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A Generalized Ring Spiral Algorithm for Coding Fullerenes and other Cubic Polyhedra [1]

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Abstract

The so-called *ring spiral* algorithm is a convenient means for generating and representing certain fullerenes and some other cubic polyhedra. In 1993 Manolopoulos and Fowler presented a fullerene on 380 vertices without a spiral. No smaller unspirable fullerene is known. In the spring of 1997, using computer, Gunnar Brinkmann found the smallest cubic polyhedron without a spiral. It has only 18 vertices. Here we generalize the ring spiral approach in order to obtain a canonical representation for arbitrary planar cubic polyhedra. Some other questions are addressed: for instance possible generalization of this method to polyhedra of higher genus and to polyhedra with vertices of arbitrary valency.

Introduction

Quite apart from the many mathematical reasons for interest in the cubic polyhedra, there are topical chemical reasons for a renewed investigation of their properties. Polyhedral carbon cages with pentagonal and hexagonal faces have been discovered [12] and have a rich and growing chemistry.

[1]Part of this paper was delivered as a talk by the third and fourth author at a conference in Kansas City in 1993

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Problems of enumeration, construction, interconversion and relative energetics are still subjects of intensive research but it appears that much of the general behaviour of fullerenes can be understood in terms of simple graph-theory-based treatments of π-electronic structure coupled to curvature-based discussion of steric strain in the σ-electronic framework [9]. Much early systematic work concentrated on the construction and enumeration of fullerene isomers, and made heavy use of the ring spiral algorithm [14]. The present paper returns to this algorithm, its successes, failures and generalisations.

The *ring spiral algorithm* for construction of a polyhedron of f faces starts with an oriented disk with a polygon of size r_1 and then attaches polygons of size $r_2, r_3, \dots, r_k, \dots r_f$ to the disk in a uniquely determined spiral in such a way that the graphs $P_1, P_2, \dots, P_k, \dots, P_f$, that are produced in this process, have all maximum valency ≤ 3. At each step of the algorithm, we can view P_k as a map (polyhedron) on the sphere with a disk removed. If flattened, P_k has a shape of a disk (with no holes). All vertices in the interior are trivalent whereas the vertices on the boundary are either 3- or 2-valent. If the boundary ∂P_k is traced according to the orientation of the disk, we can record the valencies of the s_k boundary vertices. In this way we can produce a *word* $w_k = x_{k,1}x_{k,2}\dots x_{k,s_k}$ over the symbols $\{0,1\}$, where 0 represents valency 3 and 1 represents valency 2. The word w_k can be cyclically permuted. Its actual form depends of the starting vertex on the boundary. Such a word is sometimes called the *boundary code*. For a discussion on the history, variations and improvements on the boundary code for polyhexes see [4].

Clearly, $w_1 = 11\dots1 - (r_1 - \text{times})$. If the graphs $G_{f-1} = G_f$ are trivalent then the disk closes up to the sphere and $w_{f-1} = w_f = 00\dots0 - (r_f - \text{times})$. In order to avoid ambiguity we will choose at each step of the spiral algorithm a particular cyclic permutation of the word w_k according to the following rule:

For a given ring size r one can choose any pair (z, o) as indices of entries **z**eroes and **o**nes, such that $r = z + o + 2$. The general rule reads as follows:

$$R(z, o) = 10^z1 \to 01^o0$$

This means that the word of the form

$$w_k = 10^z1v$$

is replaced by

$$u_k = v01^o0$$

If the resulting word consists of zeros only, the procedure stops and $w_{k+1} = u_k$. Otherwise, u_k is cyclically shifted to the right until the rightmost 1 arrives on the first position (leftmost position) in order to obtain w_{k+1}.

