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To the memory of
Boris Nikolaevich Delaunay

Fullerenes and disk-fullerenes

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Abstract. A *geometric fullerene*, or simply a *fullerene*, is the surface of a simple closed convex 3-dimensional polyhedron with only 5- and 6-gonal faces. Fullerenes are geometric models for *chemical fullerenes*, which form an important class of organic molecules. These molecules have been studied intensively in chemistry, physics, crystallography, and so on, and their study has led to the appearance of a vast literature on fullerenes in mathematical chemistry and combinatorial and applied geometry. In particular, several generalizations of the notion of a fullerene have been given, aiming at various applications. Here a new generalization of this notion is proposed: an *n-disk-fullerene*. It is obtained from the surface of a closed convex 3-dimensional polyhedron which has one n-gonal face and all other faces 5- and 6-gonal, by removing the n-gonal face. Only 5- and 6-disk-fullerenes correspond to geometric fullerenes. The notion of a geometric fullerene is therefore generalized from spheres to compact simply connected two-dimensional manifolds with boundary. A two-dimensional surface is said to be *unshrinkable* if it does not contain *belts*, that is, simple cycles consisting of 6-gons each of which has two neighbours adjacent at a pair of opposite edges. Shrinkability of fullerenes and n-disk-fullerenes is investigated.

Bibliography: 87 titles.

Keywords: polygon, convex polyhedron, planar graph, fullerene, patch, disk-fullerene.

Contents

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Introduction

In the 1985 paper [65] the molecules C_{60}, called *Buckminsterfullerenes*, were introduced. These molecules were discovered in the study of mass spectra of graphite vapours resulting from laser irradiation of a solid sample. Eleven years later R. Curl, H. Kroto, and R. Smalley were awarded the 1996 Nobel Prize in *Chemistry* for the discovery of *fullerenes*. The existence of the molecule C_{60} was predicted in [68] and theoretically justified in [3].

The molecule of a *chemical fullerene* can be described by a *planar cubic graph*. This graph has a unique spherical realization and splits the sphere into 5- and 6-gons. Carbon atoms are located at the vertices of the graph, and the edges represent the bonds between the atoms. A chemical fullerene is one of many possible *allotropes* of carbon C; other well-known carbon allotropes are graphite, diamond, carbon nanotubes, Lonsdaleite, graphene, and so on.

The most well-known molecule C_{60} was named *Buckminsterfullerene*, after the American architect and designer Buckminster Fuller, who proposed using 5- and 6-gons in the construction of domes. The molecule C_{60} consists of 60 carbon atoms C located at the vertices of a truncated icosahedron (see Fig. 1). A common edge of a 5-gon and a 6-gon has length 1.434 angstrom and corresponds to a single bond $C{-}C$. A common edge of two 6-gons has length 1.386 angstrom and corresponds to a double bond $C{=}C$. Therefore, the spatial model of the molecule C_{60} is not the edge skeleton of an Archimedean solid. More details on chemical fullerenes can be found, for example, in [64], [63], [68], [3], [54], [4], [5], [31], [11].

A *geometric fullerene*, or simply a *fullerene*, is the surface of a simple convex 3-dimensional polyhedron with only 5- and 6-gonal faces. From the topological point of view, a fullerene is a closed simply connected 2-dimensional manifold, that is, a sphere. From the combinatorial point of view, it is a decomposition of a sphere into 5- and 6-gons with vertices of degree $q = 3$. A fullerene with v vertices (the number v is always even) and maximal symmetry group $\operatorname{Aut} F$ will be denoted by $F_v(\operatorname{Aut} F)$. A fullerene F_v has 12 pentagonal faces and $v/2 - 10$ hexagonal faces, that is, $f_5 = 12$ and $f_6 = v/2 - 10$.

Many publications deal not only with the study of fullerenes as a whole, but also with proper parts of them called *patches* (see [57]). From the topological point of view, a patch is a simply connected 2-dimensional manifold with boundary, that is, a disk. From the combinatorial point of view, it is a decomposition of a disk into 5- and 6-gons in which all interior vertices have degree 3 and all boundary vertices have degree 3 or 2. These conditions are necessary but not sufficient for a given decomposition to be a patch.

In this paper we introduce the notion of a *disk-fullerene* (see Definition 4 in § 2.2), which generalizes the notion of a patch. From the topological point of view, a disk-fullerene is a compact simply connected 2-dimensional manifold with boundary, that is, a disk. From the combinatorial point of view, it is a decomposition of a disk into 5- and 6-gons with exactly three edges meeting at each vertex. (A fullerene with a face removed is a *special* patch, which does not have vertices of degree 2.)

There are two boundary edges and one interior edge meeting at each vertex of the boundary of a disk-fullerene. We refer to a disk-fullerene with exactly n boundary edges as an *n-disk-fullerene*. If it has v vertices and maximal symmetry group $\operatorname{Aut} DF$, then we shall denote it by n-$DF_v(\operatorname{Aut} DF)$, or simply by n-DF. Such a disk-fullerene has $n+6$ pentagonal faces and $v/2-n-5$ hexagonal faces, that is, $f_5 = n+6$ and $f_6 = v/2-n-5$. In Proposition 1 of [29] there are relations between n, v, and the minimum value of f_6 for a given n (we denote this minimum value by $m_3(n)$) guaranteeing the existence of an n-DF with 3-connected skeleton. Furthermore, the number $m_3(n)$ is found for $n \leqslant 21$, and the estimate $m_3(n) \leqslant 6$ is obtained for $n \geqslant 12$.

Only 5- and 6-disk-fullerenes can be patches, that is, proper parts of fullerenes. For $n \neq 5, 6$, no n-disk-fullerene can be extended to a fullerene.

More generally, consider decompositions of a disk and a sphere into 5- and 6-gonal cells with 3 edges meeting at each vertex. Such decompositions of a disk split into two *classes*:

- *proper* if each of them is a proper part of a sphere decomposition;
- *non-proper* if none of them are proper parts of sphere decompositions.

It would be interesting to *find a criterion* for determining the class of a given disk decomposition.

A two-dimensional surface is said to be *unshrinkable* (see Definition 9) if it does not contain *belts* (see Definition 8). Otherwise the surface is *shrinkable*. We study shrinkable and unshrinkable fullerenes and n-disk-fullerenes. A fullerene or disk-fullerene containing a belt can be shrunk by removing the interior of the belt and gluing together the two components of its boundary. As a result, the belt is replaced by a *simple zigzag* (see Definition 6). In Table 7 of [27] all 9 unshrinkable fullerenes $F_v(\operatorname{Aut} F)$ with $v \leqslant 200$ which have only simple zigzags are described. It is conjectured that no other such fullerenes exist, with any v. Among these 9 examples, the fullerene $F_{140}(I)$ has the maximal number of vertices and contains 15 simple zigzags. It is proved in Theorem 2 below that an unshrinkable fullerene has at most 15 simple zigzags; *perhaps* this bound is also valid for all zigzags.

From the combinatorial point of view, the edge skeleton of an n-disk-fullerene is a *cubic* (or 3-valent) planar graph G with only 5- or 6-gonal interior faces and the n-gonal exterior face. Recall that relations between the numbers n, v, and $m_3(n)$ guaranteeing the existence of such 3-connected graphs G are given for $n \leqslant 21$ in [29]. For $n \leqslant 11$, the values $m_3(n)$ for 3-connected graphs G are listed in Table 1 below. For $n \geqslant 12$ a series of 3-connected graphs G with $f_6 = 6$ is constructed in [29], and therefore $m_3(n) \leqslant 6$. It is conjectured that this bound is achieved on a unique n-DF, for any $n \geqslant 12$.

For $12 \leqslant n \leqslant 21$ the values $\min f_6$ for graphs G which are 2-connected but not 3-connected are given in Table 2; these values are denoted by $m_2(n)$. Starting from $n = 22$, these values repeat with period 10 (see Theorem 1).

An n-disk-fullerene with $n \geqslant 3$ has a convex realization. It is described in Remark 4 in the case of a 3-connected graph G and in Remark 5 in the case of a graph G which is 2-connected but not 3-connected. If the number of edges in the boundary of an n-disk-fullerene is equal to the number of cells adjacent to the boundary, and all these cells are 5-gons, then this n-*DF* is called an n-*thimble* (see Definition 7). According to Proposition 12, the number of simple zigzags in an unshrinkable n-thimble is at most $n + 1$.

The fullerenes and disk-fullerenes considered in this paper are closely related to 3-dimensional convex polyhedra, and therefore we have included an appendix containing three subsections at the end of the paper.

1. Convex polyhedra

The theory of fullerenes and disk-fullerenes is closely related to the theory of convex polyhedra in 3-dimensional Euclidean space $\mathbb{R}^3$. The term 'convex polyhedron' will mainly refer to the boundary 2-dimensional surface $\dot{P} = \partial P$ rather than to the 3-dimensional solid P.

We recall the basic combinatorial-topological results from the theory of convex polyhedra.

Theorem (Euler [52]). *If a convex polyhedron has v vertices, e edges, and f faces, then the numbers v, e, f satisfy the identity $v - e + f = 2$.*

Theorem (Whitney [85]). *A 3-connected planar graph has a unique spherical realization.*

Theorem (Steinitz [80]). *A graph is the 1-skeleton of a convex 3-dimensional polyhedron if and only if it is planar and 3-connected.*[1]

We follow the terminology of graph theory used in the book [60]. We use the term *skeleton* to refer to the 1-skeleton of a polyhedron (that is, its edge skeleton).

We shall also need the following three geometric theorems from the theory of convex polyhedra.

Theorem (Cauchy [8]). *Two isometric closed convex polyhedral surfaces in $\mathbb{R}^3$ are congruent if their faces corresponding under the isometry are congruent.*

Two isometric closed convex polyhedral surfaces with congruent faces can differ only in the dihedral angles at the edges corresponding under the isometry. Cauchy put the sign $+$ at an edge if the corresponding dihedral angle of the first surface is greater than that of the second, and the sign $-$ otherwise. Then he proved the following two lemmas:

- if signs $+$ and $-$ are assigned to the edges of a convex polyhedron, then among the endpoints of these edges there exists a vertex such that the sign changes fewer than four times while following a closed path around this vertex;

[1] A graph is said to be *k-connected* if it is remains connected after removing fewer than k vertices [60].

- if we follow a closed path around a vertex of the surface of a convex polyhedral angle which is being flexed, then the signs at the edges change at least four times.

From these two lemmas Cauchy concluded that the corresponding dihedral angles are equal, which implies that the polyhedral surfaces are congruent as a whole.

Let us imagine a convex polyhedron as if it is made of a carton. We enumerate the vertices of the polyhedron and write the number of each vertex on the outside of the surface inside each planar angle near the vertex. Then we dismember the polyhedron into its separate faces by cutting it along all its edges. There are only two faces among them whose edges have the same pairs of numbers at their ends. Therefore, the separate faces can be uniquely patched together into an abstract surface in which all angles with the same numbers meet at the same vertex. This abstract surface is isometric to the original convex surface and has the same *combinatorial-topological scheme* (the definition of this scheme can be found in [75]). We shall be interested in embeddings of this surface in $\mathbb{R}^3$ as a convex surface with the same faces. Under these conditions, according to the Cauchy theorem, we obtain either the original convex surface (if the numbers of the vertices appear on the outside of the surface), or the original surface turned inside out (if the numbers of the vertices appear on the inside of the surface). Clearly, the latter surface is mirror symmetric to the original one, and therefore congruent to it.

Simple polyhedron. A convex 3-dimensional polyhedron with exactly three edges meeting at each vertex is said to be *simple* or *primitive* (see, for instance, [7] and [83]).

The proof of the Cauchy theorem becomes particularly easy in the case of simple closed convex polyhedra. Namely, the dihedral angles of the polyhedron cannot change, because all the polyhedral angles have three faces, and a triangle is a rigid figure.

The Cauchy theorem for a simple convex polyhedron can easily be extended to the case of polyhedra with boundary (that is, to proper parts of closed polyhedra), though with some restrictions. Namely, assume that a 2-dimensional polyhedron P homeomorphic to a disk is embedded in $\mathbb{R}^3$ (this implies that all boundary edges form a simple edge cycle), and assume further that:

- for any boundary vertex, there is at most one adjacent interior edge;
- all interior edges form a connected graph, denoted by G;
- the graph G contains non-boundary vertices, and all of them have degree $q = 3$.

Then all embeddings of the polyhedron P in $\mathbb{R}^3$ are congruent. Here all the faces are assumed to be unchanged. Embeddings can be replaced by immersions. For example, consider the surface obtained by removing two antipodal faces of a dodecahedron. We cut it along a shortest edge path between the removed faces. As a result, we obtain a disk immersed in $\mathbb{R}^3$. It contains 10 regular pentagons and cannot be embedded in $\mathbb{R}^3$, but all its immersions in $\mathbb{R}^3$ are congruent if the pentagonal faces remain congruent.

Abstract sphere. Consider an abstract two-dimensional surface composed of Euclidean polygons. Edges which are glued together are equal. Assume that this surface is homeomorphic to the standard sphere $\mathbb{S}^2$. Under this homeomorphism, the skeleton of the surface embeds in $\mathbb{S}^2$ as a graph G. Since G is connected, each connected component of the complement $\mathbb{S}^2 \setminus G$ is simply connected. The boundary of such a connected component is an edge cycle. If an edge of G is a *bridge* (that is, the graph becomes disconnected when this edge is removed), then it enters the boundary of the adjacent domain twice, with opposite orientations. The graph G defines a cell decomposition of the sphere $\mathbb{S}^2$, with the connected components of $\mathbb{S}^2 \setminus G$ as 2-cells, the edges of G as 1-cells, and the vertices of G as 0-cells; the 2-cells are also called *faces*.

We recall that edges which are glued together must have opposite orientations (see [75]), in order to avoid Möbius bands. If two pairs of edges separate each other, then only one of these pairs can be glued together, in order to avoid handles. At most two edges can be glued together, to avoid branching at an edge. All planar angles meeting at a vertex of the surface must form a single cyclic sequence, in order for a neighbourhood of the vertex to be homeomorphic to a disk.

Theorem (Aleksandrov [1]). (i) *Any two isometric closed convex polyhedral* 2*-dimensional surfaces in* $\mathbb{R}^3$ *are congruent.*

(ii) *If all vertices of an abstract two-dimensional sphere have positive curvature, then this sphere is isometric to the surface of a convex polyhedron in* $\mathbb{R}^3$.

Recall that the curvature at a vertex is equal to 2π minus the sum of the planar angles meeting at this vertex, that is, $\omega = 2\pi - \sum \alpha$.

Part (ii) of the Aleksandrov theorem asserts the existence of a convex polyhedron. In general, the surface of this polyhedron bounds a 3-dimensional solid. However, the theorem does not exclude degenerate polyhedra, which have zero volume. In this case the surface consists of two identical convex planar (2-dimensional) polygons in $\mathbb{R}^2$ with identified boundaries. A criterion for degeneracy of a convex polyhedron was recently found in [79].

Part (i) of the Aleksandrov theorem establishes uniqueness in the class of isometric convex polyhedral surfaces, but now without assuming that the isometry takes faces to faces. A priori, the faces and edges could be completely different, but this cannot happen: Aleksandrov proved part (i) by the method originally used by Cauchy.

In practice, the vertices are uniquely determined as the points of the surface where its curvature is positive.

Theorem (Olovyanishnikov [67]). *A compact convex solid in* $\mathbb{R}^3$ *whose boundary is isometric to the surface of a closed convex polyhedron in* $\mathbb{R}^3$ *is congruent to the polyhedron.*

Olovyanishnikov proved the uniqueness of the surface of a convex polyhedron in the class of surfaces of all convex solids, rather than just in the class of surfaces of convex polyhedra. Unfortunately, no further theorems of his followed: Sergei Panteleimonovich Olovyanishnikov was killed in action in December 1941 (see [2], vol. 3, p. 676).

In summary, there are three *uniqueness theorems* for convex polyhedra: the Cauchy theorem, the Aleksandrov theorem (i), and the Olovyanishnikov theorem, and each subsequent theorem strengthens the previous one.

Platonic solids. Platonic solids are *regular* polyhedra. There are five of them: a *tetrahedron*, a *cube*, an *octahedron*, a *dodecahedron* and an *icosahedron*. The proof of this fact goes back to Euclid. All the faces of a regular polyhedron are congruent regular polygons, and furthermore, the polyhedral angles at the vertices are all congruent. The symmetry group of a regular polyhedron acts transitively on faces, edges, and vertices.

Archimedean solids. Archimedean solids are *semiregular* polyhedra. Their faces are regular polygons, and there are at least two different faces, since otherwise the polyhedron is a Platonic solid. The polyhedral angles at the vertices of an Archimedean solid are all congruent (this condition is necessary but not sufficient). The symmetry group of a semiregular polyhedron acts transitively on its vertices, which implies that the polyhedron is an *isogon*. There exist 13 special Archimedean solids (two of them have left and right forms which are mirror symmetric; crystallographers call them *enantiomorphic*) and two infinite series, *prisms* and *antiprisms*.

Poinsot solids. These are regular non-convex polyhedra, called *regular star polyhedra*. There are four of them, found by Poinsot. Cauchy proved that there are no other regular non-convex polyhedra.

Fedorov solids. Also known as *parallelohedra*, these are convex 3-dimensional polyhedra which can tessellate 3-dimensional space $\mathbb{R}^3$ by their parallel copies. There are exactly five different Fedorov solids (see [53]). Higher-dimensional parallelohedra are discussed in § 3.1.

Pictures of all the polyhedra listed above can be found in [19]. We note that one extra *pseudo-Archimedean* solid no. 13 was included in [21]. The stars of all the vertices in this polyhedron are congruent and consist of three squares and a regular triangle. Delaunay had known about this polyhedron long before (see, for example, [23]), but did not include it in the list of Archimedean solids. It can be transformed into the Archimedean solid no. 12 using a Rubik's cube-type rotation fixing a belt of squares.

Higher-dimensional polyhedra will be discussed further in §§ 3.1 and 3.2, but now we turn to fullerenes and disk-fullerenes.

2. Fullerenes and disk-fullerenes

2.1. Fullerenes and abstract fullerenes.

Definition 1. We refer to the surface of a simple closed convex 3-dimensional polyhedron as a *fullerene* if it has only 5- and 6-gonal faces.

