On Octahedral Fulleroids

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Abstract

The discovery of the fullerene has raised an interest in the study of other candidates for modeling of carbon molecules. Motivated by works of P. Fowler, Delgado Friedrichs and Deza, $O_h(a,b)$-fulleroids were defined as cubic convex polyhedra having only a-gonal and b-gonal faces and the symmetry group isomorphic with the full symmetry group of regular octahedron. In this paper we give sufficient and necessary condition for existence of $O_h(5,n)$-fulleroids depending on number n either by finding infinite series of examples to prove existence or proving nonexistence using symmetry invariants.
KEY WORDS: fulleroid, octahedral group of symmetries, convex polyhedron, cubic plane graph
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1 Introduction

Cubic convex polyhedra are suitable models for carbon molecules. These models have the following structure: vertices of such polyhedra represent the atoms of carbon, edges between vertices realise bonds between pairs of atoms. The polyhedron is cubic (every vertex is trivalent), so every carbon atom is bonded with three others. One of these bonds has to be doubled, because every carbon atom is to be associated with four bonds. This is possible because the graph of every cubic polyhedron has a 1-factor (perfect matching) that forms a Kekulé structure of the carbon molecule (double

bonds are realized along edges of this 1-factor). This can be proved by Petersen's theorem [14], the classical result of graph theory. In fact, as shown by Klein and Liu [9],[10], every cubic convex polyhedron has at least three mutually disjoint 1-factors.

The discovery of the famous fullerene C_{60} in 1985 [11] has raised an interest in other ways to model carbon molecules, see e.g. papers by Malkevitch [12] and Deza, Deza and Grishukhin [5]. Patrick Fowler in 1995, see [4],[6], asked whether a fullerene-like structure consisting of pentagons and heptagons only and exhibiting an icosahedral symmetry exist. The answer was given by Dress and Brinkmann [6]. Motivated by these examples Delgado Friedrichs and Deza [4] introduced the following definition: a *fulleroid* is a tiling of the sphere such that all its vertices have degree 3 while all its faces have degree 5 or larger. A Γ-*fulleroid* is a fulleroid on which the group Γ acts as a group of symmetries. A given Γ-fulleroid is of type (a, b) or a $\Gamma(a, b)$-fulleroid if all its faces are either a-gonal or b-gonal. The set of all $\Gamma(a, b)$-fulleroids will be denoted simply by $\Gamma(a, b)$.

In [6] $I_h(5, 7)$-fulleroids and $I(5, 7)$-fulleroids are investigated when I_h and I denotes the full icosahedral group of symmetry and its subgroup of rotational symmetries, respectively.

In [4] the authors started a research of $I(5, n)$-fulleroids for $n = 8$, 10, 12, 14, 15 and posed several questions concerning the existence of $I(5, n)$-fulleroids for any other n. Most of their questions were answered by Jendrol' and Trenkler [8], who managed to prove that for every $n \geq 8$ there exists infinitely many $I(5, n)$-fulleroids.

The question of Fowler's can be generalized in the following way: Consider any group Γ that can act as symmetry group of convex polyhedra. The list of such groups can be found e.g. in [2], or in a book [3] of Cromwell. In [8] the problem to characterize $\Gamma(a, b)$-fulleroids for all possible pairs of parameters a, b was proposed. For symmetries on fullerenes see the papers by Babić et al. [1] and Fowler et al. [7].

In this paper we focus on the case of $O_h(5, n)$-fulleroids, where O_h is a group of symmetries of the octahedron and n is arbitrary natural number greater than 3. Namely, we prove following statements:

Theorem 1 *Let $n > 3$. Then the set $O_h(5, n)$ is not empty if and only if $n \equiv 0 \pmod 4$ and $n \not\equiv 0 \pmod 5$ or $n \equiv 0 \pmod{60}$. Furthermore, the set $O_h(5, 4)$ consists of one member only and if $n > 4$ and the set $O_h(5, n)$ is not empty, then it contains infinitely many members.*

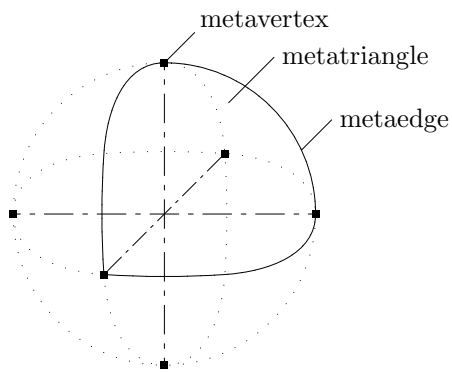

Figure 1: Metavertices, metaedges and metatriangles

2 Preliminaries

Before first results appear, let us introduce some useful notions:

Let $P \in O_h(5, n)$ be a polyhedron with full octahedral symmetry and its faces are only pentagons and n-gons. We project the polyhedron P onto the sphere whose centre is the point of central symmetry of P and explore only this projection.

