# **Extremal and Nonextendible Polycycles**

M. Deza<sup>1</sup> and M. I. Shtogrin<sup>2</sup>

Received May 2002

Abstract—We continue the analysis of (r, q)-polycycles, i.e., planar graphs G that admit a realization on the plane such that all internal vertices have degree q, all boundary vertices have degree at most q, and all internal faces are combinatorial r-triangles; moreover, the vertices, edges, and internal faces form a cell complex. Two extremal problems related to chemistry are solved: the description of (r, q)-polycycles with the maximal number of internal vertices for a given number of faces, and the description of nonextendible (r, q)-polycycles. Numerous examples of isohedral polycycles (whose symmetry groups are transitive on faces) are presented. The main proofs involve an abstract cell complex  $\mathbf{P}(G)$  obtained from a planar realization of the graph G by replacing all its internal faces by regular Euclidean r-gons.

## INTRODUCTION

Consider a planar<sup>3</sup> graph G. This graph can be embedded in the plane so that no two of its edges intersect. This embedding (a planar realization of the graph G) is a so-called flat graph. Upon adding to the flat graph all its faces, we obtain a flat map. All bounded faces of a flat map are *internal faces* of a flat graph. The vertices that do not belong to the unbounded face of a flat map are called *internal vertices* of a flat graph.

**Definition.** Suppose that a planar realization of a nonseparable planar graph G with girth r and the maximal degree of vertices q satisfies the following three conditions:

- (i) All internal faces are combinatorial r-gons with  $r \geq 3$ .
- (ii) All internal vertices have the same degree  $q \geq 3$ .
- (iii) The vertices, edges, and internal faces form a cell complex.

Then, the graph G supplemented with internal faces (taken from the given planar realization of the graph G) is called an (r, q)-polycycle and denoted by  $\Pi(G)$ 

If at least one planar realization of the planar graph G satisfies conditions (i)–(iii), where r is the girth of the graph and q is the maximal degree of vertices, we will say that the graph G admits an (r, q)-polycyclic realization. If G admits an (r, q)-polycyclic realization, then it admits exactly one such realization in the general case (see [3–6]). Only in five exceptional cases when the graph represents the edge skeleton of a Platonic body, the number of (r, q)-polycyclic realizations of G is equal to the number of faces of the Platonic body; in any of these five cases, the polycyclic realizations are isomorphic. We classify the result obtained [3–6] as a specific uniqueness theorem for a polycyclic realization. A graph G admitting an (r, q)-polycyclic realization, the (r, q)-polycyclic

<sup>&</sup>lt;sup>1</sup>CNRS/ENS, Paris, France; Institute of Statistical Mathematics, Tokyo, Japan.

E-mail: Michel.Deza@ens.fr

<sup>&</sup>lt;sup>2</sup>Steklov Institute of Mathematics, Russian Academy of Sciences, ul. Gubkina 8, Moscow, 117966 Russia. E-mail: stogrin@mi.ras.ru

<sup>&</sup>lt;sup>3</sup>The terminology related to the graph theory is borrowed from Harary's book [14].

realization of the graph G, and the (r, q)-polycycle  $\Pi(G)$  are three different concepts that are uniquely defined by each other (see above). Sometimes, we will use a common short term *polycycle* for any of these three concepts (when it is clear from the context of which concept we speak).

We have proved that, for any nonseparable flat graph, condition (iii) follows from conditions (i) and (ii). Condition (ii) implies that the degree of any internal vertex of the polycycle  $\Pi(G)$  is equal to the maximal degree of vertices of G. Naturally, the degree of any boundary vertex of  $\Pi(G)$  does not exceed the maximal degree q; it is equal to a certain number j, where  $2 \leq j \leq q$ . The set of internal vertices of the polycycle  $\Pi(G)$  may be empty (when the flat graph G is outerplanar). A separate r-gon is a special (r, q)-polycycle with parameter q = 2. As any other outerplanar graph, it can be considered as an (r, q)-polycycle with any other (greater) numerical value of the parameter q (which is useful for the classification of subpolycycles,<sup>4</sup> see Table 5 below).

It should be noted that the concept of (r, q)-polycycle  $\Pi(G)$  is introduced not only for a finite graph G but also for an infinite graph. In the case of an infinite flat graph, we always assume that there are only a finite number of vertices and edges of this graph in any finite domain of the plane. In the case of an infinite graph G, any (r, q)-polycycle  $\Pi(G)$  represents an infinite simply connected domain, generally speaking, with boundary (see below and [4, 6]); in the case of a finite graph G, any (r, q)-polycycle  $\Pi(G)$  is a disk, which is always with boundary.

An (r, q)-polycycle is called *proper* if it is a partial subgraph of the edge skeleton of a regular tiling  $(r^q)$  (i.e., a tiling of the sphere  $\mathbb{S}^2$ , Euclidean plane  $\mathbb{R}^2$ , or Lobachevskii plane  $\mathbb{H}^2$  by regular *r*-gons with angles  $\frac{2\pi}{q}$ , so that the degree of each tiling vertex is equal to q), and a *helicene* otherwise. In a full agreement with the sign of the curvature of a "plane," the parameters (r, q) are called *elliptic* if rq < 2(r+q), *parabolic* if rq = 2(r+q), and *hyperbolic* if rq > 2(r+q). If the (r,q)polycycle  $\mathbf{\Pi}(G)$  is *not* outerplanar, then these terms also correlate with the sign of the curvature of an internal vertex of the polyhedron  $\mathbf{K}(r^q)$  that is obtained from a regular tiling  $(r^q)$  upon replacing each *r*-gon by a regular Euclidean *r*-gon. Only (r, q)-polycycles  $\mathbf{\Pi}(r^q)$  with parabolic and hyperbolic parameters (r, q) do not have a boundary: they are isomorphic to the regular tilings  $(r^q)$ . In the case of elliptic parameters (r, q), even the (r, q)-polycycle  $\mathbf{\Pi}(r^q)$  has a boundary: the interior of one face  $\mathbf{F}$  is removed from the surface of a Platonic body (because a sphere cannot be completely embedded into a plane).

There is extensive literature (see, for example, [8, § 9.4; 9]) on proper (r, q)-polycycles with parabolic parameters (r, q) = (4, 4), (3, 6), and (6, 3); they are called *polyominoes*, *polyamonds*, and *polyhexes*, respectively. For instance, the first and the last types of polycycles are considered in physics and organic chemistry. All 39 proper (5, 3)-polycycles were obtained independently by chemists in [10]. However, all proper polycycles for elliptic parameters (r, q) were obtained as early as in [12]; any proper (r, q)-polycycle for these parameters has a unique *dual* (r, q)-polycycle (the one that has a common boundary with the former polycycle on the occupied sphere  $\mathbb{S}^2$ ).

General problems for arbitrary (r, q)-polycycles were considered in [1–7]. In particular, in [5, 6], a criterion was obtained for a *finite* graph to be a polycycle.<sup>5</sup> In [3, 5, 6], it was shown that any polycycle  $\Pi(G)$  is cellularly mapped into a regular tiling  $(r^q)$ ; moreover, this mapping<sup>6</sup> is uniquely defined by a flag (i.e., incident vertex, edge, and r-gon) and its image (projection) under this mapping. We should emphasize three important moments associated with the derivation of this result:

First, in the neighborhood of its internal points, the (r, q)-polycycle  $\Pi(G)$  has the same structure as the tiling  $(r^q)$ .

<sup>&</sup>lt;sup>4</sup>A polycycle P' that is a partial subgraph of a polycycle P'' is called a *subpolycycle* of the polycycle P'', while the polycycle P'' is called a *superpolycycle* relative to P' (here, we use short notation; see footnote 7).

<sup>&</sup>lt;sup>5</sup>V.P. Grishukhin pointed out that the requirement of planarity in the formulation of the criterion is redundant.

<sup>&</sup>lt;sup>6</sup>This mapping is always locally topological but not always globally topological; M.A. Shtan'ko pointed out that the term homomorphism does not apply to this case.

Second, the (r, q)-polycycle  $\Pi(G)$  is simply connected. Third, the regular tiling  $(r^q)$  has no boundary.

