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Clusters of cycles

Michel Deza [a,*], Mikhail Shtogrin [b]

[a] *CNRS and Ecole Normale Supérieure, 45 rue d'Ulm, 75005 Paris, France*
[b] *Steklov Mathematical Institute, 8 Gubkin str., 117966 Moscow, Russia*

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Abstract

A *cluster of cycles* (or (r, q)*-polycycle*) is a simple planar 2-connected finite or countable graph G of girth r and maximal vertex-degree q, which admits an (r, q)*-polycyclic realization* $P(G)$ on the plane. An (r, q)-polycyclic realization is determined by the following properties: (i) all interior vertices are of degree q; (ii) all interior faces (denote their number by p_r) are combinatorial r-gons; (iii) all vertices, edges and interior faces form a cell-complex.

An example of (r, q)-polycycle is the skeleton of (r^q), i.e. of the q-valent partition of the sphere, Euclidean plane or hyperbolic plane by regular r-gons. Call *spheric* pairs $(r, q) = (3, 3)$, $(4, 3)$, $(3, 4)$, $(5, 3)$, $(3, 5)$. Only for those five pairs, $P((r^q))$ is (r^q) without exterior face; otherwise, $P((r^q)) = (r^q)$.

Here we give a compact survey of results on (r, q)-polycycles. We start with the following general results for any (r, q)-polycycle G: (i) $P(G)$ is unique, except of (easy) case when G is the skeleton of one of the five Platonic polyhedra; (ii) $P(G)$ admits a cell-homomorphism f into (r^q); (iii) a polynomial criterion to decide if given finite graph is a polycycle, is presented.

Call a polycycle *proper* if it is a partial subgraph of (r^q) and a *helicene*, otherwise. In [ARS Comb. A 29 (1990) 5], all proper spheric polycycles are given. An (r, q)-helicene exists if and only if $p_r > (q-2)(r-1)$ and $(r, q) \neq (3, 3)$. We list the (4,3)-, (3,4)-helicenes and the number of (5,3)-, (3,5)-helicenes for first interesting p_r. Any outerplanar (r, q)-polycycle G is a proper $(r, 2q-2)$-polycycle and its projection $f(P(G))$ into (r^{2q-2}) is convex. Any outerplanar $(3, q)$-polycycle G is a proper $(3, q+2)$-polycycle.

The symmetry group *Aut*(G) (equal to *Aut*$(P(G))$, except of Platonic case) of an (r, q)-polycycle G is a subgroup of *Aut*$((r^q))$ if it is proper and an extension of *Aut*$(f(P(G)))$, otherwise. *Aut*(G) consists only of rotations and mirrors if G is finite, so its order divides one of the numbers $2r$, 4 or $2q$. Almost all polycycles G have trivial *AutG*.

Call a polycycle G *isotoxal* (or *isogonal*, or *isohedral*) if *AutG* is transitive on edges (or vertices, or interior faces); use notation IT (or IG, or IH), for short. Only r-gons and non-spheric (r^q) are isotoxal. Let $T^*(l, m, n)$ denote Coxeter's triangle group of a triangle on S^2, E^2 or H^2 with angles $\pi/l, \pi/m, \pi/n$ and let $T(l, m, n)$ denote its subgroup of index 2, excluding motions of 2nd kind.

* Corresponding author.
E-mail addresses: michel.deza@ens.fr (M. Deza), stogrin@mi.ras.ru (M. Shtogrin).

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We list all IG- or IH-polycycles for spheric (r, q) and construct many examples of IH-polycycles for general case (with *AutG* being above two groups for some parameters, including strip and modular groups). Any IG-, but not IT-polycycle is infinite, outerplanar and with same vertex-degree, we present two IG-, but not IH-polycycles with $(r, q) = (3, 5), (4, 4)$ and $AutG = T(2, 3, \infty) \sim PSL(2, Z)$, $T^*(2, 4, \infty)$. Any IH-polycycle has the same number of boundary edges for each its r-gon. For any $r \geq 5$, there exists a continuum of *quasi*-IH-polycycles, i.e. not isohedral, but all r-gons have the same 1-corona.

On two notions of extremal polycycles:

1. We found for the spheric (r, q) the maximal number n_{int} of interior points for an (r, q)-polycycle with given p_r; in general case, $(p_r/q) \leq n_{\text{int}} < (rp_r/q)$ if any r-gon contains an interior point.
2. All *non-extendible* (r, q)-polycycles (i.e. not a proper subgraph of another (r, q)-polycycle) are (r^q), four special ones, (possibly, but we conjecture their non-existence) some other finite (3,5)-polycycles, and, for any $(r, q) \neq (3, 3), (3, 4), (4, 3)$, a continuum of infinite ones.

On isometric embedding of polycycles into hypercubes Q_m, half-hypercubes $\frac{1}{2}Q_m$ and, if infinite, into cubic lattices Z_m, $\frac{1}{2}Z_m$: for $(r, q) \neq (5, 3), (3, 5)$, there are exactly three non-embeddable polycycles (including $(4^3) - e$, $(3^4) - e$); all non-embeddable (5,3)-polycycles are characterized by two forbidden sub-polycycles with $p_5 = 6$.

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1. Definition and examples

A *cluster of cycles* (a *polycycle*, for short, or (r, q)*-polycycle*) is a simple planar 2-(vertex)-connected finite or countable graph G of girth r and maximal vertex-degree q, which admits an (r, q)*-polycyclic realization* $P(G)$ on the plane.

An (r, q)-polycyclic realization is determined by the following properties:

1. all interior vertices are of degree q;
2. all interior faces are (combinatorial) r-gons;
3. all vertices, edges and interior faces form a cell-complex (i.e. the intersection of any two faces is edge, vertex or $\emptyset$).

One can show that (3) follows from (1) and (2), while neither (1) and (3) imply (2), nor (2) and (3) imply (1).

For example, $(3, q)$- and $(4, q)$-polycycles are just simplicial and cubical complexes of dimension 2.

The main example of (r, q)-polycycle is the skeleton of (r^q), i.e. of the q-valent partition of the sphere S^2, Euclidean plane R^2 or hyperbolic plane H^2 by regular r-gons. For $(r, q) = (3, 3), (4, 3), (3, 4), (5, 3), (3, 5)$, the unique (r, q)-polycycle is, respectively, Platonic tetrahedron, cube, octahedron, dodecahedron, icosahedron on S^2, *but with excluded exterior face*; for $(r, q) = (6, 3), (3, 6), (4, 4)$, it is regular partition (6^3), (3^6), (4^4) of R^2; all other (r^q)s are regular partitions of H^2.

Call a polycycle *proper* if it is a partial subgraph of (the skeleton of) the regular partition (r^q). Call a proper (r, q)-polycycle *induced* (moreover, *isometric*) if it is induced (moreover, isometric) subgraph of (r^q).

Call an (r, q)-polycycle *spheric, Euclidean* or *hyperbolic,* if (r^q) is the regular partition of S^2, R^2 or H^2, respectively. (One can also use terms *elliptic*, *parabolic* or *hyperbolic*, since $rq < 2(r+q)$, $rq = 2(r+q)$ or $rq > 2(r+q)$, respectively.) There is a literature (see e.g., Section 9.4 of [17] and [4]) about proper Euclidean polycycles (*polyhexes*, *polyamonds*, *polyominoes* for (6^3), (3^6), (4^4), respectively); the terms come from usual terms *hexagon*, *diamond*, *domino*, where the last two correspond to the case p_3, $p_4 = 2$. Polyominoes were considered first by Conway, Penrose, Colomb as tilers (of R^2, etc.; see e.g. [7]) and in the games; later they were used for enumeration in physics and statistical mechanics. Polyhexes are used widely (see e.g. [3,16]) in organic chemistry: they represent *completely condensed polycyclic aromatic hydrocarbons* (PAHs) C_nH_m with n vertices (atoms of the carbon C), including m vertices of degree 2, where atoms of the hydrogen H are adjoined. All 39 proper $(5, 3)$-polycycles were found in [8] in chemical context, but already in [18] were given all 3, 6, 9, 39, 263 proper spheric (r, q)-polycycles for $(r, q) = (3, 3), (4, 3), (3, 4), (5, 3), (3, 5)$, respectively.

