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Hyperbolic analogues of fullerenes on orientable surfaces

M. Dutour Sikirić [a], M. Knor [b,*], P. Potočnik [c], J. Širáň [d,b], R. Škrekovski [c]

[a] Department of Marine and Environmental Research, Rudjer Bošković Institute, 10000 Zagreb, Croatia
[b] Slovak University of Technology, Faculty of Civil Engineering, Department of Mathematics, Radlinského 11, 813 68, Bratislava, Slovakia
[c] Faculty of Mathematics and Physics, University of Ljubljana, and Institute of Mathematics, Physics and Mechanics, Jadranska 19, 1000 Ljubljana, Slovenia
[d] Open University, Milton Keynes, UK

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ABSTRACT

Mathematical models of fullerenes are cubic spherical maps of type $(5, 6)$, that is, with pentagonal and hexagonal faces only. Any such map necessarily contains exactly 12 pentagons, and it is known that for any integer $\alpha \geq 0$ except $\alpha = 1$ there exists a fullerene map with precisely α hexagons.

In this paper we consider hyperbolic analogues of fullerenes, modelled by cubic maps of face-type $(6, k)$ for some $k \geq 7$ on an orientable surface of genus at least 2. The number of k-gons in this case depends on the genus but the number of hexagons is again independent of the surface. We focus on the values of k that are 'universal' in the sense that there exist cubic maps of face-type $(6, k)$ for *all* genera $g \geq 2$. By Euler's formula, if k is universal, then $k \in \{7, 8, 9, 10, 12, 18\}$.

We show that for any $k \in \{7, 8, 9, 12, 18\}$ and any $g \geq 2$ there exists a cubic map of face-type $(6, k)$ with any prescribed number of hexagons. For $k = 7$ and 8 we also prove the existence of *polyhedral* cubic maps of face-type $(6, k)$ on surfaces of any prescribed genus $g \geq 2$ and with any number of hexagons α, except for the cases $k = 8$, $g = 2$ and $\alpha \leq 2$, where we show that no such maps exist.

1. Introduction

Fullerenes are carbon-cage molecules comprised of carbon atoms that are arranged on a sphere with pentagonal and hexagonal faces. The icosahedral C_{60}, well-known as buckminsterfullerene, was found by Kroto et al. [15], and later confirmed by experiments by Krätchmer et al. [14] and Taylor et al. [19]. Since the discovery of C_{60}, fullerenes have been of interest to scientists all over the world; see e.g. [3,4,7,16,17].

From a graph theoretic point of view, fullerenes can be identified with spherical embeddings of cubic 3-connected graphs, with faces bounded by cycles of length 5 and 6. Euler's formula implies that each fullerene contains exactly twelve pentagonal faces, but provides no restriction on the number of hexagonal faces. It is well-known that (mathematical models of) fullerenes with precisely α hexagonal faces exist for all non-negative values of α with the sole exception of $\alpha = 1$ [6, Section 13.4].

We will study mathematical models of fullerene analogues on orientable surfaces of higher genera. By a *hyperbolic k-gonal fullerene* we understand any trivalent map on some orientable surface of genus at least 2, with all faces bounded by cycles of length 6 or k for some fixed $k \geq 7$, that is of *face-type* $(6, k)$. The *genus* of the k-gonal fullerene is simply the genus of its supporting surface. The adjective *hyperbolic*, which will sometimes be omitted, reflects the fact that the supporting surfaces for such maps are hyperbolic in the sense that they arise as quotients by respect to suitable cocompact subgroups of the isometry group of the hyperbolic plane.

* Corresponding author.
E-mail addresses: mdsikir@irb.hr (M.D. Sikirić), knor@math.sk (M. Knor), primoz.potocnik@fmf.uni-lj.si (P. Potočnik), jozef.siran@stuba.sk (J. Širáň), skrekovski@gmail.com (R. Škrekovski).

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Analogues of fullerenes embedded on hyperbolic surfaces were considered earlier by a number of authors; see e.g. [5,20] or [21] and references therein. In most cases, the objects under investigation are restricted classes of graphite networks modelled by trivalent maps of face-type (6, 7) and (6, 8), including their geometry, stability, electronic structures, and possible applications. Constructions of higher genus fullerenes with additional symmetry properties were suggested in [12].

Suppose that a hyperbolic k-gonal fullerene of genus $g \geq 2$ has v vertices, e edges, and f faces, α of which are hexagonal and β of which are bounded by k-gons. Then, $3v = 2e = 6\alpha + k\beta$ and $f = \alpha + \beta$, which, when substituted into Euler's formula $v - e + f = 2 - 2g$, yields

$$\beta = 12(g-1)/(k-6) \quad \text{and} \quad v = 2\alpha + 4k(g-1)/(k-6). \tag{1}$$

In particular, we have no restriction on α while β is determined by k and g.

