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TOWARD 4-DIMENSIONAL FULLERENES [1]

Michel Deza and Mikhail Shtogrin

Abstract

We explore the existence of high-dimensional analogues of fullerenes F_n (i.e. of simple polyhedra with only 5- and 6-gonal faces) seen as $(d-1)$-dimensional simple manifolds (preferably, polytopal or at least spherical) with only 5- and 6-gonal 2-faces. Three infinite families of such 4-fullerenes are presented here. The Construction A gives 4-polytopes by suitable insertion of fullerenes $F_{30}(D_{5h})$ into glued 120-cells. The Construction B gives 3-spheres by growing dodecahedra and barrels F_{24} around of given fullerene. The Construction C gives 4-fullerenes from special decoration of given 4-fullerene, which add fullerenes F_{20}, F_{24}, F_{26} and $F_{28}(T_d)$ only. Finally, infinite 5-fullerenes (including a simply connected $S^3 \times R^1$) are obtained (by a variation of gluing of two regular tilings 5333 of hyperbolic 4-space).

1 Introduction

We define here *n-fullerene* as a $(n-1)$-dimensional simple (i.e. n-valent) manifold (on any surface), such that any 2-face is 5- or 6-gon. We are specially interested by the n-fullerenes, which are *spherical*, i.e. homeomorphic to the $(n-1)$-sphere, and, moreover, *polytopal*, i.e. convex. So, the dual of a n-fullerene is a $(n-1)$-dimensional simplicial manifold, such that any $(n-3)$-face is adjacent to 5 or 6 $(n-2)$-simplexes.

We will use following notation. $F_n(G)$ denotes a *fullerene*, i.e simple polyhedron with only 5- and 6-faces, having n vertices and the group of symmetry G. In particular, the regular dodecahedron $F_{20}(I_h)$ and the "hexagonal barrel" (unique F_{24}) will be also denoted as Do and B_6, respectively.

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Clearly, 120-cell is a 4-dimensional analogue of the regular *Do*. There exists a 5-dimensional analogue: simple regular tiling of the hyperbolic 4-space by 120-cells; this (infinite) tiling is denoted by 5333. 120-cell and 5333 are a 4-fullerene and a 5-fullerene, in our terms.

For any 4-polytope (moreover, for any *combinatorial* 3-sphere, i.e. a cell-complex on it), denote by (v, e, p, q) its f-vector, i.e. the number of its i-faces for $i = 0, 1, 2, 3$. The Euler's characteristic, i.e. the number $v - e + p - q$ is 0 on 3-sphere. Remind also that in any i-face of simple 3-manifold, intersect exactly 4-i (i+1)-faces; so, if it is spherical, then $e = 2v$, $p = v + q$ and the number p_5 of 5-faces is $6q$.

Because of $v - e + p - q = 0$, there is no on 3-sphere an analogue for the special role of the hexagonal (or 4-gonal) faces in simple (or 4-valent, respectively) polyhedra in terms of their cells. It is why we defined d-fullerenes in terms of their 2-faces. So, all 3-faces of polyhedral d-fullerenes are fullerenes; we want, moreover, those fullerenes to be close relatives of *Do*. Besides B_6 (unique next to *Do*, by the number of vertices), two other fullerenes with isolated hexagons, unique F_{26} and unique $F_{28}(T_d)$, are also candidates. The duals of those three polyhedra are known in Chemistry (under name Frank-Kasper polyhedra Z_{14}, Z_{15}, Z_{16}) and Physics, where they appear as dislinations (rotational defects) with respect to the vertex figure of the local icosahedral order. The fullerene $F_{30}(D_{5h})$ (1-elongated dodecahedron) will also appear below, in the Construction A.

