Combinatorics of fullerenes and toric topology

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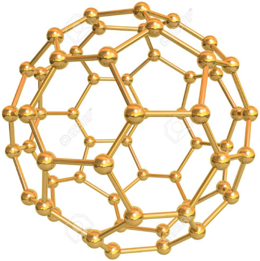
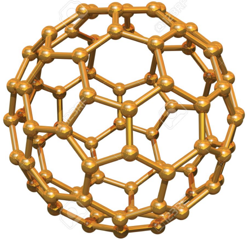
Fullerenes have been the subject of intense research, both for their unique quantum physics and chemistry, and for their technological applications, especially in nanotechnology.



C_{60}

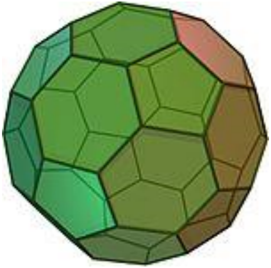


C_{80}

A fullerene is a spherical-shaped molecule of carbon such that any atom belongs to exactly three carbon rings, which are pentagons or hexagons.

Mathematical fullerenes

A convex 3-polytope is simple if any its vertex is contained in exactly 3 facets.



Truncated icosahedron combinatorially equivalent to C_{60}.

A (mathematical) fullerene is a simple convex 3-polytope with all facets pentagons and hexagons.
Each fullerene has exactly 12 pentagons.

The number of isomers

The number p_6 of hexagons can be arbitrary except for 1.

The number of combinatorial types (isomers) of fullerenes as a function of p_6 grows as p_6^9.

p_6	0	1	2	3	4	5	6	7	8	...	190
$F(p_6)$	1	0	1	1	2	3	6	6	15	...	132247999328

http://hog.grinvin.org

Toric topology assigns to each fullerene P a smooth $(p_6 + 15)$-dimensional moment-angle manifold $\mathcal{Z}_P$ with a canonical action of a compact torus T^m, where $m = p_6 + 12$.

The solution of the famous 4-*color problem* provides the existence of an integer matrix S of sizes $(m \times (m - 3))$ defining an $(m - 3)$-dimensional toric subgroup in T^m acting freely on $\mathcal{Z}_P$.

The orbit space of this action is called a quasitoric manifold $M^6(P, S)$.

We have $\mathcal{Z}_P / T^m = M^6 / T^3 = P$.

Pogorelov polytopes

A Pogorelov polytope is a simple convex 3-polytope whose facets do not form 3- and 4-belts of facets.

It can be proved that each fullerene is a Pogorelov polytope.

The class of Pogorelov polytopes coincides with the class of polytopes admitting a bounded right-angled realization in Lobachevsky (hyperbolic) 3-space (A.V. Pogorelov and E.M. Andreev).

Such a realization is unique up to isometry.

Recent results

Two Pogorelov polytopes P and Q are combinatorially equivalent if and only if there is a graded isomorphism of cohomology rings $H^*(\mathcal{Z}_P, \mathbb{Z}) \simeq H^*(\mathcal{Z}_Q, \mathbb{Z})$.

A graded isomorphism $H^*(M^6(P, S_P), \mathbb{Z}) \simeq H^*(M^6(Q, S_Q), \mathbb{Z})$ implies a graded isomorphism $H^*(\mathcal{Z}_P, \mathbb{Z}) \simeq H^*(\mathcal{Z}_Q, \mathbb{Z})$.

Main results

Let P and Q be Pogorelov polytopes.

Theorem

Manifolds $M^6(P, S_P)$ and $M^6(Q, S_Q)$ are diffeomorphic if and only if there is a graded ring isomorphism

$$H^*(M^6(P, S_P), \mathbb{Z}) \simeq H^*(M^6(Q, S_Q), \mathbb{Z}).$$

Corollary

- Two manifolds $M^6(P, S_P)$ and $M^6(Q, S_Q)$ are diffeomorphic if and only if they are homotopy equivalent.
- If the manifolds $M^6(P, S_P)$ and $M^6(Q, S_Q)$ are diffeomorphic, then polytopes P and Q are combinatorially equivalent.

For every Pogorelov 3-polytope P together with a regular 4-colouring of its facets, there is an associated hyperbolic 3-manifold of Löbell type (A.Yu.Vesnin).