It may happen that a step is not possible. In such a case the sequence $s = (r_1, r_2, \ldots, r_f)$ is not a legitimate ring-spiral sequence. If however, the algorithm succeeds then the sequence $s = (r_1, r_2, \ldots, r_f)$ is called a *ring spiral* of the trivalent polyhedron. If we choose from all possible ring spirals the one that is lexicographically first, we get the *canonical description* of the polyhedron. If there is no danger for confusion we will simplify the code to the form $s = (r_1, r_2, \ldots, r_f) = r_1 r_2 \ldots r_f$. We also use the notation ∂s_k to denote the boundary code w_k of a partial polyhedron P_k defined by the first k steps of the spiral code.

Example 1 *Let us show how one can produce the trigonal prism given its spiral code*

$$s = 34443.$$

The corresponding sequence of words is as follows:

$$s_1 = 3, \partial s_1 = w_1 = 111$$

$$s_2 = 34, \partial s_2 = w_2 = 10101$$

$$s_3 = 344, \partial s_3 = w_3 = 10010$$

$$s_4 = 3444, \partial s_4 = w_4 = 000$$

$$s = s_5 = 34443, \partial s_5 = \emptyset$$

When we attach a triangle we apply one of the following rules:

$$R(0,1) = 11 \to 010$$

$$R(1,0) = 101 \to 00$$

For a quadrilateral the rules would be:

$$R(0,2) = 11 \to 0110$$

$$R(1,1) = 101 \to 010$$

$$R(2,0) = 1001 \to 00$$

The whole process can be thus described more concisely:

$$(11)1 \stackrel{R(0,2)}{\to} (0110)1 = (101)01 \stackrel{R(1,1)}{\to} (010)01 = (1001)0 \stackrel{R(2,0)}{\to} 000.$$

Let us further abbreviate: Instead of $rr \dots r - (m - \text{times})$ can write r^m. In this case r^0 represents the empty string.

Example 2 *Hence we can abbreviate*

$$55555655655555 = 5^5 65^2 65^5$$

and

$$5555565666565555 5 = 5^5 656^3 565^5$$

If $r_k \in \{5, 6\}$, for each k, that is, if the polygons are pentagons and hexagons, we get in such a way a *fullerene.*

To generate fullerenes, we start with one of the two initial words:

$$S(5) = 11111 = 1^5$$
$$S(6) = 111111 = 1^6$$

and we apply a sequence of the following rules in any order

Pentagon:

$$R(0,3) = 11 \to 01110$$
$$R(1,2) = 101 \to 0110$$
$$R(2,1) = 1001 \to 010$$
$$R(3,0) = 10001 \to 00$$

Hexagon:

$$R(0,4) = 11 \to 011110$$
$$R(1,3) = 101 \to 01110$$
$$R(2,2) = 1001 \to 0110$$
$$R(3,1) = 10001 \to 010$$
$$R(4,0) = 100001 \to 00$$

We obtain a fullerene if the rules may be applied and we finish the process in one of the following two terminal words:

$$T(5) = 00000 = 0^5$$

$$T(6) = 000000 = 0^6$$

The spiral code has several advantages.

1. It is easy both for a human and a computer program to generate (or reconstruct) a polyhedron from its spiral code.
2. It is a concise description of a cubic polyhedron.
3. From the code one can immediately recognise the structure of faces of the polyhedron.
4. Initial sub-sequences of the code define an increasing sequence of partial polyhedra, such that each polyhedron is homeomorphic to a disk.

Unfortunately not all trivalent polyhedra (not even fullerenes!) admit ring spirals. This was shown by D.E Manolopoulos and P.W. Fowler in [14]. They produced a fullerene on 380 vertices that has no spiral. Over 400 larger fullerenes with ≤ 1000 vertices have since been found, but none smaller than the 380 vertex example [3, 20, 21].

Recently Gunnar Brinkmann [2] found the smallest trivalent planar polyhedron without a spiral, see Figure 1, while the problem of finding the smallest fullerene without a spiral remains open.