These necessary conditions for existence of a k-gonal fullerene of genus $g \geq 2$ are also sufficient for large enough values of α. More precisely, for any $k \geq 7$ and for any $g \geq 2$ such that $k - 6$ divides both $12(g-1)$ and $4k(g-1)$ there exists an $\alpha(k, g)$ such that for all integers $\alpha \geq \alpha(k, g)$ there exists a map of type $(6, k)$ on an orientable surface of genus g containing exactly α hexagonal faces and $\beta = 12(g-1)/(k-6)$ faces bounded by cycles of length k; see [10] and also [11] for more general statements. A drawback of this result is that its proof does not offer any insight into a possible determination of the *smallest* $\alpha(k, g)$ that guarantees the existence of a corresponding map. In fact, it transpires from [10] that it is the small values of α that are the hardest to work with. (A similar feature is observed in the situation when the number of t-gons is fixed, $t \neq 5, 7$, and the number of pentagons and heptagons varies; see [2].) It appears hopeless to attempt an exact determination of $\alpha(k, g)$ for all pairs $k \geq 7$ and $g \geq 2$ that satisfy the above conditions, that is, when $k - 6$ is a divisor of $12(g-1)$ and $4k(g-1)$. We therefore concentrate on the values of $k \geq 7$ that are *universal* in the sense that there is a trivalent map of type $(6, k)$ for *all* genera $g \geq 2$. In such a case, $k - 6$ must be a divisor of $12(g-1)$ for all $g \geq 2$ and hence also for $g = 2$. The only universal values of k thus are 7, 8, 9, 10, 12, and 18.

The aim of this paper is a detailed investigation of hyperbolic k-gonal fullerenes for the universal values of k. Particular attention will be given to *polyhedral* k-gonal fullerenes, that is, those satisfying the conditions that every edge lies on the boundary of two distinct faces, and the boundary cycles of any two distinct faces share at most one edge.

Our first main result, proved in Section 2, states that for any universal values of k and any $g \geq 2$ there exists a cubic map of face-type $(6, k)$ with any prescribed non-negative number of hexagons, with possible exceptions for $k = 10$ and any even value of g. This settles the problem of determining the value of $\alpha(k, g)$ for all $k \in \{7, 8, 9, 12, 18\}$ and all $g \geq 2$ to $\alpha(k, g) = 0$. The corresponding maps, however, are not polyhedral. What is more, it is not even possible for all such maps to be polyhedral. For example, no cubic octagonal map (with no hexagons at all) of genus 2 can be polyhedral since, by Euler's formula, it would have to consist of six octagons and hence some of the faces would have to share more than one edge in common.

We extend our study to polyhedral maps for the values of $k = 7$ and 8, which are likely to be the most important values for further development of the theory. We first discuss polyhexes in Section 3 which are needed for subsequent constructions. Then, in Section 4 we show that a polyhedral heptagonal fullerene of genus g with exactly α hexagonal faces exists for any $g \geq 2$ and any $\alpha \geq 0$. In the final part, Section 5, we prove that an octagonal fullerene of genus g with exactly α hexagonal faces exists whenever $g = 2$ and $\alpha \geq 3$, or $g \geq 3$ and $\alpha \geq 0$.

We would like to point out that whilst surface models of analogues of fullerenes appear to be most natural to study, one should still bear in mind that a graphite network may admit a number of topologically distinct embeddings in the Euclidean 3-space; cf. e.g. [13].

2. Non-polyhedral maps

Throughout, a *map* is any cellular embedding of a graph on an orientable surface. Our graphs may contain loops and multiple edges. Our surfaces will, for the most part, be compact and connected, with no boundary components. Nevertheless, in a few instances we will allow surfaces to be disconnected or to contain non-empty boundary components; in the latter case we will refer to a *surface with holes*. When considering a map on a surface with holes, we will always assume that each boundary component is identified with a polygon of the embedded graph.

We begin with proving the following general result.

Theorem 2.1. *Let g and α be arbitrary integers such that $g \geq 2$ and $\alpha \geq 0$. If $k \in \{7, 8, 9, 12, 18\}$ or if $k = 10$ and g is odd, then there exists a cubic map of face-type $(6, k)$ with genus g and α hexagonal faces.*

Remark 2.2. Despite all the known results summed up in the Introduction, the existence of cubic maps of face-type (6, 10) with an arbitrary number of hexagons remains open in the case of even genus.

In the proof of Theorem 2.1, we use the following general construction.

Construction A. Let M be a map on an orientable (not necessarily connected) surface with h holes, $h \geq 2$. Assume that all boundary components are identified with cycles of even length of the embedded graph, and that the degrees of the vertices in each boundary cycle form an alternating sequence $2, 3, 2, 3, \ldots$. Select a pair of holes whose boundary cycles have the same length and identify their boundaries in such a way that the vertices of degree 3 in one cycle are identified with the

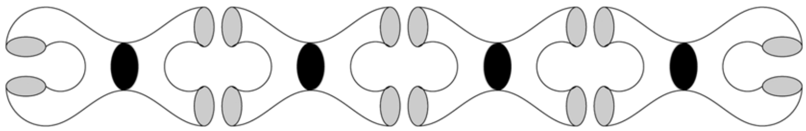

Fig. 1. Surface of genus 5 decomposed into eight "pants" (or four "double-pants").