Three axes of 4-fold rotational symmetry of P intersect the sphere in six points. Let us call these points *metavertices*. Three symmetry planes of P, each containing four metavertices, intersect the sphere in three circles, dividing the sphere into 8 parts. Let us call these parts *metatriangles*. Each circle set by one symmetry plane is divided into four parts by the metavertices. Let us call these lines *metaedges*. Together, metavertices and metaedges form an octahedron, faces of which are the metatriangles, see Figure 1.

To describe some octahedral fulleroid we will show one metatriangle of it, despite the fact it is not the elementary bit of symmetry. If the picture was supposed to become too large, only one sixth of metatriange (any of six parts obtained by dividing it according to symmetry axes) would be drawn.

Lemma 1 *Let $n > 3$. If $n \not\equiv 0 \pmod 4$, then $O_h(5, n) = \emptyset$.*

Proof. We will prove an equivalent implication: If $O_h(5, n) \neq \emptyset$, then $n \equiv 0 \pmod 4$.

Let $P \in O_h(5, n)$. We focus on one metavertex of P. It is a point of 4-fold rotational symmetry, thus the local structure of polyhedron P must have a 4-fold rotational symmetry. One can easily see that in the metavertex

a vertex or internal point of edge of P cannot be there. Strictly speaking, a vertex has 3-fold (local) rotational symmetry (all vertices of P are of degree three), and any internal point of an edge can have only 2-fold symmetry (if only it is the midpoint of the edge).

So the metavertex must lie inside some face of P. Then this face must have (local) 4-fold symmetry – if we rotate it for $\frac{\pi}{2}$ around the metavertex, in must coincide with itself.

The pentagon obivously has no 4-fold rotational symmetry, so it must be the n-gon. Finaly we see that 4 divides n. $\square$

3 Case $n \equiv 0 \pmod 4$ and $n \not\equiv 0 \pmod 5$

In this section appropriate polyhedral maps for certain classes of numbers n are constructed. In fact we will cnstruct 3-connected planar graphs G, having their group of automorphisms isomorphic to the group O_h of symmetries of regular octahedron. By theorem of P. Mani [13] (see also [15]) for each such graph G there is a convex polyhedron P such that the graph of P is isomorphic to G and the symmetry group of P is isomorphic to the automorphism group of G. In sequel we will not distinguish between polyhedron P and corresponding graph G.

From the proof of Lemma 1 we can see that every polyhedron $P \in O_h(5, n)$ has at least six n-gons, those containing metavertices.

First let us find all octahedral polyhedra with only six n-gonal faces. We already know, that all n-gons are in metavertices of symmetry meta-octahedron. The remaining space must be filled by pentagons.

For $n = 8 + 20k$ and $n = 12 + 20k$, $k \in \mathbb{N}_0$ one example can be seen on Figure 2, where applying operation from Figure 3 on each thick edge k times the number of vertices of each n-gon is increased by $20k$.

For $n = 4 + 20k$ and $n = 16 + 20k$, $k \in \mathbb{N}_0$ see Figure 4, where one metatriangle for $n = 4$ and 16 is drawn. In particular, for $n = 4$ the observed polyhedron is the cube. To extend the number n by 20, another operation (Figure 5) is available.

There is one problem about these 'polyhedra' we have got in this case. One can easily see that resulting graphs for $k > 0$ are not 3-connected, so it cannot be polyhedral maps. But this does not imply that the set $O_h(5, n)$ is empty in such cases. Convenient graphs with more than 6 n-gonal faces can be found.