It is aspherical as an orbit space of the hyperbolic 3-space $\mathbb{H}^3$ by a free action of a certain finite extension of the commutator subgroup of a hyperbolic right-angled reflection group.

Any hyperbolic 3-manifold of Löbell type can be realized as the fixed point set for the canonical involution on the quasitoric manifold $M(P, S_P)$ over P.

Main results

We prove that two Löbell manifolds are isometric if and only if their $\mathbb{Z}/2$-cohomology rings are isomorphic (V.M. Buchstaber, N.Yu. Erokhovets, M. Masuda, T.E. Panov, S. Park).

Using this result we show that two Löbell manifolds are isometric if and only if the corresponding 4-colourings are equivalent (V.M. Buchstaber and T.E. Panov).

We construct any Pogorelov polytope except for k-barrels from 5- and 6-barrel using operations of $(2, k)$-truncations and connected sum with the dodecahededron (5-barrel).
(V.M. Buchstaber, N.Yu. Erokhovets)

We construct any fullerene except for the dodecahedron and $(5, 0)$-nanotubes from the 6-barrel using 4 operations of $(2, 6)$- and $(2, 7)$-truncations such that intermediate polytopes are Pogorelov polytopes with 5-, 6- and at most one 7-gon.
(V.M. Buchstaber, N.Yu. Erokhovets)

Publications containing main results I

- V. M. Buchstaber, T. E. Panov, *Toric Topology.*, Math. Surveys and Monographs, v. 204, AMS, Providence, RI, 2015; 518 pp.
- V.M. Buchstaber, N.Yu. Erokhovets, *Construction of fullerenes.*, arXiv 1510.02948v1, 2015.
- F. Fan, J. Ma, X. Wang, *B-Rigidity of flag 2-spheres without 4-belt.*, arXiv:1511.03624 v1 [math.AT] 11 Nov 2015.

Publications containing main results II

- V.M. Buchstaber, N.Yu. Erokhovets, M. Masuda, T.E. Panov, S. Park, *Cohomological rigidity of manifolds defined by right-angled* 3*-dimensional polytopes.*, Russ. Math. Surveys, 2017, No. 2, arXiv:1610.07575v2.
- V.M. Buchstaber and T.E. Panov, *On manifolds defined by* 4*-colourings of simple* 3*-polytopes*, Russian Math. Surveys, 71:6 (2016), 1137–1139.
- V.M. Buchstaber, N.Yu. Erokhovets, *Construction of families of three-dimensional polytopes, characteristic patches of fullerenes, and Pogorelov polytopes*, Izvestiya: Mathematics, **81**:5 (2017).

Fullerenes

Fullerenes were discovered by chemists-theorists Robert Curl, Harold Kroto, and Richard Smalley in 1985 (Nobel Prize 1996).

Fuller’s Biosphere
USA Pavilion, Expo-67
Montreal, Canada

They were named after Richard Buckminster Fuller – a noted american architectural modeler.

Are also called buckyballs

Euler's formula (Leonhard Euler, 1707-1783)

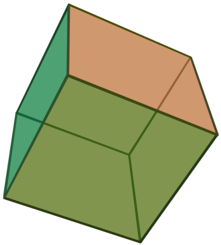
Let f_0, f_1, and f_2 be numbers of vertices, edges, and 2-faces of a 3-polytope. Then

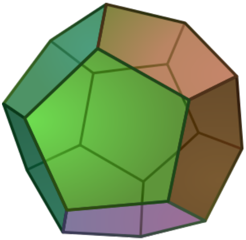
$$f_0 - f_1 + f_2 = 2$$

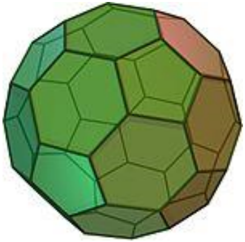
Platonic bodies

	f_0	f_1	f_2
Tetrahedron	4	6	4
Cube	8	12	6
Octahedron	6	12	8
Dodecahedron	20	30	12
Icosahedron	12	30	20

Simple polytopes







3 of 5 Platonic solids are simple.
7 of 13 Archimedean solids are simple.