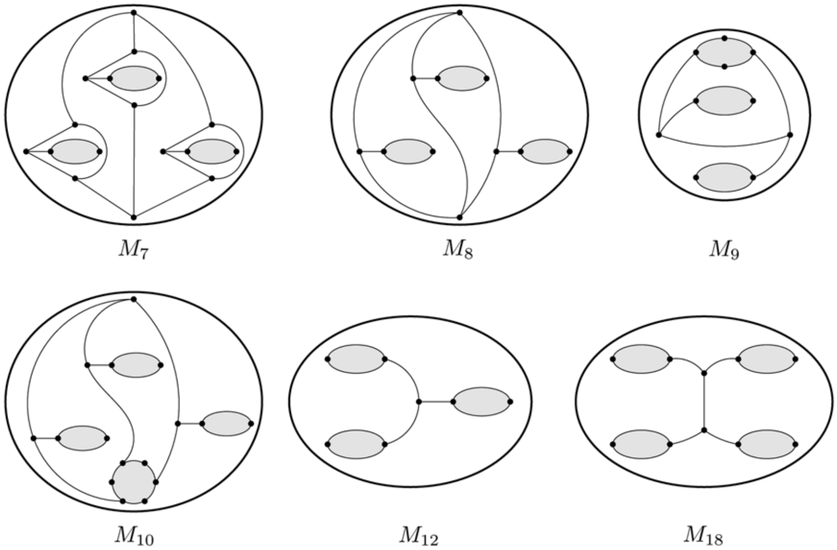

Fig. 2. Building blocks for cubic maps of type $(6, k)$, $k \in \{7, 8, 9, 10, 12, 18\}$.

vertices of degree 2 in the other cycle, retaining orientability of the resulting surface. The new map obtained this way will be denoted as M^*.

Let us include a few remarks about the resulting map M^*. Suppose that the cycles identified in the course of the construction are $A = (a_0, a_1, \ldots, a_{2k-1})$ and $B = (b_0, b_1, \ldots, b_{2k-1})$, where a_0 and b_0 have degree 2, with A and B listed in opposite orientations with respect to some fixed orientation of the underlying surface. To guarantee orientability we may assume that, for some fixed $t \in \{0, \ldots, k-1\}$ and every $i \in \{0, \ldots, 2k-1\}$, the oriented edge a_ia_{i+1} is identified with the oriented edge $b_{2t-1+i}b_{2t+i}$, subscripts being read mod $2k$. Here, different choices of the parameter t, sometimes referred to as the *twist*, may result in non-isomorphic maps.

Note that the resulting map M^* has precisely the same faces as the original map M, but the number of holes in the new underlying surface has been reduced by 2. Also, all the vertices obtained by identification have degree 3, and the degrees of the remaining vertices in M^* are the same as in M. Now assume that the original map M has face-type (k_1, k_2) and that all the vertices not lying on the boundary components of the underlying surface have degree 3. Then the map obtained by applying Construction A repeatedly until no holes remain is cubic and has face-type (k_1, k_2). Of course, Construction A can be used repeatedly until no holes remain only if the holes in the initial map can be matched into pairs with boundary cycles of equal length.

Proof of Theorem 2.1. We will make use of the well-known "pants decomposition" which decomposes an arbitrary orientable surface of genus $g \geq 2$ into $2(g-1)$ *pants*, each homeomorphic to a sphere with three holes as in Fig. 1. The surface can be re-assembled by gluing. In fact, one can do the gluing of pants in two steps. We begin with arranging the pants into pairs; in every pair we identify a single hole in each of the two pants and glue the two pants along the selected holes. This turns the original set of $2(g-1)$ pants into $g-1$ components each homeomorphic to a sphere with four holes, called *double-pants*. These can then be pasted together as shown in Fig. 1 to obtain a surface of genus g.

Let us consider the maps M_k, $k \in \{7, 8, 9, 12, 18\}$, presented in Fig. 2. Each M_k contains only holes and k-gonal faces one of which is the outer face in the figure. Note that holes are bounded by cycles of length 2. For $k \in \{7, 8, 9, 12\}$, M_k is a map on a sphere with three holes (an embedding on pants) while M_{18} is on a sphere with four holes (an embedding on double-pants), and all the holes satisfy the assumptions of Construction A. It follows that taking $2(g-1)$ copies of M_k for $k \in \{7, 8, 9, 12\}$, or $g-1$ copies of M_{18}, and identifying the holes according to Construction A and Fig. 1 yields a cubic k-gonal map on an orientable surface of genus g with no holes. This is straightforward for $k \neq 9$; if $k = 9$ we first glue pairs of pants along the holes bounded by 4-cycles to obtain the "double-pants" and then proceed as indicated.

Now assume that $k = 10$ and that g is odd. Let us take the map M_{10} embedded on the double-pants as depicted in Fig. 2. Take $g-1$ copies of this map and use Construction A repeatedly to obtain a map of genus g in which all faces are bounded by

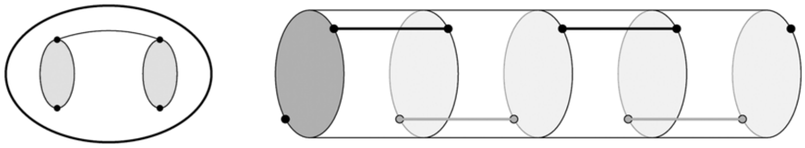

Fig. 3. Left: the map S_1; right: four copies of S_1 glued to form a cylinder.