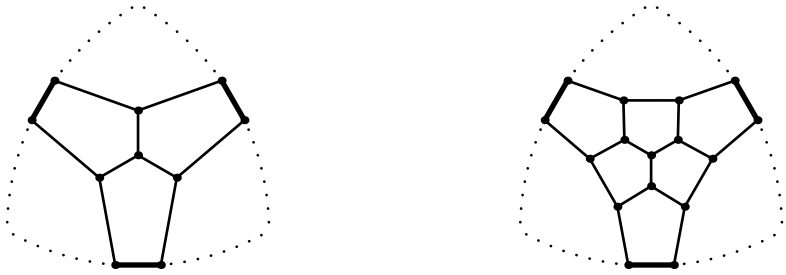

Figure 2: A metatriangle for $n = 8 + 20k$ and $n = 12 + 20k$.

Figure 3: Operation adding 5 vertices to n-gon

Figure 4: Example for $n = 4$ and $n = 16$.

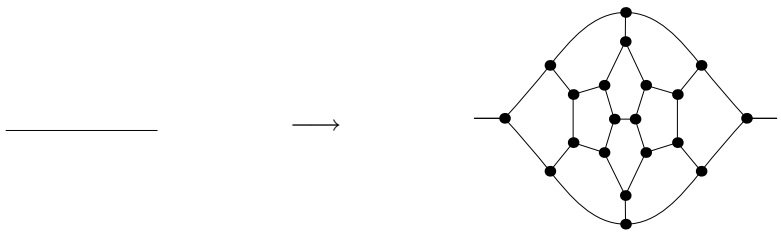

Figure 5: Operation adding 5 vertices to n-gon

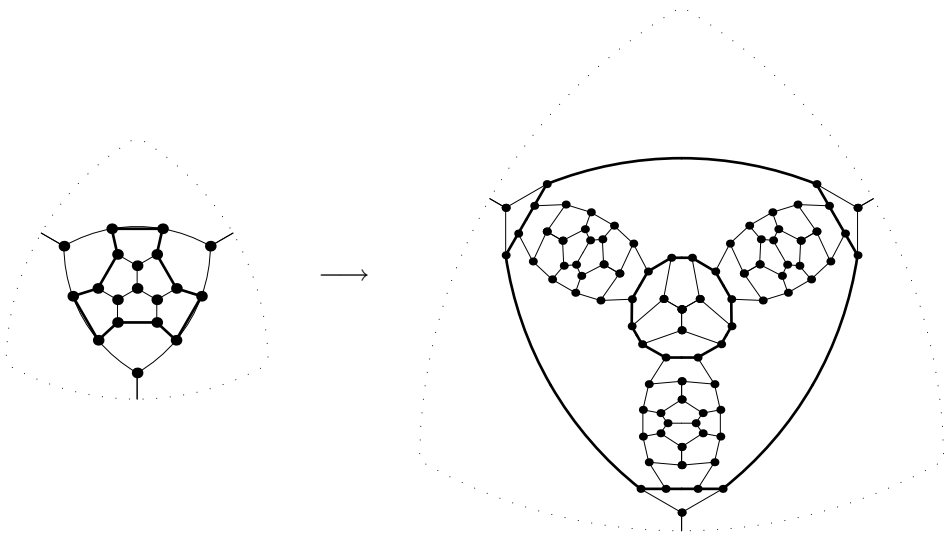

Figure 6: Generating members of $O_h(5, 16)$.

The examples above certify that the set $O_h(5, n)$ is nonempty for certain values of number n. If $n = 4$, than the cube is the only member of $O_h(5, 4)$. This can be easily observed as an outcome of Euler's theorem: If number of tetragons and pentagons is denoted by n_4 and n_5, respectively, the theorem gives the relation $2n_4 + n_5 = 12$. Together with the fact, that there must be at least 6 tetragons, we get the claim.

If $n = 16$, $n = 8 + 20k$ or $n = 12 + 20k$, to prove that the set $O_h(5, n)$ contains infinitely many members, we introduce infinite series of examples, obtained by repeating certain operation: Instead of three pentagons three n-gons are inserted, bringing certain number of new faces, within which the initial structure can be found again, see Figure 6 for $n = 16$, Figure 7 for $n = 8$ and Figure 8 for $n = 12$. Here the single thick edges joining pairs of 8-gons (or 12-gons, respectively) give us possibility to apply the expanding trick using configuration from Figure 3 as many times as desired.

