Toric Topology and Combinatorics of Fullerenes

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Abstract

- One of the main objects of the toric topology is the moment-angle functor $K \to \mathcal{Z}_K$.
- It assigns to each simplicial complex K with m vertices a space $\mathcal{Z}_K$ with an action of a compact torus T^m, whose orbit space $\mathcal{Z}_K/T^m$ can be identified with the cone CK over K.
- In the case when $K = \partial P^*$, where P is an n-dimensional convex simple polytope with m facets, the moment-angle complex $\mathcal{Z}_K$ has the structure of a smooth manifold $\mathcal{Z}_P$ with a smooth action of T^m, and the orbit space $\mathcal{Z}_P/T^m$ can be identified with P itself.

Abstract

- A mathematical fullerene is a three dimensional convex simple polytope with all 2-faces being pentagons and hexagons.
- In this case the number p_5 of pentagons is 12.
- The number p_6 of hexagons can be arbitrary except for 1.
- Two combinatorially nonequivalent fullerenes with the same number of p_6 are called isomers. The number of isomers of fullerenes grows fast as a function of p_6 .
- At that moment the problem of classification of fullerenes is well-known and is vital due to the applications in chemistry, physics, biology and nanotechnology.

Abstract

- Thanks to the toric topology, we can assign to each fullerene P its moment-angle manifold $\mathcal{Z}_P$.
- The cohomology ring $H^*(\mathcal{Z}_P)$ is a combinatorial invariant of the fullerene P.
- We shall focus upon results on the rings $H^*(\mathcal{Z}_P)$ and their applications based on geometric interpretation of cohomology classes and their products.
- The multigrading in the ring $H^*(\mathcal{Z}_P)$, coming from the construction of $\mathcal{Z}_P$, and the multigraded Poincare duality play an important role here.
- The talks is based on joint works with Taras Panov and Nikolay Erokhovets.

A convex polytope P is a bounded set of the form

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

Let this representation be irredundant, that is a deletion of any inequality changes the set. Then each hyperplane $\mathcal{H}_i = \{\boldsymbol{x} \in \mathbb{R}^n \colon \boldsymbol{a}_i \boldsymbol{x} + b_i = 0\}$ defines a facet $F_i = P \cap \mathcal{H}_i$.

Euler's formula

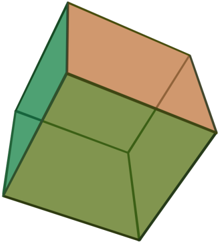
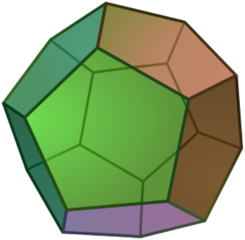
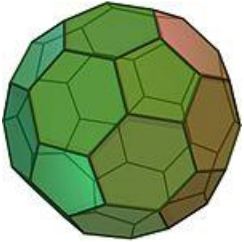
Let f_0, f_1, and f_2 be numbers of vertices, edges, and 2-faces of a 3-polytope. Then

$$f_0 - f_1 + f_2 = 2$$

	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

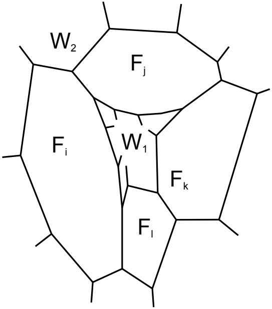
An n-polytope is simple if any its vertex is contained in exactly n facets.

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

k-belts

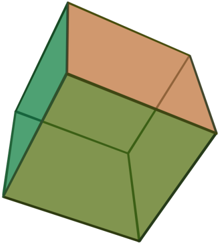
Let P be a simple convex 3-polytope. A *k-belt* *is a cyclic sequence $(F_1, \dots, F_k)$ of 2-faces, such that $F_{i_1} \cap \dots \cap F_{i_r} \neq \varnothing$ if and only if $\{i_1, \dots, i_r\} \in \{\{1,2\}, \dots, \{k-1, k\}, \{k,1\}\}$.*



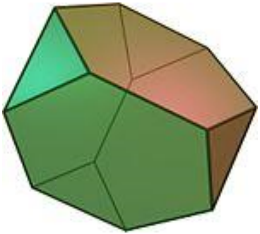
4-belt of a simple 3-polytope.

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* $F_{i_1} \cap \dots \cap F_{i_k} \neq \varnothing$.



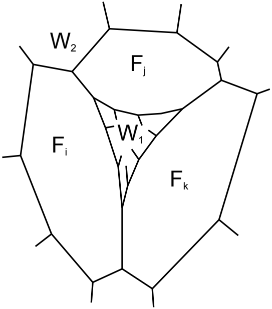
Flag polytope



Non-flag polytope

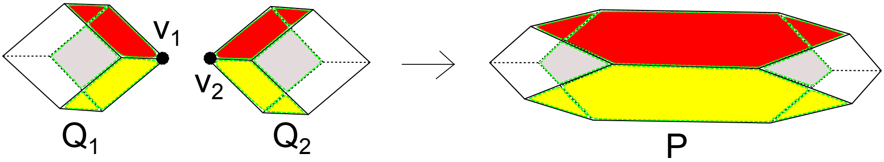
Non-flag 3-polytopes

Simple 3-polytope P is not flag if and only if either $P = \Delta^3$, or P contains a 3-belt.



If we remove the 3-belt from the surface of a polytope, we obtain two parts W_1 and W_2, homeomorphic to disks.

The existence of a 3-belt is equivalent to the fact that P is combinatorially equivalent to a connected sum $P = Q_1 \#_{v_1,v_2} Q_2$ of two simple 3-polytopes Q_1 and Q_2 along vertices v_1 and v_2.



