Hyperbolic analogues of fellerenes on orienatable surfaces

M. Knor[*], P. Potočnik[†], J. Širáň[‡], R. Škrekovski[§]

June 3, 2009

Abstract

Mathematical models of fullerenes are cubic planar maps with pentagonal and hexagonal faces. As a consequence of Eulers's formula the number of pentagons in such a map is 12. Conversly, for any integer $\alpha \geq 0$, there exists a fullerene map with precisely α hexagons unless $\alpha = 1$. In this paper, we consider hyperbolic analogues of fullerenes, which are defined as cubic maps of face-type $(6, k)$ on orientable surface of higher genus greater than 1, where by a map of face-type $(6, k)$ we mean a map with only two face lengths: 6 and k for some $k \geq 7$. It follows from Euler's formula that if k is an integer such that for any $g \geq 2$ there exists a cubic map of face-type $(6, k)$ and genus g, then $k \in \{7, 8, 9, 10, 12, 18\}$. In such a map, the number of k-gons is determined in terms of genus, with no condition on the number of hexagons. 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. Furthermore, for $k = 7$ and 8 we prove the existence of polyhedral cubic maps of face-type $(6, k)$ on surfaces of any prescribed genus $g \geq 3$ and with any number of hexagons α, with possible exceptions when $k = 8$ and either $g = 2$ and $\alpha = 4$ or $g = 3$ and $\alpha = 1, 2$.

[*]Slovak University of Technology, Faculty of Civil Engineering, Department of Mathematics, Radlinského 11, 813 68, Bratislava, Slovakia, knor@math.sk.

[†]Faculty of Mathematics and Physics, Univerity of Ljubljana, and Institute of Mathematics, Physics and Mechanics, Jadranska 21, 1111 Ljubljana, Slovenia, primoz.potocnik@fmf.uni-lj.si.

[‡]Slovak University of Technology, Faculty of Civil Engineering, Department of Mathematics, Radlinského 11, 813 68, Bratislava, Slovakia, jozef.siran@stuba.sk.

[§]Faculty of Mathematics and Physics, Univerity of Ljubljana, and Institute of Mathematics, Physics and Mechanics, Jadranska 21, 1111 Ljubljana, Slovenia, skreko@fmf.uni-lj.si.

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 at al. [9], and later confirmed by experiments by Krätchmer at al. [8] and Taylor at al. [16]. Since the discovery of the first fullerene molecule, fullerenes have been objects of interest to scientists all over the world.

From the graph theoretical point of few, fullerenes can be viewed as cubic 3-connected graphs embedded into a sphere with face lengths 5 or 6. Euler's formula implies that each fullerene contains exactly twelve pentagons, but provides no restriction on the number of hexagons. It is well known that mathematical models of fullerenes with precisely α hexagons exist for all values of α with the sole exception of $\alpha = 1$.

The aim of this paper is to investigate mathematical models of fullerene analogues, embedded on orientable surfaces of higher genera, with all faces of length 6 or k for some fixed k. In particular, 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. This problem was addressed before by Jendrol [5] in a more general setting of cubic maps with prescribed number of faces of given length, provided that the number of hexagons is large enough. (The actual smallest number of hexagons needed for the arguments of [5] to work is hard to extract.) However, it is the maps with a small number of hexagons that seem to be harder to construct.

We are particularly interested in the cases $k = 7$ and $k = 8$, where we discuss the existence of cubic maps of face-type $(6, k)$ that are, in addition, polyhedral.

In the rest of this section we introduce some terminology, needed to state our results in a rigorous mathematical manner. An *(orientable) map* is an embedding of a finite graph into an (orientable) surface (compact 2-manifold) such that the graph separates the surface into simply-connected regions, called the *faces* of the map. Unless explicitly stated otherwise, the surface is assumed to be closed (without "holes") and connected. Similarly all the graphs are connected unless stated otherwise.

The *length* of a face is the number of edges on its boundary (counted twice if the edge appears twice on the boundary of the face). Planar maps with only two face-lengths were considered in [3, 10]. If the embedded graph is regular of valence 3, then the map is also called *cubic*. A map in which each face is of length k_1 or k_2, for some fixed integers k_1, k_2, is said to be of *face-type* (k_1, k_2).

A map is called *polyhedral* if

- the underlying graph is simple (that is, it has no loops and multiple edges),
- each vertex appears at most once on the boundary of a face (or equivalently, the closure of a face is a closed disk), and

- the boundaries of two faces are either disjoint or they meet in a single vertex or in a single edge.