For $n = 24 + 20k$ and $n = 36 + 20k$ one example can be seen on Figure 9. The rectangle with number inscribed, e.g. $10 + 20k$, means repeating of the system from Figure 3 several times, now it is $2 + 4k$ times. (Number of repeating is one fifth of number inscribed).

Again, infinite series of examples can be found, using the method Jendrol' and Trenkler did in their work [8]. Instead of chain of four pentagons (the

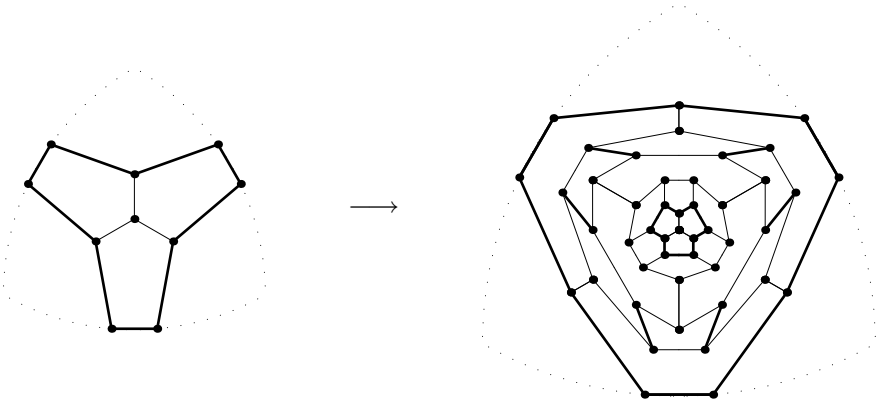

Figure 7: Generating members of $O_h(5, 8)$.

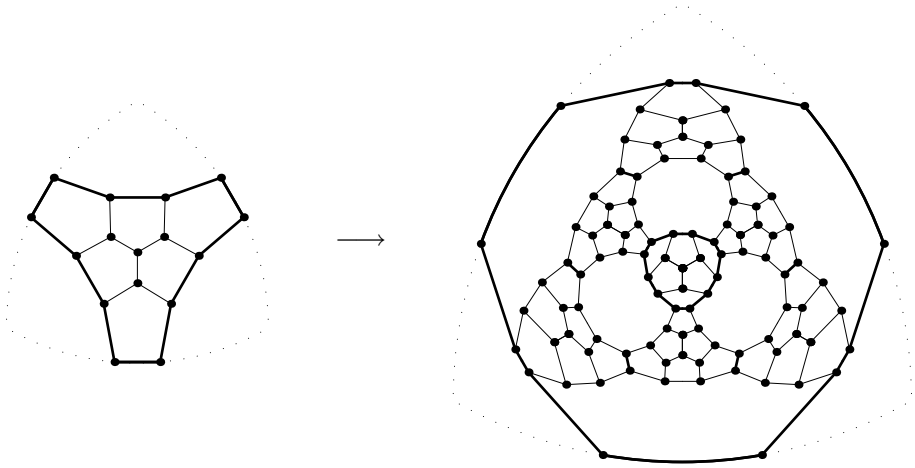

Figure 8: Generating members of $O_h(5, 12)$.

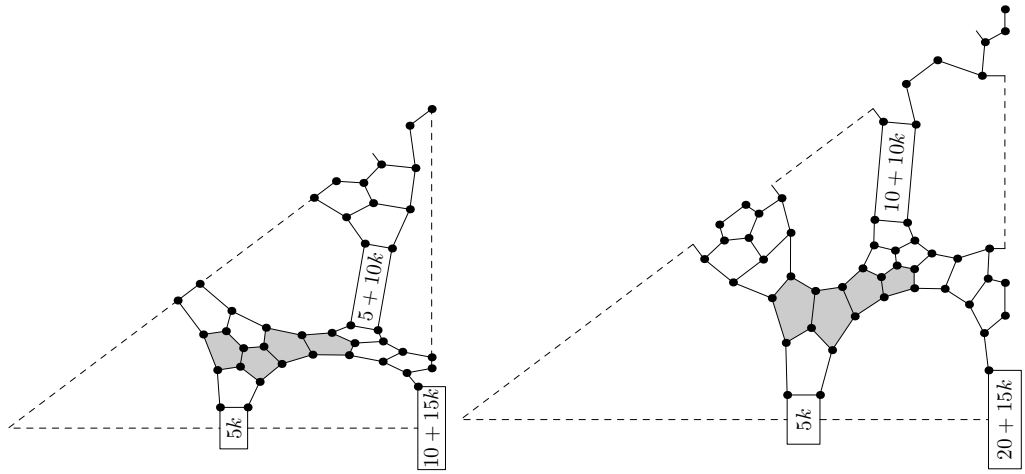

Figure 9: One sixth of metatriangle for $n = 24 + 20k$ and $n = 36 + 20k$.