The part W_i appears if we remove from the surface of the polytope Q_i the facets containing the vertex v_i, $i = 1, 2$.

Consequence 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.*

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

Realization theorems

Theorem (Eberhard, 1891)

For every sequence $(p_k | 3 \leqslant k \neq 6)$ *of nonnegative integers satisfying*

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

there exist values of p_6 *such that there is a simple* 3*-polytope* P^3 *with* $p_k = p_k(P^3)$ *for all* $k \geqslant 3$*.*

For a fixed sequence $(p_k | 3 \leqslant k \neq 6)$

- *There are infinitely many valued of* p_6*.*
- *There exist* $p_6 \leqslant 3 \left(\sum_{k \neq 6} p_k \right)$ *(J.C. Fisher, 1974)*
- *If* $p_3 = p_4 = 0$ *then any* $p_6 \geqslant 8$ *is suitable (B. Grunbaum, 1968).*

Fullerenes

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

Fullerene C_{60}
$(f_0, f_1, f_2) = (60, 90, 32)$
$(p_5, p_6) = (12, 20)$

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

Fullerenes

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

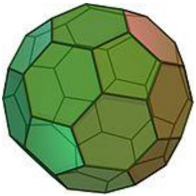
Fuller's Biosphere
USA Pavillion, Expo-67
Montreal, Canada

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

Are also called buckyballs

A *(mathematical) fullerene* *is a simple* 3*-polytope with all* 2*-facets pentagons and hexagons.*

Fullerene C_{60}



Truncated icosahedron

For any fullerene $p_5 = 12$*,*

$$f_0 = 2(10 + p_6), \quad f_1 = 3(10 + p_6), \quad f_2 = (10 + p_6) + 2$$

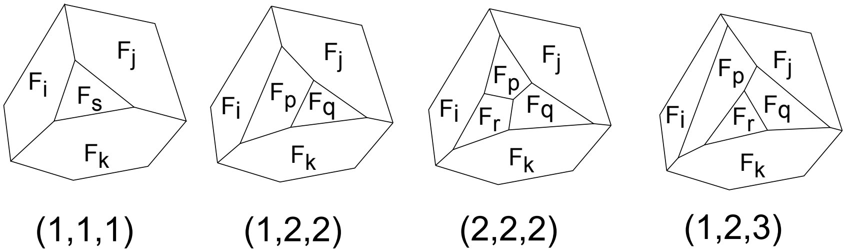
There exist fullerenes with any $p_6 \neq 1$*.*

Fullerenes as flag polytopes

Theorem (E,15)

Any fullerene has no 3-belts, that is it is a flag polytope.

The proof is based on the following result about fullerenes.
Let the 3-belt (F_i, F_j, F_k) divide the surface of a fullerene P into two parts W_1 and W_2, and W_1 does not contain 3-belts. Then P contains one of the following fragments



This is impossible since each fragment has a triangle or a quadrangle.

4-belts and 5-belts of fullerenes

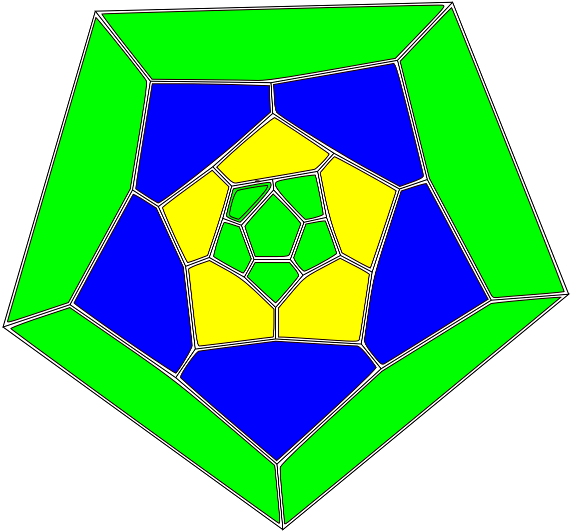
Theorem

Any fullerene has no 4-belts.

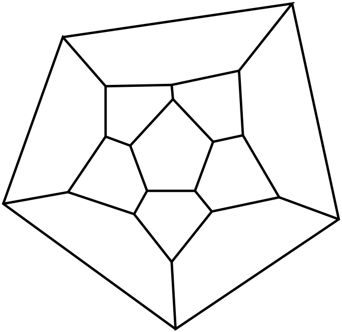
Theorem

Any fullerene P has $12 + k$ belts, where 12 belts surround 12 pentagonal faces and $k \geqslant 0$. If $k > 0$, then P consists of two "dodecahedral caps" and k hexagonal 5-belts between them, where any hexagon in a belt is incident with neighboring hexagons by opposite edges.

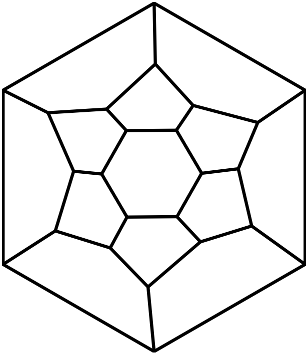
Fullerene with 2 hexagonal 5-belts



Schlegel diagrams of fullerenes

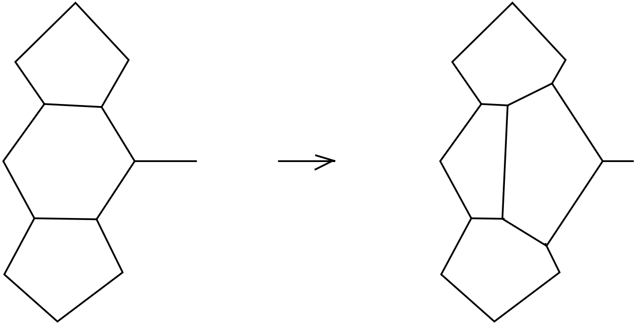


Dodecahedron
$p_6 = 0$



Barrel
$p_6 = 2$

Endo-Kroto operations



- The Endo-Kroto operation increases p_6 by 1.
- Starting from Barrel and applying a sequence of Endo-Kroto operations it is possible to obtain a fullerene with arbitrary $p_6 = k$, $k \geqslant 2$.