# EXTREMAL POLYCYCLES

Let us fix arbitrary natural numbers  $r \ge 3$  and  $q \ge 3$ . For an (r, q)-polycycle<sup>7</sup> P, denote by  $p_r(P)$ the number of its faces<sup>8</sup> and by  $n_{int}(P)$  the number of *internal* vertices. We call the number  $\frac{n_{int}(P)}{p_r(P)}$ the density of the (r, q)-polycycle P. Let us introduce one more notation:  $n(x) = \max n_{int}(P)$  for  $p_r(P) = x$ . An (r, q)-polycycle P is called *extremal* if  $n_{int}(P) = n(p_r(P))$ , i.e., if the polycycle Phas the maximum number of internal vertices  $n_{int}$  for a given number of faces  $p_r$ . In [10], all values of n(x) were obtained for (5, 3)-polycycles for  $x \le 11$ ; all extremal (5, 3)-polycycles proved to be unique and proper, and any dual of an extremal (r, q)-polycycle proved to be extremal again. In addition, a problem was posed in [10] on finding the function n(x) for  $x \ge 12$  for (5, 3)-polycycles. An exhaustive answer to this problem is given by our Theorem 1.

The cell complex consisting of all vertices, edges, and faces of an (r, q)-polycycle that are not incident with its boundary is called the *core* of this polycycle. A polycycle with nonempty connected core is called a *nontrivial elementary polycycle* if all its faces are incident with its core; no face can be removed from this polycycle without reducing the core. A separate r-gon is a *trivial elementary polycycle* with empty core.

**Lemma 1.** Any (r,q)-polycycle with elliptic parameters (r,q) is uniquely represented as a union of elementary summands, i.e., trivial and (maximal) nontrivial elementary subpolycycles that do not have pairwise common faces.

**Proof.** Consider any two vertices of an r-gon of an elliptic (r, q)-polycycle that belong to the core of this polycycle. The shortest edge path<sup>9</sup> between these vertices lies inside the union of two stars of r-gons with the centers at these two vertices; this result can easily be verified in each particular case for any elliptic parameters (r, q) = (3, 3), (3, 4), (3, 5), (4, 3), and (5, 3). Hence, any r-gon of an elliptic (r, q)-polycycle is only incident with one simply connected component of its core. All r-gons that are incident with the same nonempty connected component of the core constitute a *nontrivial elementary summand*. If nontrivial elementary summands do not exhaust all r-gons of an elliptic (r, q)-polycycle, then any of the remaining r-gons is not incident with the core; hence, any of them is a *trivial elementary summand* (with empty core). It is clear that the decomposition obtained of the elliptic polycycle into elementary summands is unique.<sup>10</sup> Lemma 1 is proved.

**Note.** For an arbitrary polycycle with elliptic parameters, all boundary vertices of any elementary summand are boundary vertices of the enveloping polycycle. Hence, any elementary summand in the enveloping elliptic polycycle is isometric (in the sense of a graphical metric).

**Remark 1.** Even for (r, q) = (6, 3), a proposition similar to Lemma 1 is not valid. Indeed, take two vertices in the tiling  $(6^3)$  that are diametrically opposite vertices of the same hexagon. Three hexagons of the tiling  $(6^3)$  surrounding the same vertex constitute one elementary polycycle, and three hexagons surrounding another vertex constitute another polycycle. These two elementary (6,3)-polycycles, which have a common hexagon, constitute together an enveloping (6,3)-polycycle<sup>11</sup> with  $p_6 = 5$ , whose core is not connected (it consists of two vertices).

<sup>&</sup>lt;sup>7</sup>For short, everywhere below, we denote an (r, q)-polycycle  $\Pi(G)$  by P.

<sup>&</sup>lt;sup>8</sup>Actually, we include only internal faces of the (r, q)-polycyclic realization of the graph G in the polycycle  $\Pi(G)$  and call them the *faces of the polycycle*  $\Pi(G)$  in what follows.

<sup>&</sup>lt;sup>9</sup>By the way, this path passes along the edges of the r-gon (see [3; 4; 6, corollary to the lemma]).

<sup>&</sup>lt;sup>10</sup>Elementary subpolycycles whose cores are parts of the same connected component of the core of a superpolycycle may have common faces; on the contrary, elementary summands do not have pairwise common faces (here, we only speak of elliptic (r, q)-polycycles.

<sup>&</sup>lt;sup>11</sup>Both (6,3)-polycycles in this enveloping polycycle are maximal elementary subpolycycles.

**Theorem 1.** Let (r,q) = (5,3). Then,

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

except for the following three cases: n(9) = 10, n(10) = 12, and n(11) = 15. The extremal polycycle is unique for  $x \le 11$  (however, this is no longer so for x = 12) and when n(x) = x;

(ii) all possible densities of (5,3)-polycycles, except for the three cases  $p_5 = 9, 10, 11$ , form the segment [0,1]. All rational densities can be realized by finite improper polycycles. All possible densities of polycycles any of whose faces contains an internal vertex form the segment  $[\frac{1}{3}, 1]$ .

**Proof.** The proof of Theorem 1 is based on Lemma 1, the list of all connected components of the cores of (5, 3)-polycycles, and the corresponding list of elementary (5, 3)-polycycles given in Table 1. The connected components of the cores are enumerated as follows. The core of the special (trivial) polycycle D is empty. The core of the polycycle  $E_1$  consists of a single vertex. If each pentagon of an elementary (5, 3)-polycycle has at most three vertices from the core that are arranged in succession along the perimeter of the pentagon, then the core does not contain pentagons and has the form of a *geodesic* (see the elementary (5, 3)-polycycles  $E_i$ ,  $i \ge 1$ ,  $B_1$ , and  $A_6$ ) or a *propeller* (see the elementary (5, 3)-polycycle  $C_3$ ). If at least one pentagon of the elementary (5, 3)-polycycle contains three vertices of the core that are arranged along the perimeter not in succession, then the whole pentagon belongs to the core. Only in the case of one or two pentagons the core can additionally contain one or two pendant edges (see  $A_5$ ,  $B_3$ ,  $C_2$  and  $A_4$ ,  $B_2$ ,  $C_1$ ). If the core contains more than two pentagons, then the total number of these pentagons can only be 3, 4, or 6 (see  $A_3$ ,  $A_2$ , and  $A_1$ ). The completeness of the list of elementary (5, 3)-polycycles is verified.

Table 1 presents all elementary (5,3)-polycycles, i.e., elementary summands of all (5,3)polycycles. The vertices of their cores are displayed in **bold** type. Using Table 1, one can easily show that any (5,3)-polycycle is obtained by gluing together elementary (5,3)-polycycles along their open edges, i.e., along the edges both of whose ends have degree 2. Here, we only deal with the gluings of elementary polycycles such that the core of every elementary polycycle coincides with a connected component of the core of their union; we treat every elementary polycycle as an elementary summand (maximal elementary subpolycycle; see Lemma 1). In Table 1, each case is denoted by a certain letter with a subscript; two numbers indicate the values of the parameters  $p_5$  and  $n_{int}$ ; for example, a triplet of the form  $(E_s, s+2, s)$  below the figure in Table 1 implies that the figure presents an elementary (5,3)-polycycle  $E_s$  with  $p_5 = s + 2$  and  $n_{int} = s$ . Only the class E consists of a countable number of elementary polycycles  $E_s$  with  $s \ge 1$ ; among the figures of Table 1, elementary polycycles  $E_s$  are indicated only for  $s \leq 5$ . Note that, for the trivial elementary polycycle, the pentagon D, any of its edges can be identified with an open edge of any other elementary polycycle, either trivial or nontrivial. If we want the pentagon D to remain an elementary summand, such an identification can be made for yet another edge of D not adjacent to the already identified one. The elementary (5,3)-polycycles  $A_1, A_2, A_3, A_4, A_5$ , and  $A_6$  (see Table 1) correspond each to its own unique (5,3)-polycycle because neither of them has open edges. The polycycles  $A_1$ ,  $A_2$ ,  $A_3$ ,  $A_4$ ,  $B_3$ , and  $A_5$  are the only extremal ones for  $p_5 = 11, 10, 9, 8, 7, 10, 6$ ; their dual polycycles are the only extremal ones for  $p_5 = 1, 2, 3, 4, 5$ , and 6. (The polycycles  $A_1, A_2$ ,  $A_3, A_4$ , and  $A_5$  are the only nontrivial polycycles that are isometric subgraphs of the skeleton  $(5^3)$ ; they are precisely those five (5, 3)-polycycles that are called *inscribed* in [10].)