By a well-known result of Robertson and Vitray [13], a map is polyhedral if the underlying graph is 3-connected and the embedding has representativity at least three.

Observe that the above conditions simplify if the map in question is cubic. In particular, an embedding of a simple cubic graph is polyhedral provided that every edge lies on the boundary of two distinct faces (i.e. no face is adjacent to itself), and that any two adjacent faces share only one edge in the boundary.

Mathematical models for fullerenes are precisely the cubic polyhedral maps of face-type $(6, 5)$. We shall generalize this notion and call a cubic polyhedral map of face-type $(6, k)$, $k \geq 7$, a *k-gonal fullerene* or a *hyperbolic fullerene* as it is embedded on an orientable surface of hyperbolic type. Constructions of higher genus fullerens (with some additional symmetry properties) have in fact been suggested earlier by Gareth Jones [6].

In this paper we resolve the question of existence of k-gonal fullerenes for $k = 7$ and 8. In particular, in Section 5 we show that a heptagonal fullerene of genus g with exactly α hexagonal faces exists for any $g \geq 2$ and any $\alpha \geq 0$. Further, in Section 6, we show that an octagonal fullerene of genus g with exactly α hexagonal faces exists whenever the following holds:

1. $g = 2$ and $\alpha = 3$ or $\alpha \geq 5$; or

2. $g = 3$ and $\alpha \geq 3$; or

3. $g \geq 4$ and $\alpha \geq 0$.

For $g = 2$ and $\alpha \leq 2$ as well as for $g = 3$ and $\alpha = 0$ octagonal fullerenes do not exist. The question of existence of octagonal fullerens remains open for $g = 2$ and $\alpha = 4$, as well as for $g = 3$ and $\alpha \in \{1, 2\}$.

2 Necessary conditions

A straightforward application of Euler's formula gives the following necessary condition for the existence of a k-gonal fullerene.

Lemma 2.1 *Let M be an n-vertex cubic map of face-type $(6, k)$, $k \neq 6$, on an orientable surface of genus g with α hexagons and β k-gons. Then,*

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

Proof. Let e and f be the number of edges and faces of the map M, respectively. Then, $f = \alpha + \beta$, $e = (6\alpha + k\beta)/2$ and $n = 2e/3$. Plugging these relations into Euler's formula $n - e + f = 2 - 2g$ gives the first relation. Inserting the first relation for β into $n = (6\alpha + k\beta)/3$ yields the second relation. ■

If we admit $k = 6$ we obtain the well-known hexagonal tessellations of the torus; these maps are also known under the name *toroidal polyhexes*, see [14, 18]. We shall therefore only consider k-gonal fullerens of genus at least 2.

Proposition 2.2 *Let k be a number such that for any $g \geq 2$ there exists a cubic map of face-type $(6, k)$ with genus g. Then $k \in \{7, 8, 9, 10, 12, 18\}$.*

Proof. If the assumption is true for some k, then, by Lemma 2.1, we have $k > 6$ and both $12(g-1)/(k-6)$ and $4k(g-1)/(k-6)$ are integers. Since we require that there exists such a map for any $g \geq 2$, even for $g = 2$, we conclude that $k - 6$ divides 12. This is satisfied only for $k \in \{7, 8, 9, 10, 12, 18\}$. ■

As we show in the next section, the necessary condition on k, given by Proposition 2.2, is also sufficient, with a possible exception when $k = 10$ and g is even. What is more, as Theorem 3.1 states, these maps exist for any prescribed number of hexagons.

Of course, it is not possible for all of these maps to be polyhedral (and thus k-gonal fullerenes). For example, a cubic map of face-type $(6, 8)$ of genus 2 and with 0 hexagons cannot be polyhedral since such a map would have 6 faces, all of length 8, implying that some of the faces would share more than one edge in common.

3 Non-polyhedral maps

In this section we prove the following theorem.

Theorem 3.1 *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. The existence of cubic maps of face-type $(6, 10)$ for arbitrary number of hexagons remains open in the case of even genus.

