Discrete Mathematics 339 (2016) 103–108

Contents lists available at ScienceDirect

Discrete Mathematics

journal homepage: www.elsevier.com/locate/disc

Hyperbolic analogues of fullerenes with face-types (6, 9) and (6, 10)

Martin Knor [a,*], Maryam Verdian-Rizi [b]

[a] Slovak University of Technology in Bratislava, Faculty of Civil Engineering, Department of Mathematics, Radlinského 11, 813 68 Bratislava, Slovakia

[b] Department of Mathematical Sciences, KAIST, 291 Daehak-ro Yuseong-gu Daejeon, 305-701, Republic of Korea

ARTICLE INFO

Article history:
Received 1 July 2014
Received in revised form 1 August 2015
Accepted 3 August 2015
Available online 24 August 2015

Keywords:
Fullerene
Polyhedral map
Face-type
Number of hexagons

ABSTRACT

Mathematical models of fullerenes are cubic polyhedral and spherical maps of face-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 polyhedral maps of face-type $(6, k)$, where $k \in \{9, 10\}$, on orientable surface of genus at least two. The number of k-gons in this case depends on the genus but the number of hexagons is again independent of the surface. For every triple $k \in \{9, 10\}$, $g \geq 2$ and $\alpha \geq 0$, we determine if there exists a cubic polyhedral map of face-type $(6, k)$ with exactly α hexagons on an orientable surface of genus g. The only unsolved cases are $k = 10$, $g = 5$ and $\alpha \leq 3$ when we are not able to say if a hyperbolic fullerene with these parameters exists.

1. Introduction

Fullerenes are carbon-cage molecules in which every atom is connected by bonds to exactly three next atoms. The well-known Buckminster fullerene C_{60} was found by Kroto et al. [14], and later confirmed by experiments by Krätschmer et al. [13] and Taylor et al. [18]. Since the discovery of C_{60}, fullerenes have attracted considerable interest of scientists all over the world, see e.g. [2,4,7,15,16].

If one replaces the carbon atoms by vertices, bonds by edges, and fills the smallest cycles (of lengths 5 and 6) by 2-cells, then a fullerene is turned into a spherical embedding of cubic 3-connected graph, with faces bounded by cycles of lengths 5 and 6. Hence, mathematical model of a fullerene is a cubic, spherical and polyhedral map of face-type $(5, 6)$.

In this paper we study mathematical models of fullerene analogues on orientable surfaces of higher genera. By a *hyperbolic k-gonal fullerene* we understand any trivalent polyhedral map on some orientable surface of genus at least two, with all faces bounded by cycles of length 6 or k for some fixed $k \geq 7$, that is of *face-type* $(6, k)$, see [3]. The *genus* of the k-gonal fullerene is simply the genus of its supporting surface. Analogues of fullerenes embedded on hyperbolic surfaces have been considered earlier by a number of authors, see e.g. [5,19] or [20] and references therein. Constructions of higher genus fullerenes with additional symmetries have been suggested in [11].

Denote by α and β the number of hexagonal and k-gonal faces, respectively, in a hyperbolic k-gonal fullerene of genus g. By Euler's formula, we have

$$\beta = 12(g-1)/(k-6), \tag{1}$$

but there is no restriction on α. Hence, we have the following problem:

* Corresponding author.
E-mail addresses: knor@math.sk (M. Knor), mverdian@gmail.com (M. Verdian-Rizi).

http://dx.doi.org/10.1016/j.disc.2015.08.001
0012-365X/

Problem 1. For every $k \geq 7$ and $g \geq 2$, characterize all α's such that there exists a hyperbolic k-gonal fullerene of genus g with exactly α hexagonal faces.

We remark that the necessary conditions for existence of a hyperbolic k-gonal fullerene of genus $g \geq 2$ are also sufficient for large enough α, see [10]. However, it seems to be impossible to determine the corresponding bound for α just using the results of [10], and moreover, the smallest values of α are the most interesting.