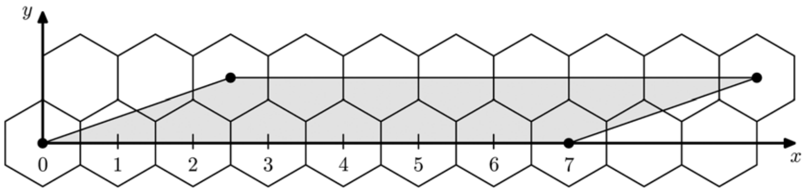

Fig. 4. Hexagonal tessellation and fundamental region for $T_{7,2}$.

10-cycles. Note that here we need $g-1$ to be even, for otherwise the hexagonal holes would not match up and the resulting surface would still have at least one hole.

It remains to extend the maps constructed thus far from α hexagons. To achieve this, take one hexagon and glue together a pair of its opposite edges to obtain a cylinder S_1 as on the left-hand side of Fig. 3. Take α copies of S_1 and paste them together according to Construction A to obtain a cylinder S_α with α hexagons as on the right-hand side of Fig. 3. We can now attach S_α according to Construction A at any one of the holes bounded by a cycle of length 2 at any stage of our gluing process, not affecting the numbers of pants or double-pants. The result is therefore a cubic map of genus g and face-type $(6, k)$ with exactly α hexagons, where $k \in \{7, 8, 9, 12, 18\}$ and $g \geq 2$ is arbitrary, or $k = 10$ and $g \geq 3$ is odd. □

Of course, the maps obtained in the proof of Theorem 2.1 are not polyhedral. In the rest of the paper we restrict our attention to polyhedral maps only. For the development of appropriate construction tools we need to make a digression into toroidal hexagonal maps.

3. Some properties of tori polyhexes

In this section we introduce certain hexagonal toroidal tessellations that will be used later in Sections 4 and 5 in our constructions of heptagonal and octagonal fullerenes.

Let us consider a tessellation of a plane by regular hexagons of side length $\frac{\sqrt{3}}{3}$ shown in Fig. 4. Take a pair of integers $a \geq 1$ and $b \geq 0$ and consider the parallelogram with vertices $(0, 0)$, $(a, 0)$, $(\frac{1}{2}+b, \frac{\sqrt{3}}{2})$, and $(\frac{1}{2}+b+a, \frac{\sqrt{3}}{2})$, as in Fig. 4. Identifying pairs of parallel sides in a standard way one obtains a cubic map $T_{a,b}$ on the torus with precisely a hexagonal faces. Note that $T_{a,b}$ corresponds to what is usually called a *tori polyhex* $H(a, 1, b)$; see e.g. [13,18,22].

For any i such that $0 \leq i < a$ let f_i be the face of $T_{a,b}$ centered at the point $(i, 0)$. Since the points $(x, 0)$ and $(b+\frac{1}{2}+x, \frac{\sqrt{3}}{2})$ have been identified, the center of f_i may also be identified with $(b+\frac{1}{2}+i, \frac{\sqrt{3}}{2})$.

In our constructions of polyhedral k-gonal fullerenes for $k \in \{7, 8\}$ we begin with the maps $T_{a,b}$. It is therefore useful to be able to determine which of these maps are polyhedral. Note that the underlying graph of $T_{a,b}$ contains no loops since it is bipartite. Further, it contains no parallel edges provided that $a > 1$ and $b \notin \{0, a-1\}$.

Proposition 3.1. *The map $T_{a,b}$ with $a > 2$ and $0 \leq b \leq a-1$ is polyhedral if and only if $b \notin \{a-2, a-1, 0, 1\}$ and $2b \notin \{a-2, a-1, a\}$.*

Proof. Observe that the face f_0 is adjacent to $f_1, f_{a-b}, f_{a-b-1}, f_{a-1}, f_b$ and f_{b+1} where subscripts are read mod a. Since $T_{a,b}$ is a face-transitive map, it suffices to consider only adjacencies and self-adjacency of the face f_0. Clearly, f_0 is not adjacent to itself if and only if none of the neighboring faces is equal to f_0, which occurs if and only if $1 \neq 0$, $a-b \neq 0$, $a-b-1 \neq 0$, $a-1 \neq 0$, $b \neq 0$ and $b+1 \neq 0$, all mod a. This is equivalent to $a > 1$, $b \neq 0$, and $b \neq a-1$.

Next, observe that f_0 has more than one edge in common with some other face f_c if and only if at least two entries in the sequence $L = (1, a-b, a-b-1, a-1, b, b+1) \bmod a$ are identical and equal to c. Checking all pairs of entries in L we see that two members in L coincide if and only if one of the following holds: $a = 1$, $a = 2$, $b = a-2$, $b = a-1$, $b = 0$, $b = 1$, $2b = a-2$, $2b = a-1$, $2b = 0$. Combining this with the facts in the previous paragraph we obtain the result. □

The previous statement has the following straightforward consequence.