Consequences of Euler's formula for simple 3-polytopes

Let p_k be a number of k-gonal 2-faces of a 3-polytope.

For any simple 3-polytope P

$$3p_3 + 2p_4 + p_5 = 12 + \sum_{k \geqslant 7} (k-6)p_k$$

Corollary

- *If* $p_k = 0$ *for* $k \neq 5, 6$*, then* $p_5 = 12$*.*
- *There is no simple 3-polytopes with all faces hexagons.*

Consequences of Euler's formula for simple 3-polytopes

Proposition

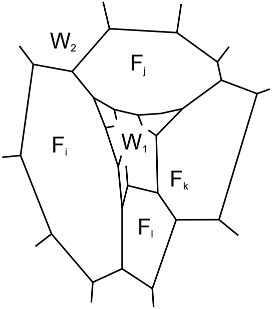
For any simple polytope

$$f_0 = 2\left(\sum_k p_k - 2\right) \quad f_1 = 3\left(\sum_k p_k - 2\right) \quad f_2 = \sum_k p_k$$

Proposition

- for any fullerene
  - $p_5 = 12$;
  - $f_0 = 2(10 + p_6)$, $f_1 = 3(10 + p_6)$, $f_2 = (10 + p_6) + 2$;
- there exist fullerenes with any $p_6 \neq 1$.

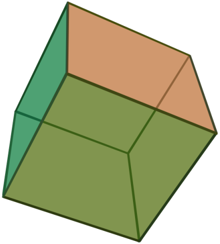
Let P be a simple convex 3-polytope. A *k-belt* *is a cyclic sequence $(F_{j_1}, \ldots, F_{j_k})$ of 2-faces, such that $F_{i_{j_1}} \cap \cdots \cap F_{i_{j_r}} \neq \varnothing$ if and only if $\{i_1, \ldots, i_r\} \in \{\{1,2\}, \ldots, \{k-1, k\}, \{k,1\}\}$.*



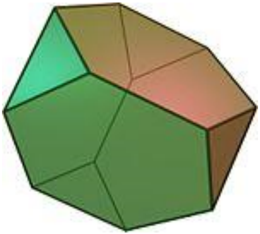
4-belt of a simple 3-polytope.

Flag polytopes

A simple polytope is called flag if any set of pairwise intersecting facets $F_{i_1}, \dots, F_{i_k}$: $F_{i_s} \cap F_{i_t} \neq \varnothing$, $s, t = 1, \dots, k$, has a nonempty intersection $F_{i_1} \cap \dots \cap F_{i_k} \neq \varnothing$.

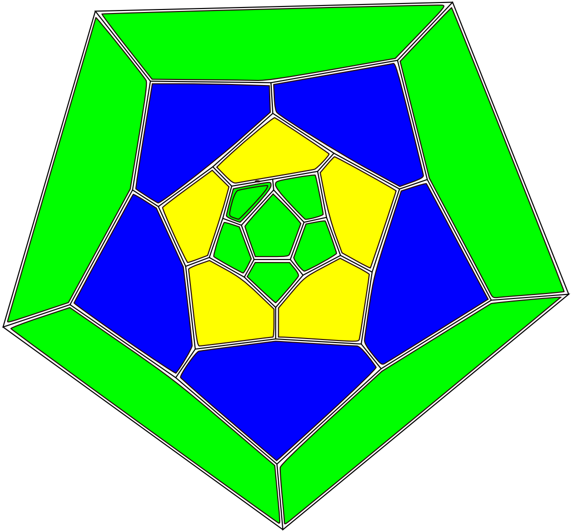


Flag polytope



Non-flag polytope

Fullerene with 2 hexagonal 5-belts



Definition

An *IPR*-fullerene (Isolated Pentagon Rule) is a fullerene without pairs of adjacent pentagons.

Let P be some *IPR*-fullerene. Then $p_6 \geqslant 20$.

An *IPR*-fullerene with $p_6 = 20$ is combinatorially equivalent to Buckminsterfullerene C_{60}.

There are 1812 fullerenes with $p_6 = 20$.