Under the conditions of Definition 1, we have

$$v = v_3, \quad 2e = 3v_3, \quad f = f_5 + f_6, \quad 2e = 5f_5 + 6f_6, \tag{1}$$

where v, e, and f denote the number of vertices, edges, and faces, respectively, and f_k denotes the number of k-gonal faces. Adding the identities (1) with coefficients 6, -2, 6, -1, respectively, and using the Euler formula, we obtain

$$f_5 = 12. \tag{2}$$

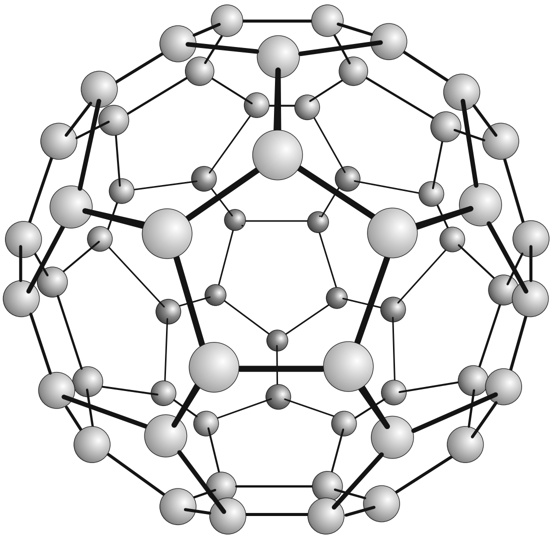


Figure 1. Buckminsterfullerene C_{60}

Using (2), we can rewrite the identities (1) as follows:

$$v = 2(f_6 + 10), \quad e = 3(f_6 + 10), \quad f = 1(f_6 + 10) + 2. \tag{3}$$

The number of different fullerenes with fixed f_6 is finite. The numbers v, e, f are minimal when f_6 is minimal. A fullerene with $f_6 = 0$ is a combinatorial dodecahedron.

A fullerene with v vertices and maximal symmetry group $\operatorname{Aut} F$ will be denoted by $F_v(\operatorname{Aut} F)$. It follows from (2) and (3) that F_v has 12 pentagonal and $v/2 - 10$ hexagonal faces. The first fullerene discovered by chemists was $F_{60}(I_h)$. The molecule corresponding to this fullerene is denoted by C_{60} and consists of 60 carbon atoms C. Its standard model is shown in Fig. 1.

Definition 2. An abstract sphere (that is, an abstract two-dimensional surface homeomorphic to the sphere $\mathbb{S}^2$) is called an *abstract fullerene* if:

(i) it is composed of regular 5- and 6-gons;
(ii) all its vertices have degree $q = 3$.

The skeleton of an abstract fullerene is embedded in $\mathbb{S}^2$ as an edge graph G in such a way that each connected component of the domain $\mathbb{S}^2 \setminus G$ is a 5- or 6-gon, possibly with some edges or vertices identified. The decomposition of the sphere $\mathbb{S}^2$ into the connected components of $\mathbb{S}^2 \setminus G$ also satisfies (1)–(3). This implies that G is connected and $v \geqslant 20$. We prove that each cell in this decomposition is bounded by a simple edge cycle:

Proposition 1. *For any abstract fullerene,*

(i) each cell is bounded by a simple edge cycle;
(ii) the intersection of any two cells is connected.

Proof. (i) The proof is by contradiction. Assume that a cell is bounded by a non-simple edge cycle. Then some edges and/or vertices of a 5- or 6-gon are identified. But if only vertices of a two-cell are identified, then we get a vertex of degree at least 4, which is impossible. Two adjacent edges also cannot be identified, since then their common vertex would have degree 1. If a pair of adjacent edges is identified with another pair of adjacent edges (in the same or a different cell), then the common vertex in the pair would be of degree 2, which is also impossible.

Now assume that two non-adjacent edges of a cell are identified. If this cell is a 5-gon, then the boundary of this cell consists of two circles joined by a bridge, and one of the circles contains another vertex. Then the circle without an extra vertex is the boundary of a 1-gon. This 1-gon must be a cell because $q = 3$, but this contradicts the assumption that there are only 5- and 6-gonal cells. If non-adjacent edges are identified in a 6-gonal cell, then the boundary of the cell again consists of two circles joined by a bridge. Here there are two possibilities.
Case 1. One of the circles has two extra vertices (that is, the identified edges of the 6-gon are neither adjacent nor opposite). Then we get a 1-gonal cell, which is impossible because $q = 3$ (see Definition 2).
Case 2. Each of the two circles contains an extra vertex (that is, the identified edges of the 6-gon are opposite). In this case there is either a 5-gon or a 6-gon attached to the given 6-gonal cell along each of the two circles. However, a 5-gon cannot be attached, since we then get a 1-gon. Therefore, there is an attached 6-gon. This 6-gon also has two opposite edges identified. Starting from this new 6-gon, we obtain a repeating pattern in our fullerene. This contradicts the assumption that the fullerene is finite. Therefore, non-adjacent edges of a 6-gon cannot be identified. Thus, any cell is bounded by a simple edge cycle.

(ii) Assume that two 6-gons have three pairs of common edges. Then our sphere decomposition has three 2-gons (because $q = 3$), which is impossible. Assume that two cells have two pairs of common edges. Then these two cells form an *annulus* (homeomorphic to the lateral surface of a round cylinder). Its boundary consists of two circles. Besides the vertices on the common edges, the two circles can contain more vertices. If one of the circles has 4 extra vertices, then there is a 2-gon adjacent to the second circle, which is impossible. If one of the circles has 3 extra vertices, then the other circle has at most one extra vertex, giving either a 2-gon or a 1-gon, which is again impossible. If both circles have two extra vertices, then we again obtain a 1-gon by the finiteness of the edge graph. It follows that any two cells intersect at a unique edge, or do not intersect at all. □

Corollary 1. *The skeleton of an abstract fullerene is isomorphic to the skeleton of a fullerene.*

Proof. Proposition 1 and the Steinitz theorem [80][2] imply that there exists a convex polyhedron whose skeleton is *isomorphic* to the skeleton of an abstract fullerene. Indeed, this skeleton is a planar 3-connected cubic graph: removing three vertices adjacent to another vertex makes the graph disconnected, but it remains connected if only two vertices are removed. □

Our further study uses the notion of a *polycycle*.

[2]This is a manuscript from Steinitz' heritage, completed and published by Rademacher.

Definition 3. Assume that two natural numbers $r \geqslant 3$ and $q \geqslant 3$ are given. A decomposition of a disk into r-gons is called an (r, q)-*polycycle* if:

(i) the degree of any interior vertex is q;

(ii) the degree of any boundary vertex is at most q.

We note that the definition from [36] included the extra condition

(iii) the cells of the decomposition form a cell complex,

which follows from (i) and (ii) (see [36]). It also follows that the degree of any vertex is at least two.

Remark 1. Any (r, q)-polycycle can be decomposed into so-called *elementary summands*. A list of elementary summands of $(5, 3)$- and $(3, 5)$-polycycles is given in [35]. We say that a (r, q)-polycycle is *unextendable* if it is not a proper part of another (r, q)-polycycle. It is proved that there are only 7 unextendable (r, q)-polycycles: 5 *proper* ones (the surfaces of the five Platonic solids with one face removed) and 2 *improper* (an octahedron with a split vertex and an icosahedron with a split vertex, shown in Fig. 2). If follows that there exists only one finite unextendable $(5, 3)$-polycycle: a dodecahedron with a face removed. No $(5, 3)$-polycycle can have only one vertex of degree 2. Also, if a $(5, 3)$-polycycle has exactly two boundary vertices of degree 2, then these two vertices cannot be adjacent or separated by one vertex of degree 3. See the details in [36], [35], [32].

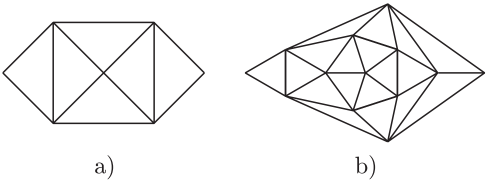


Figure 2. A vertex splitting: a) an octahedron, b) an icosahedron

Now we return to fullerenes.

Proposition 2. (i) *There are no fullerenes with* $f_6 = 1$.

(ii) *There exist fullerenes with any given* $f_6 \geqslant 2$.

Proof. This was proved in [58]. We give a new proof, since the same approach and pictures will be also used below (in Theorem 1).

(i) The proof is by contradiction. Assume that $f_6 = 1$. Then the complement of the 6-gon consists solely of 5-gons and therefore is a finite unextendable $(5, 3)$-polycycle. But this polycycle cannot be a dodecahedron with a face removed (see Remark 1), a contradiction. Thus, $f_6 \neq 1$.

(ii) A fullerene $F_{24}(D_{6d})$ with $f_6 = 2$ is shown in Fig. 3, a); it is called a *barrel*.

Two patches of types a) and b), that is, two Endo–Kroto *ambiguous* patches (see [57]) are shown in Fig. 4. Their interiors are different, but the boundaries are the same. Denote by φ the transformation turning a patch of type a) into a patch of type b). Assume that a fullerene F_v contains a patch of type a). After application of the transformation φ, the fullerene F_v turns into a fullerene F_{v+2} containing a patch of type b). Therefore, the operation φ increases the number f_6 by one.

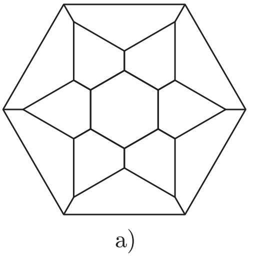


Figure 3. A barrel and convex embeddings of it: a) a Steinitz (combinatorial) embedding; b) an Aleksandrov embedding (a metric embedding with regular 5- and 6-gons). More precisely, the picture shows Schlegel diagrams of these embeddings

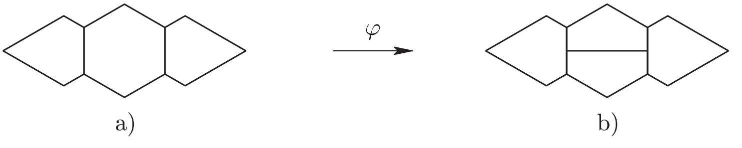


Figure 4. Two Endo–Kroto ambiguous patches

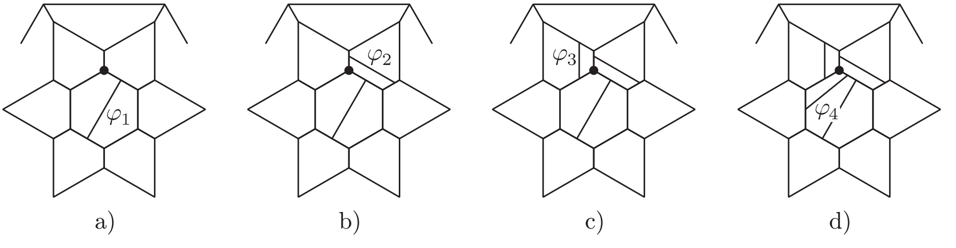


Figure 5. Carousel of operations φ_i

The barrel fullerene $F_{24}(D_{6d})$ shown in Fig. 3, a) has exactly two 6-gonal faces. It contains a patch of type a) (see Fig. 4). By applying the transformation φ we obtain a fullerene with three 6-gons.

Fig. 5, a) shows the first annulus (the *corona*) of a 6-gon (with one 5-gon from the second annulus added) and the first application of the transformation φ. Denote this transformation by φ_1. It splits the 6-gon into two 5-gons. As a result, we obtain a new 6-gon adjacent to the labelled vertex. A new patch of type a) is formed by this new 6-gon and a 5-gon adjacent to the labelled vertex and not involved in the transformation φ_1 (see Fig. 4). By applying the transformation φ_2 to this new patch (see Fig. 5, b)) we obtain a new fullerene with four 6-gons. In this way the operation φ can be iterated indefinitely around the labelled vertex (see Fig. 5). Each time a new 6-gon is added. Therefore, for any given natural number $N \geqslant 2$ there exists a fullerene with $f_6 = N$. $\square$

We can prove that the barrel is the only fullerene with $f_6 = 2$. Indeed, the first annulus around a 6-gon does not contain other 6-gons. (Otherwise there would be two adjacent 6-gons in the fullerene, and by removing these two 6-gons together with their common edge we would obtain an unextendable $(5,3)$-polycycle, which cannot exist; see Remark 1 and [35].) The second annulus around the original 6-gon also does not contain 6-gons. (Otherwise, by removing both 6-gons and splitting the bridge between them into two new edges with two new vertices, we would obtain an elementary $(5,3)$-polycycle, which cannot exist.) Therefore, we have the first annulus of six 5-gons around one 6-gon and the first annulus of six 5-gons around another 6-gon. Together this gives two 6-gons and twelve 5-gons, which form a unique fullerene.

Remark 2. A barrel, whose skeleton is shown in Fig. 3 (a), has two bases, which are congruent regular 6-gons, and twelve lateral faces, which are all 5-gons. Removing from the lateral surface of the barrel two 5-gons with a common edge not intersecting the bases, we obtain a disk embedded in $\mathbb{R}^3$. If the 5-gons were regular, then this surface would have been immersed rather than embedded in $\mathbb{R}^3$ (more precisely, in the lateral surface of a dodecahedron, as described above). Therefore, the 5-gonal faces cannot be regular, because a barrel is not a dodecahedron.

We note that there exists only one fullerene $F_{26}(D_{3h})$ with $f_6 = 3$ (see [54]).

Remark 3. Consider an abstract two-dimensional sphere consisting of regular Euclidean 5- and 6-gons with $q = 3$. When can this sphere be realized as the surface of a convex polyhedron in $\mathbb{R}^3$? Because all the cells are Euclidean and regular, such a realization would provide a special metric of non-negative curvature. By the Aleksandrov theorem (ii) (see § 1), there exists a unique convex polyhedron *isometric* to the given abstract sphere. The vertices of this polyhedron are points where the curvature of the surface is positive. If three regular 6-gons meet at a point of the abstract sphere, then this point cannot be a vertex of the corresponding convex polyhedron. Each edge of a convex polyhedron is the shortest path between two vertices of the polyhedron. However, the converse is not true: not every shortest path between two vertices of an abstract sphere becomes an edge. Only in rare cases is it possible to recognise those shortest paths between vertices of an abstract sphere of positive curvature which become edges in its realization as a convex polyhedron.

Recently a criterion for degeneracy of a convex polyhedron was found in [79]. The edges of a degenerate convex polyhedron can be characterized as simple shortest paths between vertices. By using this criterion, a new proof of the Zilberberg theorem [86] was found. This theorem asserts the existence of a non-degenerate convex polyhedron with any prescribed curvatures at the vertices of its surface.

We remark that the fullerene $F_{60}(I_h)$ with $f_6 = 20$ can be realized as the surface of an Archimedean solid. The molecule C_{60} is modelled on the surface of a truncated icosahedron (with the same symmetry group I_h) whose 6-gonal faces are not regular (see Fig. 1).

The fullerene $F_{80}(I_h)$ with $f_6 = 30$, like any other fullerene, can be realized as the surface of a convex polyhedron by the Steinitz theorem. A dodecahedron with edges cut off provides such a realization (see [56]). Fullerenes were already considered in [56], under the name *medial polyhedra*. The 6-gonal faces of $F_{80}(I_h)$

are also not regular. The edges which are not equivalent under the action of the group I_h can have arbitrary lengths.

A fullerene $F_{80}(I_h)$ cannot be realized with regular 5- and 6-gonal faces. A convex polyhedron with regular 5- and 6-gonal faces, which exists by the Aleksandrov theorem, is a rhomboicosadodecahedron. It is combinatorially equivalent to an icosahedron with vertices and edges cut off. In the metric of this polyhedron, each rectangular face together with 2/3 of the triangular faces form a regular hexagon bent along two diagonals. The convex hull of this bent hexagon is bounded by two bent hexagons: the original one and another hexagon formed by two trapezoids.

We remove this convex hull from the rhomboicosadodecahedron. As a result, the bent 6-gon consisting of a rectangle and two triangles is replaced by a bent 6-gon consisting of two trapezoids. We apply this transformation to all bent regular 6-gons. As a result, our convex polyhedron transforms into a non-convex polyhedron consisting of regular 5-gons and bent 6-gons. This gives another realization of $F_{80}(I_h)$ as a (non-convex) surface in $\mathbb{R}^3$. The intrinsic metric of this realization is different: the curvature is negative at vertices where '6-gons' (bent and non-regular) meet.

The edge skeletons of both realizations are the same if we do not regard diagonals of '6-gons' as edges. The boundary edges of a '6-gon' are non-coplanar. It is *not known* whether the edges of a '6-gon' in the molecule $C_{80}(I_h)$ are coplanar.

2.2. Disk-fullerenes and abstract disk-fullerenes.

Definition 4. An *n-disk-fullerene*, or simply a *disk-fullerene*, is the surface obtained by removing the interior of an n-gonal face from the surface of a simple closed convex 3-dimensional polyhedron whose other faces are 5- or 6-gons. A disk-fullerene with $n = 5$ or 6 is said to be *special*.

By putting the n-gonal face back, we obtain a convex polyhedron with

$$v = v_3, \quad 2e = 3v_3, \quad f = f_5 + f_6 + f_n, \quad 2e = 5f_5 + 6f_6 + nf_n, \tag{4}$$

where $f_n = 1$ when $n \neq 5, 6$. Adding the identities (4) with coefficients 6, -2, 6, -1, respectively, and using the Euler formula, we obtain

$$f_5 = n + 6. \tag{5}$$

Using (5), we can rewrite the identities (4) as follows:

$$v = 2(f_6 + n + 5), \quad e = 3(f_6 + n + 5), \quad f = 1(f_6 + n + 5) + 2. \tag{6}$$

The identities (6) imply that for any fixed n the numbers v, e, and f are minimal when f_6 is minimal. A polyhedron with $f_6 = 0$ is a combinatorial dodecahedron with a face removed.

An n-disk-fullerene with v vertices and maximal symmetry group $\operatorname{Aut} DF$ will be denoted by n-$DF_v(\operatorname{Aut} DF)$, or simply by n-DF. Any n-DF_v contains $n + 6$ pentagonal faces and $v/2 - n - 5$ hexagonal faces, that is, $f_5 = n + 6$ and $f_6 = v/2 - n - 5$. It is a proper part of a fullerene if and only if $n = 5$ or $n = 6$.

Definition 5. An abstract n-disk-fullerene is an n-gon ($n \geqslant 3$) composed of 5- and 6-gons in such a way that there are exactly 3 edges meeting at any vertex (that is, $q = 3$).

Proposition 3. *For an abstract n-disk-fullerene*:
(i) *any cell is bounded by a simple edge cycle*;
(ii) *the intersection of any two cells is connected.*

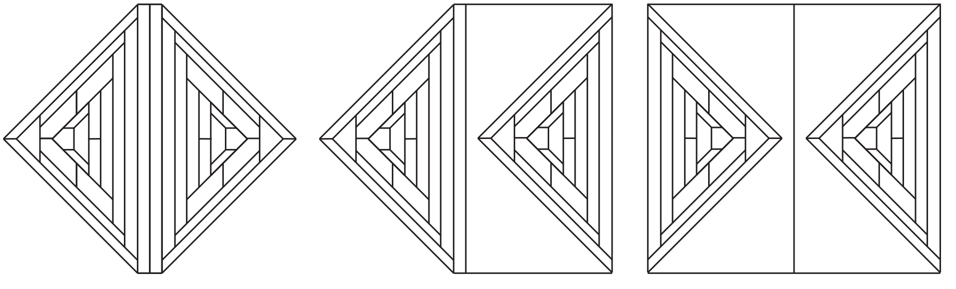
Proof. (i) Although Definition 5 does not assume that 5- and 6-gonal cells are bounded by simple edge cycles, this can be proved in exactly the same way as for abstract fullerenes, taking into account the inequality $n \geqslant 3$. Therefore, any cell of an abstract n-DF is homeomorphic to a disk.
(ii) This is proved in exactly the same way as for abstract fullerenes. □

Proposition 3 is an analogue of Proposition 1, and the latter implies Corollary 1. However, there is no analogous corollary of Proposition 3; more precisely, it does not cover all n-DFs.