Corollary 3.2. *The map $T_{a,2}$ is polyhedral if and only if $a \geq 7$. The map $T_{a,3}$ is polyhedral if and only if $a \geq 9$.*

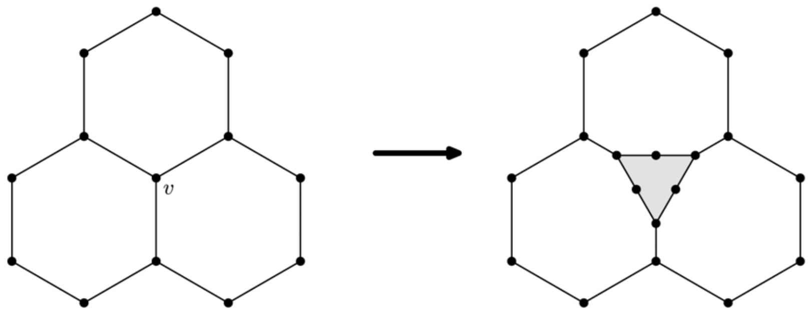

Fig. 5. Creating a hole bounded by a 6-cycle at the position of vertex v.

4. Cubic polyhedral maps of face-type (6, 7)

In this section we construct cubic polyhedral maps of face-type $(6,7)$ using the following construction that takes k toroidal polyhexes as input.

Construction B. Suppose that we have k maps $T_{a_1,b_1},\ldots,T_{a_k,b_k}$. In each such map, select a set $\mathcal{F}$ of $2h$ faces so that each face of the map is adjacent to at most one face in $\mathcal{F}$. Cut out the faces in $\mathcal{F}$ from the (generally disconnected) surface $T = T_{a_1,b_1} \cup \cdots \cup T_{a_k,b_k}$. This way, we obtain $2h$ holes, which are bounded by 6-cycles of the underlying cubic graph. Subdivide each edge in these 6-cycles to obtain 12-cycles whose vertices have degrees alternately 2 and 3. This results in an orientable map M of face-type $(6,7)$ with $2h$ holes. Finally, apply Construction A to M repeatedly h times to obtain a connected cubic map M^* of face-type $(6,7)$ with no holes.

Note that no matter how the holes of M are matched up, the map M^* will always have genus $h+1$. We may now use the maps $T_{a,2}$ to produce heptagonal fullerenes with any admissible number of hexagons and any genus.

Theorem 4.1. *For arbitrary integers $\alpha \geq 0$ and $g \geq 2$ there exists a heptagonal fullerene of genus g with exactly α hexagonal faces.*

Proof. Let $G_2,\ldots,G_{g-1}$ be disjoint copies of $T_{14,2}$. In each G_i, $2 \leq i \leq g-1$, denote by f_0^i and f_7^i the faces centered at $(0,0)$ and $(7,0)$, respectively. Next, let G_1 and G_g be disjoint copies of $T_{7,2}$ and $T_{7+\alpha,2}$, and let f_0^1 and f_7^g be the faces of G_1 and G_g centered at $(0,0)$ and $(7,0)$, respectively. Now, use Construction B by identifying f_0^i with f_7^{i+1} for each $i \in \{1,\ldots,g-1\}$ to obtain a map M^* of genus g. Note that the holes have been chosen carefully enough so as to assure that the resulting map is polyhedral (see also Corollary 3.2).

It remains to show that M^* has exactly α hexagonal faces. Note that during the construction, the edges of each of the f_0^i's and f_7^i's have been subdivided. Hence the hexagons adjacent to any one of the f_0^i's and f_7^i's are transformed into heptagons. Since every face of $G_1,\ldots,G_{g-1}$ other than the f_0^i's and f_7^i's is adjacent to one of these, the only hexagons in M^* are those coming from $G_g = T_{7+\alpha,2}$. Since G_g has $7+\alpha$ faces, precisely α of them remain hexagons in M^*. □

5. Cubic polyhedral maps of face-type (6, 8)

In this final section we describe a generic construction of octagonal fullerenes. In three cases for small values of α we have used the program CGF ([8], available from [1]) that allows us to enumerate maps, polyhedral or not, of a fixed genus with a fixed combination of face sizes.

Construction C. In a toroidal polyhex $T_{a,b}$ select $2h$ vertices in such a way that every face of $T_{a,b}$ is incident with at most one of the selected vertices. Truncate every one of the selected vertices, creating $2h$ triangles. Cut these $2h$ triangles out of the surface and subdivide every edge in the boundary cycle of the resulting holes (see Fig. 5). This results in an orientable map M of face-type $(6,8)$ with $2h$ holes each bounded by a 6-cycle with vertices of degrees alternately 2 and 3. Now apply Construction A to M repeatedly h times to obtain a cubic map M^* of face-type $(6,8)$ with no holes.