Take a simple polytope

$$P = \{\boldsymbol{x} \in \mathbb{R}^n \colon \boldsymbol{a}_i\boldsymbol{x} + b_i \geqslant 0, i = 1, \ldots, m\}.$$

Using the embedding $\quad j_P \colon P \longrightarrow \mathbb{R}^m_{\geq} \;:\; j_P(x) = (y_1, \ldots, y_m)$ where $y_i = \boldsymbol{a}_i\boldsymbol{x} + b_i$, we will consider P as the subset in $\mathbb{R}^m_{\geqslant}$.

Definition (V.Buchstaber, T.Panov, N.Ray)

A moment-angle manifold $\hat{\mathcal{Z}}_P$ is the product of $\mathbb{C}^m$ and P over $\mathbb{R}^m_{\geqslant}$ described by the pullback diagram:

$$\begin{array}{ccc} \hat{\mathcal{Z}}_P & \xrightarrow{j_{\mathcal{Z}}} & \mathbb{C}^m \\ {\scriptstyle \rho_P}\downarrow & & \downarrow{\scriptstyle \rho} \\ P & \xrightarrow{j_P} & \mathbb{R}^m_{\geqslant} \end{array}$$

where $\rho(z_1, \ldots, z_m) = \left(|z_1|^2, \ldots, |z_m|^2\right)$.

Stanley–Reisner ring of a simple polytope

Let $\{F_1, \ldots, F_m\}$ *be the set of facets of a simple polytope* P*.*
Then a Stanley-Reisner ring of P *over* $\mathbb{Z}$ *is defined as*

$$\mathbb{Z}[P] = \mathbb{Z}[v_1, \ldots, v_m]/J_{SR}(P).$$

Here $J_{SR}(P) = (v_{i_1} \ldots v_{i_k},\ \text{where } F_{i_1} \cap \cdots \cap F_{i_k} = \varnothing)$ *is the Stanley-Reisner ideal.*

- $\mathbb{Z}[\Delta^2] = \mathbb{Z}[v_1, v_2, v_3]/(v_1 v_2 v_3)$

Theorem

The Stanley-Reisner ring of a flag polytope is quadratic:

$$J_{SR}(P) = \{v_i v_j : F_i \cap F_j = \varnothing\}.$$

Stanley-Reisner ring of a simple polytope

Theorem (W. Bruns, J. Gubeladze, 1996)

Two polytopes are combinatorially equivalent if and only if their Stanley-Reisner rings are isomorphic.

Corollary

Fullerenes P_1 and P_2 are combinatorially equivalent if and only if there is an isomorphism $SR(P_1) \cong SR(P_2)$

Let

$$R^*(P) = \Lambda[u_1, \dots, u_m] \otimes \mathbb{Z}[P]/(u_i v_i, v_i^2)$$

Theorem (V.Buchstaber, T.Panov, 1998)

There is a multigraded ring isomorphism

$$H^*(\mathcal{Z}_P; \mathbb{Z}) = H[R^*(P), d]$$

where
$du_i = v_i,\ dv_i = 0,\ \mathrm{mdeg}\, u_i = (-1, 2\{i\}),\ \mathrm{mdeg}\, v_i = (0, 2\{i\})$.

B-rigidity

Definition (V.M. Buchstaber, 2006)

A simple polytope P is said to be B-rigid if the following condition holds:
Let P' be another simple polytope such that there is a graded ring isomorphism

$$H^*(\mathcal{Z}_P;\mathbb{Z}) \cong H^*(\mathcal{Z}_{P'};\mathbb{Z}).$$

Then P' is combinatorial equivalent to P.

Theorem (T.Doslić, 2003)

Any fullerene is flag and has no 4-belts.

Theorem (F.Fan, J.Ma, X.Wang, 2015)

Any flag simple polytope without 4-belts is B-rigid.

Corollary

Every fullerene is B-rigid.

Definition

The combinatorial quasitoric data (P, Λ) consists of

- an oriented combinatorial simple polytope P;
- an integer $(n \times m)$-matrix Λ defining a characteristic map

$$\ell \colon \{F_1, \dots, F_m\} \to \mathbb{Z}^n,$$

such that for any vertex $v = F_{i_1} \cap \cdots \cap F_{i_n}$ the columns

$$\lambda_{i_1} = \ell(F_{i_1}), \dots, \lambda_{i_n} = \ell(F_{i_n})$$

of Λ form a basis for $\mathbb{Z}^n$.