It is natural to ask whether it is possible to generalize the spiral algorithm in such a way as to generate all planar trivalent polyhedra and such that the conventional ring spiral - if it exists - would be lexicographically the best among all descriptions. In [2] Brinkmann proposed an efficient generalization of such a code which shares almost all advantages of the original code.

The smallest trivalent planar polyhedron without a spiral turned out to be a truncated trigonal prism. It was shown by Brinkmann and Fowler [3] that this is not a coincidence.

Theorem 1 (Brinkmann and Fowler, [3].) *The truncate of any trivalent planar polyhedron P does not have a spiral unless P is the tetrahedron.*

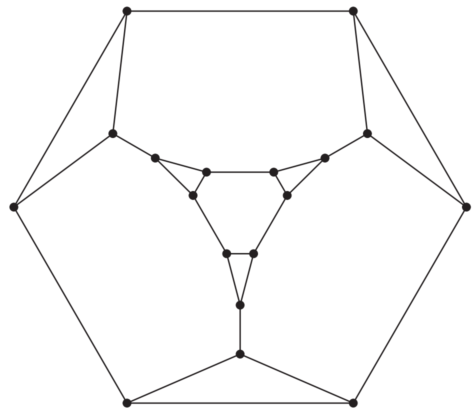

Figure 1: The smallest trivalent planar polyhedron without a ring spiral, determined by Gunnar Brinkmann, is a truncated trigonal prism.

Obviously it would be interesting to explore spiral properties of truncations of four-valent polyhedra, in particular those that arise as truncations of medials of other polyhedra. For a definition of the *medial transformation*, see for instance [8].

Generalized Spiral Code

The generalization that we propose here is different from the *Brinkmann code*, first published in [2]. While both generalizations have comparable characteristics our approach has one minor advantage. Since our partial polyhedra during reconstruction process are simply connected the generation of the polyhedron from our code may be more suitable for hand calculations.

As in the conventional ring spiral algorithm, we choose positive orientation of the disk. We will assume that the ring spiral step attaches the polygon to the disk at *position* 1. If, instead, we slide the polygon along the perimeter of the disk to the next position, we call that *position* 2, etc. We are considering the gap between two consecutive 1's on the boundary; see Figure 2.

Formally, the *generalized ring spiral* is a sequence:

$$s_f = (p_1, p_2, \ldots, p_f; r_1, r_2, \ldots, r_f)$$

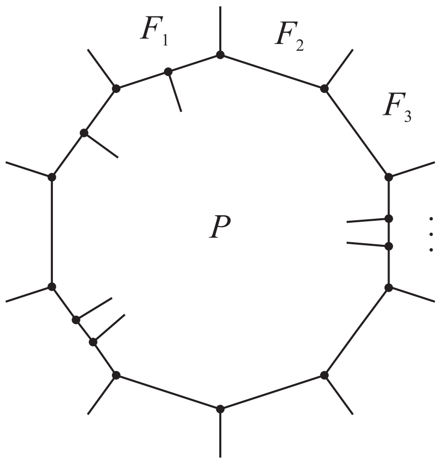

Figure 2: A partial polyhedron P and positions along the boundary ∂P where other faces $F_1, F_2, \ldots$, can be attached. If $F_1 \neq F_i$, for $i \neq 1$, the spiral step is possible.

with the following interpretation: At step k the polygon r_k is attached to the partial polyhedron P_{k-1} at the position p_k. By convention $p_1 = p_2 = p_f = 1$.

We can simplify the notation if there is no danger of confusion. If a face of size r is attached at position p, we can write this as r_p. We will also omit subscript 1 in order to shorten the notation. Hence $r_1 = r$. If $p = 1$ we say that k is a *spiral step*.

In order to compare the sequences, we consider the full form of s_f:

$$s_f = (p_1, p_2, \ldots, p_f, r_1, r_2, \ldots, r_f)$$

and the sequences are ordered lexicographically.