Observe that the number of hexagonal faces in M^* is $a-6h$ and the number of octagonal faces is $6h$. Further, since $T_{a,b}$ is a toroidal map and each identification of boundaries of a pair of holes increases the genus by 1, the genus of M^* is $h+1$.

In the next two theorems we construct cubic polyhedral maps of face-type $(6,8)$ for every genus $g \geq 2$. We start with $g=2$.

Theorem 5.1. *There are no octagonal fullerenes of genus 2 with exactly α hexagonal faces if $\alpha \leq 2$. On the other hand, if $\alpha \geq 3$, then there exists an octagonal fullerene of genus 2 with exactly α hexagonal faces.*

Proof. By (1), a cubic map of face-type $(6,8)$ and of genus 2 must have exactly six octagonal faces. If the map is polyhedral then the eight faces adjacent to every octagon must be distinct. Therefore we have at least nine faces in the map, and so $\alpha \geq 3$, which proves the first part of the statement.

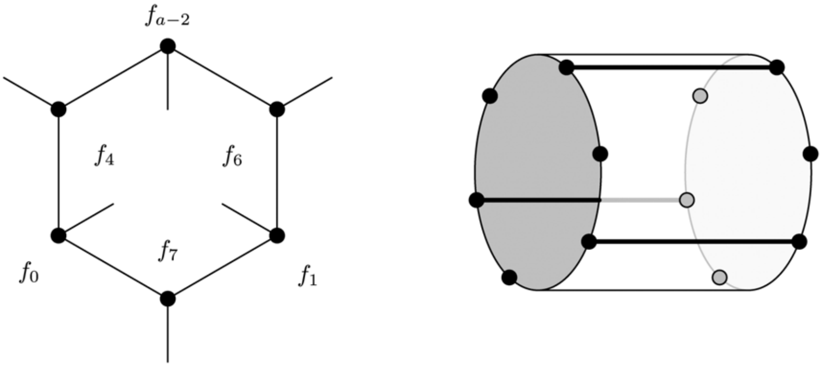

Fig. 6. Left: gluing the holes for $g = 2$ and $\alpha \geq 6$; right: R_3.

Table 1
A rotation scheme for a polyhedral octagonal fullerene of genus 2 with $\alpha = 4$.

1:2 3 4	6:2 13 14	11:5 19 20	16:7 20 23	21:13 17 24
2:1 5 6	7:3 15 16	12:5 9 8	17:8 10 21	22:14 24 15
3:1 7 8	8:3 17 12	13:6 21 20	18:10 23 19	23:16 24 18
4:1 9 10	9:4 12 15	14:6 19 22	19:11 18 14	24:21 22 23
5:2 11 12	10:4 17 18	15:7 22 9	20:11 13 16	

Now suppose that $\alpha \geq 6$ and consider $T_{a,2}$, where $a = 6 + \alpha$. In this polyhex let us select vertices v_1 and v_2 with coordinates $v_1 = (\frac{1}{2}, \frac{\sqrt{3}}{6})$ and $v_2 = (\frac{1}{2} + 6, \frac{\sqrt{3}}{6})$; see Fig. 4. Then v_1 is incident with faces f_0, f_1 and f_{a-2}, while v_2 is incident with f_4, f_6 and f_7, where f_i is the face the centered at $(i, 0)$. Since $a \geq 12$, the faces $f_0, f_1, f_{a-2}, f_4, f_6$ and f_7 are distinct. Hence, Construction C, applied to $T_{a,2}$ with $\{v_1, v_2\}$ as the set of the chosen vertices, gives a cubic map M^* of face-type (6, 8). By Corollary 3.2, $T_{a,2}$ is a polyhedral map, although this may not be the case for the map M^*. However, if none of f_0, f_1 and f_{a-2} are adjacent to any of f_4, f_6 and f_7, then the map M^* is polyhedral. As we show now, this can be achieved by selecting the twist (parameter t) in Construction C appropriately.

Denote by L_i the list of faces adjacent to f_i. Then $L_0 = \{f_1, f_{a-2}, f_{a-3}, f_{a-1}, f_2, f_3\}$, $L_1 = \{f_2, f_{a-1}, f_{a-2}, f_0, f_3, f_4\}$ and $L_{a-2} = \{f_{a-1}, f_{a-4}, f_{a-5}, f_{a-3}, f_0, f_1\}$. Let us consider the possibility of having one of f_4, f_6 or f_7 in these lists. Let $V_2 = \{f_4, f_6, f_7\}$. Since $a \geq 12$, we have $L_0 \cap V_2 = \emptyset$, $L_1 \cap V_2 = \{f_4\}$, $L_{a-2} \cap V_2 = \{f_7\}$ if $a = 12$, and $L_{a-2} \cap V_2 = \emptyset$ if $a > 12$. Thus, it is possible to construct a required 8-gonal fullerene if one can glue the boundaries of the holes corresponding to v_1 and v_2 in such a way that f_1 will not be adjacent to f_4 and f_{a-2} will be not adjacent to f_7 on this boundary.

