurations. Case (12) is excluded since it has 5 pentagons around a central pentagon, giving 6 pentagons. Finally Case (13) has 5 pentagons and one hexagon around a hexagon and, like cases (10) and (11), admits a pair of pentagons joined by a (2)-hexpath through the central hexagon and thus is not minimal.

Now we must confront the case where there is only one pentagon f on the boundary. Since f must be incident with every other face, Ω has 1 or 2 sides; if it has 2 sides f must meet both sides and hence must be a corner. In either case if f is a corner, its removal leaves a pseudoconvex patch Π with 3 or 4 pentagons but all hexagons on its boundary. If Π admits two pentagons joined by a (n)-hexpath with $n > 1$ or an (n, m)-hexpath with $mn > 1$, then Ω is not minimal. Hence, Π contains a pseudoconvex patch Π' consisting of one of Ω_{3a}, Ω_{3b}, Ω_3, Ω_{4a} or Ω_{4b} surrounded by a ring of hexagons. Using Lemma 4.2, it is straight forward but somewhat tedious to verify that, in each case, f is joined to some pentagon in Π' by a (n, m)-hexpath where $mn > 1$.

All that remains to consider is the case where Ω has one side and only one pentagonal, non-corner face f on that side. In this case the interior of Ω contains a copy Ω_{4a} or Ω_{4b}. As above it is straight forward but somewhat tedious to eliminate the possibility that f is not adjacent to a face of this core. Assume then that f shares an edge with a face of Ω_{4a} or Ω_{4b}. Again, one easily checks that none of these possibilities is minimal. $\square$

One last task before we can state and prove the main result of our paper is to introduce two infinite families of exceptional similarity classes, $\mathcal{S}_{[1,1,n,n]}$, $n > 1$, (Figure 6) and $\mathcal{S}_{[0,2,n,n+1]}$, $n > 2$, (Figure 7), and one additional exceptional similarity class $\mathcal{S}_{[2,2,2]}$ (Figure 8). Each of these similarity classes contain exactly two pseudoconvex patches neither of which can be transformed into the other by a sequence of $\alpha, \beta, \alpha^{-1}$ and β^{-1} steps. Specifically the arrangements of the pentagons precludes applying α or β and there are not sufficient bounding hexagons to apply α^{-1} or β^{-1}. The patches in Figure 8 have asymmetric boundaries and the symmetries of the patches in Figure 6 do not match the Stone-Wales transformation at the tip.

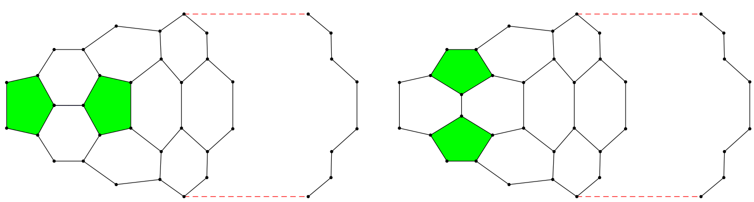


Figure 6: The only two patches in $\mathcal{S}_{[1,1,n,n]}$, $n > 1$.

Theorem 4.10. *Let $\mathcal{S}$ be a nonempty similarity class of pseudoconvex patches different from $\mathcal{S}_{[2,2,2]}$, $S_{[1,1,n,n]}$, and $\mathcal{S}_{[0,2,n,n+1]}$, and let Π and Π' be two pseudoconvex patches in $\mathcal{S}$. Then there is a sequences of α, β, α^{-1} and β^{-1} steps that transform Π into Π'.*

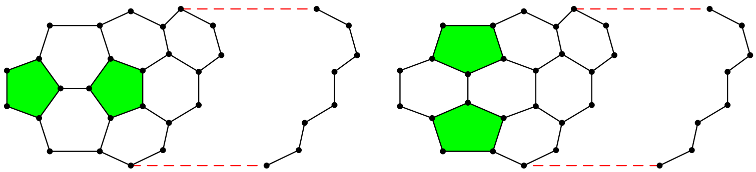


Figure 7: The only two patches in $\mathcal{S}_{[0,2,n,n+1]}$, $n > 2$.