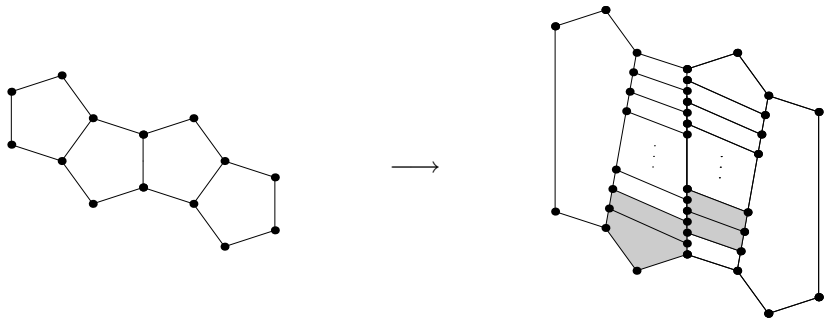

Figure 10: Operation adding two new n-gons.

grey ones on Figure 9), two n-gons and several new pentagons are inserted (see Figure 10). As above, the initial structure can be found again, e.g. the four grey pentagons on Figure 10, so infinite series is generated by induction.

Of course, there are simplier polyhedra for some numbers n. If $n \equiv 0 \pmod 3$, then one n-gon can be placed in the center of each metatriangle to receive polyhedra such as on the Figure 11.

4 The case $n \equiv 0 \pmod{20}$

We have already proved that $O_h(5, n) \neq \emptyset$ for n such that $n \equiv 0 \pmod 4$ and $n \not\equiv 0 \pmod 5$ by finding (at least) one polyhedron from $O_h(5, n)$.

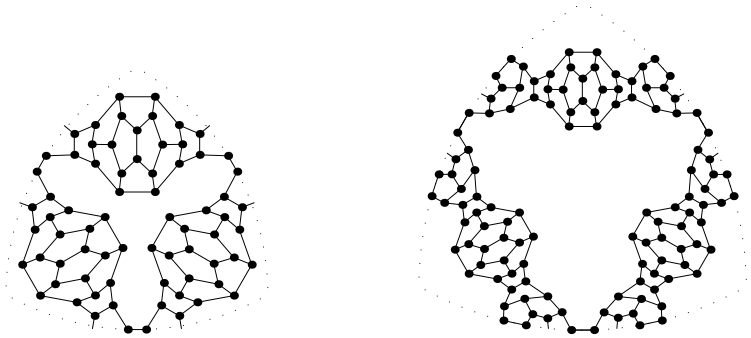

Figure 11: One metatriangle of special polyhedra for $n = 24$ and $n = 36$.

In this section we will focus on $n \equiv 0 \pmod{20}$. Our aim is to prove that in this case $O_h(5, n) = \emptyset$ for $n \not\equiv 0 \pmod 3$ and $|O_h(5, n)| = \infty$ for $n \equiv 0 \pmod 3$.

We will do it in three steps. First, we will prove that every polyhedron with pentagonal and n-gonal faces (where $n \equiv 0 \pmod 5$) can be mapped onto a dodecahedron. Then, we will investigate the projection of objects (vertices, edges, etc.) laying on one metaedge and on its axis of symmetry to find some useful invariants. At the end, we will check for infinite series of examples for admissible numbers n.

Lemma 2 *Let $n \equiv 0 \pmod 5$ and P be a polyhedron with pentagonal and n-gonal faces only and all vertices of degree 3. Then there exists the homomorphism $\Psi : P \to D$, where D denotes the dodecahedron.*

By homomorphism $\Psi : P \to D$ we mean the mapping of vertices, edges and faces of the polyhedron P onto those of the polyhedron D, respecting the incidence structure. That means if two vertices (edges, faces) of P are adjacent, then also their images are adjacent in D.

Proof. Let P be a polyhedron satisfying premise of lemma. We will make one mapping $\Psi : P \to D$ and then prove it is a homomorphism.