Let us orient the map $T_{a,2}$ counter-clockwise. Then the faces around v_1 appear in the cyclic order f_0, f_1, f_{a-2}, while those around v_2 appear in the order f_4, f_6, f_7. Therefore the pasting can be organized in such a way that f_1 is "opposite" to f_4 and f_{a-2} is "opposite" to f_7, preserving the orientability of the surface; see Fig. 6. The constructed map M^* is then polyhedral.

Suppose now that $\alpha = 5$ and consider $T_{8,2}$. In this polyhex let us select vertices $v_1 = (8 + \frac{1}{2}, \frac{\sqrt{3}}{6})$ (which may also be thought of as vertex $(8 + \frac{1}{2}, \frac{\sqrt{3}}{6})$) and $v_2 = (\frac{1}{2} + 4, \frac{\sqrt{3}}{6})$. Then v_1 is incident with f_0, f_1 and f_6, while v_2 is incident with f_2, f_4 and f_5. Thus, after creating holes at the locations of v_1 and v_2 we obtain a map M of face-type (6, 8) with two holes. Let R_3 be the cylindrical map with three hexagons shown in Fig. 6. Then R_3 is a map on the sphere with two holes (i.e., on a cylinder), where each hole is bounded by a 6-cycle with vertices of degrees alternately 2 and 3. It follows that one can paste the two holes of this cylinder to the two holes of M according to Construction A. Since the faces incident to v_1 are different from the faces incident to v_2, in this way we obtain a polyhedral map M^* on a double torus with $\alpha = 5$.

In the case $\alpha = 4$ the CGF program [1] found two maps. A rotation scheme for one of them is given in Table 1.

Finally suppose that $\alpha = 3$. Note that the graph $K_9 - K_3$, the complete graph on nine vertices with three edges forming a triangle removed, can be embedded on the orientable surface with genus 3 due to Heffter [9]; see also [23, pp. 199]. Moreover, this embedding is a triangulation with three vertices of degree 6 and six vertices of degree 8. Its dual is a polyhedral cubic map of genus 2 of type (6, 8) with three hexagons. □

Theorem 5.2. *Let g and α be integers such that $g \geq 3$ and $\alpha \geq 0$. Then there exists an octagonal fullerene of genus g with exactly α hexagonal faces.*

Proof. Consider the polyhex $T_{a,3}$ for $a = 6(g-1) + \alpha$ and select in it the vertices u_i and v_i, $1 \leq i \leq g-1$, with coordinates $u_i = (\frac{1}{2} + 6(i-1), \frac{\sqrt{3}}{6})$ and $v_i = (2 + 6(i-1), \frac{\sqrt{3}}{3})$. Since u_i is incident with faces f_{6i-6}, f_{6i-5} and f_{6i-9}, while v_i is incident with faces f_{6i-4}, f_{6i-7} and f_{6i-8}, the two vertices u_i and v_i are incident with $f_{6i-9}, f_{6i-8}, f_{6i-7}, f_{6i-6}, f_{6i-5}$ and f_{6i-4}. As $a \geq 6(g-1)$, each face of $T_{a,3}$ is incident with at most one of the selected vertices. Thus, applying Construction C on $T_{a,3}$ with the selected vertices gives a cubic map of face-type (6, 8). In the remaining part of the proof we show that if we pair up the holes appearing at u_i and v_i carefully, then the resulting map M is polyhedral.

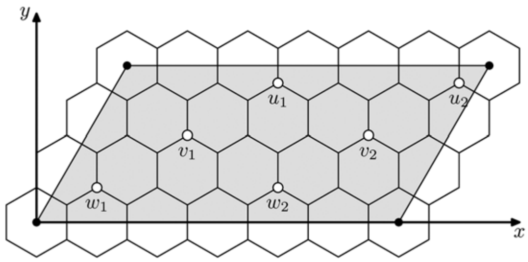

Fig. 7. Initial toroidal map for $g = 4$ and $\alpha = 0$.

Table 2
Rotation schemes for two polyhedral octagonal fullerenes of genus 3 corresponding to $\alpha = 1$ and $\alpha = 2$.

1:2 3 4	8:3 12 17	15:7 25 26	22:11 26 31	29:17 30 18
2:1 5 6	9:4 18 16	16:7 9 27	23:12 32 33	30:20 29 34
3:1 7 8	10:4 19 20	17:8 28 29	24:13 33 18	31:22 27 28
4:1 9 10	11:5 21 22	18:9 29 24	25:14 34 15	32:23 27 34
5:2 11 12	12:5 8 23	19:10 26 13	26:15 22 19	33:23 28 24
6:2 13 14	13:6 24 19	20:10 30 21	27:16 31 32	34:25 30 32
7:3 15 16	14:6 21 25	21:11 20 14	28:17 31 33	
1:2 3 4	9:4 19 20	17:8 30 25	25:12 15 17	33:21 35 36
2:1 5 6	10:4 21 22	18:8 31 32	26:12 21 34	34:26 32 27
3:1 7 8	11:5 23 24	19:9 32 29	27:13 34 20	35:28 33 31
4:1 9 10	12:5 25 26	20:9 27 31	28:14 35 15	36:29 33 30
5:2 11 12	13:6 27 24	21:10 33 26	29:16 19 36	
6:2 13 14	14:6 23 28	22:10 30 23	30:17 36 22	
7:3 15 16	15:7 28 25	23:11 22 14	31:18 35 20	
8:3 17 18	16:7 24 29	24:11 13 16	32:18 34 19	