This means that if a polyhedron admits a spiral then its canonical form will reflect this fact.

Note that the sequence $433_2 3_p, \ldots$ is not realizable for any position p.

Some codes for small fullerenes are listed in Table 1, rewritten from [10] in our shorthand notation.

The C_{380} fullerene without a spiral can be described as follows:

$$C_{380} = 5^3 6^{133} (5^2 6^8)^2 5^2 6^7 5_2 6^6 5_3 6^6 5_3 6^{12}$$

The Tutte graph [1] is:

C_{20}	5^{12}
C_{24}	$5^5 6 5^2 6 5^2$
C_{26}	$5^5(65)^3 5^4$
C_{28}	$5^3(65)^3 5^6 6$
C_{30}	$5^6 6^4 5^6$
C_{30}	$5^5 6 5 6^3 5 6 5^5$
C_{30}	$5^4(6^2 5)^2 5^6 6$

Table 1: A rewriting of a part of Table 2 of [10], giving the canonical codes of all fullerenes on ≤ 30 vertices.

$$T = 5^2 4 5^3 10 9 10 4_2 5^3 5_2 (54)^2 5_2 5 4 5_3 5 10$$

An undergraduate student Darja Gartner from Ljubljana wrote a computer program for generating a cubic polyhedron from its generalized spiral code. Her program has formed part of the Vega package since February 1994; see [16].

Theorem 2 *Every convex cubic polyhedron can be described by a generalized ring spiral.*

Proof. We give only a sketch. If false, there must be a smallest counterexample. Let us build a partial polyhedron P using the ordinary spiral. The inability to continue results from the fact that at some point adding a polygon F to the boundary ∂P would make the new partial polyhedron Q non-simply connected, see Figure 4. Let $(p_1 = 1, p_2, ..., p_k)$ be positions at which F meets P. There must be a gap between p_i and p_{i+1}. Take the boundary component of ∂Q that is the first after the edge where the face F was attached to P. This boundary component is composed of positions $p_1 + 1, p_1 + 2, ..., p_2 - 1$. Now proceed with the next face F' in a spiral-like step within this boundary component. This means F' touches P at step $p_1 + 1$. If the resulting partial polyhedron $P + F'$ is simply connected, then we succeeded to make another step in our generalized procedure, otherwise we repeat the argument but now the boundary component has the part belonging to ∂P shorter than before since P and F' may intersect only at some

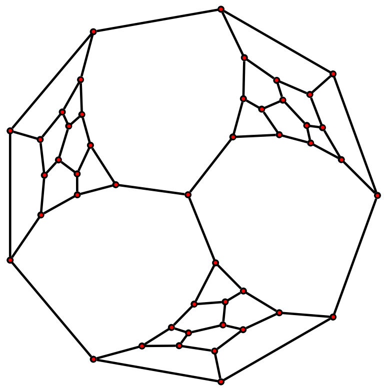

Figure 3: The Tutte graph

of the positions: $p_1+1, p_1+2, ..., p_2-1$. This follows from the renowned Jordan curve theorem from topology. Since we are working with integers, there are only a finite number of steps possible before we have to find a solution and make a step forward. After filling all but the last boundary component of Q by disks, we attach face F to the resulting partial polyhedron.

QED

Theorem 3 *The generalized ring spiral code for a convex cubic polyhedron can be computed in time $O(n^2)$.*

Proof. Since there are $O(n)$ starting positions we have only to show that one code - not necessarily the canonical one - can be found in linear time.

The key idea lies in efficient data structures, for instance cross-linked doubly-linked lists connecting the edges. In addition we present here the Algorithm P, a recursive procedure for patching holes.

- Algorithm P. [Patching a hole].
- Input: A hole H with lower and upper boundaries (+ global information about the unused faces)
- Recursive step: Add a face F at A.