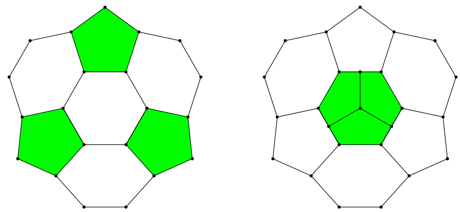


Figure 8: The only two patches in $\mathcal{S}_{[2,2,2]}$. The patch on the left is Ω_3.

Proof. Let Π and Π' be two pseudoconvex patches in $\mathcal{S}$. Then by Lemma 4.9, there is a sequence of α and β steps taking Π to a cone tip patch or a patch containing Ω_3 in $\mathcal{S}$ and a sequence of α and β steps taking Π' to a cone tip patch or a patch containing Ω_3 in $\mathcal{S}$. If both sequences of steps end in the same patch, concatenating one sequence with the reverse of the other is the sequence we seek. By Lemma 4.8 the only cases in which the terminal patches could be different are: $\mathcal{S}$ equals $\mathcal{S}_{[\ell_1,\ell_2,\ell_3]}$ where ℓ_1, ℓ_2 and ℓ_3 have the same parity and $S_{[\ell_1,\ell_2,\ell_3,\ell_4]}$ where $(\ell_1 + \ell_3) \equiv (\ell_2 + \ell_4)$ mod 3. In these cases, there are two distinct possibilities for the terminal patch. All that remains to show that, for the similarity classes in these cases but different from the excluded case, there is a short sequence of α, β, α^{-1} and β^{-1} steps that takes one of the terminal patches into the other. These steps are illustrated in Figures 9 and 10. In both cases, the necessity of avoiding the excluded patches forces additional hexagonal faces providing sufficient room to transform one patch into the other. $\square$

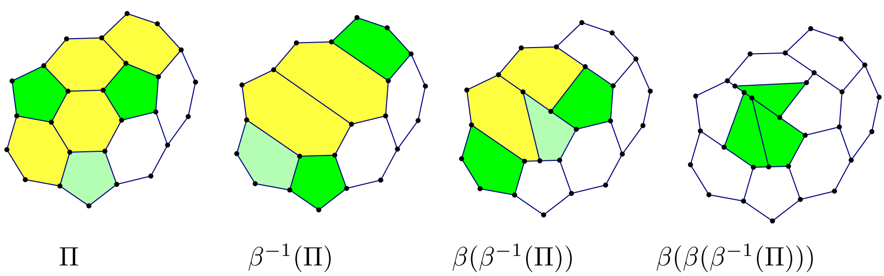
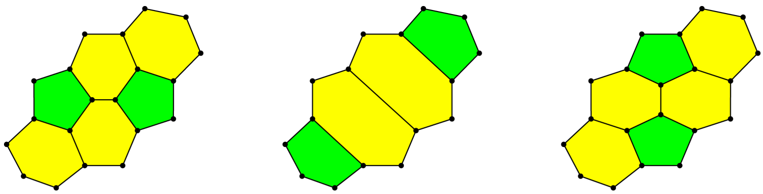


Figure 9: A patch Π with exactly three pentagons containing the exceptional case and at least two more faces.



Π $\alpha^{-1}(\Pi)$ $\alpha(\alpha^{-1}(\Pi))$

Figure 10: A patch Π with two pentagons in configuration Ω_{2b} and the transformation to the rotated configuration Ω_{2b}. Only the shaded hexagons are necessary for the transformations; the others are "spectator" faces.

Using the terminology from [3], we have the following corollaries for cones.

Corollary 4.11. *If Θ and Φ are two equivalent cones then there is a sequences of α, β, α^{-1} and β^{-1} steps that transform Θ into Φ.*

Corollary 4.12. *With the exception of the patches with side parameters $[1,1,1,1]$ or $[2,2,2]$, any symmetric or near-symmetric patch in a cone may be transformed into any other symmetric or near-symmetric patch with the same boundary by a sequence of α's, β's, α^{-1}'s, and β^{-1}'s.*

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