Quasitoric manifold $M(P, \Lambda)$

Given a characteristic map $\ell\colon \{F_1, \dots, F_m\} \to \mathbb{Z}^n$ without loss of generality we can assume that $F_1 \cap \cdots \cap F_n \neq \varnothing$, $\Lambda = (I_n, \Lambda_*)$.

Then the matrix $S = (-\Lambda, I_{m-n})$ gives the $(m-n)$-dimensional subgroup

$$K(\Lambda) = \{(e^{2\pi i\psi_1}, \dots, e^{2\pi i\psi_m}) \in \mathbb{T}^m\},\ i = \sqrt{-1},$$

where

$$\psi_k = -\sum_{j=n+1}^{m} \lambda_{k,j}\varphi_j,\ k = 1, \dots, n,\ \psi_{n+k} = \varphi_k,\ k = 1, \dots, m-n.$$

$K(\Lambda)$ acts freely on $(m+n)$-dimensional manifold $\mathcal{Z}_P$.

Definition

The quasitoric manifold $M = M(P, \Lambda)$ is the quotient $\mathcal{Z}_P/K(\Lambda)$. It is a $2n$-dimensional smooth manifold with an action of the n-dim torus $\mathbb{T}^m/K(\Lambda)$.

Four color problem

Classical formulation: Given any partition of a plane into contiguous regions, producing a figure called a map, two regions are called adjacent if they share a common boundary that is not a corner, where corners are the points shared by three or more regions.

Problem

No more than four colors are required to color the regions of the map so that no two adjacent regions have the same color.

History of the four color problem

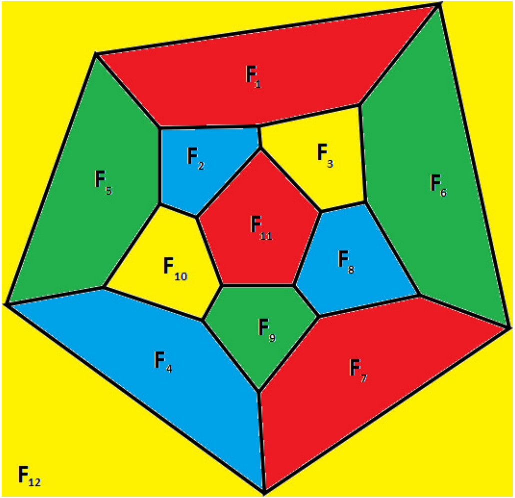
The problem was first proposed on October 23, 1852, when Francis Guthrie, while trying to color the map of counties of England, noticed that only four different colors were needed.

The four color problem became well-known in 1878 as a hard problem when Arthur Cayley suggested it for discussion during the meeting of the London mathematical society.

The four color problem was solved in 1976 by Kenneth Appel and Wolfgang Haken.

The four color problem became the first major problem solved using a computer.

Coloring of the dodecahedron



Characteristic function for simple 3-polytopes.

Let P be a simple 3-polytope. Then ∂P is homeomorphic to a sphere S^2 partitioned into polygons $F_1, \dots, F_m$.

By the four color theorem there is a coloring $\varphi\colon \{F_1, \dots, F_m\} \to \{1, 2, 3, 4\}$ such that adjacent facets have different colors.

Let e_1, e_2, e_3 be the standard basis for $\mathbb{Z}^3$, and $e_4 = \sum_{k=1}^{3} e_k$.

Proposition

The mapping $\ell\colon \{F_1, \dots, F_m\} \to \mathbb{Z}^3 : \ell(F_i) = e_{\varphi(F_i)}$ is a characteristic function.