A general theory of polycycles is considered in [10–15,21,22], namely proofs can be found as follows: Theorem 1 in [21,22], Theorems 2 and 3 in [10,12,13], Theorems 4–6 in [14], Theorems 7–9 in [15] and Theorem 10 in [11,14].

2. Criterion and unicity

Theorem 1. *Let G be any finite connected graph of girth r, different from the skeleton of* (3^3), (3^4), (4^3), (3^5), (5^3); *let v, e, f be its number of vertices, edges and r-cycles, respectively. Then G is* (r, q)*-polycycle if and only if it holds.*

1. *Any edge belongs to one or two r-cycles of the graph G.*
2. *All edges, belonging to exactly one r-cycle of G, form a simple cycle.*
3. *The intersection of any two different r-cycles is an edge, a vertex or* $\emptyset$.
4. $v - e + f = 1$.
5. *All r-cycles with common vertex can be organized into a sequence, such that any two neighbors have the common edge, containing the common vertex, and this sequence has at most q members with equality if and only if it is closed (i.e. the sequence form a cycle).*

It is clear that: (1) implies that G is 2-connected, (5) implies that any interior vertex of G has degree q and that for $q = 3$ the condition (5) is implied by (1)–(4) with exclusion in (3) of the case of intersection in a vertex.

Theorem 2. *Let G be an* (r, q)*-polycycle. Then*

1. *If G is the skeleton of one of the five Platonic polyhedra, then the number of* (r, q)*-polycyclic realizations of G is equal to the number of faces of the Platonic polyhedron and all those realizations are isomorphic.*

2. *Any other polycycle G has unique* (r, q)*-polycyclic realization and the number of its interior faces (which are all should be r-gons) is the number of r-cycles of G.*

The (r, q)-polycyclic realization $P(G)$ of a non-Platonic (r, q)-polycycle G is, in general, not unique *planar* realization of polycycle G.

3. Proper polycycles versus helicenes

First, we list all (3,3)-, (4,3)-, (3,4)-polycycles. Clearly, all (3,3)-polycycles are (3^3), (3^3)-v and (3^3)-e (i.e. a vertex with incident edges, or an edge is deleted); the last one is not induced.

We denote by P_n a path with n vertices and by P_N, P_Z infinite paths in one or both directions. All (4,3)-polycycles are: (4^3), (4^3)-v, (4^3)-e, $P_2 \times P_n$ for any natural n and two infinite ones: $P_2 \times P_N$, $P_2 \times P_Z$. Only (4^3), (4^3)-v, $P_2 \times P_2$, $P_2 \times P_3$, $P_2 \times P_4$, (4^3)-e are proper; the last two are not induced.

The number of (3,4)-polycycles is also countable, including two infinite ones (nine of the (3,4)-polycycles are proper and five of the proper ones are induced), namely all (3,4)-polycycles are: proper ones (3^4), (3^4)-v, (3^4)-e, (3^4)-P_3, (3^4)-C_3, G_n $(1 \le n \le 4)$ and unproper ones G_n ($n \ge 5$ and $n = N, Z$) and the *vertex-split* (3^4), defined below. Here $G_n = A_{n/2}$ if n is even, $G_n = B_{(n+1)/2}$ if n is odd, $G_n = A_n$ if $n = N, Z$, where A_m is (4,3)-polycycle $P_2 \times P_m$ with parallel diagonals, added one on each square, and B_m is A_m without a vertex of degree 2.

For all other (r, q), there is a continuum of (r, q)-polycycles and the number of finite ones among them is countable.

Call *vertex-split* (3^4), a (3,4)-polycycle, coming from (3^4) as follows: let $K_{x,\{a,b,c,d\}}$ be induced 4-wheel in (3^4), then replace the edges (x, a), (x, b) of (3^4) by the edges (x', a), (x', b), where x' is a new vertex of degree 2. (Curiously, this plane graph is the logo of the HSBC, Hong Kong and Shanghai Banking Corporation.)

Call *vertex-split* (3^5), a (3,5)-polycycle, coming from (3^5) as follows: let $K_{x,\{a,b,c,d,e\}}$ be induced 5-wheel in (3^5), then replace the edges (x, a), (x, b) of (3^5) by the edges (x', a), (x', b), where x' is a new vertex. See both polycycles in Section 5.2.

3.1. Cell-homomorphism into (r^q) and helicenes

Theorem 3. *Any* (r, q)*-polycyclic realization* $P(G)$ *admits a cell-homomorphism into* (r^q) *and such homomorphism is defined uniquely by a flag* (*i.e. incident vertex, edge and interior face of* $P(G)$) *and its image*.

Clearly, the above homomorphism is an isomorphism if and only if G is a proper polycycle (i.e. if the map $P(G) \to (r^q)$ is topologic: there is no pair of vertices or of edges, having the same image). In view of Theorem 3, any unproper (r, q)-polycycle is called (r, q)*-helicene*.

It is easy to check that (r, q)-helicenes exist if and only if $(r, q) \neq (3, 3)$ and $p_r \ge (q-2)(r-1)+1$ with equality only for the helicene being a belt of r-gons, going around an r-gon. All (4,3)-helicenes are two infinite ones: $P_2 \times P_N$, $P_2 \times P_Z$ and $P_2 \times P_n$ for any $n \geq 5$; given above full description of all (3,4)-polycycles, permit also to list all (3,4)-helicenes. We counted that the number of (5,3)-helicenes is 1, 7, 29 for $p_5 = 5, 6, 7$ and the number of (3,5)-helicenes is 1, 4, 20, 74 for $p_3 = 7, 8, 9, 10$.

A natural parameter to measure an (r, q)-helicene will be the degree of the corresponding homomorphism into (r^q) (on vertices, edges and faces). For $q \geq 4$, helicenes appear with vertices, but not edges, having same homomorphic image. The vertex-split (3^4) is unique such maximal helicene for $(r, q) = (3, 4)$ (x, x' are such vertices). There is a finite number of such helicenes for $(r, q) = (3, 5)$; one of them is the vertex-split (3^5).

3.2. Cell-complexes $P(G)$, $K(G)$, $X(G)$ and the curvature

Denote by $K(G)$ the abstract two-dimensional polyhedron with a metric, such that all r-gons of $P(G)$ became planar Euclidean regular r-gons; clearly, there is combinatorial cell-isomorphism between $K(G)$ and $P(G)$. The map $K(G) \to K(r^q)$ is a geometric realization of the combinatorial map $P(G) \to (r^q)$, such that the homomorphism is locally homeomorphic, i.e. it is continuous cell-map with isomorphic ϵ-neighborhood for sufficiently small ϵ (*homeomorphic* means *isometric* and *global* homeomorphism means *isomorphism*).