It is sufficient to define mapping of faces, then prove it is a homomorphism, and the mapping of edges and vertices induced by this mapping will be homomorphism since P and D are both polyhedra such that all vertices are of degree three and every two faces meet in an edge or do not meet.

We begin with one pentagon and one by one add all other faces. In each step we will observe the closed walk bounding the set of faces already added;

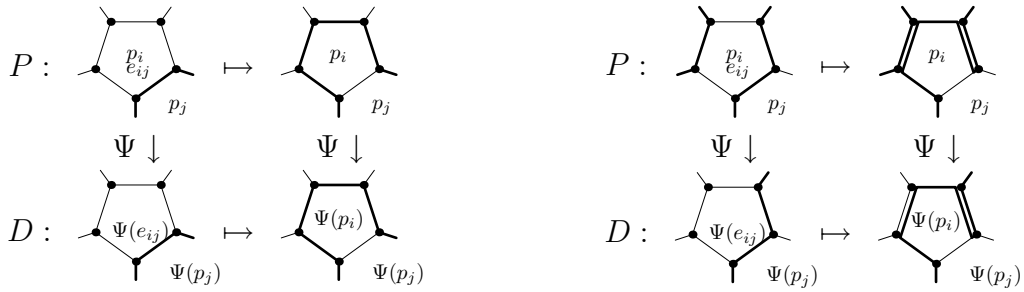

Figure 12: Adding the face p_i

let us call it C. The projection of this closed walk onto the dodecahedron will be $\Psi(C)$.

At the beginning, both C and $\Psi(C)$ are empty. As the process follows, all the faces of P move from outer part bounded by C into the inner part. At the end, the outer part will be face-empty.

Firstly we map one pentagon. There must be at least one pentagon on P, since there are only pentagons and n-gon where $n \geq 10$. (If $n = 5$, then the only polyhedron made of pentagons with all vertices of degree three is the dodecahedron and lemma is trivial.) We map this first pentagon onto any one of pentagons on D. Both C and $\Psi(C)$ become 5-cycles on P and the D, respectively.

Now we will use two operations:

- mapping one face
- simplifying the walk C (and, consequently, $\Psi(C)$)

Mapping of one face:

If there is any face p_i adjacent to some face p_j already mapped, that has not been mapped yet, we will add it. Instead of the edge e_{ij} between p_i and p_j in C we put the complement in p_i. The image of the face p_i will be the face, that is adjacent to $\Psi(p_i)$ via $\Psi(e_{ij})$. If p_i is a pentagon, the same has to be done with $\Psi(C)$, see Figure 12, left. If p_i is adjacent to more faces already mapped, we can choose anyone of them, see Figure 12, right, where image of second part of C is omitted.

If p_i is not a pentagon, we do it by similar way. Instead of certain edge its complement is put into C, the image of this complement has to be circling round the image $\Psi(p_i)$ as on Figure 13; it fits because the number n is a multiple of 5.

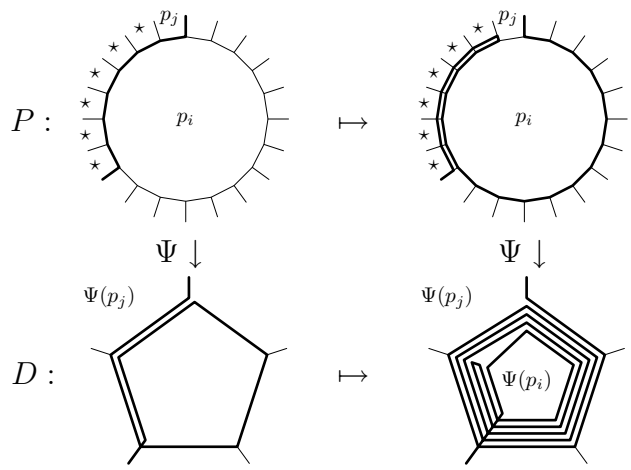

Figure 13: Adding the 20-gon

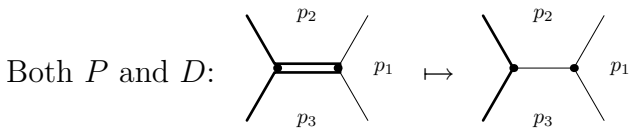

Figure 14: Simplifying the walk C

Simplifying the closed walk C:

If the path C includes the same edge two times consequently, as on Figure 14 (endings do not have to be different), we will omit this couple of edges. We can do this without any harm on $\Psi(C)$, because image of this pair of (the same) edges is the same edge in D. This can be observed easily, no matter in what order the faces p_1, p_2 and p_3 were added.