Number of combinatorial types of fullerenes

Two combinatorially nonequivalent fullerenes with the same number p_6 are called isomers.

Let $F(p_6)$ be the number of isomers with given p_6.
It is known that $F(p_6) = O(p_6^9)$.

There is an effective algorithm of combinatorial enumeration of fullerenes using supercomputer (Brinkman, Dress, 1997).

p_6	0	1	2	3	4	5	6	7	8	...	75
$F(p_6)$	1	0	1	1	2	3	6	6	15	...	46.088.148

IPR-fullerenes

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}.

The number $F_{IPR}(p_6)$ of isomers of *IPR*-fullerenes also grows fast as a function of p_6.

p_6	20	21	22	23	24	25	26	27	28	...	97
F_{IPR}	1	0	0	0	0	1	1	1	2	...	36.173.081

Canonical correspondence

Simple polytope P		moment-angle manifold $\mathcal{Z}_P$
$\dim P = n$	$\longrightarrow$	$\dim \mathcal{Z}_P = m + n$
number of facets $= m$		canonical T^m-action
$P_1 \times P_2$	$\longrightarrow$	$\mathcal{Z}_{P_1} \times \mathcal{Z}_{P_2}$

- The canonical correspondence gives a tool to build manifolds important for algebraic topology and complex geometry in terms of the combinatorics of polytopes.

- Algebraic-topological invariants of moment-angle manifolds $\mathcal{Z}_P$ give combinatorial invariants of polytopes P.

Let $L(P)$ be the face lattice of P and $\{F_1, \ldots, F_m\}$ – the set of facets.

$$\mathcal{Z}_P = \bigcup_{F \in L(P) \setminus \{\varnothing\}} \prod_{i\colon F_i \supset F} D_i^2 \times \prod_{j\colon F_j \not\supset F} S_j^1 \subset D_1^2 \times \cdots \times D_m^2.$$

is the moment-angle complex of a simple polytope P.

- $\mathcal{Z}_P$ has a structure of an $(m+n)$-dimensional smooth manifold and is also called a moment-angle manifold.
- $P = \Delta^n \Longleftrightarrow \mathcal{Z}_P = S^{2n+1}$.

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 over $\mathbb{Z}$ is defined as

$$\mathbb{Z}[P] = \mathbb{Z}[v_1, \ldots, v_m]/(v_{i_1} \ldots v_{i_k} = 0, \text{ if } F_{i_1} \cap \dots \cap F_{i_k} = \varnothing).$$

- The Stanley-Reisner ring of a flag polytope is quadratic: the relations have only the form $v_i v_j = 0$: $F_i \cap F_j = \varnothing$.
- Two polytopes are combinatorially equivalent if and only if their Stanley-Reisner rings are isomorphic.

Multigraded complex

Let

$$R^*(P) = \Lambda[u_1, \ldots, u_m] \otimes \mathbb{Z}[P]/(u_i v_i, v_i^2),$$
$$\mathrm{mdeg}\, u_i = (-1, 2\{i\}), \mathrm{mdeg}\, v_i = (0, 2\{i\}), du_i = v_i, dv_i = 0$$

be a multigraded differential algebra.

Theorem (Buchstaber-Panov)

We have an isomorphism

$$H[R^*(P), d] \simeq Tor^{*,*}_{\mathbb{Z}[v_1,\ldots,v_m]}(\mathbb{Z}[P], \mathbb{Z}) \simeq H^*(\mathcal{Z}_P, \mathbb{Z})$$

Moreover, this isomorphism defines the structure of a multigraded algebras in *Tor* and $H^*(\mathcal{Z}_P, \mathbb{Z})$.

Cohomology of moment-angle manifold

Let $P_\omega = \bigcup_{i\in\omega} F_i$ for a subset $\omega \subset [m]$.

Theorem (Buchstaber–Panov)

There are the isomorphisms:

$$H^l(\mathcal{Z}_P, \mathbb{Z}) \to \bigoplus_{\omega\subset[m]} \widetilde{H}^{l-|\omega|-1}(P_\omega, \mathbb{Z}).$$

Set

$$\beta^{-i,2\omega} = \operatorname{rank} \widetilde{H}^{|\omega|-i-1}(P_\omega, \mathbb{Z})$$

where $H^{-1}(\varnothing, \mathbb{Z}) = \mathbb{Z}$.