The Gaussian curvature of a point in $K(G)$ is $2\pi - q((r-2)/r)\pi$ in each interior vertex (since in each interior vertex meet q angles of regular Euclidean r-gons) and 0 in any other point (since $K(G)$ is a disc glued from Euclidean r-gons). So the global curvature of $K(G)$ is the sum of its curvatures in interior vertices:

$$n_{\text{int}}\left(2\pi - q\left(\frac{r-2}{r}\right)\pi\right) = n_{\text{int}}\frac{\pi}{r}(2(r+q) - rq).$$

For example, the curvature of G is 3π for $G = (3^5), (5^3)$, 2π for $G = (4^3), (3^4)$ and π for $G = (3^3)$ (while the curvature of the sphere S^2 is 4π).

Denote by $X(G)$ the metric space of *constant* curvature, obtained from $P(G)$ by introducing a metric on it, which is locally spheric, locally Euclidean or locally hyperbolic, if (r^q) is a regular partition of S^2, R^2 or H^2, respectively. $X(G)$ has also cell structure, glued from, in general, non-Euclidean faces, but here we consider it as an abstract cell-complex. Clearly, $X(G) = K(G)$ for $(r, q) = (4, 4), (6, 3), (3, 6)$. In general, both complexes are homeomorphic as manifolds and have the same curvature, but it is non-zero only on interior vertices of $K(G)$ and it is constant on all points of $X(G)$. There is cell-isomorphism amongst complexes $X(G)$, $K(G)$, $P(G)$ and each of them admits cell-homomorphism on corresponding complex of (r^q). $X(G)$ is also simply connected two-dimensional manifold, which is homeomorphic to a disc if G is finite and non-compact, otherwise. The manifold $X(G)$ has no boundary only if G is the skeleton of partition (r^q) of Euclidean or hyperbolic plane. All faces of the complex $X(G)$ are regular r-gons with angles $(2\pi)/q$, while the faces of complex $K(G)$ are regular Euclidean r-gons with angles $(r-2)\pi/r$.

3.3. Outerplanar polycycles

Call a polycycle *outerplanar* if it has no interior points, i.e. $n_{\text{int}} = 0$; clearly, it is an (r, q')-polycycle for any q' not less than the maximal degree of vertices. The following theorem show that, in a way, outerplanar polycycles are close to proper polycycles.

Theorem 4.

1. *Any outerplanar* (r, q)*-polycycle G is a proper* $(r, 2q-2)$*-polycycle and its projection* $f(P(G))$ *into* (r^{2q-2}) *is convex* (*on* S^2, R^2 *or* H^2).
2. *Any outerplanar* $(3, q)$*-polycycle is a proper* $(3, q+2)$*-polycycle.*

The proof uses the fact that the projection on (r^q) of polycyclic realization of the graph, being simply connected, is convex if and only if all boundary angles are less than π (the boundary will be a union of convex polygons).

Remark that already for $p_3 = 7$, there are outerplanar (3,4)- and (3,5)-polycycles, which remain unproper in (3^5), (3^6), respectively. A *fan* of $(q-1)$ r-gons with q-valent common (boundary) vertex, is an example of outerplanar (r, q)-polycycle, which is a proper *non-convex* $(r, 2q-3)$-polycycle.

3.4. Proper and reciprocal polycycles

For a proper polycycle, we are interested when it is induced (or, moreover, isometric) subgraph of (r^q). For $(r, q) = (3, 3), (4, 3), (3, 4)$, any induced (r, q)-polycycle for $(r, q) = (3, 3), (4, 3), (3, 4)$ is isometric, but, e.g., the path of the three pentagons is induced non-isometric (5,3)-polycycle. Any isometric polycycle is embeddable (see Section 7), but already for $p_5 = 6$, there exists a non-embeddable induced (5,3)-polycycle.

Other possible property of a proper (r, q)-polycycle is being convex in (r^q) (see Theorem 4 and remark after lemma below). Consider now the notion of reciprocity, defined for some proper polycycles.

Let P be a proper bounded (r, q)-polycycle. Consider the union of all (r-gonal) faces of (r^q) outside of P. Easy to see that this union will be an (r, q)-polycycle (and call it then *reciprocal to* P) if and only if, either P is spheric, or P is infinite and has connected boundary. Call a polycycle *self-reciprocal* if it admits the reciprocal polycycle and is isomorphic to it.

All self-reciprocal (r, q)-polycycles with $(r, q) = (3, 3), (4, 3), (3, 4), (5, 3)$ are (3^3)-e, (4^3)-v, $P_2 \times P_3$, (3^4)-v, (3^4)-C_3, (3^4)-$2K_2$ and nine (out of 11) (5,3)-polycycles with $p_5 = 6$, including six chiral ones. An example of self-reciprocal $(3, q)$-polycycle for any $q \geq 3$ is a $(3, q)$-polycycle on one of the two shores of *zigzag path*, cutting (3^q) in two isomorphic halves; it includes (3^3)-e and (3^4)-C_3 and infinite for $q \geq 6$.

4. Symmetries of polycycles

The symmetry group *AutG* of an (r, q)-polycycle G is a subgroup of *Aut*(r^q) if it is proper and an extension of *Aut*(*HomG*), otherwise; here *HomG* denotes the cell-homomorphism projection of $P(G)$ into (r^q). We have *AutG* = *AutP*(G), except of the case of G being one of the five Platonic (r^q). If an (r, q)-polycycle G is finite and $P(G)$ has a fixed point inside it, then *Aut*(G) consists only of rotations and mirrors around this point. So its order divides $2r$, 4 or $2q$, depending on what *AutG* fixes: the center of an r-gon, the center of an edge or a vertex (the corresponding groups are D_{rh}, D_{2h}, D_{qh}). (Above *AutG* is given, for finite polycycle G, as a space group, i.e. we discard plane mirror.) None of the (3,3)-, (3,4)-, (4,3)-polycycles, but almost all (r, q)-polycycles for any other (r, q), have trivial *AutG*. The number of *chiral* (i.e. with *AutG* containing no mirrors) proper (5,3)-, (3,5)-polycycles is 12, 208 (amongst, respectively, all 39, 263).

Call a polycycle G *isotoxal* (or *isogonal*, or *isohedral*) if *AutG* is transitive on edges (or vertices, or interior faces); use notation IT-(or IG-, or IH-), for short.

Let $T^*(l, m, n)$ denote Coxeter's *triangle group* of a fundamental triangle with angles $\pi/l, \pi/m, \pi/n$. Let $T(l, m, n)$ denote its subgroup of index 2, excluding motions of 2nd kind (i.e. those changing orientation); see e.g. [20, pp. 81,90,107,176,183]. Now, $T^*(2, 2, \infty) = pmm2$, $T(2, 2, \infty) = p112 \approx pm11 \approx pma2$. (Remark that $p1m1$ also has index 2 in $T^*(2, 2, \infty)$, but it is not isomorphic to $T(2, 2, \infty)$.) On the other hand, $T(2, 3, \infty) \approx PSL(2, Z)$ (the modular group) and $T^*(2, 3, \infty) \approx SL(2, Z)$. For all but one (the last in Fig. 4) known families of infinite IG- or IH-polycycles, *AutG*, if it is not a strip group, is one of the above two groups $T(l, m, n)$, $T^*(l, m, n)$ for some parameters. For all known such polycycles with strip group *AutG* (see Fig. 3), this group is isomorphic to one of $T^*(2, 2, \infty)$, $T(2, 2, \infty)$.

Only r-gons and non-Platonic (r^q) are isotoxal; their respective symmetry groups are D_{rh} and $T^*(l, m, n)$. $Aut(r^q) = D_{rh}$ in five Platonic cases; none is IT-, IG- or IH-polycycle, except isohedral (3^3).