Some relevant facts and analogues are:

(i) It is well-known (see, for example, [Bok95]) that the boundary of the 120-cell is unique simple equifacetted 3-sphere with (combinatorial) facet F_{20}. But [She66] has shown that every 4-polytope can be approximated arbitrary closely (in the Hausdorff distance) by a polytope whose facets are projective images of the dodecahedron. Remind also that 120-cell is the universal polytope in the sense that any regular $\leq$ 4-polytope, including star-polytopes, can be inscribed (vertices into vertices) in it ([Cox73], page 269); moreover, ([vOs15]) one of them ($\frac{5}{2}33$, in Schläfli notation) is isomorphe to 120-cell = 533. [FTo64] in Chapter 10, conjectures that 120-cell is isoperimetrically *best* (i.e. it has the least volume among 4-polytopes of unit in-radius, having 120 cells) and proves that it is locally best. See also [Con67], [Miy90] for some operations on 120-cell.

(ii) Pasini [Pas98] proved non-existence of *4-dimensional football*, i.e. equifacetted 4-fullerene with (combinatorial) facet $F_{60}(I_h)$. Clearly, any equifacetted spherical 4-fullerene with (combinatorial) facet F_n, has $v = \frac{qn}{4}$ vertices. Perhaps, 120-cell is unique such 4-fullerene.

(iii) All finite 3-fullerenes have (because of $v - e + p = 2(1 - g)$, where

g is the genus of the surface) $12(1-g)$ pentagonal faces; so, either they are usual spherical fullerenes, or $g=1$ and they are partitions of the torus or the Klein bottle by hexagons.

(iv) There exists (non-simple, of course) a tiling of Euclidean 3-space by (116 polyhedra isomorphic to) the Do; the question about tiling of 4-space by 4-polytopes isomorphic to the 120-cell, is open (see [Sch84]). Irregular pentagonal dodecahedra together with B_6 (also with $F_{28}(T_d)$ or B_6 and F_{26}) fill Euclidean 3-space. Those space-fillings were used (in [Wel84] on pp. 74, 136-139, 659-664) for description of clathrate crystal structures of some ice-like or silicate compounds. The hexagonal barrel B_6 tiles alone the hyperbolic 3-space; it is the fundamental polyhedron of a compact hyperbolic manifold, called the Löbell space (Löbell, 1931), which was considered also in Cosmology; see, for example, [Got80].

(v) We can show, using Theorem 6 from [DSt97], that the skeleton of the dual of any 4-fullerene does not embed isometrically (up to a scale) in any cubic lattice; 120-cell also does not embed ([DGr97]).

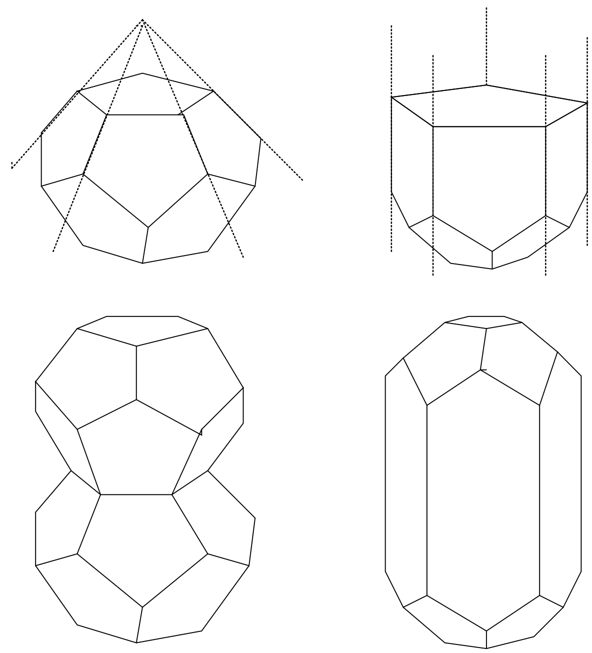
The Table below present three families of 4-fullerenes, constructed in this note.