A multigraded Poincare duality implies

$$\beta^{-i,2\omega} = \beta^{-(m-n-i),2([m]\setminus\omega)}.$$

Cohomology ring

Theorem (Buchstaber–Panov)

There is the ring isomorphism

$$H^*(\mathcal{Z}_P) \simeq \bigoplus_{\omega\subset[m]} \widetilde{H}^*(P_\omega)$$

where the ring structure on the right hand side is given by the canonical maps

$$\widetilde{H}^{k-|\omega_1|-1}(P_{\omega_1}) \otimes \widetilde{H}^{l-|\omega_2|-1}(P_{\omega_2}) \to \widetilde{H}^{k+l-|\omega_1|-|\omega_2|-1}(P_{\omega_1\cup\omega_2})$$

for $\omega_1 \cap \omega_2 = \varnothing$ *and zero otherwise.*
The canonical maps are given by the isomorphisms:

$$H^{k-|\omega|-1}(P_\omega) \simeq H^{k-|\omega|}(P, P_\omega).$$

Examples

Let P be a simple-polytope

$$H^1(\mathcal{Z}_P) = H^2(\mathcal{Z}_P) = 0,$$

$$H^3(\mathcal{Z}_P) \simeq \bigoplus_{|\omega|=2} \widetilde{H}^0(P_\omega),$$

$$H^4(\mathcal{Z}_P) \simeq \bigoplus_{|\omega|=3} \widetilde{H}^0(P_\omega),$$

$$H^5(\mathcal{Z}_P) \simeq \bigoplus_{|\omega|=3} \widetilde{H}^1(P_\omega) + \bigoplus_{|\omega|=4} \widetilde{H}^0(P_\omega).$$

$$H^6(\mathcal{Z}_P) \simeq \bigoplus_{|\omega|=4} \widetilde{H}^1(P_\omega) + \bigoplus_{|\omega|=5} \widetilde{H}^0(P_\omega).$$

For a 3-polytope $P \neq \Delta^3$ nonzero Betti numbers are

$$\beta^{0,2\varnothing} = \beta^{-(m-3),2[m]} = 1,$$

$$\beta^{-i,2\omega} = \mathrm{rank}\,\widetilde{H}^0(P_\omega,\mathbb{Z}) = \beta^{-(m-3-i),2([m]\setminus\omega)} = \mathrm{rank}\,\widetilde{H}^1(P_{[m]\setminus\omega},\mathbb{Z}),$$
$$|\omega| = i+1,\, i = 1,\dots,m-4$$

For $|\omega| = i+1$ the number $\beta^{-i,2\omega}+1$ is equal to the number of connected components of the set $P_\omega \subset P$.

Define $\beta^{-i,2j} = \sum\limits_{|\omega|=j} \beta^{-i,2\omega}$.

$\beta^{-1,4} = \frac{m(m-1)}{2} - f_1 = \frac{(m-3)(m-4)}{2}$;

3-belts and 4-belts and Betti numbers

Theorem

$\beta^{-1,6}$ is equal to the number of 3-belts.

There is a bijection $(F_i, F_j, F_k) \longleftrightarrow [u_i v_j v_k]$ between 3-belts and elements of an additive basis in $H^{-1,6}$.

Theorem

Let P be a simple 3-polytope without 3-belts, that is $\beta^{-1,6} = 0$. Then $\beta^{-2,8}$ is equal to the number of 4-belts.

There is a bijection $(F_i, F_j, F_k, F_l) \longleftrightarrow [u_i u_j v_k v_l]$ between 4-belts and elements of an additive basis in $H^{-2,8}$.

5-belts and Betti numbers

Theorem

Let P be a simple 3-polytope without 3-belts and 4-belts, that is $\beta^{-1,6} = \beta^{-2,8} = 0$. Then $\beta^{-3,10}$ is the number of 5-belts.

There is a bijection $(F_i, F_j, F_k, F_l, F_r) \longleftrightarrow [u_i u_j u_k v_l v_r]$ between 5-belts and elements of an additive basis in $H^{-3,10}$.

Relations between Betti numbers

Theorem

For any simple polytope P with m facets

$$(1-t^2)^{m-n}(h_0+h_1t^2+\cdots+h_nt^{2n})=\sum_{-i,2j}(-1)^i\beta^{-i,2j}t^{2j},$$

where $h_0+h_1t+\cdots+h_nt^n=(t-1)^n+f_{n-1}(t-1)^{n-1}+\cdots+f_0$.

Corollary

Set $h=m-3$. For a simple 3-polytope $P\neq\Delta^3$ with m facets

$$(1-t^2)^h(1+ht^2+ht^4+t^6)=$$

$$1-\beta^{-1,4}t^4+\sum_{j=3}^{h}(-1)^{j-1}(\beta^{-(j-1),2j}-\beta^{-(j-2),2j})t^{2j}+$$

$$(-1)^{h-1}\beta^{-(h-1),2(h+1)}t^{2(h+1)}+(-1)^ht^{2(h+3)}$$

For any simple 3-polytope P we have

- $\beta^{-1,4}$ – the number of pairs (F_i, F_j), $F_i \cap F_j = \varnothing$;
- $\beta^{-1,6}$ – the number of 3-belts;
- $\beta^{-2,6} = \sum\limits_{i<j<k} s_{i,j,k}$, where $s_{i,j,k} + 1$ is equal to the number of connected components of the set $F_i \cup F_j \cup F_k$;
- $\beta^{-3,8} = \sum\limits_{i<j<k<r} s_{i,j,k,r}$, where $s_{i,j,k,r} + 1$ is equal to the number of connected components of $F_i \cup F_j \cup F_k \cup F_r$.

Theorem

For any simple 3-polytope P

- $\beta^{-1,4} = \frac{h(h-1)}{2}$;
- $\beta^{-2,6} - \beta^{-1,6} = \frac{(h^2-1)(h-3)}{3}$;
- $\beta^{-3,8} - \beta^{-2,8} = \frac{(h+1)h(h-2)(h-5)}{8}$.