In the proof of Theorem 3.1, 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 the holes are bounded by cycles of even length and that the degrees of the vertices in each boundary cycle are alternatingly $2, 3, 2, 3, \ldots$. Pick two 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 vertices of degree 2 in the other cycle, and so that the resulting surface remains orientable. Then we donote the resulting map by M^*.*

A few remarks about the resulting map M^* are in place. Suppose that the identified cycles 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, and where A is listed in a clockwise and B in the counter-clockwise orientation (with respect to some fixed orientation of the underlying surface). In order to obtain an orientable surface, we will assume that, for some fixed $t \in \{0, \ldots, k-1\}$ and every $i \in \{0, \ldots, 2k-1\}$ the oriented edge $a_i a_{i+1}$ is identified with the oriented edge $b_{2t-1+i} b_{2t+i}$ (the addition in the subscripts being modulo $2k$). 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, however the number of holes in the underlying surface was decreased by 2. Also, the vertices obtained by identification all 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 is of face-type (k_1, k_2) and that all the vertices which do not lie on the boundary of the underlying surface (holes) have degree 3. Then the map obtained by applying Construction A repeatedly until no holes remain is cubic and is of face-type (k_1, k_2). Of course, Construction A can be used repeatedly until no holes remain only if the original holes can be arranged into pairs where the boundary cycles in each pair have equal length.

Proof of theorem 3.1. In the proof we use the well-known "pants decomposition" which decomposes an arbitrary orientable surface of genus g, $g \geq 2$, into $2(g-1)$ "pants", where by "pants" one means the sphere with 3 holes (see Figure 1). In fact, one can do the gluing of pants in two steps. First arrange the pants into pairs and in every pair glue two pants together by one hole in each. This gives from $2(g-1)$ pants exactly $g-1$ "double pants", where by "double pants" we mean a sphere with four holes. These can then be glued together (as shown in Figure 1) to obtain a surface of genus g.

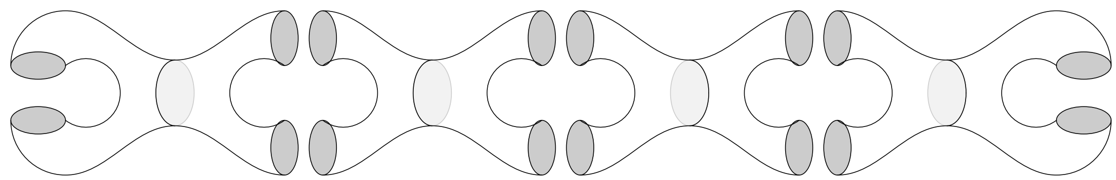

Figure 1: Surface of genus 5 decomposed into 8 "pants" (or 4 "double pants").

Let us consider the maps M_k, $k \in \{7, 8, 9, 12, 18\}$, presented in Figure 2. In all these maps, M_k contains only holes and k-gonal faces, one of the faces being the outerior one. For $k \in \{7, 8, 9, 12\}$ the M_k is a map on a sphere with three holes (i.e., it is embedded on "pants"), while M_{18} is embedded on a sphere with 4 holes (i.e., it is embedded on "double pants"), and all the holes satisfy the assumptions of Construction A. Hence, if one takes $2(g-1)$ of M_k for $k \in \{7, 8, 9, 12\}$, or $g-1$ of M_{18}, and identifies the holes according to Construction A and Figure 1, then the resulting structure is a cubic map on an orientable surface of genus g (without holes), all of whose faces are k-gons. (In the case $k = 9$ we first glue pairs of "pants" along the holes bounded by 4-cycles to obtain the "double pants".)