In the Table the columns 1, 2 give the number of vertices and 2-faces; the number of edges is $2V$, clearly. The next 5 columns give the number of corresponding fullerenes among cells of a 4-fullerene; here F_{20}, F_{24} are Do, B_6 while F_{28}, F_{30} are unique fullerenes with symmetry T_d, D_{5h}, respectively, and such number of vertices. The last column F' gives: the number of 3-cells F, when it is a fullerene in the Construction B, and the number of 3-cells *in* F, when it is a 4-fullerene in the construction C. The symbols v, $p=(p_5,p_6)$, q denote the number of vertices, of 2-faces and (for the Construction C) of cells of F.

Table. f-vectors of some "4-dimensional fullerenes"

	V	P	F_{20}	F_{24}	F_{28}	F_{30}	F'
120−	600	720	120	0	0	0	
A_i	$560i+40$	$666i+54$	$94i+26$	0	0	$12i-12$	
$B(F)$	$30v$	$\frac{71v}{2}+10$	$\frac{7v}{2}+48$	$2v-40$	0	0	2
$C_1(F)$	$20v$	$20v+3p$	$2p_5$	$2p_6$	v	0	q

2 Construction of polytopal 4-fullerenes A_i



It will be a 4-dimensional analogue of the following simple construction of the i-layered dodecahedron F_{20+10i}; see Figure above for such F_{30}. Stellate a face t of Do (i.e. extend face-planes of its 5 neighbors until their intersection; so we got a 5-pyramid on the face). Then do a projective transformation, sending the apex of 5-pyramid to infinity so that the 5-pyramid became right regular 5-prism. The image of our regular dodecahedron will be inscribed in the continuation of above 5-prism. The face t became larger and its opposite became smaller, but the both remain regular 5-gons; all other faces became irregular. Only one of six 5-axes of symmetry of Do will remain. Take the mirror reflection of such modified dodecahedron on the face-plane of t. Two such dodecahedra glued by the "large" regular face, obtained from t, form the convex 3-polytope $F_{30}(D_{5h})$. It has exactly two regular 5-gonal faces: "small" ones from both modified dodecahedra. On each of them we can continue same procedure and get general i-layered dodecahedron F_{20+10i} with symmetry D_{5d} for even $i > 0$ and D_{5h} for odd i. (This tube is the dual of 2-capped pile of i 5-anti-prisms.)

Apply same procedure to the 120-cell in 4-space. Stellate a dodecahedral face t until we get a pyramid on it. By a projective transformation, sending the apex to infinity, it will be transformed into right prism, having Do as a base. 120-cell will be modified: t became larger, its opposite became smaller, but both remain regular; all other dodecahedral cells became irregular. Take the mirror reflection of modified 120-cells on the 3-space, containing t; we get (from two modified 120-cells, glued by the "large" regular dodecahedron) the convex 4-polytope $A_1(120 - cell)$. It have exactly two faces Do, "small" Do's of two modified 120-cell, other dodecahedra are irregular. The continuation of this procedure on each of "small" Do gives the 4-polytope $A_i(120 - cell)$. See its f-vector in the Table above; exactly $30i - 30$ its 2-faces are hexagons.

We can apply the construction A to any *non-exposed* dodecahedral cell of a $A_i(120 - cell)$, i.e. having only dodecahedral neighbors: we obtain 3-spheres, but now there is no guarantee of convexity. When operation A is applied to several non-exposed dodecahedra, no two of them should have same dodecahedral neighbor. In order to enumerate such possibilities, the solution of following extremal problem will be of interest (we give it in dual form for 600-cell): estimate the maximal number of vertices in 600-cell with all pairwise distances (in the skeleton, having the diameter 5) at least 3. It is at most 9, clearly, and at least 6: take 3 suitable vertices on each of two 10-gons (among all 12), which lie in two orthogonal planes.

In Chapter 4 (Sections 1.7 and 1.8) of [SaM97] are constructed (from 600-cell, by inverting the Hopf fibration of the 3-sphere) 4-fullerenes, having each 144 dodecahedral cells and $12k$ cells B_6 for $k = 2, 3, 4, 6$. Also in Chapter 7 (Sections 2.7, 3 and 4.2) of [SaM97] are given crystall agregats, which can be used to construct 4-fullerenes.