We conjecture that all polycycles, which are isogonal and isohedral, but not isotoxal, are the infinite (3,4)-polycycle from 3rd column in Fig. 1 and $(2k, 3)$-*cactuses* for any $k \geq 2$ (with $AutP = T^*(2, k, \infty)$) and we checked this conjecture for spheric (r, q). In fact, only other IG-, but not IT-polycycle in Fig. 1 of all spheric IH-polycycles, is $P_2 \times P_Z$, i.e. the (4,3)-cactus. The cactuses are infinite polycycles obtained by the procedure, which is clear from Figs. 2 and 4. The $(2k, 3)$-cactuses for any $k \geq 3$ correspond to the case $a = 0$ of the first family in Fig. 4; they are only isogonal polycycles in Fig. 4.

Theorem 5.

1. *Any IG-, but not IT-polycycle is infinite, outerplanar and with the same vertex-degree.*
2. *There exist two IG-, but not IH-polycycles with* $(r, q) = (3, 5), (4, 4)$ (*see Fig.* 2; *their groups are* $T(2, 3, \infty)$, $T^*(2, 4, \infty)$) *and this* (3,5)-*polycycle is unique, such spheric polycycle.*

Theorem 6. *Let P be an isohedral* (r, q)*-polycycle. Then*

1. *P has the same number t of non-boundary edges for each its r-gon*;
2. *if* $t = 0, r$ *or* 1, *then P is r-gon,* (r^q) (*with* $(r, q) \neq (4, 3), (3, 4), (5, 3), (3, 5)$) *or a pair of adjacent r-gons* (*and* $AutP = D_{2h}$);
3. *if* $t = 2$, *then P is either a star of q r-gons with one common interior vertex, or an infinite outerplanar polycycle*;
4. *there exist exactly two infinite isohedral* $(3, q)$*-polycycles: both infinite polycycles from the 5th column in Fig.* 1 (*both with* $AutP = pma2 \approx T(2, 2, \infty)$);

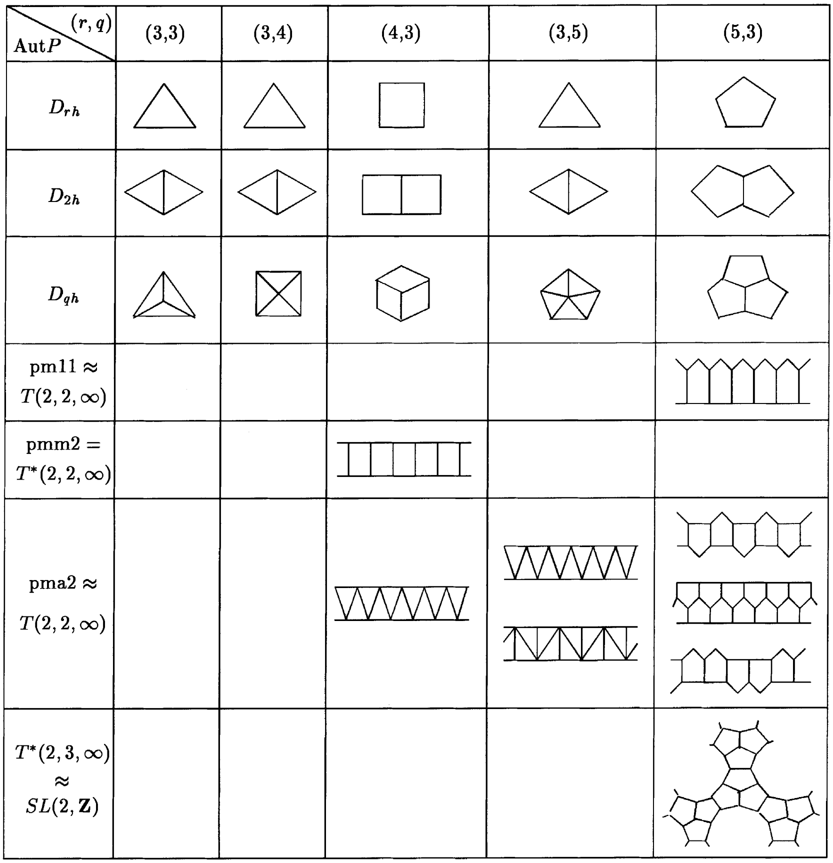
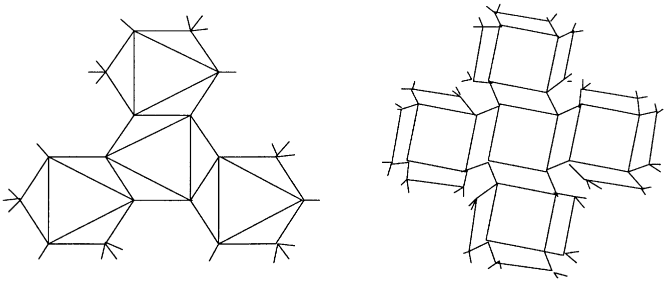


Fig. 1. All isohedral spherical polycycles (only r-gons and two infinite ones with r, q different from 5, are isogonal).



3,5
$T(2, 3, \infty)$

4,4
$T^*(2, 4, \infty)$

Fig. 2. Examples of isogonal but not isohedral polycycles.

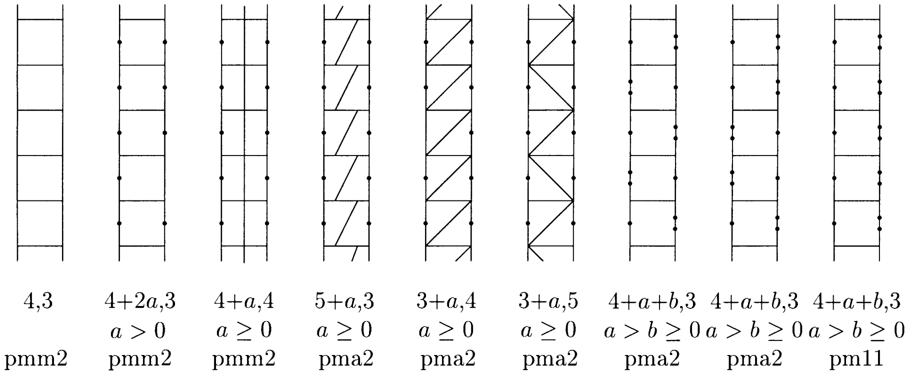


Fig. 3. Examples of isohedral polycycles with strip groups.