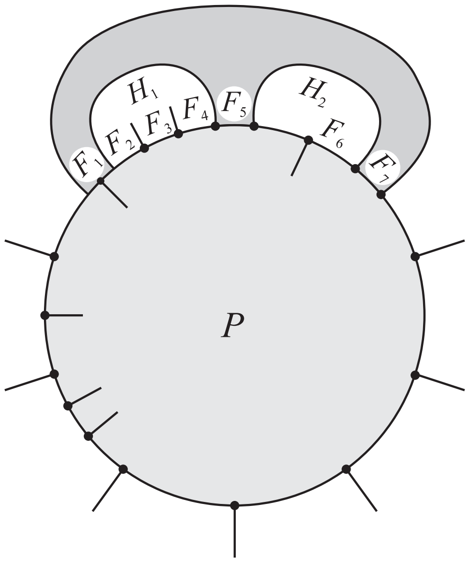

Figure 4: Attaching a face to a partial polyhedron may result in a multiply connected region.

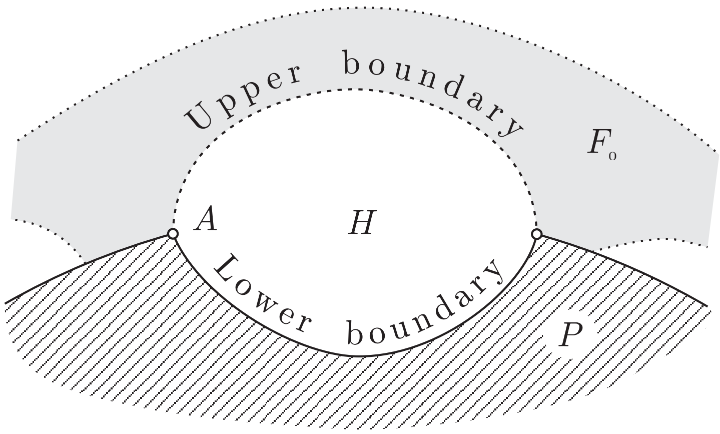

Figure 5: The hole H prevents the face F_0 from being attached to the partial polyhedron P.

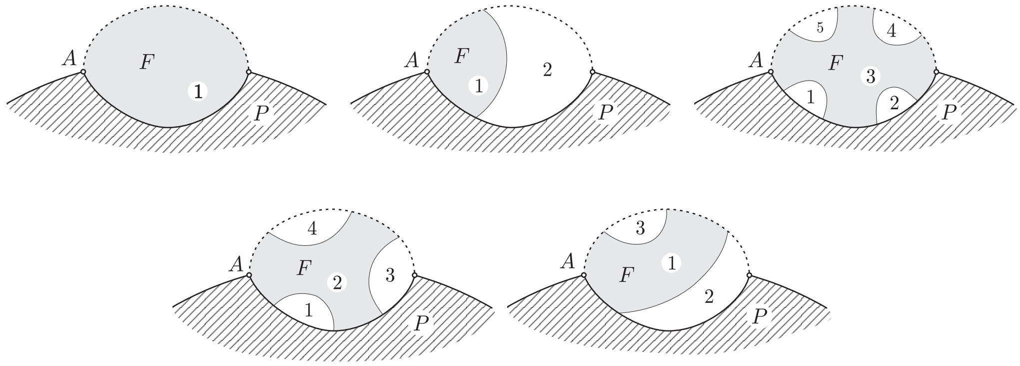

Figure 6: When trying out the face F at A, the remainder of the hole H breaks down into some lower and upper holes. The order of patches in typical cases is shown by the numbers inside the faces.

1. Try out the face F in order to determine new lower and upper holes.
2. Patch each lower hole
3. Patch F [Print out the size of F and its relative position along the current boundary]
4. Patch all upper holes.