Theorem

For a fullerene P

- $\beta^{-1,6} = 0$ – *the number of* 3*-belts.*
- $\beta^{-2,8} = 0$ – *the number of* 4*-belts.*
- $\beta^{-3,10} = 12 + k$, $k \geqslant 0$ – *the number of* 5*-belts.*
  If $k > 0$*, then* $p_6 = 5k$*.*

Corollary

The product map $H^3(\mathcal{Z}_P) \otimes H^3(\mathcal{Z}_P) \to H^6(\mathcal{Z}_P)$ *is trivial.*

Theorem

For any fullerene

- $\beta^{-1,4} = \frac{(8+p_6)(9+p_6)}{2}$;
- $\beta^{-2,6} = \frac{(6+p_6)(8+p_6)(10+p_6)}{3}$;
- $\beta^{-3,8} = \frac{(4+p_6)(7+p_6)(9+p_6)(10+p_6)}{8}$.

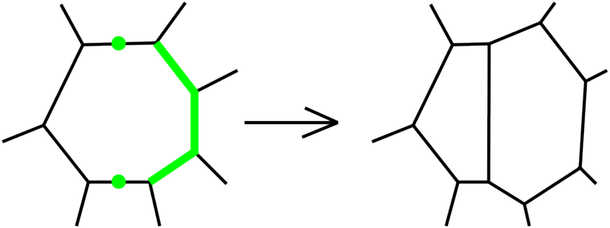
Constructions of fullerenes.

(s, k)-truncations

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

- *choose s subsequent edges of F_i;*
- *rotate the supporting hyperplane of F_i 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.

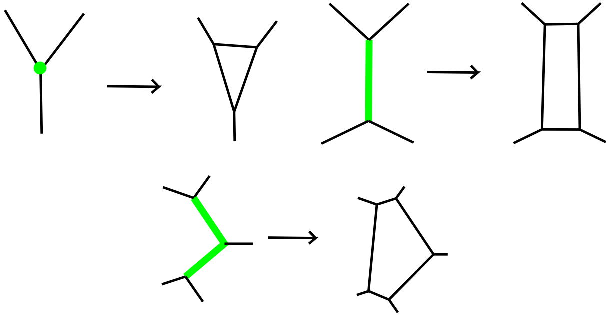


$(3, 7)$-truncation

Construction of simple 3-polytopes

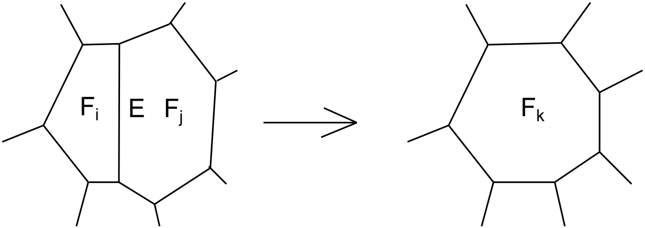
Theorem (Eberhard, Brückner, XIX)

Any simple 3-polytope is combinatorially equivalent to a polytope that is obtained from the tetrahedron by a sequence of vertex, edge and $(2, k)$-truncations.



Straightening along the edge

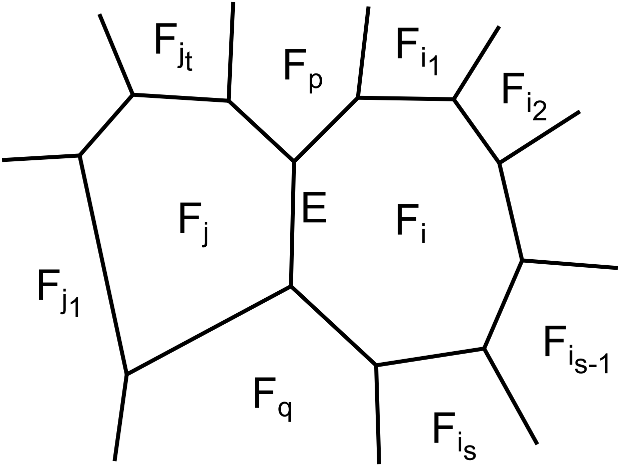
Let $E = F_i \cap F_j$ be an edge such that p-gon F_i and q-gon F_j do not belong together to any 3-belt. Then there is a combinatorial operation of straightening along E.



The result is a combinatorial polytope with a $(p+q-4)$-gonal face F_k obtained from F_i and F_j.

The straightening is an inverse operation to $(p-3, p+q-4)$- or $(q-3, p+q-4)$-truncations along edges of F_k.

Possibility of strengthening



It is possible to apply the straightening along the edge $E = F_i \cap F_j$ *if and only if* $\{F_{i_1}, \ldots, F_{i_s}\} \cap \{F_{j_1}, \ldots, F_{j_t}\} = \varnothing$.

Construction of flag 3-polytopes

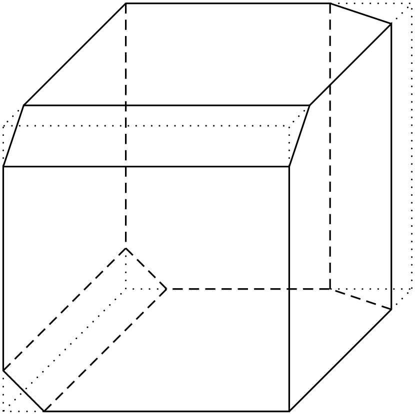
Proposition (V. Volodin, 2011)

A simple 3-polytope P is flag if and only if it admits the straightening along any edge E of P.

Theorem (E, 15)

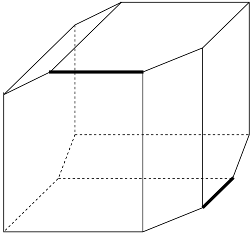
A simple 3-polytope is flag if and only if it is combinatorially equivalent to a polytope obtained from the cube by a sequence of edge truncations and $(2, k)$-truncations, $k \geqslant 6$.