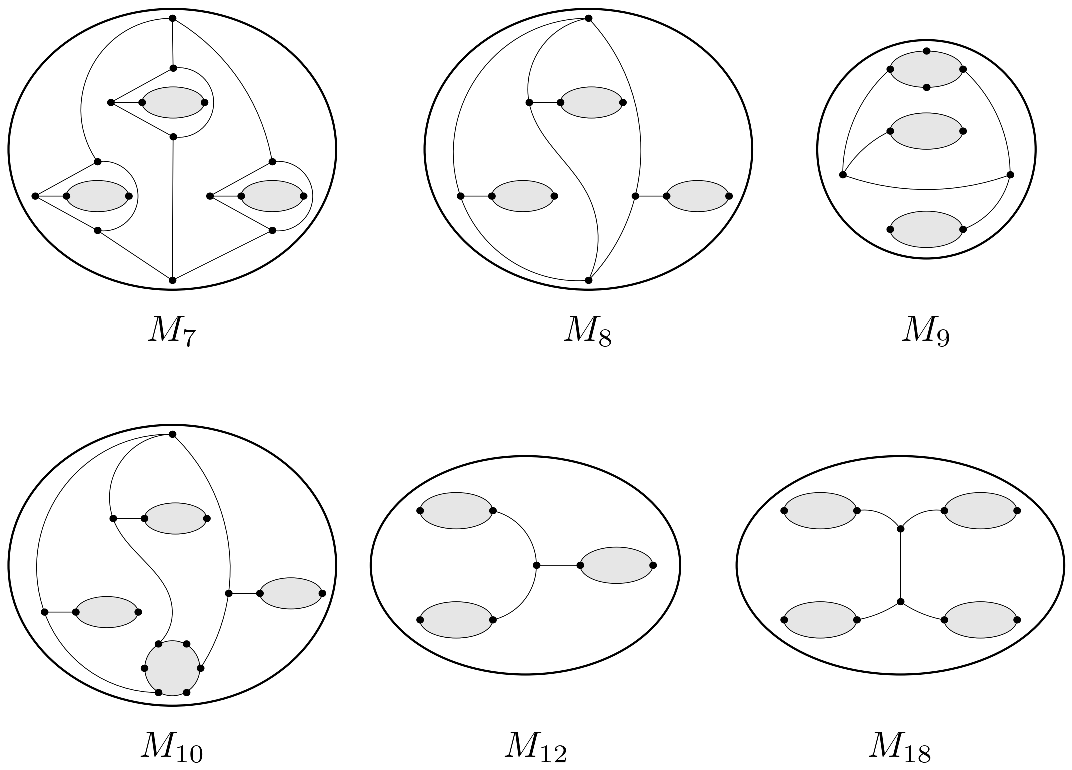

Figure 2: Building blocks for cubic maps of type $(6, k)$, $k \in \{7, 8, 9, 10, 12, 18\}$.

Now assume that $k = 10$ and that g is odd. Let us take the map M_{10} embedded into the "double pants" (that is, the sphere with four holes) depicted in Figure 2. Take $g-1$ copies of this map and use Construction A repeatedly to obtain a map of genus g in which all the faces are bounded by 10-cycles. Note that here we need that $g-1$ is an even integer, for otherwise the "hexagonal" holes would not pair up and the resulting surface would still have at least one hole.

It remains to add to the map α hexagons. Take one hexagon and glue together a pair of its opposite edges to obtain a cylinder. This cylinder is a sphere with two holes, and the map is denoted by S_1 (see the left-hand side of Figure 3). Now take α maps S_1 and glue them together according to Construction A to obtain

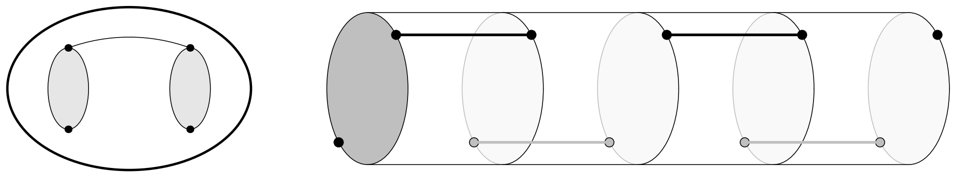

Figure 3: Left: the map S_1; Right: Four copies of S_1 glued to form a cylinder.

a connected map with just two holes (see the right-hand side of Figure 3). The resulting map is a cylinder with α hexagons and we can attach this cylinder according to Construction A at any one of the holes bounded by a cycle of length 2 at any stage of our gluing process. This does not affect the number of "pants" (or "double pants"), so that the resulting map is a cubic map of genus g with α hexagons of face-type $(6, k)$, where $k \in \{7, 8, 9, 12, 18\}$, or $k = 10$ if g is odd. ■

Of course, the maps obtained in the proof of Theorem 3.1 are not polyhedral. In the rest of the paper we restrict our attention to polyhedral maps only.

4 Some properties of tori polyhexes

In this section we present hexagonal tessellations of torus, that are used for constructing of heptagonal and octagonal fullerens.

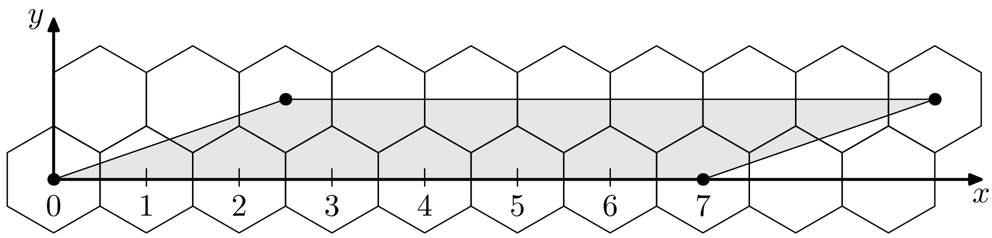

Figure 4: Hexagonal tessellation and fundamental region for $T_{7,2}$.

