Elementary polycycles and their decompositions

Mathieu Dutour Sikirić

Institute Rudjer Bošković, Croatia and Universität Rostock

April 24, 2014

I. (R, q)-polycycles

### Definition

Given  $q \in \mathbb{N}$  and  $R \subset \mathbb{N}$ , a (R, q)-polycycle is a non-empty 2-connected plane, locally finite graph G with faces partitionned in two sets  $F_1$  and  $F_2$  ( $F_1$  is non-empty), so that:

- ▶ all elements of F<sub>1</sub> (called proper faces) are combinatorial *i*-gons with *i* ∈ *R*;
- all elements of F<sub>2</sub> (called holes) are pair-wisely disjoint, i.e. have no common vertices;
- ► all vertices have degree within {2,..., q} and all interior vertices are q-valent.

#### Examples with one hole



## Examples with two holes or more



# $({3}, 3)$ -polycycles

Any ( $\{3\},3$ )-polycycle is one of the following

Tetrahedron (with no hole):



► 3 following polycycles (with one hole):



# $({4}, 3)$ -polycycles

## Any ( $\{4\}, 3$ )-polycycle is one of the following

Cube (with no hole):



3 following polycycles (with one hole)



Following infinite family (with one hole):



# $({4}, 3)$ -polycycles

The infinite family Prism<sub>n</sub> (with two holes)



► Following two infinite ({4},3)-polycycles:



# ( $\{3\}, 4$ )-polycycles

Octahedron (with no hole):



Following polycycles (with one hole)



# $({3}, 4)$ -polycycles

Following infinite family (with one hole):



▶ The infinite family *APrism<sub>n</sub>* (with two holes)



▶ Following two infinite ({3},4)-polycycles:



singly infinite polycycle

doubly infinite polycycle

#### Curvature conditions

- ► A (*R*, *q*)-polycycle is called elliptic, parabolic or hyperbolic if  $\frac{1}{q} + \frac{1}{\max_{i \in R}{i}} \frac{1}{2}$  is positive, zero or negative, respectively.
- Elliptic cases:
  - q = 3 and R with  $\max_{i \in R} i \le 5$
  - q = 4 and R with  $\max_{i \in R} i \leq 3$
  - q = 5 and R with  $\max_{i \in R} i \leq 3$
- Parabolic cases:
  - q = 3 and R with  $\max_{i \in R} i = 6$
  - q = 4 and R with  $\max_{i \in R} i = 4$
  - q = 6 and R with  $\max_{i \in R} i = 3$
- All other cases are hyperbolic.

Limit case  $F_2 = \emptyset$ ,  $R = \{r\}$ 

Elliptic ({r}, q)-polycycles: 5 Platonic solids





Tetra-CubeOcta-Icosa-Dodeca-hedronhedronhedronhedronhedron

Parabolic ({r}, q)-polycycles: 3 regular plane tilings





► Hyperbolic ({*r*}, *q*)-polycycles: infinity

Generalization and (r, q)-polycycles

- ▶ A generalization of (*R*, *q*)-polycycle is (*R*, *Q*)-polycycles: the valency of interior vertices belong to a set *Q*. All the theory extends to this case.
- A (r, q)-polycycle is a ({r}, q)-polycycle with only one hole (the exterior one). Their theory has additional features:
  - ► There exist a canonical model of them in the form of (r<sup>q</sup>) regular partition.
  - ► For any (r, q)-polycycle P, simple connectedness of P ensures the existence of a canonical map from P to (r<sup>q</sup>).

# Main examples of (r, q)-polycycles

	Elliptic	Parabolic	Hyperbolic
(r,q)	(3,3), (3,4), (4,3)	(4, 4)	all
	(5,3), (3,5)	(3,6),(6,3)	others
Exp.	$\alpha_3$ , $\beta_3$ , $\gamma_3$ , Do, Ico	$(4^4), (6^3), (3^6)$	( <i>r</i> <sup><i>q</i></sup> )
reg.part	of sphere $S^2$	of Euclidean	of hyperbolic
		plane $\mathbb{R}^2$	plane $\mathbb{H}^2$



Polyominoes: Conway, Penrose, Colomb (games, tilers of  $\mathbb{R}^2$ , etc.), enumeration (in Physics, Statistical Mechanics). Polyhexes: application in Organic Chemistry. II. Decomposition into elementary polycycles

# Elementary polycycles

- ► A bridge of a (R, q)-polycycle is an edge, which is not on a boundary and goes from a hole to a hole (possibly, the same).
- An elementary (R, q)-polycycle is one without bridges.
- Examples:





An elementary  $({5}, 3)$ -polycycle

# Open edges

► An open edge of an (*R*, *q*)-polycycle is an edge on a boundary such that each of its end-vertices have degree less than *q*.