3 Construction of spherical 4-fullerenes B(F)

Fix a fullerene F with v vertices, $p = \frac{v}{2} + 2$ faces and $e = \frac{3v}{2}$ edges. From an interior point o of F take on the ray through each vertex b a point b' with distance $d(o, b') = d(o, b) + 1$. Put on each face of F dodecahedra Do on 5-gons and barrels B_6 on 6-gons, so that their lateral sides coincide. (Always in this construction Do and B_6 are combinatorial.) We got *1-corona*: F itself and n polyhedra of *1-st floor*. The surface of 1-corona consists of p *1-anti-faces*, i.e. opposite ones to the faces of F and others, which are organized in n 3-hedral triples of 5-gons with the central vertex b' (for each of v vertices b of F). Put n new Do into those n 3-hedral angles, one Do for each. We got 2-corona with the 2-nd floor, consisting of v dodecahedra. Each of them is adjacent to 1-corona in 3 faces (of its 3-hedral angle) and to 3 neighbors on the 2-nd floor; so 6 remaining faces are free. Each of 12 5-gonal (or $p-12$ hexagonal) 1-anti-faces is incident to 5 (or 6,respectively) dodecahedra of the 2-nd floor. Those 5 (or 6) 5-gons form a half-dodecahedron (or a half-barrel, respectively). Add for each of them the second half in order to obtain p new polyhedra; they form 3-rd floor. We got 3-corona. The surface of 3-corona consists of p 2-anti-faces (i.e. the faces, opposite to 1-anti-faces) and e *quadruples*, i.e. two edge-adjacent 5-gons and two other 5-gons, edge-adjacent to the first two via each vertex of the edge of their adjacency. First two 5-gons are from the surface of 2-corona, two others are from the surface of the 3-corona. Take now two copies of 3-corona. (Remind, that each i-corona is a 3-ball in 3-space.) Now we will join them in 4-space, putting between them e new dodecahedra, which will form 4-th floor for each copy. Also corresponding 2-anti-faces of them will coincide. Each Do of the 4-th floor is incident to each copy of 3-corona by a quadruple and to four neighbors on the 4-th floor.

Clearly, $B(Do)$ is the 120-cell itself and $B(B_6)$ consists only of two (combinatorial) fullerenes Do and B_6.

In fact, the construction B can be similarly applied to any simple 3-polytope with, say, v vertices and any given *p-vector* $(p_3, p_4, ...)$, where p_i is the number of i-gonal faces for any $i \geq 3$. Above construction will give simple 3-sphere with $30v$ vertices, $60v$ edges, $\frac{71v}{2}+10$ 2-faces (including $5p_i$ i-faces for each i, except 5) and $\frac{11v}{2}+10$ cells, including 2 original 3-polytopes, $4p_i$ i-gonal barrels B_i (p_i on both 1-st and both 3-rd floors) and $\frac{7v}{2}$ dodecahedra (v on each of both 2-nd floors and $\frac{3v}{2}$, i.e. the number e of edges, on the common 4-th floor). Note that B_5 is Do and so, $4p_5 + \frac{7v}{2}$ is the number of all dodecahedra.

It looks difficult to determine when the construction B leads to 4-polytopes (i.e. the convex 3-spheres) even when applied to such polyhedra as the regular tetrahedron, the cube or the barrel B_i. B_3 is a cube with two opposite vertices truncated; B_4 is the dual of 2-capped 4-antiprism (one of all 8 polyhedra whose faces are regular triangles). B_3 (in general, B_i) are called in [BoS95] *Dürer octahedron* (in general, *the spindle with two i-gons*); among constructions, given in [BoS95], there are two simple equifacetted 3-manifolds: one with 10 facets B_3 and other with 26 facets B_4 (the first is a non-polytopal 3-sphere).