Let us consider a tessellation of a plane by regular hexagons shown in Figure 4. Note that the hexagons have sides of length $\frac{\sqrt{3}}{3}$. Now let $a \geq 1$ and $b \geq 0$ be two integers. Consider the parallelogram with vertices $(0, 0)$, $(a, 0)$, $(\frac{1}{2} + b, \frac{\sqrt{3}}{2})$ and $(\frac{1}{2} + b + a, \frac{\sqrt{3}}{2})$ (see Figure 4). If the two pairs of parallel sides are identified appropriately, one obtains a cubic map $T_{a,b}$ on the torus, which has precisely a hexagonal faces. Notice that $T_{a,b}$ corresponds to what is usually called a tori polyhex $H(a, 1, b)$.

Denote the face of $T_{a,b}$ whose center is at $(i,0)$ by f_i, $0 \le i < a$. Since we identify the points $(x,0)$ with $(b+\frac{1}{2}+x, \frac{\sqrt{3}}{2})$, the center of f_i is also at $(b+\frac{1}{2}+i, \frac{\sqrt{3}}{2})$.

In our constructions of polyhedral k-gonal fullerenes, $k \in \{7,8\}$, we start from 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 4.1 *The map $T_{a,b}$ with $a > 2$ and $0 \le b \le a-1$ 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} (the addition in subscript being modulo a). Since $T_{a,b}$ is face-transitive, it suffices to consider only the face f_0.

The face f_0 is not adjacent to itself if and only if none of the neighbouring faces is f_0, which happens if and only if $1 \ne 0$, $a-b \ne 0$, $a-b-1 \ne 0$, $a-1 \ne 0$, $b \ne 0$ and $b+1 \ne 0$ (all equalities being modulo a). This is equivalent to $a > 1$, $b \ne 0$ and $b \ne a-1$.

Now observe that f_0 has more than one edge in common with some other face f_c if and only if c is equal to at least two values from the set $L = \{1, a-b, a-b-1, a-1, b, b+1\}$ (equality again being modulo a). By considering all pairs of values in L, we see that two members in L coincide if and only if one of the following holds: $a = 1$, $a = 2$, $b = a-2$, $b = a-1$, $b = 0$, $b = 1$, $2b = a-2$, $2b = a-1$, $2b = 0$. This, combined with the previous paragraph, yields the desired result. ■

The previous statement has the following straightforward corollary.

Corollary 4.2 *The map $T_{a,2}$ is polyhedral if and only if $a \ge 7$. The map $T_{a,3}$ is polyhedral if and only if $a \ge 9$.*

5 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.

Construction B. *Suppose that we have k maps $T_{a_1,b_1}, \ldots, T_{a_k,b_k}$. In these maps, select a set $\mathcal{F}$ of $2h$ faces so that each face is adjacent to at most one face in $\mathcal{F}$. Cut out the faces in $\mathcal{F}$ from the (generally not connected) surface $T = T_{a_1,b_1} \cup \ldots \cup T_{a_k,b_k}$. In this way we obtain $2h$ holes, which are bounded by 6-cycles of the underlying cubic graph. Now subdivide each edge in these 6-cycles to obtain 12-cycles whose vertices have degrees 2 and 3 alternatingly. This results in an orientable map M of face-type $(6,7)$ with $2h$ holes. Now apply Construction A to M consecutively h times to obtain a connected cubic map M^* of face-type $(6,7)$ which does not have holes.*

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

Theorem 5.1 *Let $\alpha \geq 0$ and $g \geq 2$ be arbitrary integers. Then 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, $i \in \{2, \ldots, g-1\}$, denote by f_0^i and f_7^i the faces with centres 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 with centres in $(0,0)$ and $(7,0)$, respectively. Now, use Construction B by identifing each f_0^i and f_7^{i+1} for each $i \in \{1, \ldots, g-1\}$ to obtain a map M^* of genus g. Note that the holes were chosen carefully enough so as to assure that the resulting map is polyhedral (see also Corollary 4.2).

Finally we show that the number of hexagons is α. Note that during the construction, the edges of each of f_0^i's and f_7^i's are subdivided. Hence the hexagons neighbouring one of 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 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 the number of faces in G_g is precisely $7+\alpha$, precisely α of them remain as hexagons in M^*. ■

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

In this final section we consider the octagonal fullerens and provide a generic construction thereof.