Corollary

Any simple 3-polytope P has combinatorial data (P, Λ) and the quasitoric manifold $M(P, \Lambda)$;

Theorem [Davis-Janiszkiewicz]

We have $H^*(M(P,\Lambda)) = \mathbb{Z}[v_1,\dots,v_m]/(J_{SR}(P) + I_{P,\Lambda})$, where $J_{SR}(P)$ is the Stanley-Reisner ideal generated by monomials $\{v_{i_1}\dots v_{i_k} : F_{i_1}\cap\dots\cap F_{i_k} = \varnothing\}$, and $I_{P,\Lambda}$ is the ideal generated by the linear forms $\lambda_{i,1}v_1+\dots+\lambda_{i,m}v_m$ arising from the equality

$$\ell(F_1)v_1+\dots+\ell(F_m)v_m = 0.$$

Corollary

- If $\Lambda = (I_n, \Lambda_*)$, then
$$H^2(M^{2n}) = \mathbb{Z}^{m-n}$$
with the generators $v_{n+1},\dots,v_m$.
- The abelian group $H^*(M(P,\Lambda))$ has no torsion.

C-rigidity

Definition (M.Masuda, D.Y.Suh, 2008)

Let P be a simple convex polytope admitting at least one characteristic function. Then P is said to be cohomologically rigid (or C-rigid) if for any quasitoric manifold $M(P, \Lambda)$, and any other quasitoric manifold $M' = M(P', \Lambda')$ over a simple convex polytope P' a graded ring isomorphism

$$H^*(M) \cong H^*(M').$$

implies a combinatorial equivalence of P' and P.

Theorem (S.Choi, T.Panov, D.Y.Suh)

Let P be a simple polytope and there exists
a quasitoric manifold $M = M(P, \Lambda)$.
Then if P is B-rigid, then P is C-rigid.

Corollary

Every Pogorelov polytope P is C-rigid.

Let P be a Pogorelov polytope, M be some quasitoric manifold over P, and $v_1, \dots, v_m$ be the chosen canonical elements generating $H^2(M)$.
Let P' be some other 3-polytope, M' some quasitoric manifold over P', and $v'_1, \dots, v'_{m'}$ the corresponding elements.

C-rigidity

If there is a graded ring isomorphism

$$\varphi\colon H^*(M) \xrightarrow{\cong} H^*(M'),$$

then $m = m'$ and P is combinatorially equivalent to P'.

Theorem

We have $\varphi(v_i) = \pm v'_{\sigma(i)}$ for some permutation $\sigma\colon [m] \to [m]$.

Theorem

The permutation $\sigma\colon [m] \to [m]$ above has the following remarkable properties

- It defines a combinatorial equivalence $P \to P'$.
- For characterictic functions we have: $\Lambda' = A \cdot \Lambda \cdot B$, where $A \in Gl_n(\mathbb{Z})$, and B is the matrix of the mapping $e_i \to \pm e_{\sigma(i)}$ for the standard basis $e_1, \ldots, e_m$ of $\mathbb{Z}^m$, and the signs are the same as $\varphi(v_i) = \pm v'_{\sigma(i)}$.

Let P be a Pogorelov polytope (for example, a fullerene) and M be a quasitoric manifold over it.

Let P' be some other simple 3-polytope and M' be a quasitoric manifold over it.

Corollary

There is

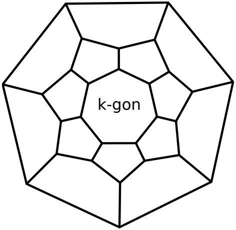
- *an automorphism* $\psi\colon T^3 \to T^3$*;*
- *a diffeomorphism* $f\colon M \to M'$*;*

such that $f(tx) = \psi(t)f(x)$ *for any* $t \in T^3$, $x \in M$

if and only if

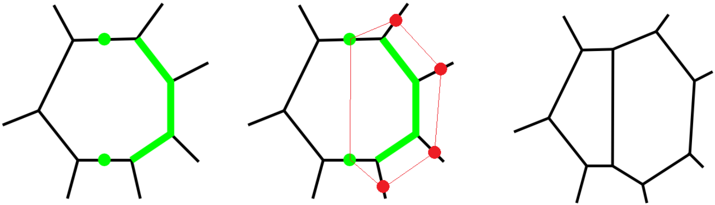
there is a graded ring isomorphism

$$H^*(M) \simeq H^*(M').$$



- The *k*-barrel ia a Pogorelov polytope for $k \geqslant 5$;
- the 5-barrel is the dodecahedron;
- the 6-barrel is a fullerene.