Indeed, consider 8-$DF_{74}(C_{2\nu})$. It is shown in Fig. 6 as a *non-normal* decomposition of a disk (that is, a decomposition containing cells whose intersection is not a whole edge). A small perturbation turns it into a normal decomposition. However, it cannot be realized as the surface of a convex polyhedron with an 8-gonal face removed, because there is a disconnected intersection of a 6-gon with the 8-gonal boundary. The skeleton of this 8-DF_{74} is a 2-connected planar graph which is not 3-connected (see footnote [1]). The skeleton becomes disconnected after removing two vertices on the vertical symmetry axis of the disk-fullerene 8-$DF_{74}(C_{2\nu})$, but it remains connected if only one vertex is removed.

Therefore, when we pass from usual n-disk-fullerenes to abstract ones, some *unusual disk-fullerenes* appear. The latter contain at least one cell whose intersection with the boundary of the n-DF is disconnected.

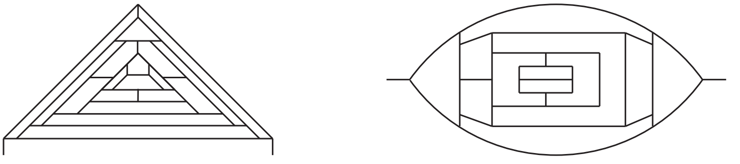
The unusual disk-fullerenes 8-$DF_{74}(C_{2\nu})$, 9-$DF_{74}(C_{\nu})$, and 10-$DF_{74}(C_{2\nu})$ with isomorphic skeletons are shown in Fig. 6. The reason why these skeletons are isomorphic is that they are 2-connected but not 3-connected. For another reason, we can get two different disk-fullerenes with isomorphic skeletons by removing different 5- or 6-gonal faces from the same fullerene. However, if the skeleton of an n-DF is 3-connected and $n \neq 5, 6$, then the Whitney theorem implies that this n-DF has a unique planar realization with the n-gonal outer face (see [85]).



8-$DF_{74}(C_{2\nu})$ 9-$DF_{74}(C_{\nu})$ 10-$DF_{74}(C_{2\nu})$

Figure 6. Three disk-fullerenes with isomorphic skeletons

If the skeleton of an n-$DF_v(\mathrm{Aut}\ DF)$ is a 2-connected graph G which is not 3-connected, then we have $\mathrm{Aut}\, DF \subset \mathrm{Aut}\, G$, but these two automorphism groups do not necessarily coincide. For example, in Fig. 7 two fragments of a disk-fullerene with the same symmetry groups are shown. However, these symmetry groups are differently disposed with respect to the two edges on which the fragments are suspended in the disk-fullerene. In the case b) the group $\operatorname{Aut} DF$ is a proper subgroup of $\operatorname{Aut} G$.



a) b)

Figure 7. Two fragments of an unusual disk-fullerene

Remark 4. According to Definition 4, an n-DF can be realised as a closed polyhedral surface with an n-gonal face removed. This surface lies in $\mathbb{R}^3$ but not in $\mathbb{R}^2$. However, we can use a central projection to project the polyhedron onto the n-gonal face from a point O in $\mathbb{R}^3$ outside the polyhedron and sufficiently close to an interior point of the n-gonal face. As a result, we obtain another convex realization of the n-DF as a convex 2-dimensional n-DF in $\mathbb{R}^2$, namely, a primitive decomposition of an n-gon into 5- and 6-gons ('primitive' means that there are 3 edges meeting at each vertex). This projection together with its decomposition is called a *Schlegel diagram*. Its skeleton is a planar cubic graph with an n-gonal outer face.

Along with an abstract n-DF we considered an abstract sphere, obtained by putting the n-gonal face back. We can also consider arbitrary abstract spheres which have cubic skeletons and are composed of 5- and 6-gons and one n-gon with $n \geqslant 3$. In this case we also have a graph G on the sphere $\mathbb{S}^2$. This graph defines a cell decomposition of the sphere, where 2-cells are the components of the domain $\mathbb{S}^2 \setminus G$, 1-cells are the edges of G, and 0-cells are the vertices of G. The relations (4)–(6) also hold in this case. However, removing the interior of the n-gonal cell from the sphere does not produce a disk fullerene in the case when the n-gonal cell on $\mathbb{S}^2$ is bounded by a non-simple edge cycle (that is, when the skeleton is 1-connected but not 2-connected).

For example, consider the two 3-DFs shown in Fig. 17 of [29]. We realize each of these disk-fullerenes on the sphere $\mathbb{S}^2$ inside the triangle of the other one. Take one extra vertex on the boundary edge of each 5-gon adjacent to the boundary. Joining these vertices by an edge (more precisely, by a *bridge*), we obtain a decomposition of $\mathbb{S}^2$ into 5-, 6-gons, and one 10-gonal cell bounded by a non-simple edge cycle. Removing the 10-gonal cell does not produce a 10-DF. The decomposition of the sphere cannot be realized as a convex polyhedron in $\mathbb{R}^3$ with a 10-gonal face, and it does not have a 10-gonal Schlegel diagram in $\mathbb{R}^2$. The reason is that the skeleton is 1-connected but not 2-connected: removing the vertex on the bridge makes the skeleton disconnected. (See also Example 2 in § 2.4.)

Therefore, if the skeleton of an abstract sphere is:

- 1-connected but not 2-connected, then it does not correspond to an n-disk-fullerene;
- 2-connected but not 3-connected, then it corresponds to an unusual n-disk-fullerene;
- 3-connected, then it corresponds to a usual n-disk-fullerene.

In the last two cases the skeleton of the abstract sphere is isomorphic to the skeleton of an abstract n-DF. In what follows we shall assume that the boundary of the n-gon on an abstract sphere is a simple edge cycle. This implies that removing the interior of the n-gon from the sphere produces an abstract n-DF. It is isomorphic to a usual n-DF if its skeleton is 3-connected, or to an unusual n-DF if the skeleton is 2-connected but not 3-connected. The next proposition follows from Definition 5, Proposition 3, and Remark 4:

Proposition 4. *If the skeleton of an abstract n-disk-fullerene is* 3*-connected, then it has a convex realization in $\mathbb{R}^3$ that does not lie in $\mathbb{R}^2$, and also a convex realization in $\mathbb{R}^2$.*

Criterion 1. *An abstract n-disk-fullerene is isomorphic to a usual n-disk-fullerene if and only if the intersection of its boundary with any cell is connected, that is, if its skeleton is* 3*-connected.*

Remark 5. If the skeleton of an abstract n-DF is 2-connected but not 3-connected, then the n-DF has a convex realization in $\mathbb{R}^2$. It can also be realized in $\mathbb{R}^3$ as a convex polyhedral surface with boundary, but the boundary is not planar. Furthermore, there is a realization in $\mathbb{R}^3$ as a non-convex polyhedral surface. It can be obtained as follows. Denote the convex realization by P. The surface P contains a cell Q which has a disconnected intersection with the boundary $\dot{P} = \partial P$. The complement $P \setminus Q$ is also disconnected. By reflecting one of the connected components of $P \setminus Q$ in the plane of Q, we obtain a non-convex realization. Any unusual n-DF has such a non-convex realization.

Therefore, any abstract n-DF has a convex realization. It is described in detail in Remarks 4 and 5.

Proposition 5. *If the skeleton of an n-disk-fullerene is* 3*-connected and $n \geqslant 7$, then $f_6 \geqslant 2$.*

Proof. The proof is by contradiction. Assume that $f_6 = 0$. Then the n-DF is a finite unextendable $(5,3)$-polycycle. However, there exists only one finite unextendable $(5,3)$-polycycle, a dodecahedron with a face removed (see Remark 1). It has $n = 5$, which contradicts the assumption $n \geqslant 7$. Hence $f_6 \neq 0$.

Assume now that $f_6 = 1$. Then there are two cases.

1) The intersection of the 6-gon with the boundary of the disk-fullerene is non-empty. Then this intersection is a single edge, because the skeleton is a cubic 3-connected graph. Removing this edge, we obtain a $(5,3)$-polycycle with two vertices of degree 2. This polycycle is unextendable because $n \geqslant 7$, and it cannot be a dodecahedron with a face removed, since the latter has $n = 5$.

2) The 6-gon does not intersect the boundary. Then the first annulus (the *corona*) around it consists of six 5-gons, and the intersection of each of them with the 6-gon

is connected. Any two neighbouring 5-gons are adjacent, that is, have a common edge. Any two 5-gons which are not neighbouring in the corona do not intersect. Indeed, the vertices of the outer boundary of the corona have alternating degrees 3 and 2. Two vertices of degree 3 cannot coincide, since otherwise we get a vertex of degree at least 4, which is impossible for a disk-fullerene. Two vertices of degree 2 also cannot coincide, since otherwise two of their adjacent edges would also coincide, and the other ends of these edges have degree 3. A vertex of degree 2 and a vertex of degree 3 in non-adjacent 5-gons also cannot coincide, since otherwise two adjacent edges of the shortest path between them on the boundary of the corona would also coincide. This is impossible, since the ends of these edges belong to adjacent 5-gons.

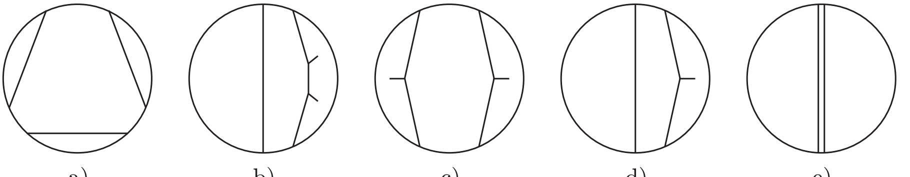
It follows that all 12 vertices on the outer boundary of the corona are different. Half of these vertices have degree 2 in the corona, and they are adjacent to 6 edges of the disk-fullerene which do not belong to the boundary of the corona. No two of these 6 edges can coincide: two coinciding neighbouring edges would produce a triangle, and two coinciding non-neighbouring edges would produce a self-intersecting polygon. The ends of these edges are also different, since otherwise we would get a 4-gon or a self-intersecting polygon. Therefore, any two neighbouring edges (out of the 6) together with two edges from the outer boundary of the corona (the first annulus of the 6-gon) are edges of a 5-gon belonging to the second annulus. Its outer boundary has 6 edges. Each vertex of this outer boundary has degree 3, so we get $n=6$, which contradicts the assumption that $n\geqslant 7$. Thus, $f_6\neq 1$. □

In the process of this proof we found a unique n-DF with $f_6=0$ (the dodecahedron with a face removed) and a unique n-DF with $f_6=1$ (the barrel $F_{24}(D_{6d})$ with a base removed, that is, 6-$DF_{24}(C_{6\nu})$). We stress that these are the only n-DFs with $f_6<2$, for any $n\geqslant 1$.

In the case of a 3-connected skeleton, a series of n-DFs with $n\geqslant 12$ and $f_6=6$ was constructed in [29]. This justifies the estimate $m_3(n)\leqslant 6$, which is conjectured to hold for any $n\geqslant 12$.

Proposition 6. *If the skeleton of an n-disk-fullerene is* 2*-connected but not* 3*-connected and $n\geqslant 12$, then $f_6\geqslant 4$.*

Proof. The given conditions imply that there exists a cell whose intersection with the boundary of the n-DF is disconnected. Possible schemes of these intersections are shown in Fig. 8, a)–d).



a) b) c) d) e)

Figure 8. a)–d): all possible disconnected intersections of a cell with the boundary of the disk; e) a chord splits the disk into two segments

In the case a), a 6-gonal cell intersects the boundary in three edges. The other three edges are *chords*, which cut three *segments* from the disk. We shall prove by contradiction that each disk segment contains a 6-gon. Assume that there exists a segment without 6-gons. We join the centre of the 6-gon to the centres of its edges on the boundary, and replace each disk segment containing a 6-gon by a segment without 6-gons. As a result, we obtain a finite unextendable $(5,3)$-polycycle, that is, a dodecahedron with a face removed, and it does not have a chord, a contradiction. Therefore, each segment of the disk contains a 6-gon, and the whole disk contains four 6-gons.

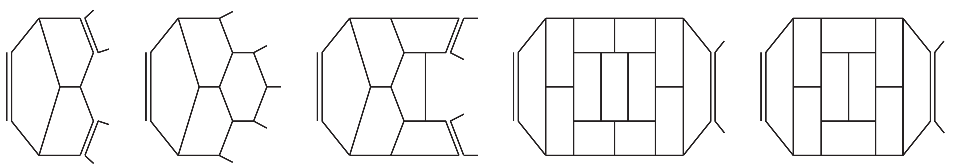
In the case b) we assert that the right disk segment contains another 6-gon (see Fig. 8, b)). Indeed, join the centre of the chord by radii to the boundary vertices of the 6-gon which do not belong to the chord. These two radii cut a 5-gon from the 6-gon. If the original right disk segment does not contain another 6-gon, then the sector containing the cut 5-gon is a $(5,3)$-polycycle with a single vertex of degree 2. But such a $(5,3)$-polycycle does not exist (see Remark 1). Therefore, the right disk segment contains another 6-gon. If there is an adjacent 6-gon on the left of the chord, then the disk contains four 6-gons. If there is an adjacent 5-gon on the left, then see the case d).

In the case c) we join the centres of the sides of the 6-gon on the boundary of the disk by an additional edge, and then consider the case d).

In the case d) we first prove that the right disk segment contains a 6-gon (see Fig. 8, d)). Indeed, if the right disk segment does not contain a 6-gon, then it together with the disk segment symmetric to it with respect to the chord form a finite unextendable $(5,3)$-polycycle, which is impossible. Therefore, the right disk segment contains a 6-gon. Next we show that it contains another 6-gon.

If the given 6-gon intersects the boundary of the disk, then it follows from the cases a), b), c) (see Fig. 8) that we can assume that the intersection consists of a single edge. In this case we remove this edge from the disk segment and construct an identical copy symmetric with respect to the centre of the chord, as shown in Fig. 8, e). If the right disk segment does not contain a second 6-gon, then we obtain a decomposition of the disk into 5-gons. This decomposition is a finite unextendable $(5,3)$-polycycle with four vertices of degree 2. But such a $(5,3)$-polycycle does not exist.

Now assume that the 6-gon does not intersect the boundary of the disk. Let us look at the structure of the disk segment. Since all the boundary cells are 5-gons, the 5-gon adjacent to the original chord is also adjacent to two other 5-gons. If the intersection of each of these 5-gons with the boundary of the disk is disconnected (see Fig. 9, a)), then the right part of the disk segment contains two smaller disk segments. Each new disk segment contains a 6-gon, which is what was to be proved.



a) b) c) d) e)

Figure 9. A disk segment with a 5-gon adjacent to the chord

Assume that the intersection of each of the two 5-gons with the boundary of the disk is connected but that they are adjacent to a 6-gon (see Fig. 9, b)). Draw a line segment between the two vertices of the 6-gon which are adjacent to its left vertex, thereby splitting the 6-gon into a 3-gon and a 5-gon. We replace the 3-gon and three 5-gons from the left part of the disk segment by a new 5-gon with a vertex of degree 2 (which can be placed at the centre of the chord). If the original disk segment did not contain a second 6-gon, then the resulting decomposition would be a $(5,3)$-polycycle with a single vertex of degree 2, which is impossible. It follows that the original segment contains a second 6-gon.

Assume that the intersection of each of the two 5-gons with the boundary of the disk is connected, and they are not adjacent to a 6-gon but are adjacent to a 5-gon which is adjacent to the boundary (see Fig. 9, c)). Then the right part of the disk segment contains two smaller segments. Each of these smaller segments contains a 6-gon, as was to be proved.

Assume now that the intersection of each of the two 5-gons with the boundary of the disk is connected, and the 5-gons are not adjacent to a 6-gon but are adjacent to a 5-gon which is adjacent to a 6-gon (see Fig. 9, d)). If there is no other neighbouring 6-gon, then the disk segment has a chord. Hence, the disk segment contains a smaller segment with another 6-gon, as was to be proved.

Finally, assume that the intersection of each of the two 5-gons with the boundary of the disk is connected, and the 5-gons are not adjacent to a 6-gon but are adjacent to a 5-gon which is adjacent to another 5-gon (see Fig. 9, e)). Then the original disk segment has another chord, and hence it contains a smaller segment. We can repeat the above argument for this smaller disk segment by considering the five cases shown in Fig. 9, including the case e). This last case can occur only finitely many times. Also, the process cannot stop at the case e), because in this case the disk segment has a chord which cuts off a smaller disk segment. All other cases lead to two 6-gons in the original disk segment. $\square$

The proof above shows that each disk segment which is cut off the disk by a chord contains two 6-gons, that is, $f_6 \geqslant 2$. In some particular cases the estimate in Proposition 6 can be improved. For example, the disk shown in Fig. 8, a) has seven 6-gons, and the disk in Fig. 8, c) has five 6-gons. The estimate can be improved not only for disks, but also for their segments. For example, the disk segments shown in Fig. 9, a) and c) have four 6-gons each, and the disk segment in Fig. 9, d) has three 6-gons.

We continue our study of the number $\min f_6$ for arbitrary n by finding the value of $\min f_6$ for disk segments whose boundary consists of only a few edges. We have $f_6 \geqslant 2$ for any such disk segment. Assume that the disk segment cut off from the disk by a chord has j edges on the boundary of the disk. Then the cyclic sequence of the degrees of its boundary vertices[3] has the form $(2,2,3,\dots,3) = (2)^2(3)^{j-1}$. It is easy to see that $j \geqslant 4$. It turns out that $f_6 = 2$ for $j = 7, 8$. The 15-disk-fullerene shown in Fig. 10, a) is split into two such disk segments.

For $j = 7$ there exists another disk segment in which the chord is adjacent to a 5-gon, and this 5-gon is adjacent to two 6-gons. The right disk segment in Fig. 10, a) has $j = 8$. Removing an edge from this disk segment makes it mirror

[3]It is called the *boundary code* (see [30], [59], [28] and Definition 12 in § 2.5).

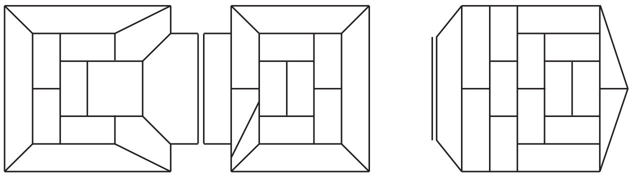


Figure 10. a) 15-$DF_{48}(C_1)$ split into two disk segments; b) a disk segment with $f_6 = 3$

symmetric but now with $j = 7$. For $j = 17$ a disk segment with $f_6 = 2$ has a chord which cuts off a smaller segment. For $j = 15$ a disk segment with $f_6 = 3$ contains a 6-gon whose intersection with the boundary is disconnected.