Theorem 1 is proved by the enumeration of all possible gluings of elementary (5,3)-polycycles with open edges. For example, for  $p_5 \equiv 0 \pmod{10}$ , an extremal polycycle is obtained by gluing only the copies of the polycycle  $C_1$ , while, for  $p_5 \equiv 9 \pmod{10}$  or  $p_5 \equiv 8 \pmod{10}$ , one should glue together the copies of the polycycle  $C_1$  and one or two copies of the polycycle  $B_2$  (always



• • •

at a deadlock). An elementary polycycle  $E_{x-2}$  is extremal for  $n(x) = x - 2 \ge 10$ ; however, even for x = 12, there is another extremal (5,3)-polycycle that is obtained by gluing the elementary polycycle  $C_1$  together with two copies of the elementary polycycle D along open edges; for x =13, 14, and 15,  $C_1 \bigcup E_1$ ,  $C_1 \bigcup E_2$ , and  $C_1 \bigcup E_3$  are also extremal. A more detailed enumeration of gluings shows that all rational numbers from the segment  $[\frac{1}{3}, 1]$  can be realized as densities of finite polycycles without involving the pentagon D in the gluing. For example, density  $\frac{1}{3}$  is realized by the proper polycycle  $E_1$ , density 1 is realized by the improper polycycle  $C_1$ , and all intermediate densities are realized by appropriate gluings of the copies of these two polycycles taken in necessary proportions. In this case, irrational densities are obtained by gluing an infinite number of copies of the polycycles  $E_1$  and  $C_1$ . Moreover, if we admit copies of the pentagon D in the gluings, then all densities from the segment  $[0, \frac{1}{3}]$  will also be realized. Theorem 1 is proved.

**Remark 2.** If an (r,q)-polycycle P can be obtained from an (r,q)-polycycle P' by adding one r-gon, we denote this as  $P' \to P$ . Using this notation, one can express all such relations between elementary (5,3)-polycycles from Table 1 as follows:  $E_s \to E_{s+1}$  for  $s \ge 1$ ;  $E_3 \to C_3, A_5 \to B_3 \to C_2, A_4 \to A_3 \to A_2 \to A_1$ ;  $E_5 \to C_2, A_4 \to B_2 \to A_2, C_1$ ;  $E_4 \to B_3$ ;  $E_6 \to B_2$ ;  $E_7 \to C_1$ ; and  $B_1 \to B_1$ .

All (3, 3)-, (4, 3)-, and (3, 4)-polycycles were obtained in [12] (proper) and [2] (improper); in the case of (r, q) = (3, 3), the pairs  $(p_r, n_{int})$  are (1, 0), (2, 0), and (3, 1); in the case of (r, q) = (4, 3), the pairs  $(p_r, n_{int})$  are (m, 0) for any  $m \ge 1$ ,  $(|\mathbb{N}|, 0)$  and  $^{12}(|\mathbb{Z}|, 0)$ , (3, 1), (4, 2), and (5, 4); in the case of (r, q) = (3, 4), the pairs  $(p_r, n_{int})$  are (m, 0) for any  $m \ge 1$ ,  $(|\mathbb{N}|, 0)$  and  $^{13}(|\mathbb{Z}|, 0)$ , (4, 1), (5, 1), (6, 1), (6, 2), and (7, 3). Among these pairs, those with  $n_{int} \ge 1$ , except for the pair  $(p_r, n_{int}) = (6, 1)$ , are realized only by proper polycycles; all improper polycycles, except for the case  $(p_r, n_{int}) = (6, 1)$ , have  $n_{int} = 0$ ; i.e., they are outerplanar.

**Theorem 2.** Let (r, q) = (3, 5). Then,

(i) if  $x \equiv 0, 1 \pmod{18}$ , then  $n(x) = \lfloor \frac{x}{3} \rfloor$  except that n(18) = 8 and n(19) = 9; if  $x \neq 0, 1 \pmod{18}$ , then  $n(x) = \lfloor \frac{x-2}{3} \rfloor$  except that  $n(x) = \lfloor \frac{x+1}{3} \rfloor$  for x = 10, 12, 13, 14, 28, 30, 31, 33, 35 and  $n(x) = \lfloor \frac{x+4}{3} \rfloor$  for x = 15, 16, 17, 34;

(ii) all possible densities of (3,5)-polycycles, except those excluded in (i), form the segment  $[0,\frac{1}{3}]$ . All rational densities are realized by finite improper polycycles;

(iii) for  $p_3 \leq 19$ , we have n(x) = 0 for  $0 \leq x \leq 4$ , n(x) = 1 for  $5 \leq x \leq 7$ , n(8) = n(9) = 2, n(10) = n(11) = 3, n(12) = n(13) = 4, n(14) = 5, n(15) = n(16) = 6, n(17) = 7, n(18) = 8, and n(19) = 9. All extremal polycycles with  $p_3 \leq 19$  are proper and, except for the cases  $p_3 = 9$ , 11 (two polycycles for each  $p_3$ ) and  $p_3 = 4$ , 7, 13, 16 (three polycycles for each  $p_3$ ), unique; any polycycle complementary to an extremal (proper) one is also extremal.

**Proof.** To prove Theorem 2, we apply the same strategy as for Theorem 1 except that now enumerations are larger (see Table 2 of elementary (3,5)-polycycles and their cores). A new difficulty consists in the fact that one has to use a special (trivial) elementary polycycle, a triangle d (with empty core), to glue certain elementary (3,5)-polycycles. In this case, a polycycle is glued together with the triangle d along a weakly open edge, i.e., along an edge whose ends have degrees 3 and 4 or 4 and 4. Along a strongly open edge, i.e., along an edge both of whose ends have degree 3, any elementary polycycle can be glued together with any other elementary polycycle. Again, we only speak of those gluings of elementary polycycles for which the core of every elementary polycycle coincides with a connected component of the core of their union; i.e., every elementary polycycle is

<sup>&</sup>lt;sup>12</sup>Here we distinguish two cases that are formally denoted by  $(|\mathbb{N}|, 0)$  and  $(|\mathbb{Z}|, 0)$  depending on whether a polycycle (considered as a chain) is infinite only in one direction or in two opposite directions; if we used a unified formal notation  $(\aleph_0, 0)$  or  $(\infty, 0)$ , we would have lost this additional information.

<sup>&</sup>lt;sup>13</sup>See the preceding footnote.



• • •

#### DEZA, SHTOGRIN

**Table 3.** Minimal nonembeddable (5, 3)- and (3, 5)-polycycles



an elementary summand of the enveloping polycycle. An outerplanar (3,5)-polycycle consists only of triangles d, i.e., of trivial elementary summands with empty cores.

The completeness of Table 2 is also proved by a simple enumeration of the cores. The core of the polycycle d is empty. The core of the polycycle  $e_1$  consists of a single vertex. If there are at most two vertices from a core in each triangle, then the core does not contain triangles and has the form of a *geodesic* (see  $e_i$ ,  $i \ge 1$ , as well as  $b_1$  and  $a_6$ ). If there is one triangle in a core, the latter may additionally have one pendant edge (see  $c_4$  and  $b_4$ ). If there are two triangles in a core, the latter may additionally have one or two pendant edges (see  $c_3$ ,  $b_3$ , and  $b_2$ ). If there are more than two triangles in a core, then their total number may only be 3, 4, 5, 6, 8, or 10 (see  $a_1$ ,  $a_2$ ,  $a_3$ ,  $a_4$ ,  $a_5$ ,  $c_1$ , and  $c_2$ ). The completeness of Table 2 is proved.

In Table 2, each elementary (3, 5)-polycycle is denoted by a certain letter with a subscript; two numbers indicate the values of the parameters  $p_3$  and  $n_{int}$ . Only the class e consists of a countable number of elementary polycycles  $e_s$  with  $s \ge 1$ , and a triplet of the form  $(e_s, 3s+2, s)$  below a figure in Table 2 indicates that the polycycle  $e_s$  has the parameters  $p_3 = 3s + 2$  and  $n_{int} = s$ ; Table 2 presents elementary polycycles  $e_s$  with subscripts  $s \le 6$  only. The rest is analogous to the proof of Theorem 1.