(s, k)-truncation

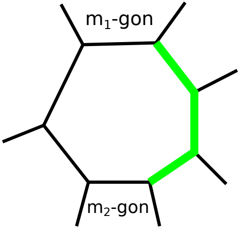


Let F be a k-gonal face of a simple 3-polytope P.

- choose s subsequent edges of F;
- rotate the supporting hyperplane of F around the axis passing through the midpoints of adjacent two edges (one on each side);
- take the corresponding hyperplane truncation.

We call it (s, k)-truncation. This is a combinatorial operation.

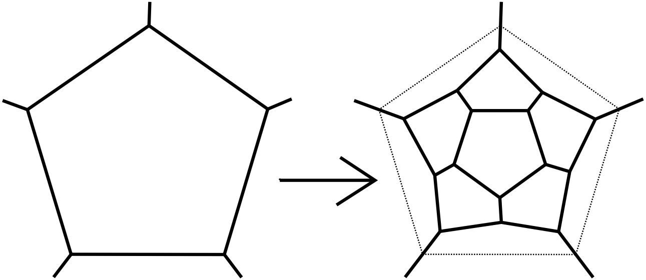
$(s, k; m_1, m_2)$-truncations



If the facet F is adjacent to an m_1 and m_2-gons by edges next to cutted one, then we also call the corresponding operation an $(s, k; m_1, m_2)$-truncation.

Connected sum along k-gonal facets

A connected sum of two simple 3-polytopes P and Q along k-gonal facets F and G is a combinatorial analog of glueing of two polytopes along congruent facets perpendicular to adjacent facets.



Connected sum with the dodecahedron along 5-gons.

Construction of Pogorelov polytopes

- Let P be a Pogorelov polytope. Then any (s, k)-truncation, $2 \leqslant s \leqslant k-4$, gives a Pogorelov polytope.
- Let P and Q be two Pogorelov polytopes. Then their connected sum along k-gonal facets is a Pogorelov polytope.

Theorem (T. Inoue, 2008)

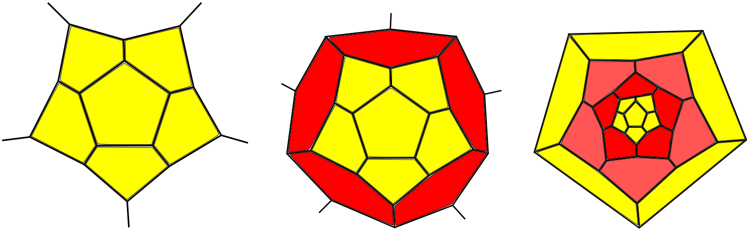
Any Pogorelov polytope can be obtained from q-barrels, $q \geqslant 5$, by a sequence of (s, k)-truncations, $2 \leqslant s \leqslant k-4$, and connected sums along p-gons, $p \geqslant 5$.

Construction of Pogorelov polytopes

Theorem (V.M. Buchstaber, N.Yu. Erokhovets, 2017)

Any Pogorelov polytope except for q-barrels can be obtained from the 5- or the 6-barrel by $(2, k)$-truncations, $k \geqslant 6$, and connected sums with dedecahedra along 5-gons.

Family $\mathcal{F}_1$, $(5,0)$-nanotubes for $k \geqslant 1$



a) b) c)

1. Start with the patch a);
2. add a hexagonal 5-belt;
3. the new patch has the same boundary;
4. make $k \geqslant 0$ steps;
5. finish with the patch a) to obtain a fullerene D_{5k}.

D_0 is the dodecahedron. A fullerene $D_{5(k+1)}$ is the connected sum of D_{5k} with D_0 along 5-gons surrounded by 5-gons.

Construction of fullerenes

Theorem (V.M. Buchstaber, N.Yu. Erokhovets, 2017)

Any fullerene not in $\mathcal{F}_1$ *can be obtained from the* 6*-barrel by a sequence of operations of* $(2,6;5,5)$-, $(2,6;5,6)$-, $(2,7;5,6)$-, $(2,7;5,5)$*-truncation such that all intermediate polytopes are either fullerenes or Pogorelov polytopes with facets* 5-, 6- *and one* 7*-gon with the* 7*-gon adjacent to some* 5*-gon.*

Thank You for the Attention!