The time complexity of Algorithm P is indeed linear. Clearly each face is considered only once and all vital information about its intersection with the boundary is stored and used later. Identification of lower and upper holes is computed at a cost that is constant per edge. Since each edge is considered only a constant number of times in the run of the entire algorithm our claim follows. In cubic planar polyhedra the number of edges and the number of faces is $O(n)$.

From the proof of the previous theorem we can deduce both the correctness of the algorithm and the fact that there is no need for backtracking. QED

Proper Generalized Spirals

The generalized spiral algorithm generates all sequences that are of interest here, in the planar case.

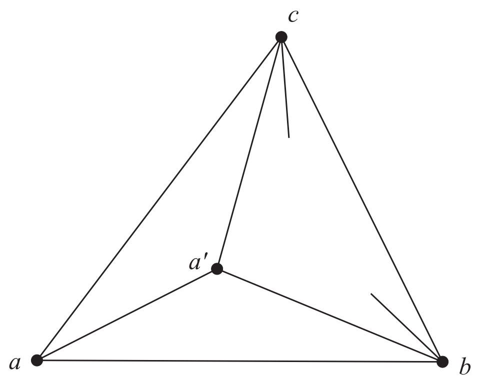

Figure 7: The cases 122 and 123 result in a smaller separating triangle $a'bc$.

A generalized spiral is called *proper* if the face r_{k+1} shares an edge with the face r_k. Note, that a ring spiral is always a generalized proper spiral.

There is an old result of Tutte that each four-connected planar graph is hamiltonian; see [18]. This means that a planar triangulation (deltahedron) without separating triangles is four-connected and hence hamiltonian as shown even earlier by Whitney; see [19]. Since the dual of a planar triangulation is a cubic map, a generalized spiral in a cubic map corresponds to a hamilton path in its dual. Hence, if a cubic map has the property that any three faces that are mutually adjacent are adjacent only along three edges with a common vertex, then such a map has a generalized spiral.

Actually we have:

Proposition 1 *A cubic map has a proper generalized spiral if and only if its dual has a Hamilton path.*

This is probably known but we include a proof in order to convince the reader.

Proposition 2 *No dual of a fullerene has a separating triangle.*

Proof. Let F^* be a triangulation, dual to a fullerene. Then F^* has vertices of valency 5 and 6, [15]. Let T, with vertices a, b, c be a separating triangle in F^*. At each corner of T we put a label, denoting the valency of that vertex that leads inside the triangle. Since T is separating, each label

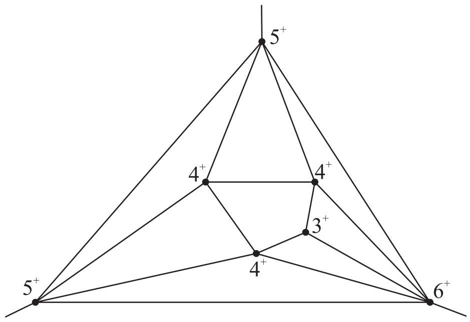

Figure 8: The case 223 would lead to a vertex of valency < 5.

is at least 1. Since F^* is a fullerene, each label is at most 3. The following are all possible cases:

$$111, 112, 113, 122, 123, 133, 222, 223, 233, 333.$$

Note that the label 11x implies 111 and the interior of T is capped. Since the interior vertex is of valency 3, F^* would not be a fullerene. The following cases remain:

$$122, 123, 133, 222, 223, 233, 333.$$

A label 3 inside implies a label 1 outside. Reversing the roles of inside and outside we rule out all cases 33x. The following cases remain:

$$122, 123, 222, 223.$$

Without loss of generality we may assume that T does not have a separating triangle in its interior.

This rules out 222. Case 12x leads to a smaller separating triangle. The only remaning case is 223 and is impossible since it would yield a vertex of valency < 5 inside T. QED

Corollary 1 *The dual of a fullerene is 4-connected.*

This gives us the following result.