**Remark 3.** In [7], we considered isometric (or with a certain scale  $\lambda$ ) embeddings of (r, q)polycycles (regarded as metric spaces of vertices in a graph with the shortest distances between
them) into hypercubes. In particular, in that paper, we pointed out two proper (5,3)-polycycles
with  $p_5 = 6$  such that any (5,3)-polycycle different from (5<sup>3</sup>) is embeddable (with scale  $\lambda = 2$ )
if and only if it does not contain any of these two polycycles as an induced subgraph:  $E_4$  and  $D \cup E_2 \cup D$  (see [7, Theorem 2] and Table 3).

The following analogue of this theorem holds for (3,5)-polycycles.

**Theorem 3.** Any (3,5)-polycycle different from the edge skeleton of the icosahedron  $(3^5)$  and the skeleton of the icosahedron with one vertex removed  $(3^5) - v$  is embeddable (with scale  $\lambda = 2$ ) if and only if it does not contain, as an induced subgraph, any of the two proper (3,5)-polycycles with 10 vertices shown in Table 3, namely,  $c_3$  and  $d \cup e_2 \cup d$ .

The proof of Theorem 3, based on [15], is given in [16].

**Remark 4.** Theorem 3 completes the solution of the embeddability problem for all (r, q)-polycycles. For  $(r, q) \neq (5, 3), (3, 5)$ , only three polycycles are nonembeddable: the cube without an edge, the octahedron without an edge, and the octahedron with a split vertex. All parabolic and hyperbolic (r, q)-polycycles are embeddable. Parabolic regular tilings  $(r^q)$  are embeddable into a finite-dimensional lattice, and hyperbolic regular tilings  $(r^q)$  are embeddable into an infinite-dimensional lattice. Certain (r, q)-polycycles with parabolic parameters (r, q) cannot be embedded into a finite-dimensional lattice, while, with hyperbolic parameters, they can.

**Remark 5.** The polycycles in Table 3 are partial but not isometric subgraphs in  $(5^3)$  and  $(3^5)$ ; among these polycycles, only the elementary polycycles  $E_4$  and  $c_3$  are induced subgraphs, which are also shown in Tables 1 and 2. Among the polycycles shown in Tables 1 and 2, only the polycycles  $A_1 \supset A_5, C_3 \supset E_3 \supset E_2 \supset E_1 \supset D$  and  $a_1 \supset a_5 \supset b_4 \supset c_4, e_3 \supset e_2 \supset e_1 \supset d$  are isometrically

125

embeddable into half-cubes (i.e., are embeddable into hypercubes isometrically with scale  $\lambda = 2$ ); here, the symbol  $\supset$  means that "a superpolycycle contains a subpolycycle." One can easily verify that any embeddable finite (r, q)-polycycle is embeddable into a  $(\frac{k}{2} + z)$ -dimensional cube for even rand is embeddable with scale  $\lambda = 2$  into a (k+z)-dimensional cube for odd r; here, k is the perimeter of the polycycle and z is the number of closed zones (i.e., cycles consisting of opposite edges of faces that do not contain the outer face). For example, among all embeddable polycycles of Tables 1 and 2, only  $A_1$ ,  $a_1$ , and  $a_5$  have z > 0; namely, z = 5, z = 3, and z = 1, respectively.

The method described above is based on the fact that, for the elliptic parameters (r, q) = (5, 3) and (3, 5), Lemma 1 and Tables 1 and 2 provide a convenient description of polycycles. However, this is not the case for nonelliptic (r, q).

**Theorem 4.** For parabolic and hyperbolic parameters (r, q), there exists a continuum of nonisomorphic elementary (r, q)-polycycles.

**Proof.** Consider a right semi-infinite chain of squares that fill a strip between two parallel rays. Inside the two horizontal sides of each square of the chain, we put r-5 and one decorated vertices to obtain an r-gon instead of a square. There are two alternatives: either r-5 decorated vertices are placed on the upper side and one on the lower side or vice versa, one decorated vertex is placed on the upper side and r-5 on the lower. Such a choice is made independently on each square when we move to the right along this chain. Therefore, there is a continuum of various (nonisomorphic) chains of this kind. All of them are chains in the tiling  $(r^q)$  for  $r \ge 7$  and  $q \ge 3$ , as well as for r = 5 and  $q \ge 4$ . It is also clear that this (r, q)-polycycle is the core of an elementary (r, q)-polycycle consisting of this polycycle supplemented with all r-gons that are incident to it in the tiling  $(r^q)$ . For  $r \ge 7$  and  $q \ge 4$ , this elementary polycycle is proper; moreover, the projection of its polycyclic realization on the tiling  $(r^q)$  is convex in the hyperbolic plane  $\mathbb{H}^2$ .

Now, consider the case of parabolic parameters (r, q), i.e., (r, q) = (6, 3), (4, 4), and (3, 6). In the square lattice, i.e., in the regular tiling  $(4^4)$  of the Euclidean plane  $\mathbb{R}^2$ , we construct a chain of squares semi-infinite in the upper right direction. On each step of this construction, there are two alternatives for choosing the next square: one can choose an adjacent square either on the right on the same level or one level higher. It is clear that there is a continuum of various (nonisomorphic) chains of this kind in the tiling  $(4^4)$  and each of these chains is the core of a certain elementary (4, 4)-polycycle. Infinite chains of hexagons in the tiling  $(6^3)$  are constructed analogously. As for the tiling  $(3^6)$ , combining two adjacent triangles in it into a rhomb and transforming the entire tiling  $(3^6)$  into a rhombic lattice combinatorially equivalent to the tiling  $(4^4)$ , one can apply the same line of reasoning as in the case of the square lattice. The cores of the parabolic polycycles constructed are outerplanar. They can be interpreted as the cores of hyperbolic polycycles (by increasing the value of the parameter q). Theorem 4 is proved.

In spite of the negative result of Theorem 4, one can easily obtain the following general estimates.

**Theorem 5.** For any finite (r, q)-polycycle P with a nonempty core such that each r-gon contains a vertex from the core, the following estimate is valid:

$$\frac{1}{q} \le \frac{n_{\text{int}}}{p_r} < \frac{r}{q}$$

**Proof.** Take an arbitrary polycycle P satisfying the hypotheses of Theorem 5. Since the number of r-gons that meet at an internal vertex of the polycycle P is equal to q and each r-gon contains at least one internal vertex of the polycycle P, the number  $n_{int}q$  counts each r-gon of the polycycle at least once; hence,  $p_r \leq n_{int}q$ . Next, we tile each r-gon by 4-gons by connecting its center with the midpoints of the sides; the number of 4-gons in each r-gon is equal to r; the number of 4-gons incident to any internal vertex is equal to q. Then, the number of 4-gons adjacent only

to internal vertices of the polycycle P is equal to  $n_{int}q$ , while the total number of 4-gons is equal to  $rp_r$ . Hence,  $n_{int}q < rp_r$ . Theorem 5 is proved.

Both estimates in Theorem 5 are, generally speaking, sharp. For example, the lower estimate is attained on a q-star of r-gons with the center at any internal vertex of an (r, q)-polycycle. To show the sharpness of the upper estimate, we consider a square with the side m + 1. Let us partition it into  $(m+1)^2$  unit squares. We obtain an (r, q)-polycycle with parameters r = q = 4 that has exactly  $m^2$  internal vertices. For a sequence of such (4, 4)-polycycles, we obtain the following relation in the limit as  $m \to \infty$ :

$$\frac{n_{\rm int}}{p_r} = \frac{m^2}{(m+1)^2} \to 1;$$

hence, the upper estimate in Theorem 5 is also sharp.

Theorem 5 shows that  $n_{int}(p_r)$  has a linear growth order in  $p_r$ ; however, we leave open the question of the exact parameters of the growth order of the function  $n_{int}$ .

We suppose that, for any nonelliptic parameters (r, q), there are proper polycycles among extremal (r, q)-polycycles; this is true for any elliptic parameters: all known extremal (r, q)-helicenes Pwith elliptic parameters (r, q) have  $p_r(P) > p_r(r^q)$ .