Examples



#### Decomposition theorem

- Theorem: Any (R, q)-polycycle is uniquely decomposed into elementary (R, q)-polycycles along its bridges.
- In other words, any (R, q)-polycycle is obtained by gluing some elementary (R, q)-polycycles along open edges.



# Summary

- Elementary (R, q)-polycycles provide a decomposition of (R, q)-polycycles.
- ► In order for this to be useful, we have to classify the elementary (R, q)-polycycles.
- For non-elliptic cases, there is no hope of classification (there is a continuum of elementary ones):



III. Classification
 of elementary
({2,3,4,5},3)-polycycles

## With at least one 2-gon

All elementary  $(\{2,3,4,5\},3)$ -polycycles, containing a 2-gon, are those eight ones:



# Totally elementary polycycle

- Call an elementary (R, 3)-polycycle totally elementary if, after removing any face adjacent to a hole, one obtains a non-elementary (R, 3)-polycycle.
- Examples:



A totally elementary polycycle



A non-totally elementary polycycle

# Classification result I



# Classification result II

(iii) the following doubly infinite ({5},3)-polycycle, denoted by  $Barrel_{\infty}$ :



(iv) the infinite series of  $Barrel_m$ ,  $m \ge 2$ :



# Classification methodology

- If an elementary polycycle is not totally elementary, then it is obtained from another elementary one with one face less.
- So, from the list of elementary ({3,4,5},3)-polycycles with n faces, one gets the list of elementary ({3,4,5},3)-polycycles with n + 1 faces.



## Full classification

Theorem: Any elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycle is one of: (i) 204 sporadic polycycles with 4 to 11 proper faces (ii) an element of the infinite series of  $Barrel_m$ ,  $2 \le m \le \infty$ . (iii) six  $(\{3, 4, 5\}, 3)$ -polycycles, infinite in one direction: δ  $\alpha$ ε  $\gamma$  $\mu$ 

(iv)  $21 = \binom{6+1}{2}$  infinite series obtained by taking two endings of the above infinite polycycles and concatenating them.

See below three examples in the infinite series  $\beta \varepsilon$ 



# Subcase of $({5}, 3)$ -polycycles

 $C_2$ 

(i) Sporadic elementary ({5}, 3)-polycycles:



 $A_1$ 









 $A_3$ 









 $C_3$ 



(ii) The infinite series of elementary ( $\{5\}, 3$ )-polycycles  $\alpha \alpha$ :



(iii) The infinite series of elementary ( $\{5\}, 3$ )-polycycles  $Barrel_q$ ,  $q \ge 3$ :



(iv) The only elementary infinite ({5},3)-polycycle are  $\textit{Barrel}_\infty$  and  $\alpha$ 

IV. Classification of elementary ({2,3},4)-polycycles

# The classification

Any elementary  $(\{2,3\},4)$ -polycycle is one of the following eight:



V. Classification of elementary ({2,3},5)-polycycles

# The technique

- Take an elementary ({2,3},5)-polycycle. If v is a vertex on the boundary, then we can consider all possible ways to make this vertex an interior vertex in an elementary ({2,3},5)-polycycle.
- ▶ From the list of elementary ({2,3},5)-polycycles with n interior vertices, one can obtain the list of elementary ({2,3},5)-polycycles with n + 1 interior vertices.



## The classification

Any elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycle is one of:

- (i) 57 sporadic  $(\{2,3\},5)$ -polycycles.
- (ii) three following infinite  $(\{2,3\},5)$ -polycycles:



# (iii) the following 5-valent doubly infinite ({2,3},5)-polycycle, called snub ∞-antiprism:



(iv) the infinite series of snub *m*-antiprisms,  $m \ge 2$  (two *m*-gonal holes):



(v) six infinite series of ({2,3},5)-polycycles with one hole (they are obtained by concatenating endings  $\alpha$ ,  $\beta$ ,  $\gamma$ )

Subcase of ( $\{3\}, 5$ )-polycycles I

(i) Sporadic elementary ( $\{3\}, 5$ )-polycycles:


# Subcase of $({3}, 5)$ -polycycles II



(ii) The infinite series of elementary ({3}, 5)-polycycles  $\alpha\alpha$ :