Construction B can be applied also to any simple partition of Euclidean or hyperbolic plane. In, particular, take, as original F, the following infinite fullerene: half-space bounded by a plane, partitioned by regular hexagons (i.e. (63)= graphite).

4 Construction C of 4-fullerenes $C_j(F)$

We give this construction in the dual terms of general simplicial 3-manifold; it was inspired by [MoS84], [SaM85]. Apply to the simplicial 3-manifold $F*$, which is the dual to given simple 3-manifold F, following four operations:

1) Transform each edge into a 4-path of three edges, by addition of two new edges on each edge, and subdivide each tetrahedron, using new edges, into four tetrahedra and one truncated tetrahedron.

2) By projection of all its faces from an interior point, subdivide each truncated tetrahedron into four tetrahedra and four 6-pyramids.

3) Glue each two 6-pyramids with common base into a 6-bipyramids (cf. two 4-pyramids, glued into the octahedron in transition to f.c.c. lattice A_3).

4) Subdivide each 6-bipyramid into six tetrahedra with common edge, linking its apexes.

Denote obtained simplicial complex by $C_1(F)$; iterating above procedure j times produces $C_j(F)$. If F has v vertices, p 2-faces (including p_5 5-gonal and p_6 6-gonal ones), q cells , then $C_1(F)$ has $20v + p$ 2-faces (including $2v + 3p_6$ hexagons) and only following cells: all cells of F plus $2p_5$ dodecahedra, $2p_6$ hexagonal barrels B_6 and v fullerenes $F_{28}(T_d)$. So, if F is a 4-fullerene (for example, 120-cell or one obtained by above constructions A or B), then any $C_j(F)$ is also 4-fullerene.

If original simplicial manifold $F*$ is spherical, then its j-th simplicial subdivision, described above, is also spherical. But the question of preserving convexity is difficult. Operations 1), 2), 3) could be arranged in order to preserve it. (For example, chosen interior points of the tetrahedra should be moved "out" within 4-th dimension in order to get edges between neighbors, then suitable two points *around* of each edge should be found and so on.) But the operation 3) can destroy convexity. Moreover, four above topological operations can be seen separately, which is not the case of their metrical contreparts.

The dualization of another decoration of 600-cell, given in [MoS84] and [SaM85], produces another infinite family of spherical 4-fullerenes, having now, as cells, only dodecahedra, B_6 and the fullerene $F_{32}(D_{3h})$. Similarly to the construction $C_j(F)$, one can generalize it on a construction (say, $D_j(F)$), which, starting from a 4-fullerene F, gives an infinite family of 4-fullerenes, having, besides of cells of F, only cells B_6 and $F_{32}(D_{3h})$. A mixed construction (choosing suitably operation C or D on each step) gives asymptotically non-periodic 4-fullerenes, having, besides of cells of F, only cells B_6, $F_{28}(T_d)$ and $F_{32}(D_{3h})$.

5 Some 5-fullerenes

The regular tiling 5333 of hyperbolic 4-space by 120-cells is a 5-fullerene: all its 2-faces are 5-gons. All 2-faces of following simple manifolds are 6-gons: the simple regular tiling 63 of Euclidean plane by hexagons and non-compact simple regular tiling 633 of hyperbolic 3-space by tilings 63. Both above infinite 3- and 4-fullerenes are simply connected; following 3-fullerenes - the simple tilings by hexagons of (unlimited in both directions) cylinder, Möbius surface, torus and Klein bottle - are not.

The following is an infinite family of 5-fullerenes, having both 5-gonal and 6-gonal 2-faces. Take two copies of the tilings 5333 and glue them in some pairs of corresponding 120-cells. Delete now from the manifold the interiors of those 120-cells. For each of them, any corresponding pair (from both 5333) of neighboring 120-cells glue in a 4-polytope A_1, described in the Section 1. If the tilings are glued in only one 120-cell, the 4-manifold is the direct product of the 3-sphere and the Euclidean line; so it is simply connected.

We doubt that d-fullerenes with large d exist.

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