**Remark 6.** Extremal polycycles represent the opposite extreme case of outerplanar polycycles. For given r, q, and  $p_r$ , an extremal polycycle maximizes the number of internal vertices  $n_{int}$  and the number of *internal* (i.e., those not belonging to the boundary) edges  $e_{int}$ ; it also minimizes the number of boundary edges (perimeter) k, the total number of edges e, and the total number of vertices n. Indeed, the Euler formula  $(n_{int} + k) - (e_{int} + k) + (p_r + 1) = 2$  and the equality  $rp_r = 2e_{int} + k$  imply the relations

$$n_{ ext{int}} = e_{ ext{int}} - p_r + 1 = -rac{k}{2} + rac{p_r(r-2)}{2} + 1 = -e + p_r(r-1) + 1 = -n + p_r(r-2) + 2,$$

which confirm the aforesaid.

The extremal animals mentioned in [11] are, in our terms, proper (4, 4)-, (6, 3)-, and (3, 6)polycycles with the minimum number of edges e and, hence, with the maximum number  $n_{\text{int}}$ . In [11], it was proved that such polycycles have  $e = 2p_4 + \lceil 2\sqrt{p_4} \rceil$ ,  $e = 3p_6 + \lceil \sqrt{12p_6 - 3} \rceil$ , and  $e = p_3 + \lceil \frac{p_3 + \sqrt{6p_3}}{2} \rceil$  edges, respectively, and that, among them, there are always polycycles that grow like a spiral.

### NONEXTENDIBLE POLYCYCLES

Consider another natural concept of maximality of polycycles. An (r, q)-polycycle is called *nonextendible* if it is not a partial subgraph of any other (r, q)-polycycle, i.e., if an addition of any new r-gon removes it from the class of (r, q)-polycycles. It is clear that a polycycle defined by the skeleton of any tiling  $(r^q)$  is nonextendible, while all other nonextendible polycycles are helicenes. It is also clear that any 3-connected (r, 3)-polycycle is nonextendible.

It turned out that Tables 1 and 2 also facilitate the determination of nonextendible (r, q)-polycycles for spherical (r, q).

**Theorem 6.** All nonextendible polycycles different from the skeleton  $(r^q)$  are given by four improper (r,q)-polycycles (two finite and two infinite ones) depicted in Table 4 and a continuum of infinite improper (r,q)-polycycles for any pair  $(r,q) \neq (3,3), (3,4), (4,3)$ .

**Proof.** The case (r, q) = (3, 3), (3, 4), (4, 3) follows immediately from the list of these polycycles given in [2]. It is clear that doubly-infinite and nonperiodic (at least in one direction) sequences of glued copies of the elementary polycycles  $b_2$  and  $e_6$  (from Table 2) yield a continuum of infinite

**Table 4.** Examples of nonextendible elliptic (r, q)-polycycles



nonextendible (3, 5)-polycycles. The same is true for the gluings of copies of the elementary polycycle  $C_2$  (from Table 1) and  $C'_2$  (obtained from  $C_2$  by rotation through  $\pi$ ), which yield a continuum of infinite nonextendible (5, 3)-polycycles.

In nonelliptic cases, i.e., for  $(r,q) \neq (3,3), (3,4), (3,5), (4,3), (5,3)$ , we consider infinite nonextendible polycycles obtained from  $(r^q)$  by rejecting certain nonadjacent *r*-gons followed by taking a universal covering. If we reject a countable number of *r*-gons using nonperiodic sequences of rejected *r*-gons, then (due to an ambiguous choice of the rejected *r*-gons at each step, similar to the choice of squares of the infinite chain in the tiling  $(4^4)$  in the proof of Theorem 4), we obtain a continuum of different polycycles. It is clear that, when rejecting different (noncongruent) sequences of *r*-gons, the universal coverings prove to be different (see Theorem 2 from [3] and [6] on a one-to-one cellular mapping, which is precisely up to congruence).

For the parameters (r,q) = (3,5), we succeeded in proving that there do not exist nonextendible finite polycycles except for one,<sup>14</sup> which is depicted in the second figure in Table 4 (where the icosahedron and octahedron with a split vertex are presented). For (r,q) = (5,3), this result follows from the data of Table 1, Lemma 1, and Remark 1.

It remains to prove the nonexistence of *finite* nonextendible polycycles for nonelliptic parameters (r, q). Here, it is convenient to return to the old, although more cumbersome, notations, which were mentioned at the beginning of the paper. In [3–6], each (r, q)-polycycle  $\Pi(G)$  and the standard tiling  $(r^q)$  were put in one-to-one correspondence with an abstract two-dimensional polyhedron  $\mathbf{P}(G)$  and a standard polyhedron  $\mathbf{K}(r^q)$ , respectively,<sup>15</sup> that are combinatorially isomorphic to the above polycycle and tiling and are composed of isometric regular Euclidean *r*-gons, and the existence of a continuous locally isometric cellular mapping  $f: \mathbf{P}(G) \to \mathbf{K}(r^q)$  was proved.

Since the angle of a regular r-gon is equal to  $(r-2)\pi/r$  and the number of regular r-gons that meet at an internal vertex of the polyhedron  $\mathbf{P}(G)$  is equal to q, the curvature of any internal vertex of the polyhedron  $\mathbf{P}(G)$  is equal to

$$\omega = 2\pi - \frac{r-2}{r}q\pi.$$

Hence, the total curvature of the polyhedron  $\mathbf{P}(G)$  is equal to

$$\Omega = n_{ ext{int}} rac{2(r+q) - rq}{r} \pi.$$

If  $n_{\text{int}} = 0$ , i.e., an (r, q)-polycycle  $\Pi(G)$  is outerplanar, then the curvature  $\Omega$  of the corresponding polyhedron  $\mathbf{P}(G)$  is equal to zero for any parameters (r, q). If  $n_{\text{int}} > 0$ , then the curvature  $\Omega$  is

<sup>&</sup>lt;sup>14</sup>The absence of other nonextendible (3,5)-polycycles is proved by a thorough enumeration; however, we do not present it here; we are trying to make this enumeration shorter.

<sup>&</sup>lt;sup>15</sup>Here, it is pertinent to recall the following relations (see [3-5]):  $\mathbf{\Pi}(G) \cong \mathbf{P}(G)$  for any parameters (r, q);  $\mathbf{K}(r^q) \cong (r^q)$  for elliptic and hyperbolic parameters and  $\mathbf{K}(r^q) \equiv (r^q)$  for parabolic parameters (r, q); and  $\mathbf{P}(r^q) \equiv \mathbf{K}(r^q)$  for parabolic and hyperbolic parameters (r, q), but  $\mathbf{P}(r^q) \equiv \mathbf{K}(r^q) - \mathbf{F}$  for elliptic parameters (the interior of the face  $\mathbf{F}$  is removed from the surface of the Platon body; a sphere cannot be completely embedded into a plane).

positive, zero, or negative, depending on whether the parameters (r, q) are elliptic, parabolic, or hyperbolic, respectively.

Any internal edge of a polyhedron  $\mathbf{P}(G)$  belongs to exactly two r-gons, while any boundary edge belongs to only one r-gon. Therefore, the following equality holds:

$$rp_r = 2e_{\text{int}} + k,$$

where, again,  $e_{int}$  is the number of internal edges of the polyhedron  $\mathbf{P}(G)$  and k is the number of boundary edges. On the other hand, since the number of boundary vertices and the number of boundary edges of the polyhedron  $\mathbf{P}(G)$  are equal to the same number k (the perimeter of the polyhedron), these two numbers in the Euler formula cancel out, and a condensed version of this formula reads as

$$n_{\text{int}} - e_{\text{int}} + p_r = 1.$$

From the last two formulas, we obtain

$$(r-2)p_r = 2n_{
m int} + (k-2).$$

Now, let us calculate the sum of plane angles of the polyhedron  $\mathbf{P}(G)$ ; we do this in two different ways: (i) we first calculate the sum of angles in separate polygons and then sum up over all polygons and (ii) we first calculate the sum of angles at separate vertices and then sum up over all vertices, both boundary and internal. As a result, we obtain the equality

$$p_r(r-2)\pi = \sum_{i=1}^k \varphi_i + n_{\text{int}} \, \frac{r-2}{r} \, q\pi,$$

where  $\varphi_i$  denotes the total angle at the *i*th boundary vertex of the polyhedron  $\mathbf{P}(G)$ . Combining this formula with the preceding one yields

$$n_{\rm int}\left(2\pi - \frac{r-2}{r}q\pi\right) = \sum_{i=1}^{k} \varphi_i - (k-2)\pi.$$
 (1)

The geometrical meaning of this equality can be formulated as the following discrete analogue of the well-known Gauss-Bonnet theorem (see [13]).