Realization of the Stasheff polytope

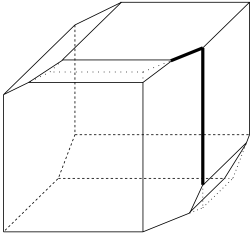


A realization of the Stasheff polytope using edge-truncations
(V. Buchstaber, 2007)

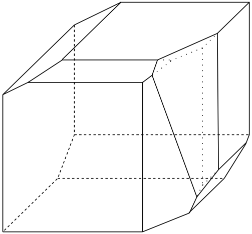
Realization of the dodecahedron



$(p_4, p_5, p_6) = (3, 6, 0)$



$(p_4, p_5, p_6) = (2, 8, 1)$



$(p_4, p_5, p_6) = (0, 12, 0)$

- first apply 3 edge-truncations to the cube to obtain the associahedron;
- then apply 2 edge-truncations of bold edges;
- at last apply $(2, 6)$-truncation of two bold edges.

Characterization of the Endo-Kroto operation

- The Endo-Kroto operation is a $(2, 6)$-truncation.
- The only (s, k)-truncation that gives a fullerene from a fullerene is an Endo-Kroto operation.

Graph-truncations of simple polytopes

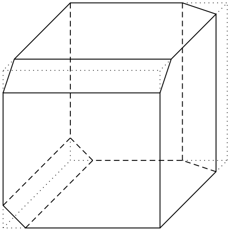
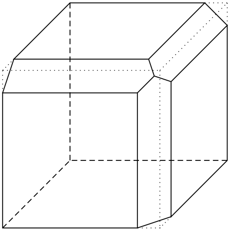
For a simple 3-polytope P let

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

be an irredundant representation and $G(P)$ be the 1-skeleton of P. Then for a subgraph $\Gamma \subset G(P)$ without isolated vertices define a graph-truncation

$$P_{\Gamma,\varepsilon} = P \cap \{\boldsymbol{x} \in \mathbb{R}^n \colon (\boldsymbol{a}_i + \boldsymbol{a}_j)\boldsymbol{x} + (b_i + b_j) \geqslant \varepsilon, F_i \cap F_j \in \Gamma\}$$

The combinatorial type does not depend on ε, if $\varepsilon > 0$ is small enough. Denote it by P_Γ.

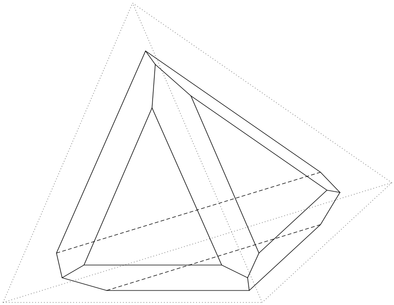
 

Different realizations of the associahedron.

Cutting off all edges

The polytope $P_{G(P)}$ is obtained from P by cutting off of all the edges.

$$p_k(P_{G(P)}) = \begin{cases} p_k(P), & k \neq 6 \\ p_k(P) + f_1(P), & k = 6 \end{cases}$$



$$(p_3, p_4, p_5, p_6) = (4, 0, 0, 6)$$

Cutting off of all the edges of a simplex.

Properties of graph-truncations

The graph $\Gamma \subset G(P)$ is admissible if any it's vertex has valency 1 or 3.

Theorem

For a simple 3-polytope P the polytope P_Γ is simple if and only Γ is admissible

Theorem

For a simple 3-polytope P and an admissible graph $\Gamma \subset G(P)$ the polytope P_Γ is flag if and only if for any 3-belt (F_i, F_j, F_k) in P one of the edges $F_i \cap F_j$, $F_j \cap F_k$ and $F_k \cap F_i$ belongs to Γ, and for any triangular face F_i the induced subgraph $\Gamma \cap F_i$ has isolates vertices.

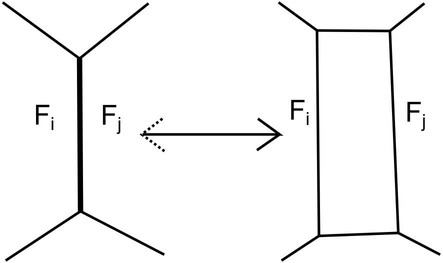
Graph-truncation and (s, k)-truncation

An edge-truncation (that is a $(1, k)$-truncation) is the only operation that is simultaneously a graph-truncation and an (s, k)-truncation.

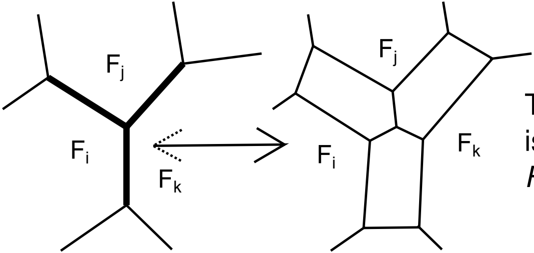
- *A graph-truncation is a monotonic operation. That is, let P be a simple polytope and $\Gamma \subset P$ be an admissible graph. Then $p_k(P_\Gamma) \geqslant p_k(P)$ for all k and there exists l such that $p_l(P_\Gamma) > p_l(P)$.*
- *(s, k)-truncation is not a monotonic operation. For example, let Q be a polytope such that the dodecahedron P is obtained from Q by a $(2, 6)$-truncation. Then*

$$p_4(Q) = 2 \geqslant 0 = p_4(P), \quad p_5(Q) = 8 \leqslant 12 = p_5(P),$$
$$p_6(Q) = 1 \geqslant 0 = p_6(P).$$

First nontrivial graph-truncations



The inverse operation
is applicable if and only if
$F_i \cap F_j = \varnothing$



The inverse operation
is applicable if and only if
$F_i \cap F_j = F_i \cap F_k = F_j \cap F_k = \varnothing$

"Eberhard's theorem for flag polytopes"

Theorem (E,14)

For every sequence $(p_k | 4 \leqslant k \neq 6)$ *of nonnegative integers satisfying*

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

there exists an integer p_6 *and a flag simple 3-polytope* P^3 *with* $p_k = p_k(P^3)$ *for all* $k \geqslant 4$.

