Toric Topology of Fullerenes

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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.
- The number of combinatorial types of fullerenes grows rapidly 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.

Thanks to 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.

In our talk 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 $\mathcal{Z}_P$, plays an important role here.

Convex polytopes

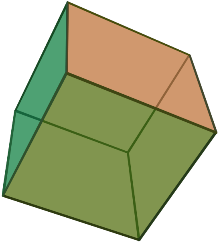
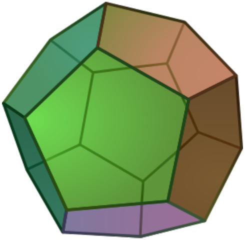
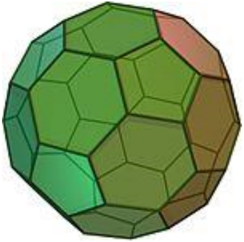
A convex polytope P is a bounded set of the form

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

Let this representation be irredundant, that is 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 $F_i = P \cap \mathcal{H}_i$.

Simple polytopes

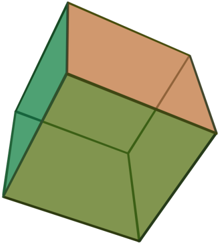
An n-polytope is simple if any its vertex is contained in exactly n facets.

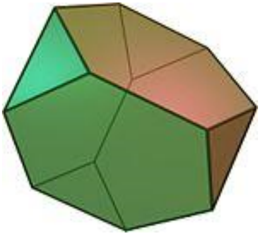
3 of 5 Platonic solids are simple.
7 of 13 Archimedean solids are simple.

Flag polytopes

A simple polytope is called flag *if any set of pairwise intersecting facets* $F_{i_1}, \ldots, F_{i_k}$ *:* $F_{i_s} \cap F_{i_t} \neq \varnothing$ *has a nonempty intersection* $F_{i_1} \cap \cdots \cap F_{i_k} \neq \varnothing$*.*



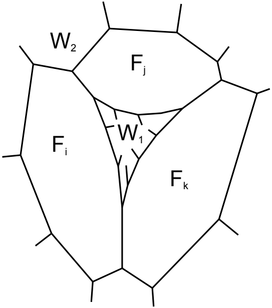
Flag polytope



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: collection of facets (F_i, F_j, F_k) with $F_i \cap F_j, F_j \cap F_k, F_k \cap F_i \neq \varnothing$, and $F_i \cap F_j \cap F_k = \varnothing$.



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

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

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

Corollary

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

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

Eberhard's theorem

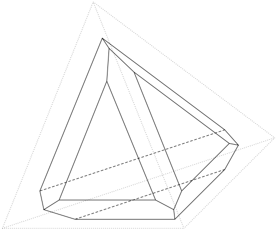
Theorem (Eberhard, 1891)

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

Theorem (E,14)

For every sequence $(p_k | 4 \leqslant k \neq 6)$ *of nonnegative integers satisfying* $2p_4 + p_5 = 12 + \sum_{k \geqslant 6}(k-6)p_k$*, there exists integer* p_6 *and a flag simple* 3*-polytope* P^3 *with* $p_k = p_k(P^3)$ *for all* $k \geqslant 4$*.*

Idea of the proof:

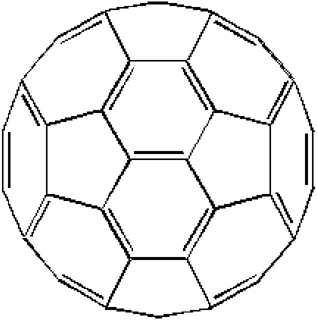


Cutting off of all edges of a simple polytope P without triangles gives a flag polytope $\widehat{P}$

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

Buckminsterfullerene

Fullerene C_{60}



Truncated icosahedron
with a Kekule structure

Carbon atoms, closed in hexatomic rings with single and double bonds alternately.

$$(f_0, f_1, f_2) = (60, 90, 32), \quad (p_5, p_6) = (12, 20)$$

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

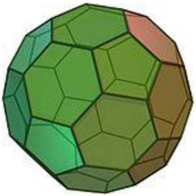
They were named after Richard Buckminster Fuller – a noted american architectural modeler.