The excess of the sum of angles of a geodesic k-gon (as compared with the sum of angles of a plane k-gon) is equal to its curvature; i.e., if  $\varphi_1, \ldots, \varphi_k$  are the angles of a geodesic k-gon that is the boundary of the polyhedron  $\mathbf{P}(G)$  and  $\omega_1, \ldots, \omega_{n_{\text{int}}}$  are the curvatures of internal vertices of the polyhedron  $\mathbf{P}(G)$ , then

$$\sum_{i=1}^k \varphi_i - (k-2)\pi = \sum_{j=1}^{n_{\text{int}}} \omega_j.$$

In our case,  $\omega_1 = \ldots = \omega_{n_{\text{int}}} = \omega$ , where  $\omega = 2\pi - (r-2)q\pi/r$ .

Let  $k_j$  be the number of vertices of degree j, where j = 2, 3, ..., q-1, q, that are situated on the boundary of the polyhedron  $\mathbf{P}(G)$  and k be the total number of vertices of the boundary polygon of the polyhedron  $\mathbf{P}(G)$ , i.e., its perimeter. Then,

$$k = k_2 + k_3 + \ldots + k_{q-1} + k_q.$$
<sup>(2)</sup>

Let us calculate the sum  $\sum_{i=1}^{k} \varphi_i - (k-2)\pi$  on the right-hand side of equality (1) for a finite polyhedron  $\mathbf{P}(G)$  considered as a geodesic k-gon. Since

$$\sum_{i=1}^{k} \varphi_i = \left\{ 1 \cdot k_2 + 2 \cdot k_3 + \ldots + (q-2) \cdot k_{q-1} + (q-1) \cdot k_q \right\} \frac{r-2}{r} \pi,$$

PROCEEDINGS OF THE STEKLOV INSTITUTE OF MATHEMATICS Vol. 239 2002

by formula (2) we obtain the equality

$$\sum_{i=1}^{k} \varphi_i - (k-2)\pi = \left\{ \left( 1 \cdot \frac{r-2}{r} - 1 \right) k_2 + \left( 2 \cdot \frac{r-2}{r} - 1 \right) k_3 + \dots + \left( (q-2) \cdot \frac{r-2}{r} - 1 \right) k_{q-1} + \left( (q-1) \cdot \frac{r-2}{r} - 1 \right) k_q \right\} \pi + 2\pi.$$
(3)

For nonelliptic pairs (r, q), the regular tilings  $(r^q)$  are not unique infinite nonextendible (r, q)-polycycles; there exists a continuum of other (r, q)-polycycles such that every vertex has degree q. However, this is not so in the finite case.

Consider a particular case of a finite polyhedron  $\mathbf{P}(G)$  in which each vertex has degree q. In this case, 2e = qn, where n is the total number of vertices and e is the total number of edges of  $\mathbf{P}(G)$ ; in view of the equality  $2e = rp_r + k$ , we can rewrite the Euler formula  $n - e + p_r = 1$  as

$$n\frac{2(q+r)-qr}{2r} = 1 + \frac{k}{r}$$

Hence, 2(q+r) - qr > 0; i.e., the parameters (r,q) are elliptic. For any of the five elliptic pairs (r,q) = (3,3), (3,4), (3,5), (4,3), (5,3), we directly verify that the equality k = r holds and that the polyhedron  $\mathbf{P}(G)$  is in fact the surface of a Platon body without one face.

Now, let a finite polycycle  $\Pi(G)$  be nonextendible but different from the skeleton of a regular tiling  $(r^q)$ . In this case, there certainly exist vertices on the boundary of the polyhedron  $\mathbf{P}(G)$  whose degrees are less than q.

**Lemma 2.** If a finite polyhedron  $\mathbf{P}(G)$  has a vertex whose degree is less than q, then the total number of these vertices is at least two.

**Proof.** We will prove Lemma 2 by contradiction. Suppose that a finite polyhedron  $\mathbf{P}(G)$  has only one vertex whose degree is less than q. Denote this vertex by  $A_1$ . All the other boundary vertices  $A_2, A_3, \ldots, A_k$  (the numbering corresponds to moving along the boundary) have degree q. Choose a flag  $\mathbf{\Phi}$  in the polyhedron  $\mathbf{P}(G)$  that consists of the vertex  $A_1$ , edge  $A_1A_2$ , and r-gon incident to them and construct a continuous locally isometric cellular mapping  $f: \mathbf{P}(G) \to \mathbf{K}(r^q)$ (see [3, 5, 6]). The mapping f is uniquely defined by the flag  $\mathbf{\Phi}$  in the polyhedron  $\mathbf{P}(G)$  and its image  $f(\mathbf{\Phi})$  in the polyhedron  $\mathbf{K}(r^q)$ .

Let us take the restriction of this mapping onto a two-dimensional chain consisting of r-gons of the polyhedron  $\mathbf{P}(G)$  incident to its boundary and try to find out what is the image of this chain under the mapping f.

Consider a closed edge path  $A'_1A_2A_3...A_kA''_1$  whose beginning  $A'_1$  and end  $A''_2$  are situated at the same vertex  $A_1$ . Moving along this path, we enumerate<sup>16</sup> all *r*-gons of  $\mathbf{P}(G)$  incident to it; we start the enumeration from the flag  $\Phi$ . Thus, we obtain a sequence of *r*-gons in which all neighboring *r*-gons are adjacent along a side. The set of all *r*-gons of this sequence constitutes a closed chain. The image of this chain under the mapping f must also be closed.

Since the edge path  $A'_1A_2A_3...A_kA''_1$  is closed, its image under the mapping f is also closed. Hence, the equality<sup>17</sup>  $f(A''_1) = f(A'_1)$  holds, and, henceforth, we will split neither the vertex  $A_1$  nor its image  $f(A_1)$ .

Now, we pass on to the analysis of the mappings of stars. All r-gons of the polyhedron  $\mathbf{P}(G)$  incident to a vertex A constitute a *star*; we denote it by **St**A. Let us show that the following relations hold:

$$\mathbf{St}f(A_j) = \mathbf{F} \cup f(\mathbf{St}A_j), \qquad j = 2, 3, \dots, k,$$

<sup>&</sup>lt;sup>16</sup>It is convenient first to cut off the vertices of the polyhedron  $\mathbf{P}(G)$  and then enumerate all *r*-gons encountered while moving along the smoothed boundary in the sequential order.

<sup>&</sup>lt;sup>17</sup>This equality implies that the perimeter k satisfies the relation  $k = mr, m \in \mathbb{N}$ .

where **F** is a fixed r-gon of the polyhedron  $\mathbf{K}(r^q)$ , which is the same for any  $j = 2, 3, \ldots, k$ . Indeed, f maps the flag  $\mathbf{\Phi}$  to its image  $f(\mathbf{\Phi})$ . Denote by **F** the r-gon from the polyhedron  $\mathbf{K}(r^q)$  that is adjacent to  $f(\mathbf{\Phi})$  along the edge  $f(A_1A_2)$ . Since the number of r-gons of the star  $\mathbf{St}A_2$  in  $\mathbf{P}(G)$  is equal to q-1 and the number of r-gons of the star  $\mathbf{St}f(A_2)$  in  $\mathbf{K}(r^q)$  is equal to q, the r-gon **F** has one more edge  $f(A_2A_3)$  on its boundary; hence, we obtain the equality  $\mathbf{St}f(A_2) = \mathbf{F} \cup f(\mathbf{St}A_2)$ . For the same reason, the r-gon **F** has the edge  $f(A_3A_4)$  on its boundary, whence we obtain the equality  $\mathbf{St}f(A_3) = \mathbf{F} \cup f(\mathbf{St}A_3)$ , and so on. Thus, the relations presented are proved.