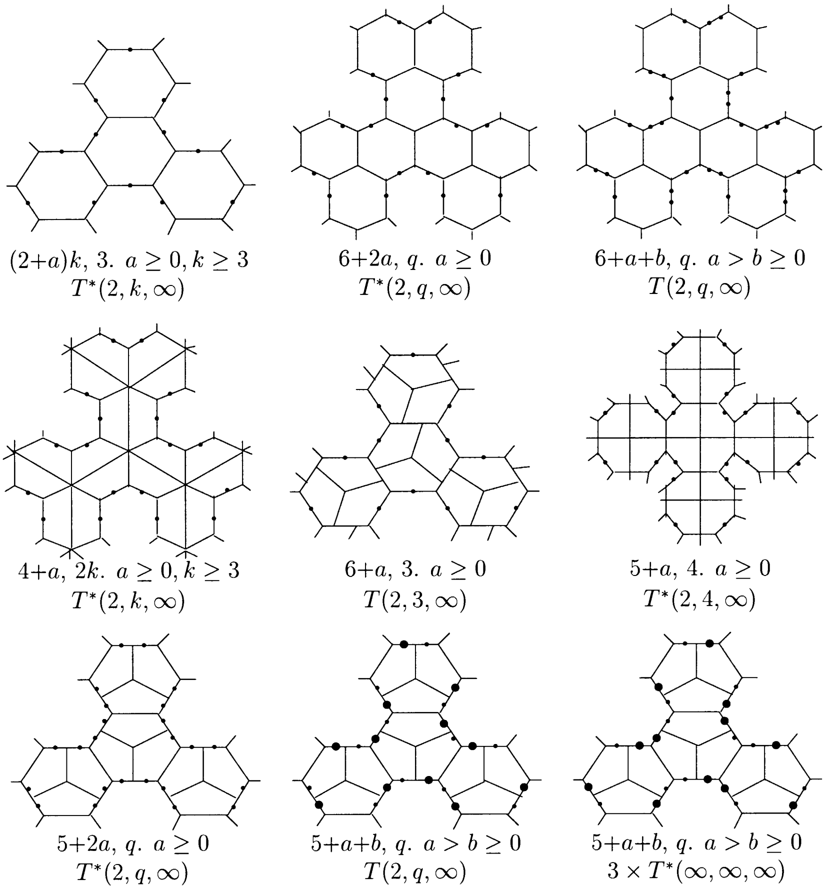


Fig. 4. Examples of families of isohedral cactuses.

5. *if* $1 \le t \le r-3$, *then P is infinite; for any r, there exists isohedral* $(r, 4)$*-polycycle with* $t = r-1$ (*take an r-gon with right angles and AutP, generated by mirrors from all but one of its sides*);
6. *all spheric isohedral polycycles are* (*see Fig.* 1): *11 finite ones* (*see* (2) *above*) *and eight infinite ones* ($P_2 \times P_Z$), *six its decorations* (*all with strip groups AutP*) *and the (5,3)-cactus with AutP* $= T^*(2, 3, \infty)$;
7. *eight families of isohedral decorations of* $P_2 \times P_Z$ *are given in Fig.* 3; nine *families of isohedral decorations of* (r, q)*-cactuses are given in Fig.* 4.

Remark that 1st, 2nd decorations in Fig. 3 are the case $k = 2$ of, respectively, 1st, 4th cactuses in Fig. 4. Amongst the eight decorations in Fig. 3, only the case $a = 0$ of the 4th one is isogonal.

The group of the last family in Fig. 4 is in 1–1-correspondence with $T(2, 2, \infty)$, but different from it. It is the product of $T^*(\infty, \infty, \infty)$ and the group (of order 3) of congruence of the triangle with all vertices in infinity.

For any $r \ge 5$, there exists a continuum of *quasi*-IH-polycycles, i.e. not isohedral, but all r-gons have the same 1-corona. In fact, let T be an infinite, in both directions, path of regular r-gons, such that for any of them, the edges of adjacency to its neighbors are at distance $\lfloor (r-3)/2 \rfloor$ and the sequence of (one of the two possible) choices of joining each new r-gon, is aperiodic and different from its reversal. There is a continuum of such T for any $r \ge 5$. Any T is quasi-isohedral and its group of automorphism is trivial. Also, T is embeddable (see Section 7); it is unproper if $r = 5, 6$ and isometric if $r \ge 7$.

5. Two extremal properties

5.1. Maximal number of interior points

Recall that $p_r(P)$, $n_{\text{int}}(P)$ denote the number of interior faces and interior vertices of given finite (r, q)-polycycle P. Call $(n_{\text{int}}(P))/(p_r(P))$ the *density* of P and denote by $n(x)$ the maximum of $n_{\text{int}}(P)$ over all (r, q)-polycycles P with $p_r(P) = x$; call *extremal* any (r, q)-polycycle P with $n_{\text{int}}(P) = n(x)$. So, extremal polycycles represent opposite case to outerplanar ones (see Section 3.3), with the same p_r. Clearly, an extremal polycycle also maximizes the number e_{int} of non-boundary edges and minimizes the number Per (for *perimeter*) of boundary edges (or boundary points), as well as the number n of all vertices and the number e of all edges. In fact, Euler formula

$$(n_{\text{int}} + \text{Per}) - (e_{\text{int}} + \text{Per}) + (p_r + 1) = 2,$$

and equality $rp_r = 2e_{\text{int}} + \text{Per}$, imply

$$\begin{aligned} n_{\text{int}} &= e_{\text{int}} - p_r + 1 = -\tfrac{1}{2}\text{Per} + \tfrac{1}{2}p_r(r-2) + 1 = -e + p_r(r-1) + 1 \\ &= -n + p_r(r-2) + 2. \end{aligned}$$

For (5,3)-polycycles with $x \le 11$, $n(x)$ was found in [8]; all extremal (5,3)-polycycles turn out to be proper and unique. Moreover, the (5,3)-polycycles, which are reciprocal to any such extremal one, turn out to be also extremal. Cyvin et al. [8] asked about $n(x)$ for $x \geq 12$; this section answers this question for any x and for all spheric (p, q).

First, consider three trivial cases of (r, q). All pairs (p_r, n_{int}) for $(p, q) = (3, 3)$ are (1,0), (2,0), (3,1); for $(p, q) = (4, 3)$: $(n, 0)$ for all $n \geq 1$, (3,1), (4,2), (5,4); for $(p, q) = (3, 4)$: $(n, 0)$ for all $n \geq 1$, (4,1), (5,1), (6,1), (6,2), (7,3).

Call *kernel* of a polycycle, the cell-complex of vertices, edges and faces of the polycycle, which are not incident with its boundary. Call a polycycle *elementary* if it is a r-gon or if it has non-empty connected kernel, such that the deletion of any face from the kernel will diminish it (i.e. any face of the polycycle is incident to its kernel).

Lemma

1. *Any* (r, q)*-polycycle with* $(r, q) = (3, 3), (3, 4), (4, 3), (3, 5), (5, 3)$ *is a union of elementary polycycles without common faces.*
2. *For* $(r, q) = (6, 3), (4, 4), (3, 6)$ *and for the case* $r \geq 7$, $q \geq 3$, *there is a continuum of connected* (*components of*) *kernels of* (r, q)*-polycycles.*

In the above lemma (2) and for $r \geq 7$, $q \geq 4$, one can find, moreover, a continuum of elementary (r, q)-polycycles, which are proper and convex on the hyperbolic plane.

The part (1) of the above lemma does not hold already for $(r, q) = (6, 3)$: two elementary polycycles, having each a single point as the kernel, can be glued into a (6,3)-polycycle with $p_6 = 5$, having two isolated vertices as (disconnected) kernel, but elementary polycycles, having those vertices as kernels, have a common 6-gon.

We believe that for each non-spheric (r, q), amongst extremal (r, q)-polycycles there exist a proper one; in fact, each known extremal (r, q)-helicene P has $p_r(P) > p_r(r^q)$.

The *extremal animals* of [19] are, in our terms, *proper* (4,4)-, (6,3)- and (3,6)-polycycles with minimal number of edges and so, maximal number of interior vertices, for a given number of interior faces. It was proved in [19] that such polycycles have $e = 2p_4 + \lceil 2\sqrt{p_4} \rceil$, $e = 3p_6 + \lceil \sqrt{12p_6 - 3} \rceil$, $e = p_3 + \lceil (p_3 + \sqrt{6p_3})/2 \rceil$, respectively, and that there are amongst them those, which grow like a spiral. In fact, the proof of [19] implies that those extremal animals are, moreover, extremal in our sense.