Corollary 2 *A fullerene has a proper generalized spiral.*

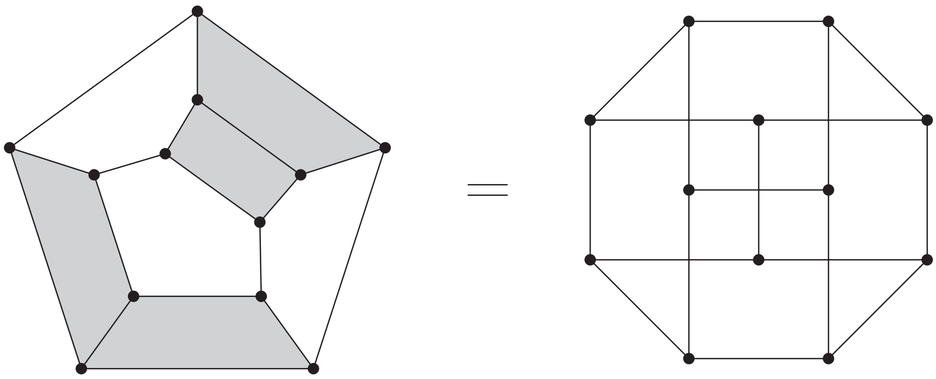

Figure 9: The smallest non-trivial omnispiral polyhedron has 12 vertices.

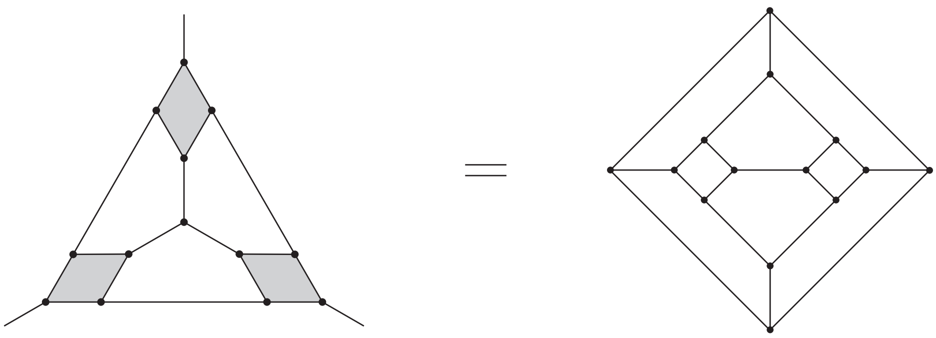

Figure 10: The next smallest non-trivial omnispiral polyhedron on 14 vertices has isolated quadrilaterals.

Omnispiral Polyhedra

One may think of polyhedra without a spiral as *the worst possible case* when each starting position leads to at least one non-spiral step. Here we take a brief look at the opposite extreme: the case where each starting position leads to a spiral. We call such a polyhedron an *omnispiral polyhedron.*

For instance, an $n-$sided prism Π_n is an omnispiral polyhedron. In general, there are three different starting positions, leading to the following codes:

- $n4^n n$

- $4^2 n 4 n 4^{n-3}$
- $4 n 4 n 4^{n-2}$

For a trigonal prism the first code is canonical while for $n > 3$ the second code is canonical.

The smallest possible case is the tetrahedron T with the (unique) code 3^4. Figures 9 and 10 depict the two smallest non-trivial omnispiral polyhedra which were found by Gunnar Brinkmann.

Non-cubic polyhedra

The generalized ring spiral code can be used to describe any regular planar polyhedron, but for non-cubic polyhedra the interpretation of the code has to be changed. For instance, a four-valent polyhedron can be built by repeatedly attaching polygons to a partial polyhedron. In case of cubic polyhedra, we used only 0 and 1 on the boundary of the disk. If we keep the meaning of 0, ie. a vertex whose valencies have been used, and interpret 1 as a vertex with one free valency, then we may introduce 2 to denote a vertex with two free valencies. Figure 11 shows how the elongated octahedron, ie. the polyhedron obtained by capping two opposite sides of a cube, can be built by a spiral.