Altogether, using these operations the path C remains closed walk, its image, $\Psi(C)$ also remains closed walk with the same number of edges and the same sequence of 'turnings right', 'turnings left' and 'turning backwards'.

At the end of the process, all faces of P are mapped. Some edges are also mapped, and some vertices can have been mapped more times as vertices of more faces. In the outer part of closed trial C, no faces must be there, and after applying second operation as many times as possible, C must become trivial (one vertex only, no edges). As in all steps the number of edges in C and $\Psi(C)$ is equal, at the end also the closed walk $\Psi(C)$ is trivial.

We have already made some mapping $\Psi : P \to D$ working at faces of P. Our next task is to prove it is well-defined and a homomorphism.

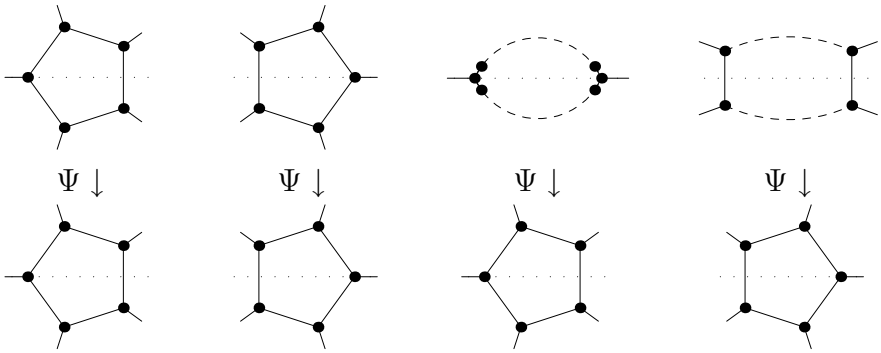

Figure 15: Possible position of pentagons and n-gons on an metaedge and their image

It is sufficient to prove that for every pair p and q of adjacent faces of P the pentagons $\Psi(p)$ and $\Psi(q)$ are also adjacent. If p and q is a pair from the first operation, then it is obvious. So let us suppose that p and q have never played a role of p_i and p_j in the first step. Since at the end both p and q have been mapped, there must be one step of the second type, where p and q act as p_2 and p_3 on Figure 14. Because all vertices of both P and D are of degree three, $\Psi(p)$ and $\Psi(q)$ are adjacent. Hence Ψ is a homomorphism.

□

Lemma 3 *Let* $n \equiv 0 \pmod{20}$ *and* $n \not\equiv 0 \pmod 3$. *Then* $O_h(5,n) = \emptyset$.

Proof. Let us suppose $O_h(5,n) \neq \emptyset$. Let $P \in O_h(5,n)$. Using the Lemma 2 we get mapping $\Psi : P \to D$, where D denotes the dodecahedron.

We will analyze one metatriangle of P and its image.

Let us focus on the image of a metavertex, the objects on an metaedge, those on axis of symmetry and the center point of the metatriangle.

As shown above, there must be a face of P placed in the metavertex. There are two possible positions of this face, distinguished by the fact whether the face meets metaedges in vertices or not.

On the metaedge, the vertices, the edges and midpoints of edges can be there. Faces intersected by metaedge can be placed the ways shown on Figure 15 only. Projection of all these objects onto the dodecahedron D can also be seen on Figure 15.

We can easily see that if a point moves along the metaedge, the image of this point moves only on one section line of D, see Figure 16.

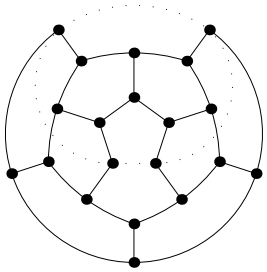

Figure 16: Section line (dotted) on the dodecahedron

On the axis of symmetry of metatriangle, the same objects can be placed as on the metaedge. So also its image is only on certain section line of D, similar to one on Figure 16.

Let us look at the metavertex once more. In the metavertex 4 metaedges and 4 symmetry axes intersect. The number of vertices (and edges) between two adjacent lines is $\frac{n}{8} = \frac{20k}{8} = \frac{5}{2}k$, so the image of all intersecting lines must lie on the same section line of the dodecahedron.