Next two theorems give a full solution of the problem for $(r, q) = (5, 3), (3, 5)$.

Theorem 7. *Let* $(r, q) = (5, 3)$. *Then*

1. *With exception of three cases* $(n(9) = 10, n(10) = 12, n(11) = 15)$, $n(x) = x$, *if* $x \equiv 0, 8, 9 (\text{mod } 10)$, $n(x) = x - 1$ *if* $x \equiv 6, 7 (\text{mod } 10)$, $n(x) = x - 2$, *otherwise, and extremal polycycle is unique if* $n(x) = x$.
2. *All possible densities of* (5,3)*-polycycles, beside exceptions for* $p_5 = 9, 10, 11$, *form the segment* $[0, 1]$.

The proof uses the above lemma and the list (found by exhaustive search) of all connected components of kernels of (5,3)-polycycles; clearly, E_i, $1 \leqslant i \leqslant 5$, are the first members of elementary (5,3)-polycycles E_i, $i \geqslant 1$, with $i + 2$ pentagons and i interior vertices. The kernels are subgraphs induced by all interior vertices of elementary (5,3)- and (3,5)-polycycles on Figs. 5 and 6. Any (5,3)-polycycle can be obtained by gluing of elementary poly-

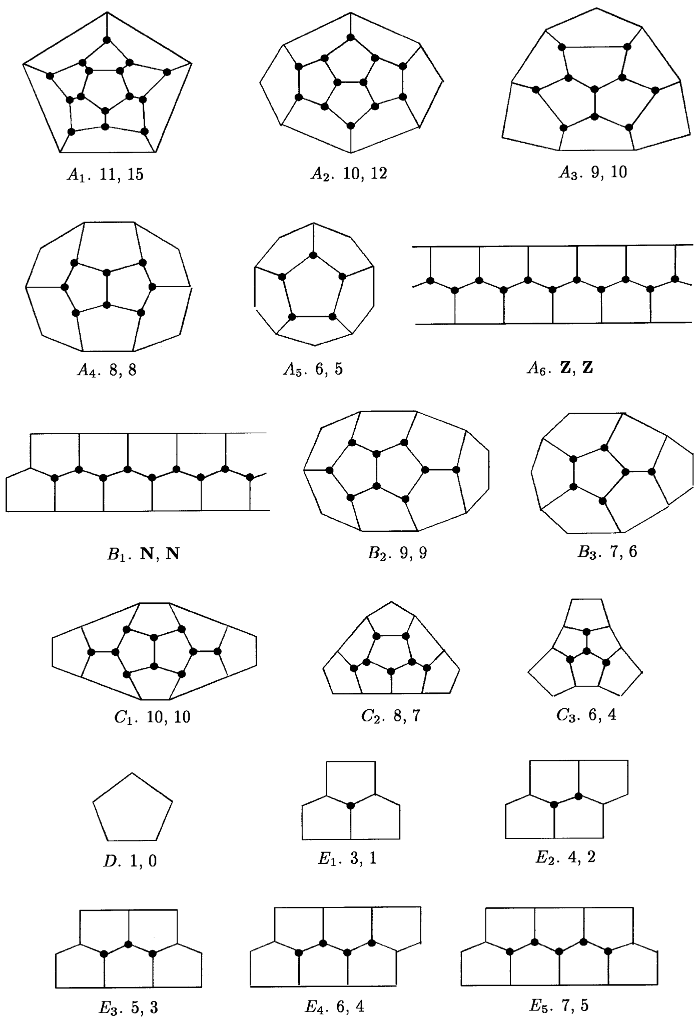


Fig. 5. Elementary (5,3)-polycycles and their kernels.

cycles by *open* (i.e. such that both vertices have degree 2) edges. Theorem 7 is obtained by consideration of all such gluings.

Theorem 8. *Let* $(r, q) = (3, 5)$. *Then*

1. $n(x) = \lfloor x/3 \rfloor$ *if* $x \equiv 0, 1 (\mathrm{mod}\, 18)$, *with exception of* $n(18) = 8$, $n(19) = 9$; *otherwise,* $n(x) = \lfloor (x-2)/3 \rfloor$, *with exception of* $n(x) = \lfloor (x+1)/3 \rfloor$ *for* $x =$ 10–14, 28, 30–33, 35, *and* $n(x) = \lfloor (x+4)/3 \rfloor$ *for* $x =$ 15–17, 34.
2. *All possible densities of* (3,5)*-polycycles, besides exceptions given in* (1) *above, form the segment* $[0, \frac{1}{3}]$; *all rational densities can be realized by finite unproper polycycles.*

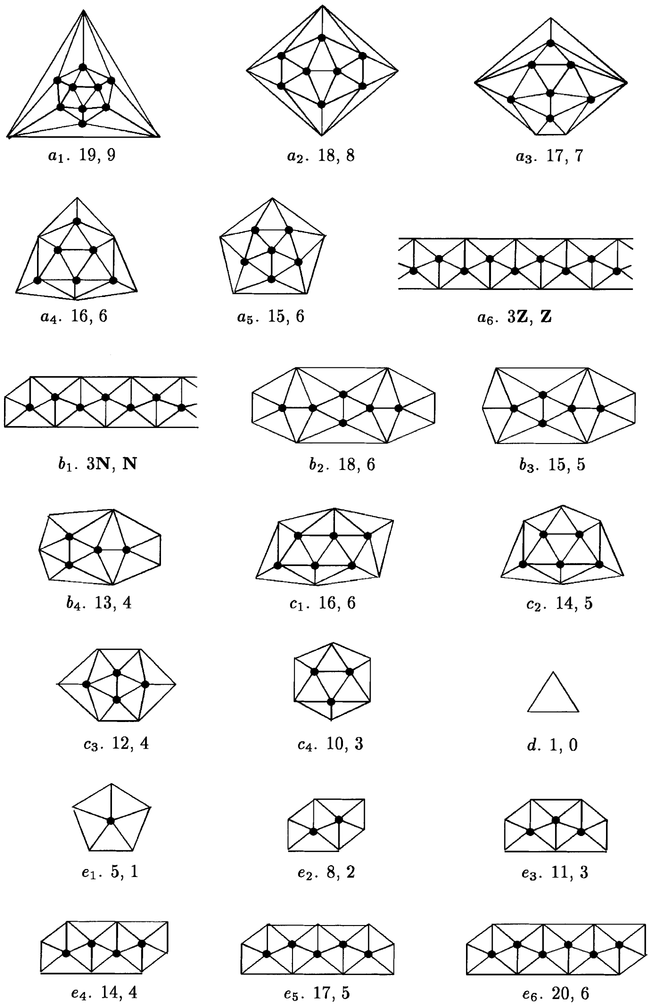


Fig. 6. Elementary (3,5)-polycycles and their kernels.

3. *For* $p_3 \leq 19$ *the following holds*: $n(x) = 0$ *if* $0 \leq x \leq 4$, $n(x) = 1$ *if* $5 \leq x \leq 7$, $n(x) = 2$ *if* $8 \leq x \leq 9$, $n(x) = 3$ *if* $10 \leq x \leq 11$, $n(x) = 4$ *if* $12 \leq x \leq 13$, $n(14) = 5$, $n(x) = 6$ *if* $15 \leq x \leq 16$, $n(17) = 7$, $n(18) = 8$, $n(19) = 9$.

Moreover, for $p_3 \leq 19$, *all extremal polycycles are proper and the reciprocal of an extremal one is also extremal; extremal ones are unique, except the cases* $p_3 = 9, 11$ (*two polycycles*) *and* $p_3 = 4, 7, 13, 16$ (*three polycycles*).