Are also called buckyballs

Fullerenes

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

Fullerene C_{60}



Truncated icosahedron

For any fullerene $p_5 = 12$,

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

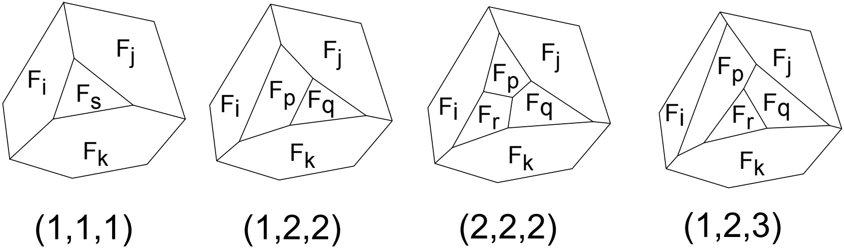
There exist fullerenes with any $p_6 \neq 1$.

Fullerenes as flag polytopes

Theorem (E,15)

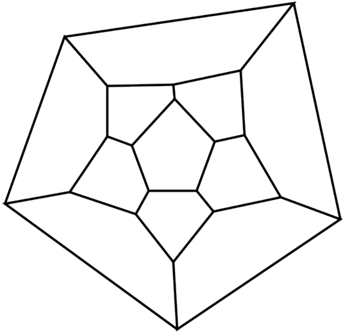
Any fullerene is a flag polytope.

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

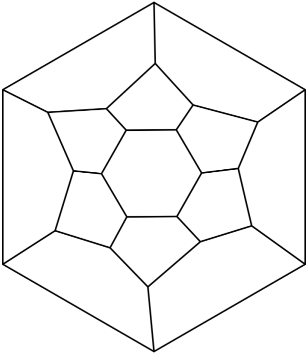


This is impossible since each fragment contains triangle or quadrangle.

Schlegel diagrams of fullerenes

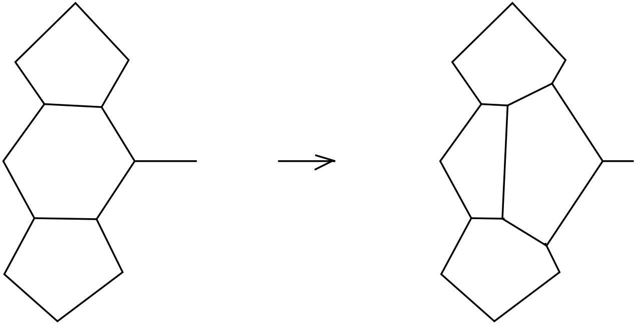


Dodecahedron
$p_6 = 0$



Barrel
$p_6 = 2$

Endo-Kroto construction



Starting from Barrel and applying a sequence of the Endo-Kroto constructions it is possible to obtain a fullerene with arbitrary $p_6 = k$, $k \geqslant 2$.
The Endo-Kroto construction is a $(2,6)$-truncation.

Number of combinatorial types of fullerenes

Let $F(p_6)$ be the number of combinatorial types of fullerenes with given p_6. In 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

Definition

IPR-fullerene (Isolated Pentagon Rule) is a fullerene having no two pentagons with common edge.

Let P be some IPR-fullerene. Then $p_6 \geqslant 20$. *IPR-fullerene with* $p_6 = 20$ *is combinatorially equivalent to Buckminsterfullerene* C_{60}.

The number $F_{IPR}(p_6)$ of combinatorial types of *IPR*-fullerenes also grows rapidly 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

Construction of *IPR*-fullerenes

The Endo-Kroto construction can not give the *IPR*-fullerene.

The operations of simultanious truncation of all edges of a fullerene P gives an *IPR*-fullerene $\widehat{P}$ with $p_6(\widehat{P}) = p_6(P) + f_1(P)$.

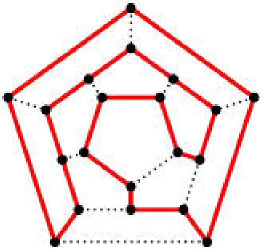
For the dodecahedron the corresponding *IPR*-fullerene C_{80} has 80 vertices and is highly symmetric.

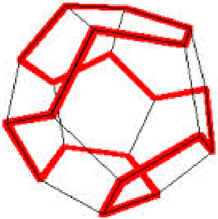
Hamiltonian cycles

A Hamiltonian cycle is a cycle in graph that passes through any vertex one and only one time.

Theorem (Kardos, 2014)

The edge graph of any fullerene has a hamiltonian cycle.