For all other j with $4 \leqslant j \leqslant 16$, the inequality $f_6 \geqslant 3$ holds. However, disk segments with $f_6 = 3$ exist only for $j = 6, 7, 8, 9, 10, 15, 16$. Such a disk segment with $j = 6$ is shown in Fig. 11, a), and the one in Fig. 10, b) has $j = 10$. The disk segment shown in Fig. 10, b) has two adjacent 5-gons whose common edge has one endpoint on the boundary and the other in a 6-gon. Replacing these two 5-gons by a single 6-gon, we obtain another disk segment with $j = 9$. Disk segments with $j = 15$ and $j = 16$ are shown in Fig. 11, b) and c).

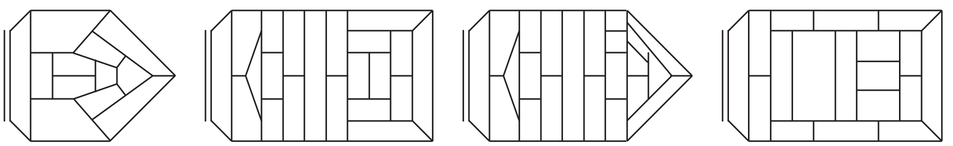


Figure 11. Four disk segments: a), b), and c) with $f_6 = 3$; d) with $f_6 = 4$

For $j = 4, 5, 11, 12, 13, 14$ we have the estimate $\min f_6 \geqslant 4$. A disk segment with $f_6 = 4$ and $j = 11$ is shown in Fig. 11, d). For $4 \leqslant j \leqslant 14$ none of these disk segments contains a smaller segment.

A series of n-DFs with 3-connected skeletons and $f_6 = 6$ is constructed in [29] for $n \geqslant 12$. It follows that for n-DFs with 3-connected skeletons and $n \geqslant 12$ the estimate $\min f_6 \leqslant 6$ holds, that is, $m_3(n) \leqslant 6$. According to Proposition 1 of [29], there exists an n-DF_v if and only if $v \geqslant 2(m_3(n) + n + 5)$, $n \geqslant 1$, except for the impossible cases $(n, v) = (1, 42), (3, 24), (5, 22)$, where $m_3(n)$ denotes the smallest value of f_6 for n-DFs with 3-connected skeletons. The values $m_3(n)$ for $3 \leqslant n \leqslant 11$ are given in Table 1.

Theorem 1. *Let $m_2(n)$ denote the smallest value of f_6 in an n-disk-fullerene whose skeleton is 2-connected but not 3-connected, for $n \geqslant 12$. Then:*

(i) $m_2(n) = 4$ *if* $n \equiv 4, 5, 6 \pmod{10}$;

(ii) $m_2(n) = 5$ *if* $n \equiv 2, 3, 7, 8 \pmod{10}$;

(iii) $m_2(n) = 6$ *if* $n \equiv 0, 1, 9 \pmod{10}$.

Table 1. The smallest value of f_6 for usual n-DFs (with 3-connected skeletons) with $3 \leqslant n \leqslant 11$.

n	3	4	5	6	7	8	9	10	11
$m_3(n)$	3	2	0	1	3	4	6	7	8

Proof. (i) A 15-$DF_{48}(C_1)$ is shown in Fig. 10, a). This 15-DF is split into two disk segments by a chord. The left disk segment together with the disk segment mirror symmetric to it with respect to the chord form a 14-DF. The right disk segment together with the disk segment mirror symmetric to it with respect to the chord form a 16-DF. Each of these three disk-fullerenes has $f_6 = 4$. An arbitrary number of the $(5,3)$-polycycles shown in Fig. 9, e) can be put between the two disk segments of these 14-, 15-, and 16-disk-fullerenes. There are no other n-DFs with $f_6 = 4$.

(ii) The case $n = 12$ is special. Two disk segments identical to the one shown in Fig. 11, a) form a 12-DF. Between its two disk segments one can put a summand shown in Fig. 9, e). Two disk segments shown in Fig. 11, a) and c) form a 22-DF. These 12-DF and 22-DF have $f_6 = 6$. However, $m_2(n)$ is not 6 for $n = 12$ and $n = 22$. Indeed, take a disk segment whose chord is adjacent to a 5-gon which is adjacent to two 6-gons, while all other cells of this disk segment are 5-gons. This disk segment has $f_6 = 2$ and $j = 7$. Two such disk segments together form a 14-DF with $f_6 = 4$. Replacing the two 5-gons which are adjacent to the chord by a 6-gon, we get a 12-DF with $f_6 = 5$ (see [29]). This is the minimal 12-$DF_{44}(C_{2\nu})$ (see Remark 9 in § 2.4).

A disk segment with $f_6 = 2$ and $j = 7$ together with the disk segment shown in Fig. 11, b) forms a 22-DF. The left disk segment shown in Fig. 10, a) and the disk segment shown in Fig. 11, a) form a 13-DF with $f_6 = 5$. In Fig. 10 the left disk segment a) together with the disk segment b) forms a 17-DF, and the right disk segment a) with the disk segment b) forms an 18-DF. In both cases $f_6 = 5$. Between the segments of each of these four n-disk-fullerenes (with $n = 22, 13, 17, 18$) one can put an arbitrary number of the $(5,3)$-polycycles shown in Fig. 9 e).

(iii) The disk segment with $f_6 = 2$ and $j = 8$ shown on the right in Fig. 10, a) and the disk segment with $f_6 = 4$ and $j = 11$ shown in Fig. 11, d) form a 19-DF with $f_6 = 6$. The two disk segments with $f_6 = 3$ and $j = 10$ shown in Fig. 10, b) form a 22-DF with $f_6 = 6$. The disk segment with $f_6 = 3$ and $j = 6$ shown in Fig. 11, a) and the disk segment with $f_6 = 3$ and $j = 15$ shown in Fig. 11 b) form a 21-DF with $f_6 = 6$. Between the segments of these disk-fullerenes one can put an arbitrary number of the $(5,3)$-polycycles shown in Fig. 9, e).

It remains only to verify that $m_2(n) \neq 5$ in the case (iii). Assume that a disk decomposition with $f_6 = 5$ does not have an edge which is a chord (see Fig. 8, c)). Then we join the centres of the opposite boundary edges of the 6-gon by a new edge. We obtain a new disk decomposition with $f_6 = 4$. Hence $j = 7$ or $j = 8$. More precisely, the terminal disk segments must have $j = 7$ or $j = 8$, and $(5,3)$-polycycles shown in 9 e) can be inserted between them. Removing the new edge, we obtain the original disk decomposition with $f_6 = 5$. The number of boundary edges is

$7+7-2=12$, $7+8-2=13$, or $8+8-2=14$. For $n=12,13$ we get $m_2(n)=5$, but $n=14$ has $m_2(n)=4$.

Assume that a disk decomposition with $f_6=5$ has a edge which is a chord. Then there are two possible cases:

- one disk segment with $f_6=2$ and another disk segment with $f_6=3$, with insertions shown in Fig. 9 e) between them;
- two disk segments with $f_6=2$, one insertion with $f_6=3$ shown in Fig. 9, d), and some possible insertions shown in Fig. 9, e).

In the second case the number of boundary edges is $7{+}7{+}12=26$, $7{+}8{+}12=27$, or $8+8+12=28$. For $n=27,28$ we get $m_2(n)=5$, but $n=26$ gives $m_2(n)=4$. The inequality $m_2(n)\neq 5$ is therefore verified.

All possible $n\geqslant 12$ are considered in the cases (i), (ii), (iii). The number of 6-gons in an n-DF can be made equal to any natural number larger than 4, 5, 6, respectively, while keeping the number of boundary edges unchanged. This is done using the carousel of operations φ_i, $i=1,2,\dots$ (see Fig. 5).

It follows that there exist arbitrarily many usual and unusual n-DFs with the boundary code $(3,3,\dots,3)=(3)^n$ for $n\geqslant 12$ (see [29], footnote [3], Table 2, and also [28] and [38]). $\square$

The values of $m_2(n)$ with $n\leqslant 21$ for n-DFs whose skeletons are 2-connected but not 3-connected are given in Table 2. All minimal n-DFs with $n\leqslant 11$ were found using a computer. They are unique except for the cases $n=9$ and 11. In the minimal exceptional n-DFs, that is, in one $1\text{-}DF_{40}(C_s)$ and one $2\text{-}DF_{26}(C_{2\nu})$, all $n+6$ pentagons are organized into a block which is opposite to the n-gon. For $n=8,9,10,11$ we have one $8\text{-}DF_{72}(C_{2v})$, two $9\text{-}DF_{62}(C_s)$s, one $10\text{-}DF_{50}(C_{2v})$, and two $11\text{-}DF_{48}(C_s)$s. All these 6 minimal unusual n-DFs resemble chemical nanotubes (oblong fullerenes). They consist of similar blocks of 5-gons separated by 6-gons (see also Remarks 9 and 10). A similar n-DF is shown in Fig. 6 a), but it is not minimal.

Table 2. Minimal values of f_6 for unusual n-DFs (with only 2-connected skeletons).

n	2	8	9	10	11	12	13	14	15	16	17	18	19	20	21
$m_2(n)$	6	23	17	10	8	5	5	4	4	4	5	5	6	6	6

Table 2 repeats periodically: we have $m_2(n)=m_2(10+n-[n/10])$ for $n\geqslant 22$, where the square brackets denote the integral part of a number. We assume that $m_3(n)=6$, which implies that $m_1(n)=m_2(n)$ for $n\geqslant 22$ (see [29]). Of course, $m_1(n)=m_3(n)$ for $n\geqslant 19$ with $n\equiv 0,1,9 \pmod{10}$. The number of n-DFs on which the value $m_1(n)$ is achieved is equal to 1 for $n=1,\dots,8$ and to 2, 3, 8 for $n=9,10,11$, respectively. The number of n-DFs on which the value $m_3(n)$ is achieved is equal to 1 for $3\leqslant n\leqslant 21$ except for $n=9,10,11$, and possibly for all $n\geqslant 22$. The values $m_2(n)$ for $n\geqslant 12$ are given in Theorem 1. See also Table 4 in § 2.5.

Let us construct an $8\text{-}DF_{72}(C_{2v})$. Take a regular 8-gon. Draw two parallel chords subdividing it into two trapezoids and a rectangle. By putting two new vertices at the centres of the chords we turn the rectangle into a 6-gon and the trapezoids into 5-gons. Then draw three bisector rays from the three degree-2 vertices of the 5-gon. The free ends of these bisector rays are the vertices of a triangle whose boundary is the inner boundary of an annulus consisting of three polygons adjacent to the boundary of the trapezoid. We turn these three polygons into 6-gons by subdividing two edges of the triangle into two edges each and subdividing the third edge into three edges. Then we attach four edges to the resulting four vertices of degree 2. The free ends of these edges are the vertices of a 4-gon whose boundary is the inner boundary of a second annulus consisting of four polygons adjacent to the first annulus. We turn these four polygons into 6-gons by subdividing three edges of the 4-gon into two edges each and subdividing the fourth edge into three edges. Then we attach 5 edges to the resulting five vertices of degree 2. The free ends of these edges are the vertices of a 5-gon whose boundary is the inner boundary of a third annulus consisting of polygons adjacent to the second annulus. We add 5 new vertices at the centres of the edges of the 5-gon, and attach 5 edges to these 5 new vertices. The free ends of these edges are the vertices of the last 5-gon.

The structure of one of the 9-$DF_{62}(C_s)$s is different from the 8-$DF_{72}(C_{2v})$: one of the two trapezoids is replaced by a regular 5-gon. It is also decomposed into cells, but its boundary has 4 adjacent hexagons and not 3 as in the case of the trapezoid. Furthermore, the two 6-gons adjacent to the central 6-gon are also adjacent to the fifth 6-gon, while all the other cells are 5-gonal.

The 10-$DF_{50}(C_{2v})$ and one 11-$DF_{48}(C_s)$ are considered in § 2.5 (see Case 1.2).

In order to prove Theorem 1 we needed to find all disk segments with $f_6 = 2$ and $f_6 = 3$ whose boundary has a connected intersection with any cell. At first glance, this task seemed very daunting, since already for $f_6 = 4$ there is an infinite series of disk segments whose boundary has a connected intersection with any cell. This series is given by the parameter $j = 13 + k$, where $k \in \mathbb{N}$. However, the problem was solved with the help of a special computer program. It was shown that in the cases $f_6 = 2$ and $f_6 = 3$ there are only 15 disk segments with the required property: three with $f_6 = 2$ and twelve with $f_6 = 3$. They are shown in Table 3.

All these 15 disk segments are generalized disk-fullerenes. They are extendable, since each of them has an edge whose ends are vertices of degree 2. However, none of them is a patch, that is, none can be extended to a fullerene.

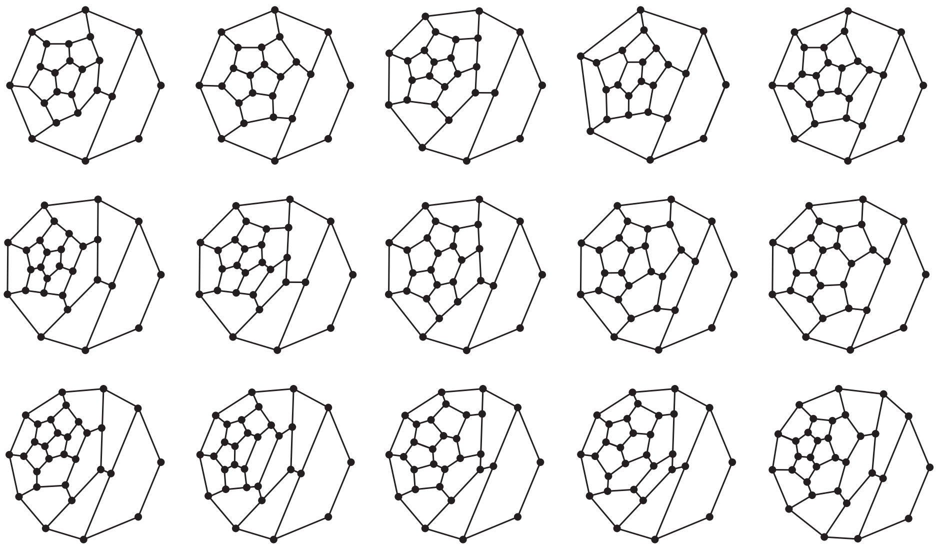
Also found were 5 analogous disk segments with $f_6 = 4$ for $j \leqslant 14$ (for $j = 14$ this is the minimal representative in the indicated series and corresponds to the smallest $k = 1$) and 11 analogous disk segments with $f_6 = 5$ for $j \leqslant 13$, but we do not list them here.

2.3. The structure of fullerenes and disk-fullerenes.

Definition 6. A closed edge path in the skeleton of a fullerene or disk-fullerene is called a *zigzag* (see the Introduction) if the left and the right turns at the vertices alternate along this path. A zigzag is said to be *simple* if it does not have self-intersections. See also [25] and [26].

It is easy to see that a simple zigzag in a fullerene or disk-fullerene consists of at least 10 edges. Therefore, if all zigzags are simple, then there are at most $e/5$ of them, since each edge belongs to at most two zigzags.

Table 3. All disk segments with $f_6 = 2$ and $f_6 = 3$ whose boundary has a connected intersection with any cell.



Remark 6. (i) If two zigzags intersect, then each connected component of their intersection consists of a single edge. In each of them the intersection is *transverse*, that is, the segments of the zigzags near their common edge are on different sides with respect to each other. This property holds also for self-intersecting zigzags.

(ii) Each of n pairs of adjacent edges on the boundary of an n-DF generates a zigzag, possibly self-intersecting. These are the only zigzags which intersect the boundary, and their number is at most n.

(iii) If an edge does not belong to the boundary of a disk-fullerene, but both ends of the edge belong to the boundary, then any zigzag containing this edge is self-intersecting. If a zigzag intersects the boundary and is simple, then in this zigzag two boundary edges alternate with at least two edges which do not belong to the boundary.

Proposition 7. *The intersection of a cell in an n-disk-fullerene* (*or fullerene*) *with a simple zigzag is connected.*

Proof. A cell in a fullerene or disk-fullerene cannot have just one common edge with a zigzag. A non-empty intersection of a 5-gon with a simple zigzag contains two and only two adjacent edges. Let us prove by contradiction that two opposite pairs of adjacent edges of a 6-gon cannot belong to a simple zigzag. We first prove this in the case of a fullerene.

Assume that two opposite pairs of adjacent edges of a 6-gon belong to a simple zigzag. Then the cell adjacent to the 6-gon along an edge which does not belong to the zigzag has a disconnected intersection with the zigzag. It follows that this cell is another 6-gon. There is a third 6-gon which is adjacent to the second and has a disconnected intersection with the zigzag, an so on. All possible ways of

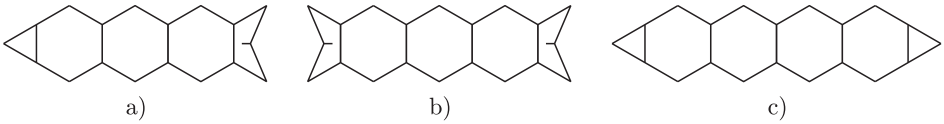


Figure 12. If the intersection of a zigzag with a 6-gon is disconnected, then there exists an m-gon with $m \neq 5, 6$

termination of this process (in any direction) are shown in Fig. 12. However, none of these cases is possible for a fullerene.

In the case of a disk-fullerene the proof is similar, but the following modification is needed. Consider the first 6-gon which intersects the zigzag in two opposite pairs of adjacent edges. If this 6-gon is on the interior side of the zigzag, then the proof is the same. Suppose now that the first 6-gon is on the exterior side. Then we choose a second 6-gon on the same side as the part of the zigzag which is interior with respect to the cycle consisting of the other part of the zigzag and an edge of the first 6-gon not belonging to the zigzag. This second 6-gon is adjacent to a third 6-gon which also has a disconnected intersection with the zigzag, and so on. As in the case of a fullerene, this process (this time in only one direction) cannot terminate at a 6-gon. □

Corollary 2. *The number of cells adjacent to a simple zigzag on any side of it is equal to half the number of its edges. There is one exception: when counting the number of cells adjacent to a zigzag on the exterior side, the boundary edges of the zigzag are not considered.*

Next we consider a special type of disk-fullerenes called *thimbles*.

Definition 7. An (abstract) n-disk-fullerene is called an (abstract) n-*thimble* if all its cells adjacent to the boundary are 5-gons and there are exactly n of them.

Remark 7. Doubling a thimble (that is, identifying the boundaries of two identical thimbles) creates a decomposition of a sphere into 5- and 6-gons. This decomposition has n vertices of degree 4. The boundary 5-gons of the two thimbles are split into pairs of 5-gons which become adjacent along a boundary edge in the decomposition of the sphere. We replace each of these pairs by a 6-gon. Interior points of the former boundary edges become interior points of the new 6-gons, and vertices of degree 4 become interior points of opposite edges of the new 6-gons. As a result, we obtain a fullerene. Each of the two original thimbles fills exactly half the fullerene, but the thimbles are not patches in the sense of [57]: the combinatorial structure of a thimble *is not preserved* when it is extended to a fullerene.