We used for the proof the same strategy as for the proof of Theorem 7, but the number of cases to consider is much larger in this case. Other difference with (5, 3)-polycycles is that we should use now (in order to glue some elementary (3, 5)-polycycles) the elementary polycycle d with empty kernel. So we give only Fig. 6 of all minimal (3, 5)-polycycles with connected kernels. Clearly, e_i, $1 \leqslant i \leqslant 6$, are the first members of the family of elementary (3,5)-polycycles e_i, $i \geqslant 1$, with $3i + 2$ triangles and i interior vertices.

Remark that the kernels of (5, 3)-polycycles A_i, $1 \leq i \leq 5$, of Fig. 5 are all non-trivial isometric (5, 3)-polycycles; they are also all *circumscribed* (5, 3)-polycycles, i.e. r-gons can be added around the perimeter, such that they will form a simple circuit. (They were found in [8]; such (6, 3)-polycycles are useful in organic chemistry.) All circumscribed (3, 5)-polycycles are the kernels of polycycles a_i, $1 \leq i \leq 5$, and c_i, $1 \leq i \leq 4$ of Fig. 6. It turns out that all polycycles G in one of Figs. 5 and 6, admitting the dual graph G^* in another one, are as follows: $A_1^* = a_5$, $A_2^* = c_3$, $A_3^* = c_4$, $A_4^* = e_2$, $A_5^* = e_1$; $E_1^* = d$ and $a_1^* = A_3$, $a_2^* = A_4$, $a_4^* = C_3$, $a_5^* = A_5$, $c_1^* = E_4$, $c_2^* = E_3$, $c_3^* = E_2$, $c_4^* = E_1$; $e_1^* = D$. A_6 occurs also in Fig. 1; its dual is infinite (3, 4)-polycycle there.

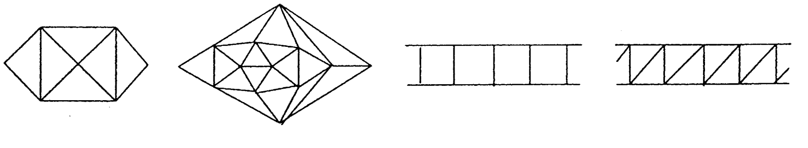
For *any* (r, q), we have only the bounds given in Theorem 9 below; they are linear with respect to p_r. The lower bound is attained, e.g., by the star of q r-gons with one common (interior) vertex. For Euclidean $(p, q) = (6, 3), (4, 4), (3, 6)$, the upper bound is attained in the limit.

Theorem 9. *Any (r, q)-polycycle, such that each of its r-gon contains an interior vertex, satisfy to $p_r/q \leq n_{\text{int}} < rp_r/q$.*

In order to prove those bounds, consider complex $X(G)$ from Section 3.2. Divide each of its face (a regular r-gon) into r 4-gons by the lines from the center to the mid-points of edges and, denoting by σ the area of 4-gon. Using that any r-gon contains at least one interior vertex, observe that $p_r\sigma \leq n_{\text{int}}q\sigma < p_r r\sigma$.

5.2. Non-extendible polycycles

Consider now another notion of maximality, appropriate to polycycles. Call an (r, q)-polycycle *non-extendible* if it is not a proper subgraph of another (r, q)-polycycle. Four examples of non-extendible polycycles, depicted below, are: vertex-split (3^4) and vertex-split (3^5) (defined in Section 3) and two infinite polycycles (Z-paths of quadrangles and of triangles; both appear also in Fig. 1).



Theorem 10. *All non-extendible (r, q)-polycycles are (r^q), four above examples, possibly (but we conjecture their non-existence) some other finite $(3, 5)$-polycycles and, for any $(r, q) \neq (3, 3), (3, 4), (4, 3)$, a continuum of infinite ones.*

For example, a continuum of non-extendible $(5, 3)$-polycycles comes as all infinite (in both directions) aperiodic sequences of glued (by doubled edges) polycycles C_2 (in the column 2 of Fig. 5) from Fig. 5, and its upside down version, say, C_2'. The same procedure, used for polycycles b_2, e_6 from Fig. 6, gives a continuum of non-extendible (3, 5)-polycycles. The $(4, 4)$-cactus from Fig. 2 is also non-extendible since all its vertices have degree 4.

The hardest part of the proof of the above theorem was to show that any finite non-extendible polycycle G is spheric. Using a discrete analog of Gauss–Bonnet formula (see [1, Theorem 1.8.2, p. 76]), applied to $K(G)$), we get that the curvature of $K(G)$ is positive: the curvature is equal to excess of the sum of angles of geodesic n-gon, bounding the disc of perimeter n, over $(n-2)\pi$, i.e. the sum of angles of Euclidean n-gon, namely using non-extendibility of finite polycycle G, we get an estimation of above sum of angles, which imply positivity of the curvature.

Finally, consider (r, q)-polycycles, such that any interior point of any interior face has degree 1 of the cell-homomorphism onto (r^q). The number of such polycycles, which are not extendible without losing this property, is equal to 0 for $(p, q) = (3, 3)$, $(3, 4)$ and equal to 1 for $(p, q) = (4, 3)$ (it is $P_2 \times P_5$). This number is finite for $(p, q) = (5, 3)$, $(3, 5)$ and infinite, otherwise.

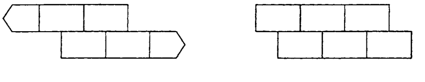
6. Metric properties of polycycles: embedding into Q_m, Z_m

Call a polycycle *embeddable* if the metric space of its vertices (with usual shortest-path metric) is embeddable isometrically, up to a scale λ, into a hypercube Q_m, $m < \infty$, or (if the graph is infinite) into a cubic lattice Z_m, $m \leq \infty$; see [9,6,11] for details. We have the following embeddings of (r^q): (3^3), (4^3) is embeddable into Q_3; (3^4) into Q_4; (3^5) into Q_6; (5^3) into Q_{10}; (4^4) into Z_2; (3^6), (6^3) into Z_3 and all others into Z_∞. So, any isometric polycycle is embeddable.

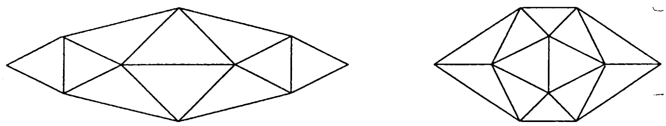
Examples of non-embeddable polycycles are: $(4^3) - e$, $(3^4) - e$, $(5^3) - e$, $(3^5) - e$, vertex-split (3^4), vertex-split (3^5) and four polycycles, given in the figures in theorem below. Amongst above 10 polycycles only vertex-split (3^4) and vertex-split (3^5) are helicenes; amongst remaining eight proper polycycles only one on the right-hand side of the figures in theorem below, are induced ones (they are E_4 and c_3 of Figs. 5 and 6, respectively).

Theorem 11.

1. *For* $(r, q) \neq (5, 3), (3, 5)$, *there are exactly three non-embeddable polycycles*: $(4^3) - e$, $(3^4) - e$ *and the vertex-split* (3^4),
2. *except* (5^3) *itself, any* $(5, 3)$-*polycycle is embeddable if and only if it does not contain, as an induced subgraph, neither of the two proper polycycles with* $p_5 = 6$, *given below*



3. *we conjecture that, except* (3^5) *and* $(3^5) - v$, *any* $(3, 5)$-*polycycle is embeddable if and only if it does not contain, as an induced subgraph, neither of the two proper 10-vertex polycycles, given below*



There are no other non-embeddable (3,5)-polycycle with $p_3 \leq 10$.