- (iii) The only elementary infinite ({3},5)-polycycles are  $\alpha$  and snub  $\infty$ -antiprism.
- (iv) The infinite series of elementary ({3},5)-polycycles snub m-antiprisms,  $m \ge 2$ :

VI. Application to extremal polycycles

### Definition

- Given a finite (r, q)-polycycle P, denote by
  - *n<sub>int</sub>(P)* the number of interior vertices
  - and  $f_1(P)$  the number of faces in  $F_1$ .
- Fix x ∈ N. An (r, q)-polycycle with f<sub>1</sub>(P) = x is called extremal if it has maximal n<sub>int</sub>(P) among all (r, q)-polycycles with f<sub>1</sub>(P) = x.
- Problem: to find  $N_{r,q}(x)$ , the maximal number of vertices.
- ► Fact: For fixed r, q, f<sub>1</sub>(P) = x extremal polycycle has also maximal n<sub>int</sub>(P), e<sub>int</sub>(P) (interior faces) and minimal n, l, Perim = n<sub>ext</sub>
- ▶ For (r, q)=(3,3), (4,3), (3,4), the question is trivial.
  8 authors, 1997: found N<sub>5,3</sub>(x) for x < 12 (unique, partial subgraph of Dodecahedron).</li>

#### Use of elementary polycycles

If a (r, q)-polycycle P is decomposed into elementary (r, q)-polycycles (EP<sub>i</sub>)<sub>i∈I</sub> appearing x<sub>i</sub> times, then one has:

$$\begin{cases} n_{int}(P) = \sum_{i \in I} x_i n_{int}(EP_i) \\ f_1(P) = \sum_{i \in I} x_i f_1(EP_i) \end{cases}$$

If one solves the Linear Programming problem

maximize 
$$\sum_{i \in I} x_i n_{int}(EP_i)$$
  
with  $x = \sum_{i \in I} x_i f_1(EP_i)$   
and  $x_i \in \mathbb{N}$ 

and if  $(x_i)_{i \in I}$  realizing the maximum can be realized as (r, q)-polycycle, then  $N_{r,q}(x)$  can be found.

# Small extremal (5, 3)-polycycles

x	$N_{5,3}(x)$	extremal	components
1	0		D
2	0		D, D
3	1		$E_1$
4	2		E <sub>2</sub>
5	3		E <sub>3</sub>

x	$N_{5,3}(x)$	extremal	components
6	5		$A_5$
7	6		B <sub>3</sub>
8	8	KH	$A_4$
9	10		A <sub>3</sub>
10	12		<i>A</i> <sub>2</sub>

x	$N_{5,3}(x)$	extremal	components
11	15		$A_1$
12	10	AT AT	$E_{1}, B_{2}$
			$D, C_1, D$
		TET	<i>C</i> <sub>1</sub> , <i>D</i> , <i>D</i>
			E <sub>10</sub>

## Extremal (5, 3)-polycycles

• Theorem: For any  $x \ge 12$ , one has

$$N_{5,3}(x) = \begin{cases} x & \text{if } x \equiv 0, 8, 9 \pmod{10}, \\ x - 1 & \text{if } x \equiv 6, 7 \pmod{10}, \\ x - 2 & \text{if } x \equiv 1, 2, 3, 4, 5 \pmod{10}. \end{cases}$$

- Extremal polycycle realizing the extremum:
  - If  $x \equiv 0 \pmod{10}$  (unique):





• If  $x \equiv 9 \pmod{10}$  (unique):









• If  $x \equiv 8 \pmod{10}$  (unique):



• If  $x \equiv 7 \pmod{10}$  (non-unique):







• If  $x \equiv 6 \pmod{10}$  (non-unique):





▶ Otherwise (non-unique): *E<sub>n</sub>* 

# Extremal (3, 5)-polycycles

#### Theorem

- $N_{3,5}(x) = \lfloor \frac{x}{3} \rfloor + 1$  for  $x \equiv 14, 16, 17 \pmod{18}$ ,
- ▶  $N_{3,5}(x) = \lfloor \frac{x}{3} \rfloor 1$  for  $x \equiv 3, 4, 6, 7, 9, 11 \pmod{18}$ , and

• 
$$N_{3,5}(x) = \lfloor \frac{x}{3} \rfloor$$
, otherwise,

but with 5 exceptions: above value plus 1 for x = 11, 15, 17 and N<sub>3,5</sub>(x) = x − 10 for 16 ≤ x ≤ 19.