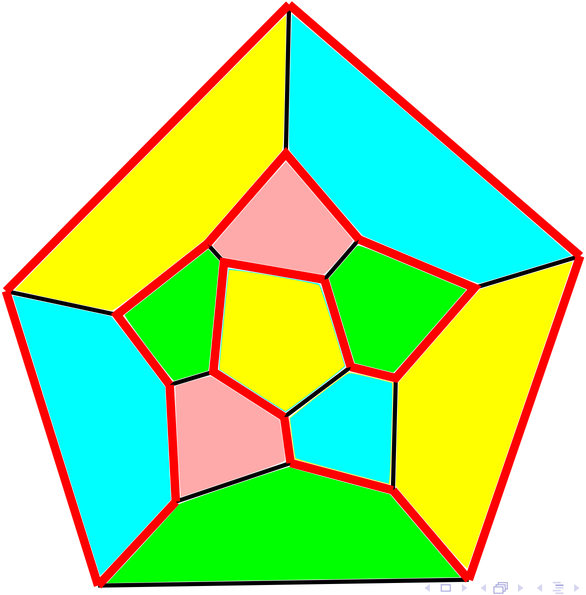
Any hamiltonian cycle defines a 4-coloring.

The cycle divides the surface of a fullerene into two disks. The dual graph of each disk is a tree, therefore each disk can be colored in two colors.

Any 4-coloring defines a characteristic function by the rule

$$1 \to \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, 2 \to \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, 3 \to \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, 4 \to \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

4-coloring of dodecahedron



Canonical correspondence

Simple polytope P $\dim P = n$ number of facets $= m$	$\longrightarrow$	moment-angle complex $\mathcal{Z}_P$ $\dim \mathcal{Z}_P = m + n$ canonical T^m-action
Combinatorics of P	$\longleftrightarrow$	Topology of $\mathcal{Z}_P$

Moment-angle complex

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

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

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

$\mathcal{Z}_P$ has a structure of $(m+n)$-dimensional smooth manifold and is also called moment-angle manifold.

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 $\mathbb{Q}$ is defined as*

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

- 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

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

be a multigraded differential algebra.

Theorem (Buchstaber-Panov)

We have an isomorphism

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

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

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:

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

Set

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

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

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:

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

Let P be a simple-polytope

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

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

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

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

3-polytopes

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

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

$$\beta^{-i,2\omega} = \dim \widetilde{H}^0(P_\omega, \mathbb{Q}) = \beta^{-(m-3-i),2([m]\setminus\omega)} = \dim \widetilde{H}^1(P_{[m]\setminus\omega}, \mathbb{Q}),$$

$$|\omega| = i+1, i = 1, \dots, m-4$$

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

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

k-belts

Let P be a simple 3-polytope. By a k-belt we call a cyclic sequence of 2-faces $(F_{i_1}, \dots, F_{i_k})$ such that $F_{i_1} \cap F_{i_2}, \dots, F_{i_{k-1}} \cap F_{i_k}, F_{i_k} \cap F_{i_1} \neq \varnothing$, and all other intersections are empty.

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 $H^{-2,8}$.

Relations between Betti numbers

Theorem

For any simple polytope P

$$h_0 + h_1 t^2 + \cdots + h_n t^{2n} = \frac{\sum_{-i,2j} (-1)^i \beta^{-i,2j} t^{2j}}{(1-t^2)^{m-n}},$$

where $h_0 + h_1 t + \cdots + h_n t^n = (t-1)^n + f_{n-1}(t-1)^{n-1} + \cdots + f_0.$

Corollary

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

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

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

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

Example

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

Theorem

For a fullerene P

- $\beta^{-1,6} = 0$ – *the number of* 3*-belts.*
- $\beta^{-2,8} = 0$ – *the number of* 4*-belts.*

Corollary

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

5-belts of fullerenes

Theorem

For a fullerene P we have $\beta^{-3,10} = 12 + k$ *is the number of 5-belts. If* $k > 0$*, then the fullerene consists of two dodecahedral caps and* k *hexagonal belts between them.*

Set of pentagons

Let P be a fullerene and $\omega^* = \{i, F_i\text{– pentagon}\}$. For convenience let $\omega^* = \{1, \ldots, 12\}$.

Betti numbers $\beta^{-i,2\omega}$, $\omega \subset \omega^*$ or $\omega \subset [m] \setminus \omega^*$, are important combinatorial invariants of fullerenes.

- $\beta^{-11,2\omega^*} = \beta^{-(m-14),2([m]\setminus\omega^*)}$.
- *P is an IPR-fullerene* $\Longleftrightarrow \beta^{-11,2\omega^*} = 11$.
- *For the dodecahedron and the barrel* $\beta^{-11,2\omega^*} = 0$.

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