Observe that as $g \geq 3$ we have $a \geq 12$, so $T_{a,3}$ is a polyhedral map by Corollary 3.2. Our intention is to paste the hole appearing at the position of u_i to the one at the position of u_{i+1} and also to paste the hole at v_i to that at v_{i+1} for some values of i. Since the underlying graph of $T_{a,b}$ is vertex-transitive, it suffices to check the pair u_1 and u_2. The faces incident with u_1 are f_0, f_1 and f_{a-3}, while u_2 is incident with f_6, f_7 and f_3. Now we have to check whether these faces are not already adjacent. As in the previous proof, denote by L_i the list of faces adjacent to f_i. Then $L_0 = \{f_1, f_{a-3}, f_{a-4}, f_{a-1}, f_3, f_4\}$, $L_1 = \{f_2, f_{a-2}, f_{a-3}, f_0, f_4, f_5\}$ and $L_{a-3} = \{f_{a-2}, f_{a-6}, f_{a-7}, f_{a-4}, f_0, f_1\}$. Further, let $V_2 = \{f_6, f_7, f_3\}$.

First, consider the case $g = 3$ and $\alpha = 0$. Then $a = 12$ and we have four selected vertices, u_1, u_2, v_1 and v_2. We would like to glue the hole appearing at the position of u_1 (v_1) to the one appearing at the position of u_2 (v_2); let us denote these match-ups for short by u_1–u_2 and v_1–v_2. In this case we have $L_0 \cap V_2 = \{f_3\}$, $L_1 \cap V_2 = \emptyset$ and $L_{a-3} \cap V_2 = \{f_6\}$. Thus, we would be able to construct a required 8-gonal fullerene if it is possible to paste the boundaries of the holes corresponding to u_1 and u_2 in such a way that f_0 will be not adjacent to f_3 on this boundary and f_{a-3} will be not adjacent to f_6. Since in the counter-clockwise rotation the faces around u_1 appear in the cyclic order f_0, f_1, f_{a-3} while those around u_2 appear in the order f_3, f_6, f_7, the gluing can be organized in such a way that f_0 is "opposite" to f_3 and f_{a-3} is "opposite" to f_6, preserving the orientability of the surface. Hence, M^* is a polyhedral map.

Now consider the case when either $g = 3$ and $\alpha \geq 3$, or g is odd and $g \geq 5$. In this case we have even numbers of u's and also even numbers of v's. Hence, we will glue them in the fashion u_1–u_2, u_3–u_4, ... and also v_1–v_2, v_3–v_4, ... Now $a \geq 15$ and $L_0 \cap V_2 = \{f_3\}$, $L_1 \cap V_2 = \emptyset$ and $L_{a-3} \cap V_2 = \emptyset$. Thus, we can glue the holes with a twist, forcing that the face f_0 will be "opposite" to f_3, which gives the required 8-gonal fullerene.

Finally suppose that g is even (i.e., $g-1$ is odd), $g \geq 4$. Moreover, suppose that if $g = 4$ then $\alpha \geq 1$, and so $a \geq 19$. We glue the holes in the fashion u_2–u_3, u_4–u_5, ..., v_1–v_2, v_4–v_5, v_6–v_7, ..., u_1–v_3. All the pairs with the exception of the last one are correct according to our previous discussion. In the last one, v_3 is incident with faces f_{14}, f_{11} and f_{10}. Let $W_3 = \{f_{14}, f_{11}, f_{10}\}$. Since $a \geq 19$, we have $L_0 \cap W_3 = \emptyset$, $L_1 \cap W_3 = \emptyset$, $L_{a-3} \cap W_3 = \{f_{14}\}$ if $a = 20$ or $a = 21$ and $L_{a-3} \cap W_3 = \emptyset$ if $a = 19$ or $a \geq 22$. Thus, we can glue the holes with a twist forcing the face f_{a-3} to appear "opposite" f_{14} in the cases $a = 20$ and $a = 21$, which gives the required octagonal fullerene.

It remains to consider three small cases. We begin with $g = 4$ and $\alpha = 0$. Here we start with a hexagonal grid with the fundamental region depicted in Fig. 7 and we paste the opposite edges in order to obtain a polyhex $M' = H(6, 3, 0)$. Select in M' the six vertices u_1, u_2, v_1, v_2, w_1 and w_2, depicted as white circles in Fig. 7. Then it is obvious that no face incident with v_1 is adjacent to any face incident with v_2, and a similar statement holds for the pair u_1 and u_2, as well as for w_1 and w_2. Therefore, supplementing Construction C on M' with gluing the pairs of holes according to the scheme u_1–u_2, v_1–v_2 and w_1–w_2 we obtain a polyhedral octagonal fullerene of genus 4 with no hexagonal faces.

For $\alpha = 1$ and 2 the CGF program [1] found a number of maps. In Table 2 we give a rotation scheme for each of the two values of α. □

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