There are several ways in which one can extend this approach to non-planar polyhedra, which could be useful for describing, say toroidal cages. However, the extensions we have found so far are not very natural and the time needed to find the canonical code may grow. Probably the most reasonable extension would be to attach faces as in the planar case but cutting the polyhedron along all those edges that would result in a non-planar polyhedron. This means that at the end one would have a disk with all faces attached correctly but on the boundary all edges would have to be pairwise identified. In this respect our code would become similar to the code proposed by Gunnar Brinkmann [2].

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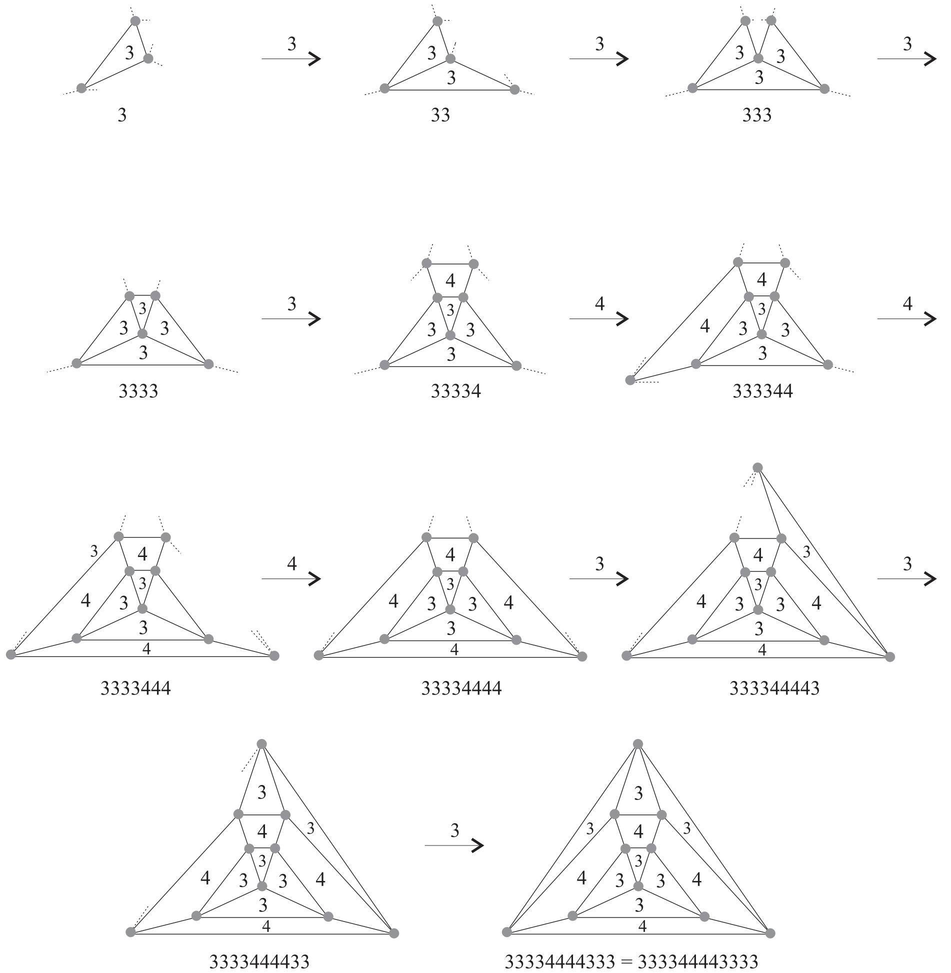

Figure 11: The elongated octahedron can be described by a generalization of the spiral code for 4-valent planar polyhedra. The sequence of face additions is shown. An obvious extension gives $3^4 4^{4m} 3^4$ for all members of the family of 4-valent planar polyhedra obtained by capping a tower of m cubes at both ends.