Two disk segments identical to the disk segment shown in Fig. 10, b) form a 20-DF all of whose boundary cells are 5-gons. Clearly, this 20-DF is not a thimble, because the number of boundary 5-gons is 18, not 20.

Example 1. Fix a number $n \geqslant 7$ and consider $n-3$ concentric circles of radii $1, 2, \dots, n-4, n-3$. Using these circles and unit segments joining some chosen vertices on the circles, we construct the edge skeleton of a thimble. Namely, we put $6, 7, 8, \dots, n-1, n, n$ unit segments between neighbouring circles, respectively.

(The number of edges in the last annulus between the circles is the same as the number of edges in the next-to-last annulus; in particular, for $n = 7$, we have 6, 7, 7 edges in the three annuluses between the circles, respectively.) These edges together with circle arcs form the skeleton of a thimble which fills the whole disk of radius $n - 3$.

Now we choose the vertices. On the circle of radius 1 we choose 6 vertices[4] which split it into 6 *elementary arcs*. We add 6 unit segments along radii starting at the chosen vertices and ending at 6 vertices on the circle of radius 2. We add 7 more vertices to the circle of radius 2 by splitting 5 elementary arcs into two parts each and the remaining arc into three parts. Then we add 7 unit segments starting at the 7 added vertices and ending at some 7 vertices on the circle of radius 3. We add 8 more vertices on the circle of radius 3 by splitting one elementary arc into three parts and the six other elementary arcs into two parts each (we cannot split more than one arc into three parts, since then we would get a 7-gon). Then we add 8 unit segments starting at the 8 added vertices and ending at some 8 vertices on the circle of radius 4. We proceed in this way until we add n unit segments whose endpoints specify n vertices on the next-to-last circle. After splitting each elementary arc of the next-to-last circle into two parts, we add n unit segments starting at the n added vertices and ending at some n vertices on the last circle. This finishes the construction.

We have five pentagons in the first annulus between the circles, one pentagon in the next-to-last annulus, and n pentagons in the last annulus. All other cells are hexagons. As a result, we obtain an n-disk-fullerene. There are n pentagons adjacent to its boundary, out of a total number of $n + 6$ pentagons (see (5)). This disk-fullerene is an n-thimble.

It can easily be seen that n-thimbles exist for any $n \geqslant 5$ but not for $n \leqslant 4$.

Lemma 1. *All the boundary* 5*-gons of a thimble form a cylinder, one of whose edges is the boundary of the thimble and the other is a simple zigzag.*

Proof. Consider the cyclic sequence of 5-gons adjacent to the boundary of a thimble. The 5-gons in this sequence are all different. Indeed, each 5-gon has a single edge on the boundary, since the number of 5-gons in the sequence is equal to the number of boundary edges. Neighbouring 5-gons in the sequence have a common edge with an endpoint on the boundary of the thimble. We need to prove that non-neighbouring 5-gons in the sequence do not intersect. Assume that they do intersect, and consider the following two cases.

Case 1. Two non-neighbouring 5-gons have a common vertex A which is opposite to the boundary edge of each 5-gon. Since $q = 3$, the two 5-gons have a common edge AB. The star of the vertex B contains a third cell, which has a common edge BC with one 5-gon and a common edge BD with the other 5-gon. The vertices C and D belong to the boundary of the thimble. Since there are only 5-gons adjacent to the boundary, the third cell in the star of B is a 5-gon, which has a disconnected intersection with the boundary. This is a contradiction.

Case 2. Two neighbouring 5-gons have a common edge AB, where the vertex A is opposite to the boundary edge of one 5-gon, and the vertex B is opposite to

[4] Another series of thimbles can be constructed in exactly the same way if we start with five vertices instead of six.

the boundary edge of the other 5-gon. The star of B contains a third cell, which has a common edge with the first 5-gon of the sequence. One of the ends of this edge belongs to the boundary of the thimble. Hence the third cell in the star of B is a 5-gon. The third and the second 5-gons have a common edge, say BC. The star of C consists of the second 5-gon, the third 5-gon, and some fourth 5-gon. The fourth and third 5-gons have a common edge CD, and so on. The sequence $ABCD\dots$ can be continued indefinitely. (Indeed, two sequences of 5-gons, one indexed by even numbers and the other by odd numbers, cannot close up into a cylinder with two boundary components, but they also cannot close up into a Möbius band with only one boundary component.) Again, we end up with a contradiction. □

Pairs of edges of boundary 5-gons with a common vertex which is opposite to a boundary edge of a 5-gon form a simple zigzag. This follows from the fact that all cells adjacent to the boundary of a thimble are different 5-gons.

If all the boundary cells of an n-DF are 5-gons, but the n-DF is not a thimble, then pairs of edges of these boundary 5-gons with a common vertex opposite to a boundary edge form a self-intersecting zigzag. But if all the boundary cells of an n-DF are 5-gons forming a cylinder whose second boundary component is a simple zigzag, then the n-DF is a thimble.

We therefore obtain the following corollary of Definition 7, Proposition 4, and Criterion 1:

Corollary 3. *The skeleton of an abstract thimble is isomorphic to the skeleton of a thimble, that is, it is* 3*-connected.*

Proposition 8. *A disk cut out from a fullerene or n-disk-fullerene by a simple zigzag contains exactly* 6 *pentagons.*

Proof (see also [26]). Let D be a disk cut out by a zigzag Z. (There are two such disks in the case of a fullerene and only one such disk in the case of a disk-fullerene.) The degrees of the vertices of the zigzag Z in D alternate between 3 and 2. We attach a 5-gon to each pair of boundary edges of D with a common vertex of degree 3. (The total number of the attached 5-gons equals half the number of edges in the zigzag.) By identifying edges of the 5-gons containing vertices of degree 2 in D we obtain a thimble. Besides the boundary 5-gons, this thimble contains exactly six 5-gons belonging to D. □

Corollary 4. *Lemma 1 and Corollary 2 imply the estimate $f_6 \geqslant n-6$ for an arbitrary n-thimble. It follows that an n-thimble with $n \geqslant 13$ is not a minimal n-DF.*

The disk D in Proposition 8 constitutes half of a fullerene: it forms a fullerene when combined with the disk mirror symmetric to it, rotated through the angle $2\pi/z$, where z is the number of edges in the zigzag. The disk D is also a patch (its combinatorial structure is *preserved* when it is extended to a fullerene; see Definition 11 below, and [57]). Recall the following definition (see the Introduction):

Definition 8. If a fullerene or a disk-fullerene contains a cyclic sequence of 6-gons in which each 6-gon is adjacent to its neighbouring 6-gons along a pair of opposite edges and is not adjacent to non-neighbouring 6-gons, then we refer to this sequence of 6-gons as a *belt*. (A belt was called a *railroad* in [36], [37], [26], [27].)

Each 6-gon in a fullerene or a disk-fullerene belongs to at most three belts. The two boundary components of a belt are identical simple zigzags.

Let us cut a fullerene with a belt along the middle line of the belt. Then each 6-gon splits into two 5-gons, and the fullerene splits into two thimbles. These thimbles are not necessarily identical, and they are not patches.

Lemma 2. *If a fullerene or a disk-fullerene has a simple zigzag such that all the adjacent cells on one of its sides are* 6*-gons, then these* 6*-gons form a belt.*

Proof. A 6-gon adjacent to a zigzag contains a pair of zigzag edges with a common vertex (see Proposition 7). The number of such 6-gons is half the number of edges in the zigzag (see Corollary 2). Take two neighbouring 6-gons in the cyclic sequence. They have a common edge. One end of this edge belongs to the zigzag. Denote the other end by A and assume that A belongs to a third 6-gon which is adjacent to the zigzag along the two edges with common vertex opposite to A. This third 6-gon is adjacent to the first two 6-gons. Let AB be the common edge of the third and second 6-gons. The vertex B belongs to some fourth cell (because $q = 3$). Since one of the ends of the common edge of the fourth and third cells belongs to the zigzag, the fourth cell is a 6-gon adjacent to the zigzag. Let BC be the common edge of the fourth and second 6-gons. The vertex C belongs to some fifth cell, which is a 6-gon adjacent to the zigzag (by the same reason as for the fourth cell). Let CD be the common edge of the fifth and fourth 6-gons. Then the vertex D belongs to a sixth 6-gon, which is adjacent to the zigzag, and so on.

If we now swap the second and the third hexagons, then we obtain two sequences of 6-gons, one indexed by even numbers and the other by odd numbers, that are adjacent along the middle polygonal line $ABCD\dots$, which is infinite. Indeed, it cannot close up, for suppose that it does close up. It has either an even or an odd number of edges. However, both cases are impossible: in the first case the two sequences of 6-gons cannot close up into a cylinder, which has two boundary components; and in the second case the two sequences cannot close up into a (forbidden; see above) Möbius band, even though it has one boundary component. We obtain a contradiction.

Therefore, adjacent 6-gons on one side of the zigzag cannot intersect unless they are neighbouring in the cyclic sequence. It follows that these 6-gons form a belt. The second boundary component of the belt is also a simple zigzag. $\square$

In Lemma 1 it is assumed that the number of boundary 5-gons is equal to the number of boundary edges. Then non-neighbouring 5-gons in the cyclic sequence do not coincide and do not intersect.

In Lemma 2 it is not assumed that the number of 6-gons adjacent to a simple zigzag from one side is equal to half the number of edges in the zigzag. Nevertheless, non-neighbouring 6-gons in the cyclic sequence do not coincide and do not intersect.

It is no coincidence that the proofs of Lemmas 1 and 2 are similar, because Lemma 1 can be viewed as a particular case of Lemma 2: one can cut the belt along its middle line and get a thimble.

Remark 8. A zigzag on a non-orientable two-dimensional surface can have either an even or an odd number of edges. However, a disk and a sphere are orientable, so zigzags on them must have even number of edges.

Proposition 9. *Assume that a fullerene has two simple zigzags which do not intersect. Then*:

(i) *the fullerene has at least one belt*;

(ii) *both zigzags have the same number of edges.*

Proof. (i) Two simple zigzags Z_1 and Z_2 cut the fullerene into two disks and an annulus. Each disk contains six 5-gons, so the annulus contains only 6-gons. By Lemma 2, there exists a belt.

(ii) Since there are only 6-gons between the zigzags Z_1 and Z_2, we can apply Lemma 2. If the first boundary component of the belt is Z_1 and the second boundary component is not Z_2, then there is another belt. If the second boundary component of the second belt is not Z_2, then there is a third belt, and so on. After a finite number of steps we get a belt whose second boundary component is Z_2. Then all the boundary components of all these belts have the same length. □

Note that adjacent edges of a cell in a disk-fullerene cannot belong to its boundary, since $q = 3$. It follows that a 6-gon has at most three edges on the boundary, and a 5-gon has at most two boundary edges.

Let us now look at thimbles more closely. The position of a simple zigzag in a thimble with respect to the boundary can vary. By Proposition 8, the intersection of a simple zigzag with the boundary of a thimble can have at most three connected components. If there are exactly three, then the disk in Proposition 8 has six 5-gons adjacent to the boundary of the thimble. This disk has symmetry group $C_{3\nu}$. If there are exactly two components in the intersection, then the disk has four boundary 5-gons and two 5-gons which are not adjacent to the boundary. If there is only one component in the intersection, then the disk has two boundary 5-gons and four non-boundary ones. If the simple zigzag does not intersect the boundary of the thimble, then all six 5-gons in the disk are not adjacent to the boundary.

Proposition 10. *If two simple zigzags in a thimble do not intersect the boundary and do not intersect each other*, *then*:

(i) *the thimble has at least one belt*;

(ii) *the two zigzags have the same length.*

Proof. (i) By Proposition 8, each simple zigzag cuts a disk containing six 5-gons off the thimble. They are all not adjacent to the boundary, because the zigzag does not intersect the boundary. If the disks cut off from the thimble by the two zigzags do not intersect, then the thimble contains 12 rather than 6 non-boundary 5-gons, which is impossible by the identity (5). Therefore, one disk is contained in the other, and all six 5-gons are contained in the smaller disk. Since there are only 6-gons between the zigzags, the existence of a belt follows from Lemma 2.

(ii) If the second boundary component of the belt does not coincide with the second zigzag, then there are only 6-gons adjacent to the belt from the other side. These 6-gons form another belt, and so on. After a finite number of steps we end up at a belt whose boundary component is the second given zigzag. Both boundary components of each belt have the same length. □

2.4. Unshrinkable fullerenes and disk-fullerenes. Since for any $n \geqslant 1$ the number of n-DFs is infinite, it makes sense to specify a basic set of n-DFs such that any n-DF can be obtained from a basic n-DF by means of some simple operation. We define the basic set as consisting of n-DFs without belts. This leads to a kind of *reduction*. We define each reduction step together with the reduction operation itself.

Reduction step. Assume that an n-disk-fullerene has a belt. Consider the operation of deleting the interior of the belt with subsequent identification of its boundary zigzags. We call this operation a *shrinking* of the n-disk-fullerene.

We should point out that this reduction step is not uniquely defined. If the belt does not intersect the boundary of the n-DF, then after deleting the interior of such a belt with inner boundary Z_1 and outer boundary Z_2 we obtain a disk with boundary Z_1 and an annulus with inner boundary Z_2. They can be united into a new n-DF in z different ways, where z is the number of edges of the simple zigzag Z obtained after identifying the zigzags Z_1 and Z_2. For example, two disk-fullerenes $7\text{-}DF_{72}(C_1)$ and $7\text{-}DF_{54}(C_1)$ are shown in Fig. 13. The first of them was found with the help of a computer program (see Remark 11, (ii) below), and the second was obtained from the first by the reduction $7\text{-}DF_{72}(C_1) \to 7\text{-}DF_{54}(C_1)$.

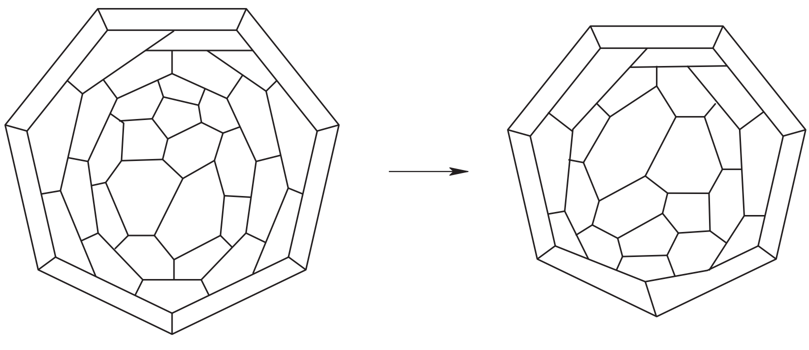


Figure 13. A shrinkable $7\text{-}DF_{72}(C_1)$ with only simple zigzags (11 zigzags in total), and one of its reductions

Here we have chosen the reduction step under which the disk with boundary Z in the $7\text{-}DF_{54}(C_1)$ is obtained from the disk with boundary Z_1 in the $7\text{-}DF_{72}(C_1)$ by a central symmetry (rotation through the angle π). This rotation is allowed precisely when the number $z/2$ is odd. In any case there are $z/2$ non-trivial rotations through an angle of the form $(2k+1)2\pi/z$ preserving the front side and $z/2$ mirror rotations swapping the front side and the reverse side. We note that the $7\text{-}DF_{54}(C_1)$ has only two zigzags, a simple zigzag of length 18 (obtained by identifying the zigzags Z_1 and Z_2) and another self-intersecting zigzag.

Assume now that Z_2 intersects the boundary of the n-DF. Then we attach an n-gon to the boundary of the n-DF, obtaining a sphere. By removing from it the interior of the belt we obtain two disks with boundaries Z_1 and Z_2. We identify them in one of z ways and remove the attached n-gon. As a result, we obtain a new n-DF.

Definition 9. A disk-fullerene with at least one belt is said to be *shrinkable*, and a disk-fullerene without belts is *unshrinkable*.

Any disk-fullerene can be turned into an unshrinkable disk-fullerene by a finite number of reductions. For example, the $7\text{-}DF_{54}(C_1)$ on the right in Fig. 13 is unshrinkable.

A disk-fullerene with a simple zigzag Z can be extended by cutting it into two parts along Z and inserting a belt joining them. The extending operation is the reverse of the shrinking operation and is also not uniquely defined. A disk-fullerene without simple zigzags cannot be extended and cannot be shrunk.

All of the above applies not only to disk-fullerenes, but also to fullerenes. The number of simple zigzags can occasionally increase under shrinking. However, the number of 6-gons always decreases. Therefore, any shrinkable fullerene can be reduced to an unshrinkable one in a finite number of steps.

Recall that for any $n \geqslant 3$ an abstract $n\text{-}DF$ is isomorphic to an $n\text{-}DF$ if and only if its skeleton is 3-connected (see Criterion 1).

For $1 \leqslant n \leqslant 6$ (the exceptional cases $n = 1, 2$ will be considered below), any cell of an abstract $n\text{-}DF$ can have at most one common edge with the n-gonal boundary. Therefore, for $3 \leqslant n \leqslant 6$ any abstract $n\text{-}DF$ is isomorphic to a usual $n\text{-}DF$. It turns out that this property also holds for $n = 7$. However, it does not always hold for $n = 8$, as is shown by the following two examples.

Example 2. Consider two $2\text{-}DF$s, each with a 5-gon as one of the two cells adjacent to the boundary, and put them on the sphere $\mathbb{S}^2$ in such a way that each $2\text{-}DF$ is inside the 2-gon of the other one. Choose one extra vertex on each edge of the 2-gons belonging to 5-gons, and join the new vertices by a bridge. We obtain a decomposition of the sphere into 5-gons, 6-gons, and one 8-gon. However, by removing the 8-gonal cell from this decomposition we do not obtain the expected abstract $8\text{-}DF$, because the skeleton of the resulting decomposition is 1-connected but not 2-connected.

Example 3. Consider two $3\text{-}DF$s, each with 5-gons as two of the three cells adjacent to the boundary, and put them on the sphere $\mathbb{S}^2$ in such a way that each $3\text{-}DF$ is inside the triangle of the other one. Choose one extra vertex on each edge of the triangles belonging to 5-gons. Consider on the boundary of each disk-fullerene a pair of new edges with the common vertex belonging to the two original 5-gons. We join the additional vertices by two new edges in such a way that each pair of new edges becomes opposite to a pair of edges of the new 6-gon. As a result, we obtain a decomposition of the sphere into 5-gons, 6-gons, and one 8-gon. The new 6-gon has two common edges with the 8-gon. By removing the interior of the 8-gon from the sphere we obtain an *unusual* $8\text{-}DF$: its skeleton is 2-connected but not 3-connected. It has a convex realization described in Remark 5.

Example 3 shows that in order to obtain an $n\text{-}DF$ for $n \geqslant 8$, we need to require additionally that each non-empty intersection of a 5-gon or a 6-gon with the n-gonal boundary be a single edge.

These conditions are satisfied for all thimbles in Example 1. None of these thimbles has belts, as is seen from the following criterion.