### Non-elliptic case

► For parabolic (r, q)-polycycles (i.e. (r, q)=(4, 4), (6, 3) or (3, 6)) the method of elementary polycycles fails (since there is no classification) but "extremal animals" of Harary-Harborth 1976 (proper ones, growing as a spiral) are extremal:



Hyperbolic cases are very difficult.

VII. Application to non-extendible polycycles

## Definition

A (r, q)-polycycle is called non-extendible if it is no proper subgraph of another (r, q)-polycycle. Examples:



Extendible (3, 4)-polycycle



## Classification

Theorem: All non-extendible (r, q)-polycycles are:

- Regular partitions (r<sup>q</sup>)
- Four following examples:



### Infinite non-extendible polycycles

• Take the two elementary (5,3)-polycycles and



form infinite word  $\dots u_{-1}u_0u_1\dots$  with  $u_i$  being  $C_2$  or  $C'_2$ . This gives a continuum of non-extendible (5,3)-polycycles.

- ► Similarly, one has a continuum of (3,5)-polycycles.
- ► For non-elliptic (r, q), one takes the infinite tiling (r<sup>q</sup>), removes an infinity of r-gonal faces sharing no edges and takes the universal cover of this (r, q)-polycycle.

#### Finite non-extendible polycycles

- ► Main lemma: all finite non-extendible (r, q)-polycycles are elliptic, i.e. <sup>1</sup>/<sub>q</sub> + <sup>1</sup>/<sub>r</sub> > <sup>1</sup>/<sub>2</sub>
- ► So, we can use decomposition of non-extendible (r, q)-polycycles into elementary (r, q)-polycycles and the classification of them.
- Given an (r, q)-polycycle P, the graph of its elementary components is denoted by el(P); its vertices are its elementary (r, q)-polycycles with two elementary (r, q)-polycycles adjacent if they share an edge:



- ► A finite ({r}, q)-polycycle P is a (r, q)-polycycle if and only if el(P) is a tree.
- Every tree is either an isolated vertex, or contains at least one vertex of degree 1.
- One checks on this vertex that there is only two possibilities:



VIII. 2-embeddable (r, q)-polycycles

#### 2-embedding

• The Hamming distance on  $\{0,1\}^n$  is defined by

$$d(x,y) = \#\{1 \le i \le n \text{ s.t. } x_i \neq y_i\}$$

- ▶ Given a connected graph G, denote by d<sub>G</sub> the shortest path distance between vertices of G
- ► A graph *G* is said to be 2-embeddable if, for some *n*, there exists a mapping

$$\psi: V(G) \rightarrow \{0,1\}^S$$
  
 $v \mapsto \psi(v)$ 

such that, for all vertices v, v' of G, one has  $d(\psi(v), \psi(v')) = 2d_G(v, v')$ 

#### Alternating zones

- In a plane graph G, an alternating zone, is a sequence of edges e<sub>i</sub> such that e<sub>i</sub> and e<sub>i+1</sub> belong to a same face F<sub>i</sub> and it holds:
  - If  $|F_i|$  is even,  $e_i$  and  $e_{i+1}$  in opposition
  - If |F<sub>i</sub>| is odd, e<sub>i</sub> and e<sub>i+1</sub> are opposed. There are two possible choices for e<sub>i+1</sub> given e<sub>i</sub> and they are required to alternate.
- ► A subgraph H of G is called convex if, for any two vertices v, v' of H, all shortest paths between v and v' are included in H.
- ► If Z is a not self-intersecting alternating zone, then G Z consists of two graphs G<sub>i</sub>. If both G<sub>i</sub> are convex, then we say that Z defines convex cut.

#### Examples

Two (3,5)-polycycles with an non-convex alternating zone:



Two (5,3)-polycycles with an alternating zone, which is not convex:



# Embedding of (r, q)-graph

- ► If the alternating zones of a plane graph G define convex cuts, then G is 2-embeddable.
- Above condition is not necessary.
- ► A (r, q)-graph is a plane graph such that all interior faces have at least r edges and all interior vertices have degree at least q.
- Chepoi et al.: (4,4)-, (3,6)- and (6,3)-graphs are 2-embeddable.
- ► So, all parabolic and hyperbolic (r, q)-polycycle are 2-embeddable.