If P has no triangles then the polytope $P_{G(P)}$ is flag.

Construction of *IPR*-fullerenes

- An Endo-Kroto operation can not give an *IPR*-fullerene.
- For a fullerene P the polytope $P_{G(P)}$ is an *IPR*-fullerene with $p_6(P_{G(P)}) = p_6(P) + f_1(P)$.
- For the dodecahedron the corresponding *IPR*-fullerene C_{80} has 80 vertices and is highly symmetric.

Fullerenes obtained by a graph-truncation

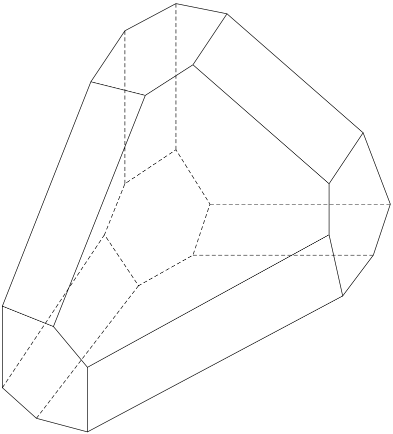
The edge E is a shout of the 2-face F, if $E \cap F$ is a vertex.

Theorem

Let P be a simple 3-polytope and $\Gamma \subset P$ be an admissible graph. Then P_Γ is a fullerene if and only if

- *Γ does not have isolated edges;*
- *$p_k(P) = 0$ for $k \geqslant 7$;*
- *any triangular face of P has two or three shouts in Γ;*
- *any quadrangular face of P has one or two shouts in Γ;*
- *any pentagonal face of P has at most one shout in Γ;*
- *any hexagonal face of P has no shouts in Γ;*

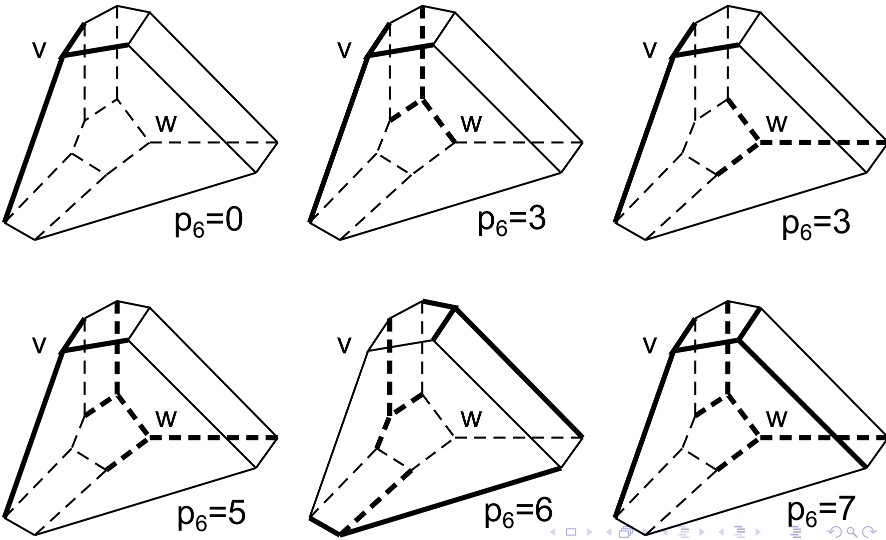
Graph-truncations of the permutohedron



Proposition

We can not obtain a fullerene as a graph-truncation of the permutohedron.

All graphs up to the symmetry on the associahedron that give fullerenes



Graph-truncations of fullerenes

Let P be a fullerene and $\Gamma \subset P$ be an admissible graph.

Corollary

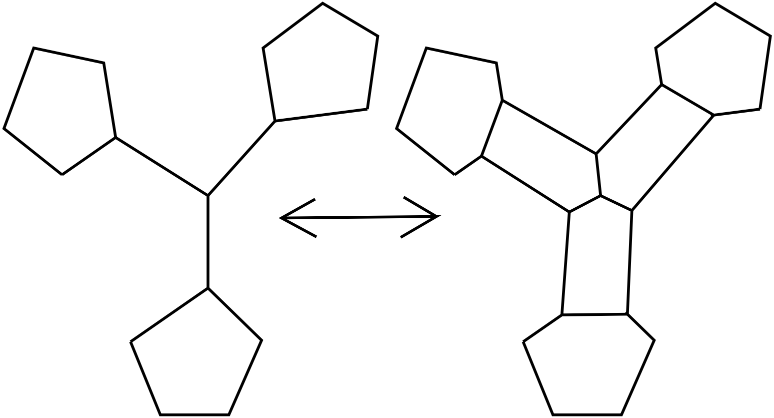
P_Γ is a fullerene if and only if

- *Γ does not have isolated edges;*
- *any hanging edge of Γ is a shout of a pentagon;*
- *different hanging edges correspond to different pentagons;*

If P_Γ is not a fullerene, then we can not obtain a fullerene from it by any sequence of graph-truncations.

Graph-truncations of fullerenes

The first nontrivial graph-truncation gives the following operation on fullerenes, which is always defined in both directions.