Moving along the chain of r-gons taken from the stars  $\mathbf{St}A_2, \mathbf{St}A_3, \ldots, \mathbf{St}A_k$ , starting from the r-gon with edge  $A_2A_1$  and ending at the r-gon with edge  $A_kA_1$ , we write out their images under the mapping f. The image of the r-gon with the edge  $A_2A_1$  lies outside the r-gon  $\mathbf{F}$  and is adjacent to it along the edge  $f(A_2A_1)$ . The image of the r-gon with the edge  $A_kA_1$  lies outside the r-gon  $\mathbf{F}$  and is adjacent to it along the edge  $f(A_2A_1)$ .

If the degree of the vertex  $A_1$  is no less than three, then at least two r-gons from the polyhedron  $\mathbf{P}(G)$  are incident to the vertex  $A_1$ . For the two of these r-gons that are adjacent to the boundary along the edges  $A_1A_2$  and  $A_1A_k$ , we have already obtained two images above; both of them lie outside the r-gon  $\mathbf{F}$ : one is incident to the edge  $f(A_1A_2)$ , while the other, to the edge  $f(A_1A_k)$ . These two images are different indeed because the total number of r-gons of the polyhedron  $\mathbf{K}(r^q)$  that are incident to the vertex  $f(A_1)$  is no less than three (the degree q of every vertex of  $\mathbf{K}(r^q)$  is greater than or equal to 3). Since the degree of the vertex  $A_1$  is less than q, these r-gons cannot both belong to the image of the star  $\mathbf{St}A_1$  under the mapping f; in the present case,  $\mathbf{St}f(A_1) \neq \mathbf{F} \cup f(\mathbf{St}A_1)$ . We obtained a contradiction.

If the degree of the vertex  $A_1$  equals two, then only one r-gon from the polyhedron  $\mathbf{P}(G)$  is incident to the vertex  $A_1$ , which is adjacent to the boundary along the edges  $A_1A_2$  and  $A_1A_k$ simultaneously. This is the flag  $\Phi$ . As before, we have already obtained two images of the flag  $\Phi$ ; both of them lie outside the r-gon  $\mathbf{F}$ : one is adjacent to  $\mathbf{F}$  along the edge  $f(A_1A_2)$ , while the other, along the edge  $f(A_1A_k)$ . These two images are different indeed because the total number of r-gons of the polyhedron  $\mathbf{K}(r^q)$  that meet at the vertex  $f(A_1)$  is no less than three  $(q \geq 3)$ . However, there must be only one image of the same r-gon (in this case, the flag  $\Phi$ ) under the mapping f. We obtained a contradiction again.

Hence, the situation when only one vertex of the polyhedron  $\mathbf{P}(G)$  has degree less than q is impossible; there must be at least two such vertices. Lemma 2 is proved.

End of the proof of Theorem 6. Consider an arbitrary finite nonextendible (r, q)-polycycle  $\Pi(G)$  and prove that the corresponding polyhedron  $\mathbf{P}(G)$  always has positive curvature, so that the parameters (r, q) are elliptic.

We will prove this by contradiction. Suppose that the parameters (r,q) are parabolic or hyperbolic, i.e., the inequality  $qr - 2(q+r) \ge 0$  holds. Then, the following estimate is valid for the coefficient of  $k_q$  in (3):  $(q-1)\frac{r-2}{r} - 1 = \frac{qr-2(q+r)}{r} + \frac{2}{r} \ge \frac{2}{r}$ . On the boundary of the finite nonextendible polycycle  $\mathbf{\Pi}(G)$ , which is different from the skele-

On the boundary of the finite nonextendible polycycle  $\mathbf{\Pi}(G)$ , which is different from the skeleton of a Platonic body, there must certainly exist vertices of degree less than q in addition to vertices of degree q; by Lemma 2, the number of such vertices must be no less than two, as the number of vertices of the corresponding polyhedron  $\mathbf{P}(G)$ . The total number of vertices on the boundary must be greater than r (see the corollary to the lemma in [3]). Any two vertices of degree less than q must be separated by at least r - 1 vertices of degree q; otherwise, our polycycle  $\mathbf{\Pi}(G)$  would be extendible.<sup>18</sup> It follows from the aforesaid and condition  $r \geq 3$ 

<sup>&</sup>lt;sup>18</sup>If, between two vertices with degrees less than q on the boundary of the polycycle  $\Pi(G)$ , there are only r-s vertices of degree q, where  $s \ge 2$ , then these vertices are connected by a boundary edge chain of length r-s+1; this chain can be closed to give a new r-gon by adding a new chain of length s-1, where  $s-1 \ge 1$ , to the old chain on the outer side of the polycycle  $\Pi(G)$ . The degree of these two vertices remains no greater than q; thus, the polycycle is extended.

that

$$k_q \ge (r-1)\sum_{j=2}^{q-1}k_j \ge 2\sum_{j=2}^{q-1}k_j.$$

Therefore, by (3), the quantity  $\sum_{i=1}^{k} \varphi_i - (k-2)\pi$  calculated for the polyhedron  $\mathbf{P}(G)$  obeys the estimate

$$\sum_{i=1}^{k} \varphi_{i} - (k-2)\pi \geq \left\{ \left( 1 \cdot \frac{r-2}{r} - 1 + 2 \cdot \frac{2}{r} \right) k_{2} + \left( 2 \cdot \frac{r-2}{r} - 1 + 2 \cdot \frac{2}{r} \right) k_{3} + \dots + \left( (q-2) \cdot \frac{r-2}{r} - 1 + 2 \cdot \frac{2}{r} \right) k_{q-1} \right\} \pi + 2\pi.$$
(4)

The coefficient of  $k_j$  on the right-hand side of inequality (4) increases as the index j increases. Since the least coefficient (that of  $k_2$ ) is positive, all the other coefficients of  $k_j$  are also positive. The values of  $k_j$  themselves are nonnegative (and there even exists one positive  $k_j$  because there are vertices on the boundary of  $\mathbf{P}(G)$  whose degree is less than q). Hence,

$$\sum_{i=1}^k \varphi_i - (k-2)\pi \ge 2\pi.$$

The positivity of the right-hand side of inequality (4) implies the positivity of the left-hand side. Thus, in view of (1), the curvature  $\Omega$  of the geodesic k-gon is positive. The resulting inequality 2(r+q) - qr > 0 contradicts the assumption made. Hence, a finite nonextendible polycycle cannot have parabolic or hyperbolic parameters (r, q); these parameters are elliptic. Theorem 6 is proved.

Note that the number of (r, q)-polycycles such that the degree of the mapping of an internal point of any face under a continuous locally isometric cellular mapping  $f: \mathbf{P}(G) \to \mathbf{K}(r^q)$  is equal to 1 and that are extendible (with the loss of this property)

- is equal to 0 for the parameters (r,q) = (3,3), (3,4);
- is equal to 1 for the parameters (r,q) = (4,3) (this is  $P_2 \times P_5$ );
- is finite for the parameters (r,q) = (5,3), (3,5); and
- is infinite for the remaining parameters (r, q).

The finiteness of this number for the parameters (r, q) = (5, 3) and (3, 5) follows from the fact that the number of 5-gons and 3-gons must be no greater than 12 and 20, respectively.

Note also that one can obtain interesting examples of infinite nonextendible (r, q)-polycycles as universal coverings for the complement to the covering of all vertices of the regular tiling  $(r^q)$ by nonadjacent *r*-gons (if such a covering exists; the cube, octahedron, and icosahedron have such coverings, while the tetrahedron and dodecahedron do not).

## EXAMPLES OF ISOHEDRAL POLYCYCLES

Following [8], we call a polycycle P isogonal or isohedral if its automorphism group (denoted by Aut P) is transitive on the vertices or faces, respectively. In [7], we gave theorems describing such (r, q)-polycycles. Tables 5–8 below display all families of such polycycles that we have obtained.

Table 5 presents all 19 isohedral (r, q)-polycycles with elliptic parameters (r, q). Among them, only 3-, 4-, and 5-gons (triangles in the three cases q = 3, 4, 5) and two infinite (r, q)-polycycles (one of them in the two cases q = 4, 5) are isogonal.<sup>19</sup> There is only one *cactus* among infinite polycycles; all the other are *ribbons*.