## Elliptic 2-embeddable (r, q)-polycycles

For elliptic (r, q) ≠ (5, 3), (3, 5) (i.e., (3, 3), (3, 4), (4, 3)), only three polycycles are non-embeddable:



- A (3,5)-polycycle different from Icosahedron {3,5} and {3,5} − v, is 2-embeddable if and only if it does not contain, as an induced subgraph, any of (3,5)-polycycles c<sub>3</sub> and d + e<sub>2</sub> + d.
- A (5,3)-polycycle different from Dodecahedron {5,3} is
  2-embeddable if and only if it does not contain, as an induced subgraph, any of (5,3)-polycycles E<sub>4</sub> and D + E<sub>2</sub> + D.

IX. Application to face-regular spheres

#### Euler formula

- Take a 3-valent plane map and denote by p<sub>k</sub> the number of faces having k edges.
- Then one has the equality

$$12 = \sum_{k=3}^{\infty} (6-k) p_k$$

- So, every 3-valent plane map has at least one face of size less than 6.
- ▶ So, 3-valent plane graphs with faces of gonality at most 5
  - have at most 12 faces,
  - have at most 20 vertices.

### Face-regular maps

- A (p, q)-sphere is a 3-valent plane graphs, whose faces are por q-gonal.
- Take G a (p, q)-sphere. Then:
  - G is called pR<sub>i</sub> if every p-gonal face is adjacent to exactly i p-gonal faces.
  - ► G is called qR<sub>j</sub> if every q-gonal face is adjacent to exactly j q-gonal faces.
- The subject of enumerating them is very large. We intend to show non-trivial results obtained by using decomposition into elementary polycycles.
- p ≤ 5. So, if one removes all q-gonal faces and all edges between any two q-gonal faces, then the result is a ({p}, 3)-polycycle.

## Polycycles of (5, q)-sphere $qR_0$

- ► The set of 5-gonal faces of (5, q)-sphere qR<sub>0</sub> is decomposed into elementary ({5}, 3)-polycycles.
- Let us see in the classification the elementary polycycles that could be ok
  - They should be finite (this eliminate  $Barrel_{\infty}$  and  $\alpha$ )
  - They should have some vertices of degree 2 (this eliminates Dodecahedron and *Barrel<sub>k</sub>*)
  - It should be possible to fill open edges so as to have no pending vertices of degree 2.









NO









NO







NO





The infinite series of elementary ({5},3)-polycycles  $\alpha\alpha$ :





# (5, q)-sphere $qR_0$

► The set of 5-gonal faces of (5, q)-sphere qR<sub>0</sub> is decomposed into the following elementary ({5}, 3)-polycycles:



- ► The major skeleton Maj(G) of a (5, q)-sphere qR<sub>0</sub> is a 3-valent map, whose vertex-set consists of polycycles E<sub>1</sub> and C<sub>3</sub>.
- ► It consists of *el*(*G*) with the vertices C<sub>1</sub> (of degree 2) being removed.



A (5, 14)-sphere  $14R_0$ 



The decomposition into elementary polycycles.



Their names in the classification of  $({5}, 3)$ -polycycles.



The graph el(G)



Maj(G): eliminate  $C_1$ , so as to get a 3-valent map

#### Results

Theorem: For a (5, q)-sphere  $qR_0$ , the gonality of faces of the 3-valent map Maj(G) is at most  $\lfloor \frac{q}{2} \rfloor$ .

- ▶ Proof: Take a q-gonal face F. Denote by x<sub>E1</sub>, x<sub>C3</sub> and x<sub>C1</sub> the number of ({5}, 3)-polycycles E<sub>1</sub>, C<sub>3</sub> and C<sub>1</sub> incident to F.
- Counting edges, one gets:

$$q = 2x_{E_1} + 3x_{C_3} + 5x_{C_3}$$

which implies  $q \ge 2(x_{E_1} + x_{C_3})$ .

▶ But x<sub>E1</sub> + x<sub>C3</sub> is the gonality of the face corresponding to F in Maj(G).
## Results

Theorem: For q < 12, we have a finite number of (5, q)-spheres  $qR_0$ .

- **Proof**: Take such a plane graph *G*.
- ► The associated map Maj(G) is 3-valent with faces of gonality at most 5.
- So, the number of  $(\{5\}, 3)$ -polycycles  $E_1$  and  $C_3$  is at most 20.
- The number of polycycles *C*<sub>1</sub> is bounded as well.
- This implies that the number of vertices of G is bounded and so, we have a finite number of spheres.

For details and extensions, see:

 M. Deza, M. Dutour Sikirić, Geometry of Chemical Graphs: Polycycles and Two-faced Maps, Cambridge University Press, Series: Encyclopedia of Mathematics and its Applications (No. 119) 2008.