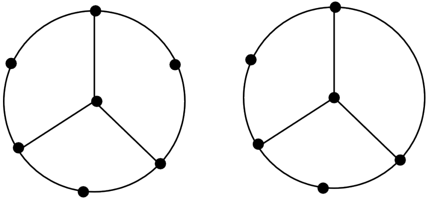


A polygonal partition of a compact 2-surface M^2 (closed or with boundary) is called ***simple****, if the intersection of any two polygons is either empty or their common edge.*

Any vertex of a simple partition has valency

- 3 if it is an interior point of a surface;
- 2 or 3 if it lies on the boundary.

Let μ_i be the number of boundary vertices of valency i.



$p_4 = 3$

$\mu_2 - \mu_3 = 0$, $\chi(M) = 1$

$2 \cdot 3 = 6 \cdot 1 + 0$

$p_3 = 1, p_4 = 2$

$\mu_2 - \mu_3 = -1$, $\chi(M) = 1$.

$3 \cdot 1 + 2 \cdot 2 = 6 \cdot 1 + 1$

Simple partitions of 2-surfaces

Let p_k be a number of k-gons in a simple partition.

For any simple partition of M^2

$$3p_3 + 2p_4 + p_5 = 6\chi(M^2) - \delta + \sum_{k \geqslant 7}(k-6)p_k, \, (*)$$

where $\delta = \mu_2 - \mu_3$

- *There are no hexagonal simple partitions of a closed surface if $\chi(M^2) \neq 0$.*
- *There exist hexagonal simple partitions of a torus and a Klein bottle.*

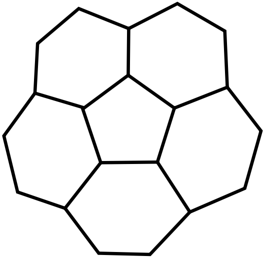
Simple partitions of a disk into 5- and 6-gons

A disk D^2 is a 2-surface homeomorphic to $\{\boldsymbol{z} \in \mathbb{C} \colon |\boldsymbol{z}| \leqslant 1\}$.

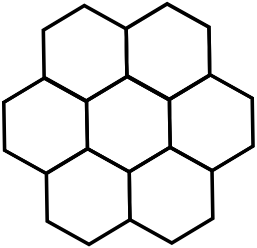
For a disk $\chi(D^2) = 1$ and the formula $(**)$ has the form

$$p_5 = 6 - \delta.$$

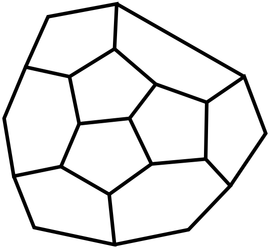
- $p_5 = 0 \Leftrightarrow \delta = 6$; $p_5 = 6 \Leftrightarrow \delta = 0$.
- There exist simple partitions of D^2 with arbitrary p_5 and p_6.



$p_5 = 1, p_6 = 5, \delta = 5$;



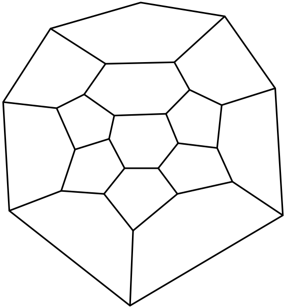
$p_5 = 0, p_6 = 7, \delta = 6$;



$p_5 = 7, p_6 = 2, \delta = -1$

Simple edge cycles on fullerenes

- A simple cycle in $G(P)$ divides a boundary of a fullerene P into two disks W_1 and W_2 with induced simple partitions.
- There is a bijection between the boundary vertices of W_1 and W_2 that maps the vertex of valency i to the vertex of valency $5-i$.
- For each disk W_1 and W_2 we have $\mu_2 \neq 1$ and $\mu_3 \neq 1$.



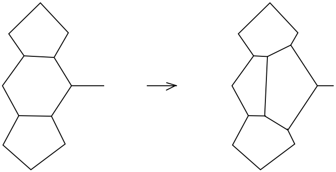
A simple partition of a disk which can not appear as W_1 or W_2.

Surgery of fullerenes

By a surgery of a fullerene we mean the operation of replacement of W_1 by a simple partition W_1' of D^2 into 5- and 6-gons such that there exists a bijection between the boundary vertices $v_1', \dots, v_p'$ of W_1' and $v_1, \dots, v_p$ of W_1 ordered cyclically that

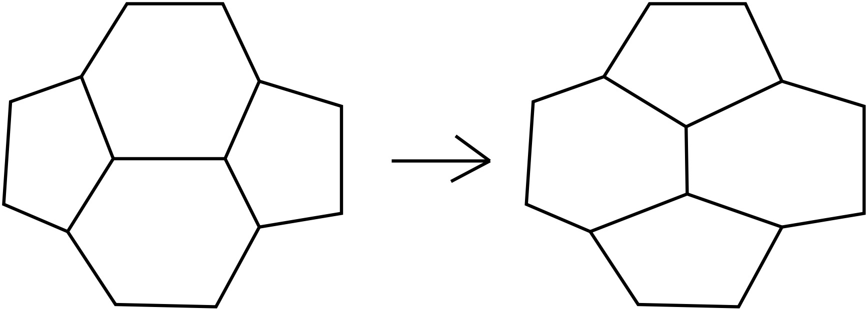
- *preserves the valences of vertices;*
- *has the form $v_i' \to v_{(s+i) \mod p}$ or $v_i' \to v_{(s-i) \mod p}$ for some s.*

The result is again a fullerene.



An Endo-Kroto operation gives a surgery of fullerenes.

Stone-Wales operation



- A Stone-Wales operation can produce an isomer;
- It is a flip;
- It is an example of a surgery.

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