Construction C. *Take $T_{a,b}$ and select $2h$ vertices, so that every face of $T_{a,b}$ is incident with at most one of the selected vertices. Now truncate all the selected vertices, which creates $2h$ triangles. Cut out these $2h$ triangles from the surface and subdivide every edge bounding the resulting holes (see Figure 5). In such a way we obtain an orientable map M of face-type $(6,8)$ with $2h$ holes, each of which is bounded by a 6-cycle whose vertices have degrees 2 and 3 alternatingly. Now apply Construction A to M consecutively h times, to obtain a cubic map M^* of face-type $(6,8)$ which does not have 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 $g = 2$.

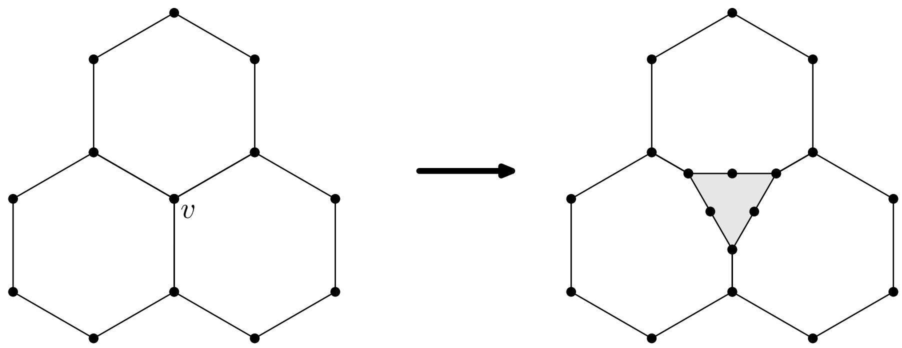

Figure 5: Creating a hole bounded by a 6-cycle at the place of vertex v.

Theorem 6.1 *If $\alpha \leq 2$ then there exist no octagonal fullerenes of genus 2 with exactly α hexagonal faces. On the other hand, if $\alpha = 3$ or $\alpha \geq 5$ then there exists an octagonal fullerene of genus 2 with exactly α hexagonal faces.*

Remark. Note that the existence of an octagonal fullerene of genus 2 with precisely 4 hexagonal faces is still an open question.

PROOF. By Lemma 2.1, a cubic map of face-type $(6, 8)$ and of genus 2 must have exactly 6 octagonal faces. If the map is polyhedral then the eight faces, adjacent to every octagon, must be distinct. Therefore we have at least 9 faces in the map, so that $\alpha \geq 3$, which gives the first part of the statement.

Now suppose that $\alpha \geq 6$ and consider $T_{a,2}$, where $a = 6 + \alpha$. 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 Figure 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 centre of which is in $(i, 0)$). 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 the set of chosen vertices being $\{v_1, v_2\}$, gives a cubic map M^* of face-type $(6, 8)$. By Corollary 4.2, $T_{a,2}$ is a polyhedral map, but this may not be the case for M^*. However, if none of f_0, f_1 and f_{a-2} is 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 selcting 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 $L_{a-2} = \{f_{a-1}, f_{a-4}, f_{a-5}, f_{a-3}, f_0, f_1\}$. Is it possible that we have f_4, f_6 or f_7 in these lists? Let $V_2 = \{f_4, f_6, f_7\}$. As $a \geq 12$, 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, there is a required 8-gonal fullerene if we can glue the boundaries of the holes, appearing on the places of v_1 and v_2, in such a way that f_1 will not be adjacent to f_4 on this boundary and f_{a-2} will be not adjacent to f_7. Let us fix a rotation on $T_{a,2}$; say we choose the anti-clockwise one. Then the faces around v_1 are in cyclic order f_0, f_1, f_{a-2}, while those around v_2 are in order f_4, f_6, f_7. Therefore the gluing 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 Figure 6. The constructed map M^* is then polyhedral.

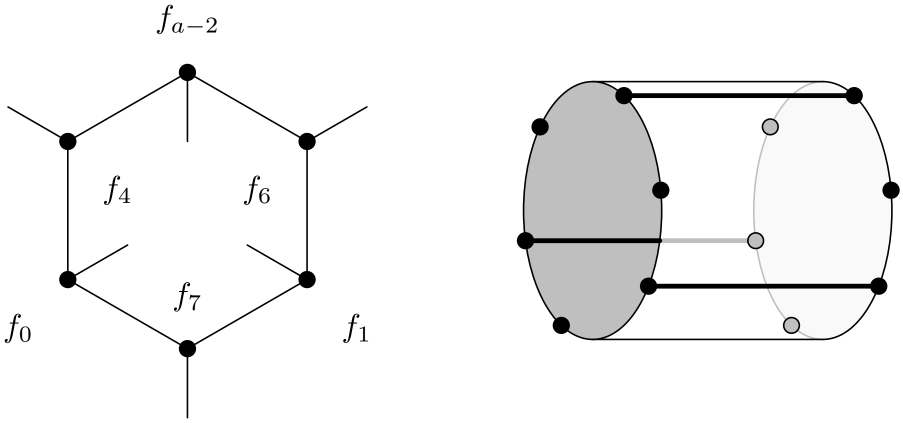

Figure 6: Left: Gluing the holes for $g = 2$ and $\alpha \geq 6$; Right: R_3.