<sup>&</sup>lt;sup>19</sup>Table 5 does not contain the following elliptic isohedra: an exceptional (r, q)-polycycle with parameters r = 2and q = 3, because condition (i) (see the definition of polycycles in the Introduction) requires that  $r \ge 3$ , and special (r, q)-polycycles with parameters  $r \ge 2$  and q = 2, because condition (ii) requires that  $q \ge 3$  (in fact, these isohedra are not polycycles but monocycles since they do not have any strictly proper subpolycycles).

## DEZA, SHTOGRIN

Table	5.	All	19	isohedral	elliptic	(r, q	)-polycycles
-------	----	-----	----	-----------	----------	-------	--------------

$\boxed{\begin{array}{c} (r,q) \\ Aut P \end{array}}$	(3,3)	(3,4)	(4,3)	(3,5)	(5,3)
$D_{rh}$					$\bigcirc$
$D_{2h}$	$\bigcirc$	$\bigcirc$		$\bigcirc$	
$D_{qh}$	$\bigwedge$		$\bigcirc$		
$pm11 \approx T(2, 2, \infty)$					
$pmm2 = T^*(2, 2, \infty)$					
pma $2 \approx T(2,2,\infty)$					
$T^*(2,3,\infty) \approx SL(2,\mathbb{Z})$					

Table 6. Examples of families of isohedral (r,q)-polycycles with a ribbon group of symmetry



PROCEEDINGS OF THE STEKLOV INSTITUTE OF MATHEMATICS Vol. 239 2002





Table 8. Examples of isogonal (but not isohedral) (r, q)-polycycles



### DEZA, SHTOGRIN

Table 6 presents, among nine figures, eight families of decorations (on the edge marked by a single dot, there are *a* decorated vertices, and, on the edge marked by two dots, there are *b* decorated vertices) of the (4,3)-polycycle  $P = P_2 \times P_{\mathbb{Z}}$  (the product of a segment and an edge line) with ribbon groups of symmetry. Only the undecorated leftmost and the middle polycycles are isogonal for a = 0.

Table 7 presents all families of nonribbon isohedral polycycles (namely, nine families of cacti) together with their parameters (r, q) and the automorphism groups Aut P. There is only one isogonal case among the polycycles of Table 7, the left polycycle in the first row for a = 0.

The automorphism group of the rightmost polycycle in the bottom row is in one-to-one correspondence with the group  $T(2,3,\infty)$  but is different from it: each central inversion is replaced with a reflection in a line. This is also a subgroup of index 2 of the group  $T^*(2,3,\infty)$ ; however, it is isomorphic to the product  $3 \times T^*(\infty,\infty,\infty)$ . It turned out that, except for this case, all known isohedral polycycles have triangular groups T(l,m,n) or  $T^*(l,m,n)$  as Aut P.

Table 8 presents two more cacti: a (3,5)-polycycle representing a universal covering of an icosahedron from which four pairwise disjoint faces are removed and a (4, 4)-polycycle representing a universal covering of a square lattice from which a square sublattice of index 4 is removed. These polycycles are isogonal but *not* isohedral; they have two orbits of faces with respect to the group Aut P: the faces of one orbit have edges on the boundary of the polycycle P, while the faces of another orbit have no edges on the boundary of the polycycle P; except for these two, we do not know any other such polycycles.<sup>20</sup>

Note that the first polycycle in Table 7 for k = 2 degenerates into a ribbon (see the second polycycle in Table 6), and the fourth polycycle in Table 7 for k = 2 also degenerates into a ribbon (see the third polycycle in Table 6). All the other polycycles in Table 6, or, more precisely, their representatives, are given in Table 5: the first; the fourth, fifth, and sixth for a = 0; and the seventh, eighth, and ninth for a = 1 and b = 0. The seventh polycycle from Table 7 for a = 0 and q = 3 is also presented in Table 5 (see the intersection of the column (r, q) = (5, 3) and row Aut  $P = T^*(2, 3, \infty)$ ).

Recall that  $T^*(l, m, n)$  denotes the Coxeter triangular group whose fundamental triangle has angles  $\frac{\pi}{l}$ ,  $\frac{\pi}{m}$ , and  $\frac{\pi}{n}$ , while T(l, m, n) denotes its subgroup (of index 2) of motions of the first kind, i.e., orientation-preserving motions. For ribbon groups, there are following relations between groups: pmm2 =  $T^*(2, 2, \infty)$ ,  $T(2, 2, \infty) = p112 \approx pma2 \approx pm11 \not\approx p1m1$ . Recall also that  $T(2, 3, \infty) \approx PSL(2, \mathbb{Z})$  (a modular group) and  $T^*(2, 3, \infty) \approx SL(2, \mathbb{Z})$ .

## ACKNOWLEDGMENTS

The second author was supported by the Russian Foundation for Basic Research (project no. 02-01-00803) and by the program "Leading Scientific Schools of the Russian Federation" (project no. 00-15-96011).

## REFERENCES

- 1. Deza, M. and Shtogrin, M.I., Embedding of Chemical Graphs in Hypercubes, *Mat. Zametki*, 2000, vol. 68, no. 3, pp. 339-352.
- Deza, M. and Shtogrin, M.I., Polycycles, Voronoi Conf. on Analytic Number Theory and Space Tilings, Kiev: Inst. Mat., Nat. Akad. Nauk Ukr., 1998, pp. 19–23.
- Deza, M. and Shtogrin, M.I., Primitive Polycycles and Helicenes, Usp. Mat. Nauk, 1999, vol. 54, no. 6, pp. 159-160.

<sup>&</sup>lt;sup>20</sup>Table 8 does not contain exceptional elliptic (r,q)-polycycles with parameters r = 2 and  $q \ge 4$  because they satisfy neither condition (i), which requires that  $r \ge 3$ , nor condition (iii), which requires that the intersection of cells should be a cell again; these polycycles are also isogonal but not isohedral; all q!/2 of their planar realizations prove to be pairwise isomorphic.

- 4. Deza, M. and Shtogrin, M.I., Infinite Primitive Polycycles, Usp. Mat. Nauk, 2000, vol. 55, no. 1, pp. 179-180.
- 5. Shtogrin, M.I., Primitive Polycycles: A Criterion, Usp. Mat. Nauk, 1999, vol. 54, no. 6, pp. 177–178.
- 6. Shtogrin, M.I., Nonprimitive Polycycles and Helicenes, Usp. Mat. Nauk, 2000, vol. 55, no. 2, pp. 155-156.
- Deza, M. and Shtogrin, M.I., Polycycles: Symmetry and Embeddability, Usp. Mat. Nauk, 2000, vol. 55, no. 6, pp. 129-130.
- 8. Grünbaum, B. and Shephard, G.C., Tilings and Patterns, New York: Freeman, 1987.
- 9. Bousquet-Mélou, M., Guttman, A.J., Orrick, W.P., and Rechnitzer, A., Inversion Relations, Reciprocity, and Polyominoes, Ann. Combin., 1999, vol. 3, pp. 223-249.
- 10. Cyvin, S.J., Cyvin, B.N., Brunvoll, J., Bremdsdal, E., Zhang Fuji, Guo Xiofeng, and Tosic, R., Theory of Polypentagons, J. Chem. Inform. Comp. Sci., 1993, vol. 33, pp. 466-474.
- 11. Harary, F. and Harborth, H., Extremal Animals, J. Combin. Inform. Syst. Sci., 1976, vol. 1, pp. 1-8.
- 12. Harborth, H., Some Mosaic Polyominoes, Ars Combin., 1990, vol. 29, pp. 5–12.
- 13. Aleksandrov, A.D., Vypuklye mnogogranniki (Convex Polyhedra), Moscow: Gostekhizdat, 1950.
- 14. Harary, F., *Graph Theory*, Reading: Addison-Wesley, 1969. Translated under the title *Teoriya grafov*, Moscow: Mir, 1973.
- Chepoi, V., Deza, M., and Grishikhin, V.P., Clin d'oeil on l<sub>1</sub>-embeddable planar graphs, *Discrete Appl. Math.*, 1997, vol. 80, pp. 3-19.
- Deza, M. and Shtogrin, M.I., Embeddability Criterion for (r, q)-Polycycles, Usp. Mat. Nauk, 2002, vol. 57, no. 3, pp. 149–150.

Translated by I. Nikitin