Criterion 2. *If at least one non-boundary* 5*-gon of a thimble is adjacent to a boundary* 5*-gon, then the thimble is unshrinkable.*

Proof. Assume that the boundary of the thimble has n edges. Then the thimble has n boundary 5-gons. Since we have a non-boundary 5-gon adjacent to a boundary 5-gon, there is a set of at least $n+1$ pentagons whose union is connected. If the thimble had a belt, all these $n+1$ pentagons would be on the same side of the belt. Then on the other side of the belt there would be at most 5 pentagons, which contradicts Proposition 8 (according to which there should be 6 pentagons). □

Therefore, Example 1 gives a thimble without belts for any $n \geqslant 7$. If none of the non-boundary 5-gons is adjacent to a boundary 5-gon, then the thimble has a belt (this follows from Lemma 2), that is, it is shrinkable.

Now we return to fullerenes. The next proposition follows from Definitions 6 and 9 and Proposition 9:

Proposition 11. (i) *If a fullerene is unshrinkable, then any two of its simple zigzags intersect.*

(ii) *A shrinkable fullerene or disk-fullerene has at least two simple zigzags of the same length.*

Lemma 3. *In a shrinkable fullerene or thimble, all the belts with pairwise non-intersecting interiors form a cylinder. Both boundary components of this cylinder are adjacent to* 5*-gons.*

Proof. We consider the cases of fullerenes and thimbles separately.
The case of a fullerene. There are two disks on the different sides of the belt, and each contains six 5-gons (see Proposition 8). Any other belt which has no common interior point with the first belt is inside one of the two disks. If two belts have no common boundary points, then there is a cylinder (an annulus) between them consisting only of 6-gons. By Lemma 2, this cylinder contains a sequence of belts in which two neighbouring belts are adjacent along a zigzag. The belts in this sequence fill another cylinder. If there are only 6-gons adjacent to this cylinder from the outside, then they form a belt by Lemma 2. We join this belt to the cylinder. After a finite number of steps we obtain a cylinder with only 5-gons adjacent to its boundary from the outside.
The case of a thimble. All n boundary 5-gons are on the same side of any belt in the thimble, because they form an annulus homeomorphic to the lateral surface of a round cylinder, and this annulus is connected. We prove by contradiction that the remaining six 5-gons are all on the other side of the belt. Assume that there are fewer than six 5-gons there. Consider the middle edge cycle splitting the belt into two cylinders. It cuts out a disk from the thimble and this disk is a new thimble. The number of 5-gons in this new thimble must be equal to the number of boundary 5-gons plus 6. However, by assumption there are fewer than six old 5-gons inside the new thimble. This is a contradiction. Therefore, there are exactly six 5-gons on the other side of the belt. All of them are not boundary cells of the thimble.

The same six 5-gons are on the disk side of another belt, because only these 5-gons are not adjacent to the boundary. Indeed, if the two indicated disks did not intersect, then the thimble would contain 12 rather than 6 non-boundary 5-gons, which is impossible by (5). Therefore, one disk is inside the other, and all six 5-gons are in the smaller disk. The complement of the smaller disk in the larger one is a cylinder.

There are only 6-gons between the belts in the cylinder. The cylinder has a sequence of belts in which any two neighbouring belts are adjacent along a zigzag. These belts fill the cylinder. (The cylinder can consist of only two original belts if they are adjacent.) There are 6 non-boundary 5-gons on one side of the cylinder, and n boundary 5-gons on the other side. If there are only 6-gons adjacent to the boundary of the cylinder from the outside, then they form a belt by Lemma 2. We attach this belt to the cylinder. After a finite number of steps we obtain a cylinder with only 5-gons adjacent to its boundary components from the outside. There is at least one non-boundary 5-gon adjacent to one of the boundary components, and all n boundary 5-gons are adjacent to the other boundary component. Therefore, all the belts constructed above form a cylinder with only 5-gons adjacent to its boundary from the outside. □

We note that all the belts in a thimble are pairwise non-intersecting and belong to a single cylinder. Each 6-gon in a thimble belongs to at most one belt. If there is a belt containing a given 6-gon, then when trying in one of the two other possible ways to construct a belt containing this 6-gon and corresponding to each of the two other pairs of edges opposite to it, we come to one of the n boundary 5-gons of the thimble.

Any other disk-fullerene can contain several cylinders. By Lemma 1 and Remark 6, (ii), the number of simple zigzags in an unshrinkable n-thimble is at least 1 and at most $n+1$.

Proposition 12. (i) *Any thimble has at least one simple zigzag which does not intersect its boundary.*

(ii) *An unshrinkable thimble has exactly one simple zigzag which does not intersect the boundary, and hence the number of simple zigzags in the n-thimble is at most $n+1$.*

Remark 9. An unshrinkable disk-fullerene must have at least two simple zigzags which do not intersect the boundary. For example, take two thimbles obtained by removing a face from a dodecahedron. We add one vertex to each edge in a pair of adjacent edges on the boundary of each thimble. We join these vertices by two edges in such a way that the new edges become opposite sides of a 6-gon uniting both thimbles into a single disk-fullerene. As a result, we obtain an unshrinkable 12-DF with two simple zigzags which do not intersect each other nor the boundary. (Incidentally, this is the minimal 12-$DF_{44}(C_{2\nu})$; see [29].) Each of the unshrinkable 8-, 9-, and 10-DFs in Fig. 6 also contains two simple zigzags which do not intersect each other nor the boundary.

Remark 10. A disk-fullerene with two non-intersecting simple zigzags but without a belt can be extended to obtain a disk-fullerene with two non-intersecting belts which do not belong to the same cylinder. (This means that Lemma 3 cannot be generalized to all disk-fullerenes.) Each of these two simple zigzags can be used independently of each other to extend the disk-fullerene any specified number of times. See also Remark 11, (iv).

Lemma 4. *Assume that an unshrinkable fullerene or thimble is given. Then each simple zigzag has at least one adjacent* 5*-gon on each side.*

Proof. If a simple zigzag in a thimble intersects the boundary, then it has at least two adjacent 5-gons on each side. Therefore, we may assume that the zigzag does not intersect the boundary.

We prove the statement by contradiction. If there are no adjacent 5-gons on some side of a simple zigzag, then all cells adjacent to it are 6-gons. By Lemma 2 they would form a belt, implying that the fullerene or thimble is shrinkable. □

Each of the 5 pairs of adjacent edges in a 5-gon belongs to a zigzag, possibly self-intersecting. Since we have $f_5 = 12$ for any fullerene, the number of zigzags adjacent to 5-gons in a fullerene is at most 60. By Lemma 4 there are at least two 5-gons adjacent to each simple zigzag of an unshrinkable fullerene. Therefore, such a fullerene has at most 30 simple zigzags. However, this bound is not the best possible.

Each of n pairs of adjacent edges on the boundary of a thimble generates a zigzag, possibly self-intersecting. This zigzag intersects the boundary and therefore has at least two adjacent 5-gons on each side. An unshrinkable thimble has no belts, hence it has only one simple zigzag which does not intersect the boundary. The total number of simple zigzags in an unshrinkable thimble is at most $n+1$. This is the best possible bound.

Lemma 5. *Assume that a fullerene has a simple zigzag with only one adjacent* 5*-gon on one of its sides. Then this fullerene also has a self-intersecting zigzag.*

Proof. Assume that there is only one adjacent 5-gon on one of the sides of a simple zigzag Z. All the other adjacent cells are 6-gons, which form an open chain. By Proposition 7, each 6-gon in this chain has only two edges in Z (equivalently, no two 6-gons in the chain have common interior points, that is, all the 6-gons in the chain are different).

Let us prove that non-neighbouring 6-gons in the chain do not intersect (in boundary points). Indeed, take two neighbouring 6-gons in the chain. They have a common edge. Only one end of this edge belongs to Z (see above). Assume that the other end of the edge (denote it by A) belongs to a third 6-gon, which is adjacent to Z along two edges with a common vertex opposite to A. Then these three 6-gons split Z into two parts.

We can assume without loss of generality that the second 6-gon is adjacent to that part of the zigzag which is adjacent only to the 6-gons from the open chain. The third 6-gon is adjacent to each of the first two. Let the edge AB be the intersection of the third and second 6-gons. Since all vertices are 3-valent, the vertex B belongs to a fourth cell. But one end of the common edge of the third and fourth cells belongs to Z. Hence the fourth cell is a 6-gon adjacent to Z. Let the edge BC be the intersection of the fourth and second 6-gons. Then the vertex C belongs to a fifth cell which is a 6-gon adjacent to Z (as in the case of the fourth cell). Let the edge CD be the intersection of the fifth and fourth 6-gons. Then, as above, the vertex D belongs to a sixth 6-gon which is adjacent to the zigzag, and so on. If we swap the second and third 6-gons, then we obtain two chains of 6-gons, one indexed by even numbers and the other by odd numbers. These two chains are adjacent along the polygonal line $ABCD\dots$, which must be infinite. This is a contradiction.

Therefore, any two 6-gons in the open chain do not have common boundary points unless they are neighbouring in the chain.

In the 6-gons of the open chain, pairs of adjacent edges that are opposite to pairs of adjacent edges belonging to Z form a polygonal line Λ which is a proper part of a zigzag containing an edge passed through twice that is in the original 5-gon and is opposite to the 5-gon's vertex at which the two of its edges belonging to Z are adjacent. (The open polygonal line Λ together with this edge forms a closed polygonal contour which is not a zigzag but is part of the zigzag.) □

The following alternative is a trivial corollary of Lemma 5.

Alternative. *If a fullerene has only simple zigzags, then among the cells adjacent to any zigzag from one side there are*

(a) *either at least two* 5*-gons,*

(b) *or no* 5*-gons* (*only* 6*-gons*).

If a fullerene has only simple zigzags and among the cells adjacent to some zigzag there are exactly two 5-gons, then both of these 5-gons are on one side of the zigzag.

Lemma 5 justifies Proposition 8 (iii) from [26].

Theorem 2. *Assume that all the zigzags in a fullerene are simple and pairwise intersecting. Then:*

(i) *there are at least two* 5*-gons adjacent to any zigzag on each side;*

(ii) *the number of all zigzags is at most* 15 (*this bound is the best possible*).

Proof. (i) Since all the zigzags are simple and pairwise intersecting, there are no belts. By Alternative (a), there are two 5-gons adjacent to any zigzag on each side.

(ii) Each 5-gon is adjacent to at most 5 zigzags. Since $f_5 = 12$, the total number of zigzags is at most $5f_5 = 60$. By (i), there are at least four 5-gons adjacent to any simple zigzag. Therefore, the fullerene has at most $5f_5/4 = 15$ zigzags. □

All the pairwise non-intersecting belts in a fullerene form a cylinder which has only 5-gons adjacent to its boundary components from the outside. Therefore, we have the following statement.

Corollary 5. *In a fullerene the number of cylinders formed by pairwise non-intersecting belts is at most* 15. (*Recall that in a thimble, the number of cylinders formed by all its belts is at most* 1.)

Theorem 3. *If an n-disk-fullerene is unshrinkable, and all the zigzags not intersecting its boundary are simple, then:*

(i) *there are two* 5*-gons adjacent to each side of any such zigzag;*

(ii) *the number of such zigzags is at most* $5(n+6)/4$.

As regards a shrinkable n-DF, if only two 5*-gons are adjacent to such a zigzag and all the zigzags are simple, then both the* 5*-gons are on the same side of the zigzag.*

The proof is similar to the proof of Theorem 2. For simplicity we only indicated a lower bound in (i).

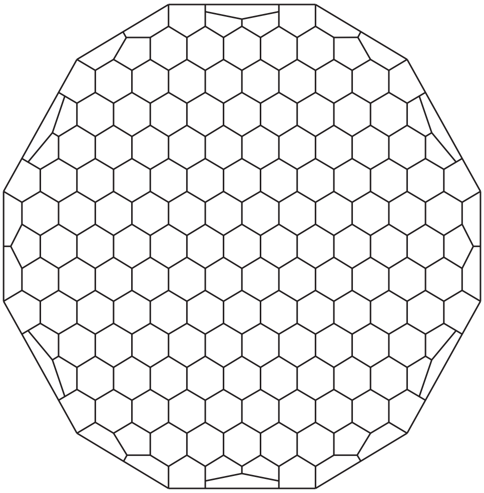


Figure 14. An unshrinkable 30-$DF_{336}(C_{6\nu})$ with only simple zigzags (there are 18 of them)

Remark 11. (i) If all the zigzags in an n-DF are simple, then their total number is at most $n + 5f_5/4 = n + 5(n+6)/4$. This follows from Theorem 3, (ii) and Remark 6, (ii) (that the number of zigzags not intersecting the boundary of an n-DF is at most n).

(ii) For $n \leqslant 15$ with $n \neq 5, 6$ and $f_6 \leqslant 25$, there is only one n-DF with only simple zigzags (see Fig. 13, on the left): the 7-$DF_{72}(C_1)$ with $f_6 = 24$ and $f_5 = 13$. It was found with the help of a computer program. Among its 11 zigzags, two have length 18 and nine have length 20, and seven zigzags of length 20 intersect the boundary. Therefore, the bound indicated in Remark 6 (ii) is achieved on this disk-fullerene. The two zigzags of length 18 do not intersect. They are the boundary components of a single belt: this disk-fullerene is shrinkable. However, there exist unshrinkable disk-fullerenes with two non-intersecting simple zigzags (see Remark 10).

(iii) An unshrinkable disk-fullerene 30-$DF_{336}(C_{6\nu})$ with $f_5 = 36$ and $f_6 = 133$ is shown in Fig. 14.

It has 18 zigzags, all of them simple: one zigzag of length 72 with symmetry group $C_{6\nu}$; two zigzags of length 66 with symmetry group $C_{3\nu}$; six zigzags of length 58 with symmetry group C_s; three zigzags of length 56 with symmetry group $C_{2\nu}$; six zigzags of length 48 with symmetry group C_s. It is not a thimble, though it also looks like a sunflower.

(iv) For any $n = 4k + 12$ with $k \in \mathbb{N}$ there exists an unshrinkable n-DF which has $2k+1$ simple zigzags. For $k = 5$ it is the 32-$DF_{154}(C_{2\nu})$ shown in Fig. 15. It has 11 simple zigzags and 4 self-intersecting zigzags. The number of self-intersecting zigzags is the same for all k. (In particular, this disk-fullerene has more than two pairwise non-intersecting simple zigzags; therefore, after extension by means of each of these zigzags it will have more than two pairwise non-intersecting belts.)

The number of simple zigzags grows with k. Therefore, the number of simple zigzags in an unshrinkable disk-fullerene can be arbitrarily large.

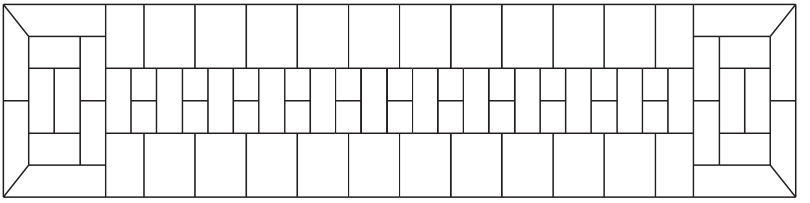


Figure 15. Unshrinkable 32-$DF_{154}(C_{2\nu})$; 11 of its 15 zigzags are simple

It would be interesting to know *for which* n there exist unshrinkable n-DFs with an arbitrarily large number of simple zigzags.

2.5. Generalized disk-fullerenes: the compact case. In the definition of a disk-fullerene there are restrictive conditions on the degrees of the vertices and on the decomposition into 5-gons and 6-gons. Now we shall weaken these restrictions. Namely, besides usual and unusual n-DFs, whose vertices have degree 3, we shall also consider generalized n-DFs, which can have vertices of degree 2 on the boundary, and exceptional n-DFs with $n = 1, 2$.

Definition 10. A *generalized* n*-disk-fullerene* is a decomposition of an n-gon into 5-gons and 6-gons in which all interior vertices have degree 3 while boundary vertices have degree 3 or 2.

In particular, the disk segments shown in Figs. 9, 10, 11 and listed in Table 3 are generalized disk-fullerenes.

Case 1: *generalized* n*-*DF*s*, $n \geqslant 3$, *with vertices of degree* 2 (*on the boundary*). By attaching an 'exterior' n-gon to the boundary of a generalized n-DF we obtain a decomposition of a sphere with

$$v = v_2 + v_3, \quad 2e = 2v_2 + 3v_3, \quad f = f_5 + f_6 + f_n, \quad 2e = 5f_5 + 6f_6 + nf_n, \tag{7}$$

where $f_n = 1$. Adding the identities (7) with coefficients 6, -2, 6, -1, respectively, and using the Euler formula, we obtain

$$f_5 = n + 6 - 2v_2. \tag{8}$$

Adding the identities (7) with coefficients 10, -3, 10, -2, we obtain

$$v_3 = 2(f_6 + n + 5 - 2v_2). \tag{9}$$

Using (8) and (9), we can rewrite the identities (7) in the form

$$v = 2(f_6 + n + 5) - 3v_2, \quad e = 3(f_6 + n + 5) - 5v_2, \quad f = f_6 + n + 7 - 2v_2. \tag{10}$$

The identities (10) imply that for a fixed n with $n \neq 5, 6$ the number of vertices, edges, and faces depend on the two parametres f_6 and v_2. (When $v_2 = 0$ we come back to usual and unusual n-DFs.)

The identities (8) together with $f_5 \geqslant 0$ imply the inequality

$$2v_2 \leqslant n+6. \tag{11}$$

In particular, when $f_5 = 0$, the inequality (11) turns into the identity

$$2v_2 = n+6. \tag{12}$$

Since all vertices of degree 2 are on the boundary, it follows that $v_2 \leqslant n$, and hence $n \geqslant 6$.

The identity (12) implies that n is even but $n \neq 2, 4, 8$. Since $f_5 = 0$, the disk consists solely of 6-gons. It is either a disk embedded in the decomposition (6^3), or a disk immersed in this decomposition. The existence of such disks implies that the bound (11) is the best possible.

We split the case under consideration into two subcases.

Subcase 1.1: *patches*, *or subfullerenes* (*proper parts of fullerenes*).

Definition 11. A decomposition of an n-gon into 5-gons and 6-gons which can be extended to a fullerene will be called a *subfullerene*; the term *patch* was used in [57]. A fullerene with a face removed will be called a *special disk-fullerene* (it is always a patch).

As before, by attaching an 'exterior' n-gon to the boundary of a patch we obtain the formulae (7)–(10). The inequalities

$$0 \leqslant f_5 \leqslant 12 \tag{13}$$

imply the following restriction on the number of vertices of degree 2:

$$\frac{n}{2} - 3 \leqslant v_2 \leqslant \frac{n}{2} + 3. \tag{14}$$

Therefore, for any fixed n the number v_2 can assume at most 7 values.

If $v_2 = n/2$ and the degrees of the vertices on the boundary strictly alternate, then the generalized n-*DF* is a patch because its boundary is a zigzag, and two such n-*DF*s together form a fullerene. Patches of this type exist for any even $n \geqslant 10$. The patch corresponding to $n = 10$ is half of the surface of a dodecahedron. For $n \geqslant 12$ the existence follows from Example 1, in which one needs to replace n by $n/2$ and also remove all 5-gons adjacent to the boundary.