Any outerplanar polycycle is embeddable, as well as any connected outerplanar graph.

Amongst 39 proper $(5, 3)$-polycycles, the embeddable ones are: (5^3), three with $p_5 = 7$, 9 with $p_5 = 6$ (all but two given in (2) above) and all 14 with $p_5 \leq 5$. Amongst $(5, 3)$-polycycles of Fig. 5, the embeddable ones are $A_1 \supset A_5$, $C_3 \supset E_3 \supset E_2 \supset E_1 \supset D$ (the sign "$\supset$" denotes here "contains as a partial subgraph"). Amongst $(5, 3)$-polycycles of Fig. 1, only the infinite one with the symmetry *pma*2 and interior vertices, is not embeddable.

Amongst $(3, 5)$-polycycles of Fig. 6, the embeddable ones are $a_1 \supset a_5 \supset b_4 \supset c_4$, $e_3 \supset e_2 \supset e_1 \supset d$. $(3, 5)$-Polycycles $a_5 = (3^5) - v$, $a_2 = (3^5) - e$ in Fig. 6 contain the forbidden $(3, 5)$-polycycles from (3) above, as induced non-isometric subgraphs.

Embeddable (r, q)-polycycles have the scale $\lambda = 1$ if r is even and 2, otherwise. Consider any finite embeddable polycycle with perimeter d and k *closed zones*, i.e. cyclic sequences of opposite (alternating) non-boundary edges, see [6,11]. Then it is embeddable into $Q_{(d/2)+k}$ if r is even (this implies that d is also even), and it is embeddable, with scale 2, into Q_{d+k} if r is odd. For example, amongst all embeddable polycycles in Figs. 5 and 6, all with $k > 0$ are A_1, a_1, a_5; they have $k = 5, 3, 1$, respectively.

There is a continuum of $(6, 3)$-polycycles, which are embeddable only into Z_∞: take all infinite (in both directions) paths of $(6, 3)$-polycycles $P := C_{0,1,\ldots,9} + (3, 8)$, glued each by its edges named (4,5) and (6,7); the choice how to glue, by edges of the same or different name, should be done aperiodically.

7. Some relatives of *(r, q)*-polycycles

It will be interesting to find some analog of the above results for a generalization of polycycles on other surfaces. The following examples illustrate arising options:

1. There is no straightforward analog of Theorem 1 for, say, "polycycles on the torus T^2": 2-connectedness of the graph does not imply that its embedding on T^2 is a simply connected union of faces (a handle can break it).
2. The ring of three (or four) hexagons is example of planar, but not simply connected "polyhex" (in a large sense used in chemistry) without any (or locally homeomorphic) homomorphism on (6^3). Theorem 3 also does not admit a generalization already on *mono*-5-(6^3), i.e. on the partition of the plane by regular hexagons around one central regular pentagon, having only vertices of degree 3 (in fact, a path of a pentagon and six hexagons, having six consecutive vertices of degree 3 on the boundary circuit, is not a subgraph of mono-5-(6^3), but it is also not a "helicene", since after mapping of its pentagon on the pentagon of mono-5-(6^3), the last hexagon of the path also maps on this pentagon). On the other hand, the cell-map of Theorem 3 exists even if we permit boundary vertices of degree greater than q, but this map will not be locally homeomorphic around those "singularities".

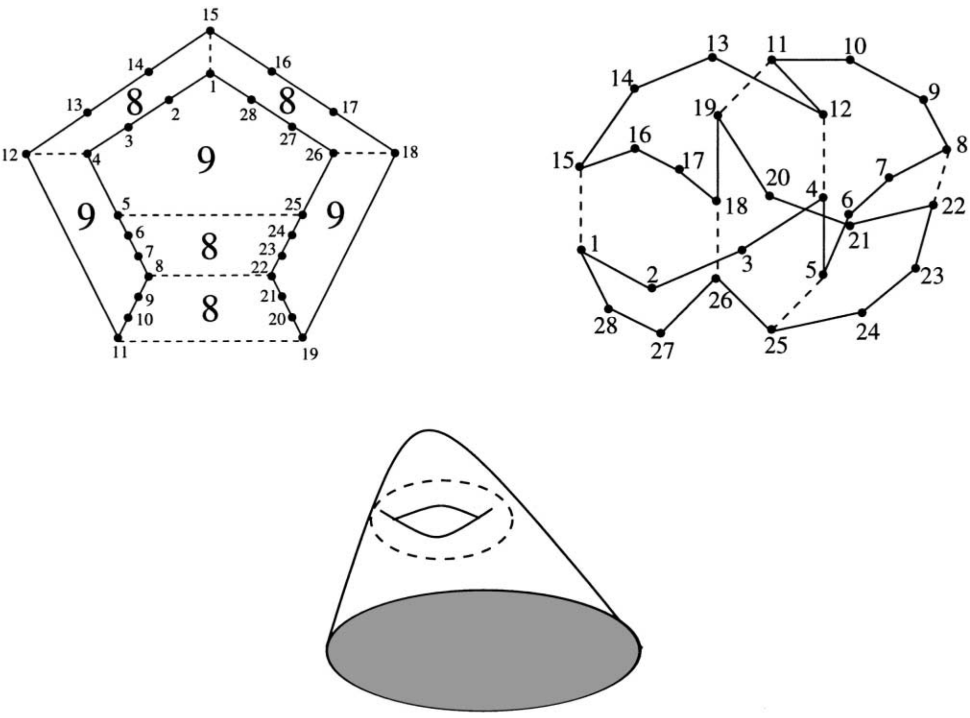


Fig. 7. Cross-ring as "not simply connected (8, 3)-polycycle".

3. Consider *cross-ring*, depicted in Fig. 7: first on R^2 as the skeleton of dual disphenoid with two new vertices added on some eight edges, and next in R^3 as the skeleton of a polyhedral (2-connected) sphere with one hole and handle. All eight planar realizations of this graph are not polycyclic: they have both 8- and 9-gonal faces. All conditions of the criterion in Theorem 1 are satisfied, except of (4): $v - e + f = 28 - 34 + 8 \neq 1$. But this polyhedral sphere permits to consider the cross-ring as "not simply connected $(8, 3)$-polycycle" with $p_8 = 5$; this polyhedron have five regular 8-gonal faces: four indicated by the number "8" on the left-hand side of Fig. 7 and one bounded by $C_{11,12,4,5,25,26,18,19}$. The handle prevents it from embedding into R^2 and from cell-homomorphism into (8^3). All vertices $1, 2, \ldots, 28$ are on the boundary of the disc.

Finally, we mention two following relatives of finite (r, q)-polycycles. See [2 and references therein] (mainly authored by M. Perkel) for the study of *strict polygonal* graphs, i.e. graphs of girth r and vertex-degree q, such that any path P_2 belongs to unique r-circuit of G. See [5, pp. 546–547 and references therein] for information on *equivelar* polyhedra, i.e. polyhedral embedding, with convex faces, of (r, q)-*map* (i.e. all faces are combinatorial r-gons and the vertex-degree of the skeleton is q) into R^3, such that all flags are equal. So, in both these cases graphs are q-regular, have girth r, Euler characteristic $v - e + f = v(6 - r)/2r$ and coincide with Platonic polyhedra in the case of genus 0. Recall that, for an (r, q)-polycycle, any non-boundary path P_2 belongs to unique r-circuit and there exist polyhedral realization in R^3 with all interior faces being regular r-gons.

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