Suppose now that $\alpha = 5$ and consider $T_{8,2}$. 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 of holes at the places 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 3 hexagons shown in Figure 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 2 and 3 alternatingly. Hence, one can glue 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 double torus with $\alpha = 5$.

Finally suppose that $\alpha = 3$. Note that the graph $K_9 - K_3$, the complete graph on 9 vertices with removed three edges that comprise a triangle, can be embedded on the orintable surface with genus 3 due to Heffter [7] (see also [17, pp. 199]). Moreover, this embbeding is a triangulation with 3 vertices of degree 6 and 6 vertices of degree 8. Its dual is a polyhedral cubic map of type $(6, 8)$ with 3 hexagons and genus 2. ∎

Theorem 6.2 *Let g and α be integers, $g \geq 3$ and $\alpha \geq 0$. Then there exists an octagonal fullerene of genus g with exactly α hexagonal faces with possible exceptions of $g = 3$ and $\alpha = 1, 2$.*

Remark. Note that the existence of octagonal fullerenes of genus 3 with precisely 1 or 2 hexagonal faces remains open.

PROOF. Consider $T_{a,3}$, where $a = 6(g-1)+\alpha$. In $T_{a,3}$ select 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 to 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 rest 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.

Observe that as $g \geq 3$ we have $a \geq 12$, so that $T_{a,3}$ is a polyhedral map by Corollary 4.2. Our intention is to glue the hole appearing at the position of u_i with the one at the position of u_{i+1} and also to glue the hole at v_i with 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 if these faces are not adjacent already. Analogously 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 $L_{a-3} = \{f_{a-2}, f_{a-6}, f_{a-7}, f_{a-4}, f_0, f_1\}$. Denote $V_2 = \{f_6, f_7, f_3\}$.

First consider the case $g = 3$ and $\alpha = 0$. Then $a = 12$ and we have 4 selected vertices, u_1, u_2, v_1 and v_2. We like to glue the hole appearing at the position of u_1 (v_1) with the one appearing at the position of u_2 (v_2). We denote this pairing of holes by $u_1 - u_2$ and $v_1 - v_2$. In this case $L_0 \cap V_2 = \{f_3\}$, $L_1 \cap V_2 = \emptyset$ and $L_{a-3} \cap V_2 = \{f_6\}$. Thus, there is a required 8-gonal fullerene if we can glue the boundaries of the holes, appearing on the places of v_1 and v_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 anti-clockwise rotation the faces around v_1 are in cyclic order f_0, f_1, f_{a-3}, while those around v_2 are in 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 number of v's. Hence, we will glue them in fashion $u_1 - u_2$, $u_3 - u_4, \ldots$ and also $v_1 - v_2$, $v_3 - v_4, \ldots$. 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 "oposite" 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 $\alpha \geq 1$. Then $a \geq 19$. We glue the holes in fashion $u_2 - u_3$, $u_4 - u_5$, $\ldots$, $v_1 - v_2$, $v_4 - v_5$, $v_6 - v_7$, $\ldots$, $u_1 - v_3$. All the pairs, but the last one, are all right due 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 that the face f_{a-3} will be "opposite" to f_{14} in the cases $a = 20$ and $a = 21$), which gives the required octagonal fullerene.

It remains to solve the case $g = 4$ and $\alpha = 0$. Here we start with a hexagonal

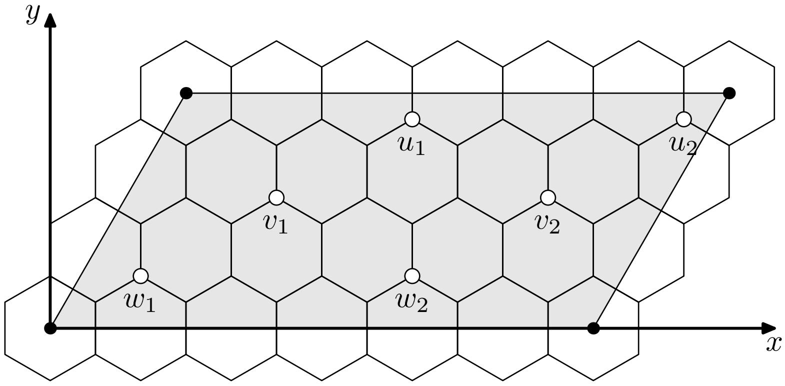

Figure 7: Initial toroidal map for $g = 4$ and $\alpha = 0$.