In this subcase we study generalized disk-fullerenes, but we shall drop the word 'generalized' for brevity. Recall that a usual n-*DF* is a generalization of a special patch (a fullerene with a face removed), that is, of a special disk-fullerene.

Therefore, a patch is a disk which is a proper part of a simple ($q = 3$) convex polyhedron with only 5- and 6-gonal faces. Here by a polyhedron we mean not the solid $P \subset \mathbb{R}^3$ but its boundary $\partial P = \dot{P}$. The proper part of the surface $\dot{P}$ defining the patch (we denote it by D) is bounded by a simple edge cycle which we denote by C. The cycle C splits the surface $\dot{P}$ into two disks D and $\dot{P} \setminus \operatorname{int} D$, where $D \cap (\dot{P} \setminus \operatorname{int} D) = C$. Therefore, both disks D and $\dot{P} \setminus \operatorname{int} D$ are patches (see Definition 11).

All the vertices of the cycle C have degree 2 in C and degree 3 on the surface $\dot{P}$. If a vertex of C has degree 2 in the disk D, then it has degree 3 in the disk $\dot{P} \setminus \operatorname{int} D$, and vice versa.

If the disk $\dot{P} \setminus \operatorname{int} D$ contains more than one face, then it has at least one interior edge separating faces. Since the skeleton of $\dot{P}$ is connected, there is an edge inside $\dot{P} \setminus \operatorname{int} D$ with an end belonging to C. This end is a vertex of degree 2 in the disk D because $q = 3$. All the vertices of D have degree 3 if and only if $\dot{P} \setminus \operatorname{int} D$ has only one face (see Definition 4).

Assume that the patch D is not special. Then D has at least one vertex of degree 2, and it belongs to the cycle C. However, a vertex of degree 2 cannot be unique. Indeed, otherwise the skeleton of the surface $\dot{P}$ would be 1-connected but not 2-connected (removing the vertex of degree 2 would violate the connectivity), and therefore the surface $\dot{P}$ would not be a fullerene.

Therefore, the number of vertices of degree 2 is at least two. It is equal to two if and only if the disk $\dot{P} \setminus \operatorname{int} D$ contains only two faces, and the vertices of degree 2 are the ends of the edge separating these two faces. (These faces are 5- or 6-gonal, because $\dot{P}$ is a fullerene.) Indeed, if the two vertices of degree 2 were not joined by an edge, then the skeleton of $\dot{P}$ would be 2-connected but not 3-connected (removing these two vertices would violate the connectivity), and $\dot{P}$ would not be a fullerene. Therefore, in general the disk D contains at least three vertices of degree 2, and the disk $\dot{P} \setminus \operatorname{int} D$ contains at least three vertices of degree 3. By interchanging D and $\dot{P} \setminus \operatorname{int} D$ we get that in general the cycle C has at least 6 edges.

In fact, C contains exactly 5 or 6 edges if and only if it is the boundary of a cell in the fullerene $\dot{P}$. In all other cases the number of edges of C is at least 8.

Definition 12. The cyclic sequence of degrees of the vertices on the boundary of a generalized disk-fullerene is called its *boundary code* (see also footnote [3]).

The next proposition summarizes the facts mentioned above.

Proposition 13. (i) *A generalized disk-fullerene with a single vertex of degree* 2 *cannot be a patch.*

(ii) *A generalized disk-fullerene with two vertices of degree* 2 *is a patch if and only if it has boundary code*

$$(2,3,3,3,2,3,3,3),\ (2,3,3,3,2,3,3,3,3),\ \textit{or}\ (2,3,3,3,3,2,3,3,3,3).$$

A special disk-fullerene is either a 5-DF with $f_5 = 11$ and boundary code $(3,3,3,3,3) = (3)^5$, or a 6-DF with $f_5 = 12$ and boundary code $(3,3,3,3,3,3) = (3)^6$. For $q = 3$ only a special disk-fullerene can be extended to a fullerene by putting back the removed face. When $q = 3$ and $n \neq 5, 6$, no other n-disk-fullerene has this property: it cannot be extended to a fullerene without changing its combinatorial structure, because the missing face is not 5- or 6-gonal.

There are infinitely many disk-fullerenes with a given boundary code (see, for example, Proposition 2, (ii) and Fig. 5).

A *trivial* patch, containing either a single cell or two cells, is uniquely determined by its boundary code, which is one of the sequences $(2,2,2,2,2)$, $(2,2,2,2,2,2)$, $(2,2,2,3,2,2,2,3)$, $(2,2,2,3,2,2,2,2,3)$, or $(2,2,2,2,3,2,2,2,2,3)$.

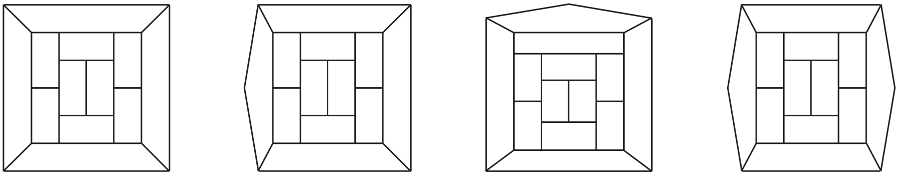


Figure 16. Disk-fullerenes which are not patches

Subcase 1.2: *generalized n-disk-fullerenes which are not patches.* By analogy with Remark 1, we say that a disk-fullerene is *unextendable* if it is not a proper part of another disk-fullerene. For example, if all vertices have degree 3, then the disk-fullerene is unextendable. Four examples are shown in Fig. 16: a) is a usual 4-DF; b) and c) are generalized 5-DFs; d) is a generalized 6-DF. None of these four disk-fullerenes are patches. The first three are unextendable. The fourth one is extendable, and it can be extended in infinitely many ways. By attaching a 6-gon to the half of the boundary with vertices of degree 2 we obtain an extendable 6-DF which again has two vertices of degree 2, but they are adjacent, that is, they are endpoints of a boundary edge. To this edge we can attach an arbitrary sequence of the $(5,3)$-polycycles shown in Fig. 9, e), as in Theorem 1. If we attach another 6-gon along the other part of the boundary, then we obtain a minimal 2-$DF_{26}(C_{2\nu})$, which is unextendable. The above two 6-DFs can be viewed as two segments with identified chords (see Fig. 8, e)), and they can be united to form an unusual 10-$DF_{50}(C_{2\nu})$. One such 6-DF together with the 7-DF in Fig. 11, a) can be united to form a minimal unusual 11-$DF_{48}(C_s)$. See also Table 4.

Example 4. Take any thimble from Example 1, and choose one extra vertex on each elementary arc of the last circle. As a result, we obtain a generalized $2n$-DF. The last annulus between circles consists of 6-gons, hence $f_5 = 6$. The last circle has n vertices of degree 3 and n vertices of degree 2. This generalized $2n$-DF constitutes half of a fullerene. Namely, a fullerene can be obtained by gluing together two mirror copies of this $2n$-DF rotated with respect to each other through the angle π/n. (The common boundary of the two $2n$-DFs becomes a simple zigzag after gluing.) Furthermore, this $2n$-DF is a patch.

Example 5. Assume that the number $n \geqslant 7$ in Example 1 is even. Then the last circle consists of an even number of arcs. We enumerate the arcs in a cyclic order. Then we add one extra vertex to each arc with an even number (arcs with odd numbers remain elementary). We get $n/2$ additional vertices on the boundary of the disk. Now the boundary has $n + n/2$ vertices: n vertices of degree 3 and $n/2$ vertices of degree 2. There are $n/2$ pentagons and $n/2$ hexagons adjacent to the boundary. We obtain a generalized $(3n/2)$-DF which is a patch when $n = 10, 12$ but not a patch for any other even number $n \geqslant 8$.

Example 6. In Example 5 we add $n/2$ unit edges with endpoints at the $n/2$ additional vertices. The other endpoints of these edges give some $n/2$ vertices on the additional circle (see Example 1). As a result, we obtain a new disk-fullerene with

$n/2$ vertices on the boundary (an $(n/2)$-DF). All its cells adjacent to the boundary are 6-gons. There are $n/2$-pentagons in the next-to-last annulus between circles.

The disk-fullerene described in Example 5 is extendable. Namely, it can be extended to the disk-fullerene constructed in Example 6.

Case 2: *usual* n-DF*s*, *unusual* n-DF*s*, *and exceptional* n-DF*s with* $n \geqslant 1$. We say that an n-DF is *exceptional* if $n = 1$ or 2. Each 5-gon in an exceptional n-DF is bounded by a simple edge cycle, as in the case $n \geqslant 3$ (otherwise we would get two 1-gons, since $q = 3$). Two 5-gons can have only one common edge (otherwise we would get two 1-gons, or two 2-gons, or a 1-gon and a 2-gon, since $q = 3$). Similarly, a 5-gon and a 6-gon can have only one common edge.

However, a 6-gon can be bounded by a non-simple edge cycle in the case when it is adjacent to the n-gon and $n = 1$. A 6-gon which is not adjacent to the 1-gon is bounded by a simple edge cycle. Two 6-gons can have two common edges if both are adjacent to the n-gonal boundary for $n = 2$, or if both are adjacent to the self-intersecting 6-gon for $n = 1$. When $n \geqslant 3$, all the 5- and 6-gons are bounded by simple edge cycles, and any two of them have at most one common edge.

Now we consider the whole collection of disk-fullerenes treated in this subsection, namely, usual n-DFs, unusual n-DFs, and exceptional n-DFs.

For $n \geqslant 8$ there exist simple ($q = 3$) decompositions of the sphere into 5-gons, 6-gons, and one n-gon with a 1-connected skeleton which is not 2-connected. However, these decompositions do not give n-disk-fullerenes.

We remark that the skeleton of an n-disk-fullerene is:

- 1-connected but not 2-connected when $n = 1$;
- 2-connected but not 3-connected when $n = 2$;
- 3-connected when $3 \leqslant n \leqslant 7$;
- 2-connected when $n \geqslant 8$.

The minimal values of f_6 for $n \leqslant 21$ are given in Tables 1 and 2.

The value $m_1(n)$, that is, the minimal value of f_6 for the given n, is achieved for $n \geqslant 2$ on an n-DF with:

- only a 3-connected skeleton for $3 \leqslant n \leqslant 10$;
- either a 3-connected or a 2-connected (but not 3-connected) skeleton for $n = 11, 19, 20, 21$, and possibly also for $n \geqslant 22$ with $n \equiv 0, 1, 9 \pmod{10}$;
- a 2-connected but not 3-connected skeleton for $n = 2, 12, \dots, 18$, and possibly also for $n \geqslant 22$ with $n \not\equiv 0, 1, 9 \pmod{10}$.

Recall also that for any $n \geqslant 1$ the number of vertices of an n-DF is minimal when f_6 is minimal, as follows from (6).

Case 3: *generalized* n*-disk-fullerenes with* $n \geqslant 1$. We first show that there is no generalized n-DF with a vertex of degree 2 when $n = 1$ or $n = 2$. Indeed, when $n = 1$, the existence of a vertex of degree 2 implies that $f_1 = 1$. When $n = 2$, the existence of two vertices of degree 2 implies that $f_2 = 1$, and the existence of only one vertex of degree 2 implies that $f_6 \geqslant 0$, $f_5 = 1$, and $f_1 = 1$. Thus, Case 3 is nothing but the formal union of Cases 1 and 2.

In all three cases we considered those disk-fullerenes which can be used for their generalizations. Now we break up all n-DFs into four families:

α: *usual* n*-disk-fullerenes* with $n \geqslant 3$, that is, n-DFs with 3-connected skeletons;

Table 4. Minimal values of f_6 for n-DFs in the families $\alpha \cup \beta \cup \gamma$, $\beta \cup \gamma$ and α.

n	1	2	3	4	5	6	7	8	9	10	11
$m_1(n)$	14	6	3	2	0	1	3	4	6	7	8
$m_2(n)$	–	6	–	–	–	–	–	23	17	10	8
$m_3(n)$	–	–	3	2	0	1	3	4	6	7	8

n	12	13	14	15	16	17	18	19	20	21	$\geqslant 22$
$m_1(n)$	5	5	4	4	4	5	5	6	6	6	$\min\{m_2, m_3\}$
$m_2(n)$	5	5	4	4	4	5	5	6	6	6	see Theorem 1
$m_3(n)$	6	6	6	6	6	6	6	6	6	6	$\leqslant 6$

β: *unusual n-disk-fullerenes* with $n \geqslant 3$ whose skeletons are 2-connected but not 3-connected;

γ: *exceptional n-disk-fullerenes*, that is, n-DFs with $n = 1$ or $n = 2$;

δ: *generalized n-disk-fullerenes* with $n \geqslant 3$ which have vertices of degree 2.

The families α, β, δ contain both patches and disk-fullerenes which are not patches. No n-DF in the family γ is a patch. The family α contains the subfamily of *thimbles* and the subfamily of *special n-DFs*. An n-DF in the latter family is obtained by removing a face from a fullerene (that is, it has $n = 5$ or $n = 6$).

We recall that an n-DF in the family δ satisfies the equalities (8) and (9), that is, $f_5 = n + 6 - 2v_2$ and $f_6 = 2v_2 + v_3/2 - n - 5$. When $v_2 = 0$, these equalities turn into the equality (5) and the first equality in (6).

We combine Tables 1 and 2 into Table 4, which contains the values of the following three functions of n:

$$m_1(n) = \min f_6|_{\alpha\cup\beta\cup\gamma}, \quad m_2(n) = \min f_6|_{\beta\cup\gamma}, \quad m_3(n) = \min f_6|_{\alpha}.$$

Cyclic sequences of n numbers 3 and 2 split into the following three types:

first type: boundary codes of patches (proper parts of fullerenes);

second type: boundary codes of n-disk-fullerenes which are not patches;

third type: all other cyclic sequences of numbers 3 and 2.

Indeed, a cyclic sequence of numbers 3 and 2 either is the boundary code of a disk-fullerene or is not. If it is the boundary code of a patch, then it cannot be the boundary code of a disk-fullerene which is not a patch, because the complement of a patch to a fullerene would also be the complement of a fullerene for a disk-fullerene which is not a patch if it had the same boundary code.

If we replace each 3 by 2 and each 2 by 3 in the boundary code of a patch, then we obtain the boundary code of another patch, since the two patches complete each other to form a fullerene. In the boundary code of a patch there are at most 4 vertices of degree 2 between any successive vertices of degree 3, and at most 4 vertices of degree 3 between successive vertices of degree 2.

If we replace each 3 by 2 and each 2 by 3 in the boundary code of a disk-fullerene which is not a patch, then we do not obtain the boundary code of another disk fullerene, since otherwise these two disk-fullerenes together would form a fullerene, so they would be patches. In the boundary code of a disk-fullerene which is not a patch there are at most 4 vertices of degree 2 between successive vertices of degree 3, but there are no restrictions on the number of vertices of degree 3 between successive vertices of degree 2.

The boundary codes of disk-fullerenes in the above families α, β, γ consist solely of numbers 3. It turned out that all cyclic sequences of n numbers 3 belong either to the first type (if $n = 5, 6$) or to the second type (if $n \neq 5, 6$).

Cyclic sequences of numbers 3 and 2 are not well understood. For example, the three cyclic sequences (2), $(2, 2)$, and $(2, 3)$ are of the third type. If the numbers 3 and 2 strictly alternate and the length of the sequence is an even number at least 10, then this sequence is of the first type (see above). It would be interesting to *find a criterion* which allows one to determine the type of a sequence of numbers 3 and 2.

We note that the necessary conditions (13) and (14) are not sufficient for a generalized n-DF to be a patch. For example, the generalized 6-DF with $v_2 = 2$ and $f_5 = 8$ shown in Fig. 16, d) is not a patch, although it satisfies the inequalities (13) and (14).

We note also that the skeleton of an n-DF with $n \neq 1, 2$ does not have loops or multiple edges, and the degree of a vertex in a generalized n-DF cannot be equal to 1.

We have been mainly concerned with n-gons put together from 5- and 6-gonal cells and with $q = 3$ in which the intersection of any cell with the boundary is connected. Each of them admits a convex realization as described in Remark 4, and they are all unextendable disk-fullerenes: they cannot be extended if $n \neq 5, 6$, and for $n = 5, 6$ they can be extended only to fullerenes, but the disk becomes a sphere in the process of this extension.

If we do not require vertices to be 3-valent, then we can obtain many other decompositions of a disk into 5- and 6-gons, for example, (r, q)-polycycles with $r = 5, 6$ and $q \geqslant 3$ (see Definition 3). All finite $(6, 3)$-polycycles are extendable and have vertices of degree 2 (see [36]). Among finite $(5, 3)$-polycycles, the only unextendable one is the dodecahedron with a face removed, that is, 5-$DF_{12}(D_{5\nu})$ with $f_6 = 0$ (see Remark 1).

Chemists also consider other analogues of fullerenes. Among them are *boron-nitrogen compounds*, whose molecules can be modelled as simple convex polyhedra with only 4- and 6-gonal faces (a cube, a 6-gonal prism, and so on) (see [62]). See [34] for an account of the embedding of chemical graphs in cubes.

Disk-octahedrites, that is, decompositions of a disk into 3- and 4-gons can be treated similarly to disk-fullerenes. An n-disk-octahedrite has $f_3 = n + 4$ and $f_4 = v - n - 3$. For $n = 3, 4$ we obtain an octahedrite (see [37]) with a face removed. Here is an example with $n \geqslant 5$. The shortest diagonals of a regular convex n-gon bound a new n-gon. The centres of all its sides except one are the vertices of an $(n - 1)$-gon. The centres of all its sides except one (the one which would produce a 5-gon) are the vertices of an $(n - 2)$-gon. Continuing this process, we end up at a 4-gon which is adjacent to three 3-gons. All n cells adjacent to the boundary are 3-gons.

2.6. Generalizations of disk-fullerenes: the non-compact case. One of the generalizations of the notion of fullerene to non-compact simply connected two-dimensional manifolds is given by the decomposition (6^3). It admits a convex realization in $\mathbb{R}^3$ which preserves the combinatorial structure of the skeleton of the decomposition (see § 3.2).

The plane $\mathbb{R}^2$ is an unbounded simply connected two-dimensional manifold, and (6^3) is a unique (from the combinatorial-topological viewpoint) simple decomposition into 6-gons (all vertices have degree $q = 3$, and the 6-gons can be assumed to be regular).

There also exist decompositions of $\mathbb{R}^2$ into 5- and 6-gons with all vertices of degree 3. The number of 5-gons in such a decomposition is bounded: $1 \leqslant f_5 \leqslant 6$. Any such decomposition can be viewed as an infinite convex polyhedron in $\mathbb{R}^3$. These are so-called *nanocones* for $1 \leqslant f_5 \leqslant 5$ and *nanotubes* for $f_5 = 6$ (see [6], [39], and also [11], where compact nanotubes in the form of oblong fullerenes are also considered). Only in the case $f_5 = 1$ is the decomposition unique from the combinatorial-topological viewpoint. When $2 \leqslant f_5 \leqslant 6$, there exist infinitely many combinatorial types of such decompositions. Incidentally, by analogy with nanocones and nanotubes, the n-disk-fullerenes considered above can be viewed as *nanodisks*. We recall that the estimate $f_6 \leqslant 6$ follows from the Aleksandrov theorem for an infinite convex polyhedron whose surface is homeomorphic to the plane and has total curvature $\Omega = \sum \omega \leqslant 2\pi$.