There are two untouched points types yet, the midpoint of some metaedge and the centre of the metatriangle. Now the important one for us is the second one. In this point, three symmetry axes intersect. We already know, that their images lie on the same section line of D. (That's because changing from axis to metaedge in one metavertex does not make difference, neither does following the metaedge to another metavertex or changing to another axis). On the other hand, the object placed here must have full 3-fold symmetry, so it must be a vertex.

But if we inspect the image of this point, the image of the three axes (three edges incident with the vertex) lie on three different sections of D, what is the contradiction.

To conclude, the set $O_h(5, n)$ must be empty. □

4.1 The case $n \equiv 0 \pmod{60}$

It seems that the Lemma 3 holds also if $n \equiv 0 \pmod 3$, but it is not true. The proof fails in the last step.

In this case in the centre of the metatriangle, there is one more possible object with 3-fold symmetry, which was not in previous: the n-gon! So we get, that necessarily there are 8 n-gons more (in the center of metatriangles).

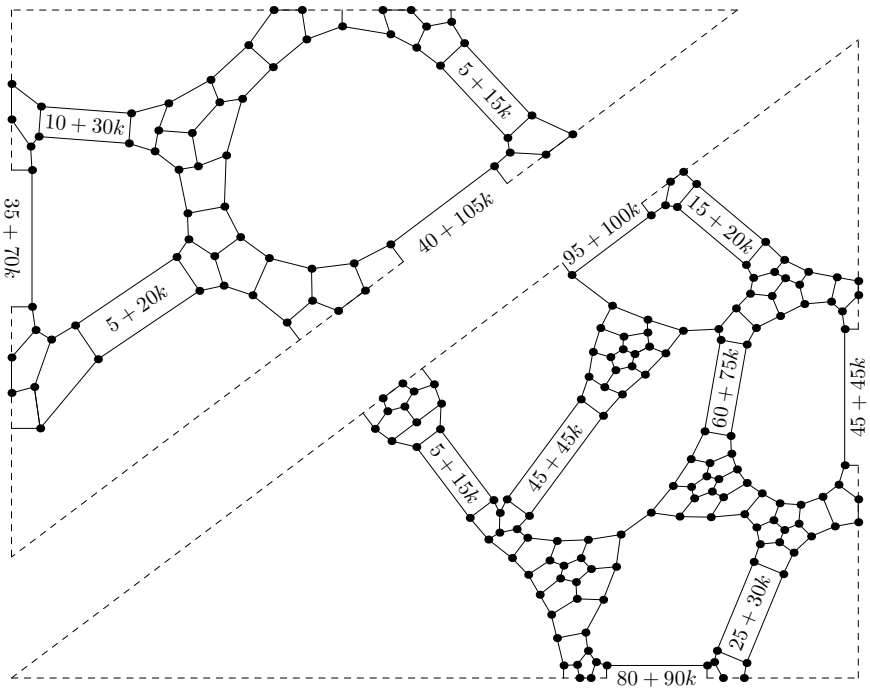

Figure 17: One sixth of a metatriangle for $n = 60 + 120k$ and $n = 120 + 120k$

One can easily prove (by listing all possibilities) that in the midpoint of every metaedge, another n-gon must be there. Thus this makes another 12 n-gons.

We will figure only one sixth of the metatriangle. On Figure 17 we can see them for two classes of number n, the rectangles with number inscribed have the same meaning as above. To make certain of existence infinitely many examples also in this case, one can use the operation from Figure 10 again, or simply use the operation shown on figure 18.

Altogether, these examples were the last missing parts of proof of the

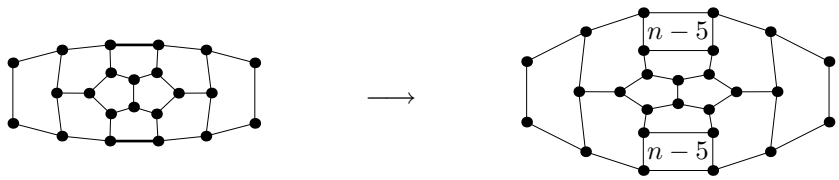

Figure 18: Operation generating more n-gons, where n is a multiple of 5

main Theorem 1.

Acknowledgements

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