grid with the fundamental region depicted in Figure 7 and we glue the opposite edges in order to obtain a tori polyhex $M' = H(6, 3, 0)$. Select in M' six vertices u_1, u_2, v_1, v_2, w_1 and w_2 (these vertices are depicted as white circles in Figure 7). Then it is obvious that no face incident with v_1 is adjacent to any face incident with v_2, and analogous statement is true for the pair u_1 and u_2, as well as for w_1 and w_2. Therefore if we provide 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 map of face-type $(6, 8)$, that is, an octagonal fullerene of genus 4 with no hexagonal faces. ■

We remark that the cases $g = 2$ and $\alpha = 4$, as well as $g = 3$ and $\alpha = 1, 2$, remain open for octagonal fullerenes.

Acknowledgement. The research for this paper was supported by the following grants: Slovenian-Slovak Bilateral project, ARRS Research Program P1-0297, ARRS Reasearch project J1-0540, VEGA Research Grant No. 1/0489/08, and APVV Research Grants No. 0040/06 and 0104/07.

References

[1] M. S. Dresselhaus, G. Dresselhaus, P. C. Eklund, Science of Fullerenes and Carbon Nanotubes, Academic Press, New York, 1996.

[2] P. W. Fowler, D. E. Manolopoulos, An Atlas of Fullerenes, Oxford Univ. Press, Oxford, 1995.

[3] B. Grünbaum, J. Zaks, *The excistence of certain planar maps*, Discrete Math. **10** (1974) 93.

[4] I. Gutman, S. J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer-Verlag, Berlin, 1989.

[5] S. Jendrol, *On face vectors of trivalent graphs*, Math. Slovaca **36** (1986) 367.

[6] G. A. Jones, *Schwazites, pants decompositions and triangle groups*, manuscript.

[7] L. Heffter, *Über das Problem der Nachbargebiete*, Math. Ann. **38** (1891) 477.

[8] W. Krätschmer, L. D. Lamb, K. Fostiropoulos, D. R. Huffman, *Solid C_{60}: a new form of carbon*, Nature **347** (1990) 354.

[9] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, *C_{60} Buckminsterfullerene*, Nature **318** (1985) 162.

[10] P. J. Owens, *Regular planar graphs with faces of only two types and shortness parameters*, J. Graph Theory **8** (1984) 253.

[11] J. Malkevitch, *Geometrical and Combinatorial Questions About Fullerenes*, in: P. Hansen, P. Fowler, M. Zheng (Eds.), Discrete Mathematical Chemistry, DIMACS Series in Discrete Mathematics and Theoretical Computer Science **51** (2000) 261.

[12] E. R. Margine, A. N. Kolmogorov, D. Stojaković, J. O. Sofo, V. H. Crespi, *Theory of genus reduction in alkali-induced graphitization of nanoporous carbon*, Physical Review B **76** (2007) 115436.

[13] N. Robertson, R. P. Vitray, *Representativity of surface embeddings*, In: Paths, Flows and VLSI-Layout, B. Korte, L. Lovasz, H.J. Prömel, and A. Schrijver, Eds., Springer-Verlag, Berlin - New York, 1990.

[14] W. C. Shiu, P. C. B. Lam, H. Zhang, *k-resonance in toroidal polyhexes*, J. Math. Chem. **38** (2005) 451.

[15] E. Steinitz, *Polyeder und Raumeinteilungen*, Enzykl. Math. Wiss., Vol. 3 (Geometrie), Part 3AB12 (1922) 1.

[16] R. Taylor, J. P. Hare, A. K. Abdul-Sada, H. W. Kroto, *Isolation, separation and characterisation of the fullerenes C_{60} and C_{70}: the third form of carbon*, J. Chem. Soc. Chem. Commum. (1990) 1423.

[17] J. W. T. Youngs, *Solution of the Map-Coloring Problem - Cases 3, 5, 6, and 9*, J. Combin. Theory **8** (1970) 175.

[18] H. Wang, D. Ye, H. Zhang, H. Wang, *The forcing number of toroidal polyhexes*, J. Math. Chem. **43** (2008) 457.