Remark 12. Two decompositions of the plane into 5- and 6-gons with vertices of degree $q = 3$ are said to be *equivalent* if they become isomorphic after removing some finite parts. The number of equivalence classes is equal to:

- 1 for $f_6 = 0, 1, 5$;
- 2 for $f_6 = 2, 3, 4$;
- ∞ for $f_6 = 6$

(see [6] and the references there).

If a nanotube [6] has a belt, then its middle line C cuts it into two parts. The part containing all 6 old 5-gons is a thimble, and together with the thimble symmetric to it with respect to C it forms a fullerene (see Remark 7). The second part, which does not contain old 5-gons, is half of a cylinder, and together with the other half of the cylinder symmetric to it with respect to C it forms a whole cylinder.

The number of boundary components of an infinite simply connected manifold, that is, of an ∞-DF, can be equal to $1, 2, \dots$. Examples are a half-plane, the strip between two parallel lines, and so on. Each of these manifolds admits decompositions into 5- and 6-gons in which all vertices have degree 3. There are no restrictions on f_5 here. The set of 5-gons can even be infinite: if we cut the decomposition (6^3) along a straight line dividing a strip of 6-gons into 5-gons, then the resulting decomposition of a half-plane would have an infinite number of 5-gons.

An infinite two-dimensional manifold with only one boundary component can have an arbitrary number of 5-gons: $f_5 = 0, 1, 2, \dots$. The case $f_5 = 0$ is obtained as the *universal covering* of the decomposition $(6^3) \setminus H$, where $H = \mathrm{int}(6\text{-gon}) \subset (6^3)$. The case $f_5 = 1$ is obtained from the universal covering of $(6^3) \setminus H$ by removing an angle $\pi/3$, as was done in a similar case in [39]. The cases $f_5 \geqslant 2$ can be obtained in the same way, since the operation of removing an angle $\pi/3$ can be iterated indefinitely on the universal covering of $(6^3) \setminus H$: each consecutive angle is removed from its corresponding sheet of the covering.

In the case of an infinite two-dimensional manifold with two or more boundary components, a decomposition exists for any fixed $f_6 = 0, 1, 2, \dots,\ f_5 = \infty$, and $q = 3$. The case $f_6 = 0,\ f_5 = \infty,\ q = 3$ corresponds to $(5,3)$-polycycles [35].

When $f_6 > 0$, there exists a continuum of different types of decompositions of a strip infinite in both directions between two boundary components. An example of such a decomposition is shown in Fig. 17 and consists of an infinite number of congruent *elementary summands*, with the second elementary summand obtained from the first by a parallel translation t, and the third elementary summand obtained from the second by a glide reflection g. As is well known, there is a continuum of infinite sequences of two symbols.

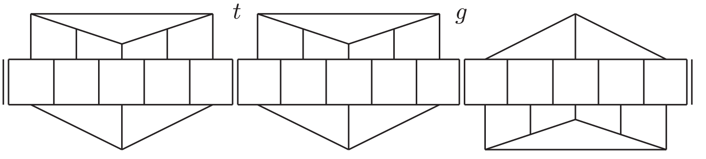


Figure 17. Three elementary summands in an infinite chain

A torus, a Klein bottle, a cylinder infinite in both directions, and an infinite Möbius band do not admit simple (that is, with $q = 3$) decompositions into 5- and 6-gons with $f_5 \geqslant 1$. Indeed, otherwise the universal covering plane would admit a simple decomposition into 5- and 6-gons with an infinite number of 5-gons. A torus and a Klein bottle only admit simple (primitive) decompositions into 6-gons. Only a sphere and a projective plane admit simple decompositions into 5- and 6-gons.

There are generalizations of the notion of fullerene to higher-dimensional manifolds [33], [14], [39], and also analogues of decompositions of $\mathbb{R}^3$ into fullerenes [55], [47], [48], but we do not consider them here.

3. Applications

3.1. Parallelohedra. A convex n-dimensional polyhedron is called a *parallelohedron* if it can tessellate the Euclidean space $\mathbb{R}^n$ by its parallel copies.

The tessellating parallelohedron is viewed as a solid, the whole space $\mathbb{R}^n$ is filled by its parallel copies, no two copies have common interior points, and any point of the space belongs to at least one copy. If the parallelohedra in a tessellation are adjacent along complete faces, then the tessellation is said to be *normal*; otherwise it is *non-normal*. The group of parallel translations of a normal tessellation always acts transitively on the parallelohedra. In the case of a non-normal tessellation into parallelohedra (into parallel copies of a fixed parallelohedron) we require additionally that the group of parallel translations act transitively on all parallelohedra. If a polyhedron admits a non-normal tessellation, then it also admits a normal one (see [82]). Any parallelohedron is centrally symmetric, and all its facets are also centrally symmetric (see [66]).

Voronoi developed the general theory of primitive parallelohedra in [83]. A normal tessellation of $\mathbb{R}^n$ into n-dimensional parallelohedra is said to be *primitive* if the number of parallelohedra meeting at any vertex of the tessellation is $n+1$. (This is the minimal number of parallelohedra meeting at a vertex; when $n = 2$, we obtain the simple decompositions ($q = 3$) considered above.) Otherwise the tessellation is non-primitive. Since a normal tessellation into parallelohedra is uniquely determined by specifying a single parallelohedron of it, we refer to this parallelohedron as primitive or non-primitive correspondingly.

Voronoi proved that a primitive n-dimensional parallelohedron has $2(2^n - 1)$ facets and that it is affinely equivalent to a *Dirichlet–Voronoi parallelohedron*. The latter is a parallelohedron all of whose interior points are closer to its centre than to the centres of all other parallelohedra in the normal tessellation. Voronoi therefore reduced the classification of primitive parallelohedra to the classification of Dirichlet–Voronoi parallelohedra.

Two parallelohedra are said to be of the same *type* if their corresponding normal tessellations have affinely equivalent dual simplicial decompositions.

Voronoi also constructed an algorithm for finding all types of primitive parallelohedra in any dimension. Using his algorithm, he found all three types of primitive 4-dimensional parallelohedra. For an arbitrary dimension he presented the *principal form of Voronoi type* I, the form of the type II, and so on. The book [16] provides a good guide to the original works [83], [84] of Voronoi.

In a normal tessellation each face of a parallelohedron is a face of the tessellation. Following [42], we say that a face of a parallelohedron is *standard* if it is the intersection of two parallelohedra in the tessellation. A standard face has a centre of symmetry, which is also a centre of symmetry of the whole tessellation. For instance, any facet of a parallelohedron is a standard face. If all the faces of a parallelohedron are standard, then the parallelohedron is a parallelepiped.

In a non-normal tessellation, some faces of the tessellation are proper parts of faces of the parallelohedron. A face of the tessellation is defined as the intersection of all the parallelohedra containing this face. A face is convex. If a face has a centre of symmetry which is also a centre of symmetry of the whole tessellation, then the face is standard. In a non-normal tessellation, such a face can be a proper part of the intersection of two parallelohedra. However, a facet of a tessellation is always the intersection of two parallelohedra. This does not depend on whether the tessellation is normal or not. Since we require that any non-normal tessellation into convex parallelohedra have a transitively acting group of parallel translations, a facet is always centrally symmetric. Furthermore, the centre of symmetry of a facet is a centre of symmetry of the whole tessellation, because a convex parallelohedron has a centre of symmetry. It follows that a facet of a non-normal tessellation is also standard.

In [42] the following two notions were defined for a tessellation of $\mathbb{R}^n$ into convex n-dimensional parallelohedra:

- the *degree of a face* is the number of parallelohedra containing this face,
- the *index of a face* is the inverse of the degree of the face.

It is shown in [42] that the sum of the indices of the standard faces is equal to $2^n - 1$.

This result immediately implies the following theorem of Minkowski: the number of $(n-1)$-dimensional faces of an n-dimensional parallelohedron is at most $2(2^n-1)$ (see [42]).

Therefore, the number of facets of an n-dimensional parallelohedron is at least $2n$ and at most $2(2^n - 1)$.

For $n = 2$ there exists only one primitive parallelogon: a centrally symmetric hexagon, and one non-primitive parallelogon: a parallelogram. A tessellation into hexagons is normal. All parallelogons in a non-normal tessellation are parallelograms.

For $n = 3$ there exists one primitive parallelohedron and 4 non-primitive ones, and they have 6, 8, 12, 12, 14 faces, respectively (see [53]). Any non-normal tessellation into 3-dimensional parallelohedra can be obtained as the limit of a normal tessellation as some dihedral angles of the parallelohedron tend to π (if the original parallelohedron is not a parallelepiped, of course). The following two cases are possible:

1) the combinatorial-topological type of the tessellation is preserved;
2) the combinatorial-topological type of the tessellation changes.

In the second case, the parallelohedron is a parallelepiped, that is, it has 6 faces. However, there are 10 parallelohedra (rather than 6) in the tessellation which are adjacent to the given parallelohedron along its 2-dimensional faces. The reason is that some adjacency takes place along proper parts of faces. These parts of faces are faces of the non-normal tessellation. We call them *decorative* faces of a non-normal parallelohedron. We obtain a convex parallelohedron with 10 faces. There are exactly two types of non-normal parallelohedra with 10 faces [78], and there are no normal parallelohedra with 10 faces.

For $n = 4$ there are three primitive parallelohedra (see [83]) and $49 = 48 + 1$ non-primitive ones (see [12], [15], and also [77]).

For $n = 5$ there are 222 types of primitive parallelohedra (see [72], [49], and also [50] and [10]). The number of non-primitive parallelohedra amounts to thousands.

We remark that the Voronoi algorithm becomes too resource-consuming for $n = 5$, so another two-stage algorithm was used in [72]. First all the adjacency types of primitive 5-dimensional parallelohedra were found. The notion of adjacency type of a parallelohedron was introduced in [71].

We also mention another result of [72]: a solution of the problem of the least dense lattice covering of 5-dimensional space by identical balls: the least dense lattice is given by the principal form of Voronoi type I.

Recall that, according to Voronoi's theorem, *a primitive n-dimensional parallelohedron is affinely equivalent to a Dirichlet–Voronoi parallelohedron.* The following elaboration was obtained in [65]: for any primitive n-dimensional parallelohedron, an affinely Dirichlet–Voronoi parallelohedron equivalent to it is unique up to a similarity. This statement is still valid when parallelohedra meet at $(n-2)$-dimensional faces in a non-primitive way, provided that any two facets can be connected by a chain of facets in which any two neighbouring facets meet at a primitive $(n-2)$-face (see [45]).

Voronoi stated his geometric constructions in an analytic form (pure geometry was not fashionable at that time). He proved that all locally densest lattice sphere packings (*limit forms*) are *perfect lattices.* He also constructed a decomposition of the cone of positive quadratic forms in n variables into perfect gonohedra [84].

The notion of a *perfect Voronoi polyhedron* $\Pi(n)$ was introduced in [81], and Voronoi's study of perfect lattices was stated in geometric terms. The polyhedron $\mu_n(m)$ dual to $\Pi(n)$ was considered in [69], where it was shown that in order to describe all equivalence classes of groups of integer $n \times n$ matrices it suffices to find the groups of integer automorphisms of the centres of gravity of pairwise inequivalent finite faces (of all dimensions) in the polyhedron $\Pi(n)$ or $\mu_n(m)$. All maximal finite groups of integer 5×5 matrices were found in [70].

The works [23], [40], [9], [41], [46] opened a new direction in the theory of normal tessellations and point systems.

3.2. The generatrissa. Let us show that the 'infinite fullerene' (6^3), that is, the tessellation of the plane $\mathbb{R}^2$ into regular 6-gons admits a convex realization in $\mathbb{R}^3$, as does any fullerene or disk-fullerene.

We put an axis perpendicular to $\mathbb{R}^2$ at the centre of one of the 6-gons in the tessellation (6^3), and then construct a *circular paraboloid* in $\mathbb{R}^3$ with this axis. On the surface of the paraboloid we take points which project parallel to the axis to the centres of the cells in the tessellation (6^3). At all these points take the tangent planes to the paraboloid. They are the planes of the faces of an infinite convex polyhedron circumscribed about the paraboloid. It is an easy fact from analytic geometry that the faces of this polyhedron project to the cells of the tessellation (6^3).

This proof uses the basic object in the proof of Voronoi's theorem, which he called the *generatrissa*. Now we describe its construction and the proof in more detail.

Consider a centrally symmetric 6-gon in $\mathbb{R}^2$ which is not inscribed in a circle, and tessellate $\mathbb{R}^2$ by parallel translations of it. On each copy of it we construct an infinite rectangular prism with this hexagon as the base. Then we construct oblique planar sections of these prisms in such a way that all these sections together form an infinite convex polyhedral surface. Namely, we choose one *original* hexagon to be left unchanged. Then we replace a hexagon adjacent to it (the first copy) by a planar section of the prism based on that copy, with the section plane chosen so that it contains the common edge of the original hexagon and its first copy. The section is sloped. The slope of its plane can be chosen arbitrarily.

By fixing this slope we obtain a unique section of the prism. This section is a 6-gon projecting onto the first copy. Now consider a second copy adjacent to the original hexagon and the first copy. The prism above the second copy contains an edge of the original hexagon and an edge of the section of the prism over the first copy. These two edges span a unique plane which intersects the prism over the second copy in a hexagon. Then we choose a third copy which is adjacent to the second copy and the original hexagon, and construct a section of the prism over the third copy in the same way. Continuing this process, we obtain sections of the prisms over all the 6 hexagons in the corona around the original hexagon. These 6 sections close up into an annulus. This follows from the fact that the original 6-gon is convex and centrally symmetric, and all its copies in the first corona are parallel to it and have common edges with it.

Sections of the prisms over the copies of the original hexagon in its second, third, ... coronas are constructed similarly. As a result we obtain an infinite convex polyhedron in $\mathbb{R}^3$ whose faces project onto cells of the original tessellation in $\mathbb{R}^2$. The surface of this polyhedron is circumscribed about an *elliptic* paraboloid which is called the *Voronoi generatrissa*. We apply an affine transformation of $\mathbb{R}^3$ which takes the elliptic paraboloid into a *circular* one while keeping its axis perpendicular to the plane $\mathbb{R}^2$. Then each cell of the tessellation consists of points of $\mathbb{R}^2$ which are closer to the centre of this cell than to the centre of any other cell.

Indeed, the projection of the line of intersection of two tangent planes of the paraboloid passes through the centre of the segment joining the projections of the points of tangency if the paraboloid is elliptic, and the projection of the line of intersection is also perpendicular to this segment if the paraboloid is circular. Therefore, the tessellation of $\mathbb{R}^2$ becomes a Dirichlet–Voronoi decomposition.

This was the way Voronoi proved his theorem that any primitive parallelohedron is an affine image of a Dirichlet–Voronoi parallelohedron. The dimension of a parallelohedron in this theorem is arbitrary. The essential feature of Voronoi's proof is the construction of a generatrissa. In the case of dimension 2 we have described the generatrissa explicitly as an infinite convex surface circumscribed about an elliptic paraboloid. The construction of a generatrissa is uniquely determined by the choice of the slope of the planar section of one of the 6-gonal prisms.

For the construction of higher-dimensional generatrisses see [83], [84].

A theory of generatrisses was developed in [73], [74], where necessary and sufficient conditions for the existence of a generatrissa were found. Both Voronoi's theorem and Zitomirskij's theorem [87] are theorems on the existence of a generatrissa which projects along the axis of an elliptic paraboloid onto a given normal tessellation. Zitomirskij's theorem is a generalization of Voronoi's theorem and states that an n-dimensional parallelohedron which is primitive at all faces of dimension $n-2$ is affinely equivalent to a Dirichlet–Voronoi parallelohedron.

According to Voronoi's conjecture, *any parallelohedron is affinely equivalent to a Dirichlet–Voronoi parallelohedron*. This conjecture is open for normal tessellations into parallelohedra with non-primitive $(n-2)$-dimensional faces (see [51], [42], [45], [44]).

3.3. Delaunay and his tetrahedric symbol. Time is running and at every instant we have to make a decision. No one can reverse time to get rid of unintended negative consequences; the train is gone.

Once B. N. Delaunay went to visit his younger grandson Borya. He took a trolley bus without looking at its route number, and the trolley bus was soon going in the wrong direction. The editor of his last paper [20] lived in that direction, so Delaunay decided to pay him a visit. When the editor opened the door and saw Delaunay, he instantly began to wave him away with both hands:

– Boris Nikolaevich, please do not come in; I have a bad case of flu!

– That's not a problem, I have not had the flu for 15 years — and he came in. They talked animatedly for more than two hours, but not about the paper, since that was discussed only at work, in the Steklov Institute. Delaunay had found a person willing to listen to his fascinating stories. After he returned home he found that he had contracted the flu. Later he suffered a hip fracture. He never recovered...

From time to time Delaunay reviewed his old papers and improved them by adding something new. For example, in the popular article [20] he elaborated on his classification of 3-dimensional lattices and, more importantly, on the *Delaunay tetrahedric symbol*, of which he was very proud. And there was a reason for this pride: the introduction of the tetrahedric symbol made the *Selling reduction step* particularly clear and simple, so that *Selling reduction* (which consists of a finite number of Selling reduction steps for each 3-dimensional lattice) was renamed *Delone reduction* by crystallographers. See details in [13], [22], [61], [17], [18], [24], [20].

Here is a quotation from Delaunay ([20], p. 170): "Unfortunately, apart from directly verifying this assertion for each of the 24 types separately, I could not find a natural general proof". After seeing this statement, the third author suggested that Delaunay replace it with the following proof. It is easy to find all *reduced Selling 4-vectorites* in a 3-dimensional lattice (see [20]). Consider rotations of the space about a point which is the origin of all four vectors in a reduced Selling 4-vectorite. The point symmetry group of the lattice consists of all such rotations taking a reduced Selling 4-vectorite to itself or to a congruent Selling 4-vectorite. The symmetry group of an arbitrary Selling 4-vectorite coincides with the symmetry group of a 3-dimensional simplex with vertices at the endpoints of the vectors of the 4-vectorite (by the way, the symmetry groups of all 3-dimensional simplices were described in [76]). However, Delaunay left the original sentence unchanged in his manuscript.

A conference dedicated to the 120th anniversary of Delaunay's birth was held in Moscow on 16–20 August 2010. The major part of the organisational work was done by N. P. Dolbilin, who continues to trace Delaunay's path in research and has published an essay on Delaunay's life and work [43]. Delaunay's daughter Anna B. (1928–2012), cheerful, friendly, and energetic like her father, and both her sons Seriozha and Borya shared their warm memories of Boris Nikolaevich Delaunay.

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