As regards the analogue of Problem 1 for classical fullerenes, that is for cubic, spherical and polyhedral maps of face-type $(5, 6)$, it is well-known that (mathematical models of) these fullerenes with precisely α hexagonal faces exist for all non-negative values of α with the sole exception of $\alpha = 1$, see [6, section 13.4]. In [3], Problem 1 is solved for the cases $k = 7$ and 8 and all $g \geq 2$:

Theorem 2. *If $k \in \{7, 8\}$, $g \geq 2$ and $\alpha \geq 0$, then there exists a hyperbolic k-gonal fullerene of genus g with exactly α hexagonal faces, except for $k = 8$, $g = 2$ and $\alpha \leq 3$, where no such maps exist.*

(In fact, for $k = 8$, $g = 2$ and $\alpha = 3$, it is claimed in [3] that a corresponding hyperbolic fullerene exists, which is false. They claim 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]", while Heffter [9] only shows that K_9 has an embedding on S_3. When Youngs [21] refers to Heffter's work, it is to resolve Heawood problem for K_9, but not to show the existence of triangular embedding for $K_9 - K_3$. On the contrary, it was shown by Jungerman [12] (using computer program) that $K_9 - K_3$ has no orientable triangular embedding.)

In this paper we consider the next two values, namely $k = 9$ and 10. Analogous to the cases $k = 7$ and 8, we give a complete solution of Problem 1 for all $g \geq 2$ with the exception of cases $k = 10$, $g = 5$ and $\alpha \leq 3$, when we are not able to state if corresponding hyperbolic 10-gonal fullerenes exist.

We remark that values $k = 7, 8, 9, 10$ are *universal* in the sense that there is a trivalent polyhedral map of face-type $(6, k)$ for all genera $g \geq 2$. The remaining universal values are $k = 12$ and 18, see [3], and it will be interesting to investigate Problem 1 for these two values of k.

In the next section we present some preliminary results and a general construction for duals of hyperbolic k-gonal fullerenes when $k \in \{9, 10\}$. Section 3 is devoted to hyperbolic 9-gonal fullerenes, and Section 4 deals with hyperbolic 10-gonal fullerenes.

2. Preliminaries

A *map* is an embedding of a graph, possibly with loops or multiple edges, into a surface, such that every face is homeomorphic to an open 2-cell. A map is *polyhedral* if the following is true, see [17, Proposition 5.5.12] and the text below.

(p1) The underlying graph of the map is simple, that is, without loops and multiple edges.
(p2) All facial walks are cycles, that is, no vertex appears more than once on the boundary of a face.
(p3) The intersection of any two faces is either empty, or it contains a unique vertex, or exactly two vertices and the edge joining them.

Let T be a map. If we shrink every face of T to a vertex and extend every vertex of T to a face, we obtain a *dual map* T^D. Then T and T^D have the same numbers of edges and every edge of T intersects exactly one edge of T^D and vice versa. By [17, Proposition 5.5.12 (b), (d)], a map is polyhedral if and only if its dual map is polyhedral.

Let T be a hyperbolic k-gonal fullerene of genus g and let T^D be its dual map. Then T^D is a polyhedral triangulation of orientable surface of genus g in which every vertex has degree either 6 or k. However, to check polyhedrality for T^D, it suffices to check (p1), as (p2) and (p3) follow. More precisely, (p2) is implied by the fact that the underlying graph for T^D does not contain loops, and (p3) is implied by the fact that this graph does not have multiple edges and the vertex degrees are greater than 2. Hence, we have the following proposition:

Proposition 3. *Let T be a triangulation of an orientable surface of genus $g \geq 2$ by a simple graph G, such that α vertices of G have degree 6 and the remaining vertices have degree k. Then the dual of T is a hyperbolic k-gonal fullerene of genus g with exactly α hexagonal faces.*

In our constructions, we do not construct hyperbolic k-gonal fullerenes directly, instead we construct their duals. By Proposition 3, this approach reasonably simplifies the check for polyhedrality. In all but finitely many cases we construct the required triangulations using triangulations of tori by 6-regular simple graphs.

For $k = 9$, take two toroidal triangulations by 6-regular simple graphs. In each of them, cut out two adjacent facial triangles together with the edge joining them. This leaves a 4-hole in each surface. These 4-holes are bounded by 4-cycles with four vertices having degrees 6 and 5 distributed alternatively around the cycle. Hence, if we glue these holes together *properly*, that is, we identify the boundary cycles so that in every case a vertex of degree 6 will be identified with a vertex of degree 5 and we identify these cycles in the opposite way (so that the resulting surface is orientable when making more gluing of this type), we obtain a triangulation of an orientable surface in which the vertex degrees are 6 and 9 only, see Fig. 1.