Fullerenes, combinatorics of polytopes, Lobachevskian geometry and applications

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Atoms of carbon, evaporating from heated surface of graphite, may form molecules representing convex polytopes.

The boundary of such polytopes is made of 6- and 5-gons, whose vertices correspond to carbon atoms.

A molecule with n carbon atoms is denoted by $\mathrm{C_n}$

Fuller's biosphere,
USA pavilion,
Expo-67,
Montreal, Canada

Fullerenes are named after american architect and philosopher R.Buckminster Fuller (1895–1983), who patented the construction of geodesic domes for covering large areas with supports only on the boundary.

In English there is a name for fullerenes: buckyballs.

Buckminsterfullerene
C_{60}

Soccer ball

R.Buckminster Fuller

Fullerenes

Fullerene C_{60} was discovered by theoretical chemists R.Curl, H. Kroto and R. Smalley in 1985 (Nobel prize, 1996).

Astronomers have found the predicted spectral lines of fullerenes in space – in the atmospheres of carbon stars.

Afterwards fullerenes were found on Earth in the flame of electric arc.

For a long time fullerenes have been obtained only in laboratories of scientific centers.

Since 1992 there are reports of occurences of fullerenes in

- circumstellar media, interstellar media, meteorites, interplanetary dust particles (IDPs), lunar rocks;
- hard terrestrial rocks from Shunga (Russia), Sudbury (Canada) and Mitov (Czech Republic), coal, terrestrial sediments from the Cretaceous-Tertiary-Boundary and Permian-Triassic-Boundary, fulgurite.

Euler formula

Leonhard Euler (1707, Basel – 1783, St-Petersburg).

Let f_0 be the number of vertices, f_1 the number of edges,

f_2 the number of facets of 3-polytopes. Then

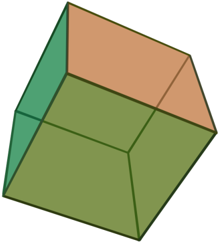
$$f_0 - f_1 + f_2 = 2$$

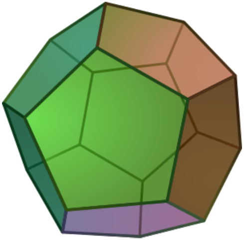
Platonic bodies

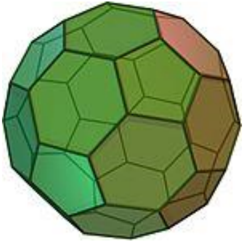
	f_0	f_1	f_2
Tetrahedron	4	6	4
Cube	8	12	6
Octahedron	6	12	8
Dodecahedron	20	30	12
Icosahedron	12	30	20

Definition

A 3-polytope is called simple, if each vertex is contained in exactly 3 edges.







Euler formula and simple polytopes

Let p_k be the number of k-gonal facets of a polytope.

For every simple polytope P there is the following relation on p_k

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

Corollary

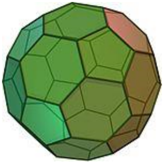
If $p_k = 0$ for $k \neq 5, 6$, then $p_5 = 12$.
There are no simple polytopes with only hexagonal facets

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

Definition

A (mathematical) fullerene is a simple 3-polytope such that all its facets are 5- or 6-gons.

Fullerene C_{60}



Truncated icosahedron (one of 13 Archimedean solids)

For each fullerene we have $p_5 = 12$,

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

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

Realizability of p-vector

Theorem (Eberhard, 1891)

For each sequence $(p_k | \ 3 \leqslant k \neq 6)$ of nonnegative integers, satisfying the relation on p_k

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

there exist p_6 and a 3-polytope P^3 such that $p_k = p_k(P^3)$ for all $k \geqslant 3$.

Problem

Which $p_6 = p_6(P^3)$ could be realized for a given sequence $(p_k | \ 3 \leqslant k \neq 6)$.

Realizability of f-vector

Theorem (E.Steinitz, 1906)

A triple (f_0, f_1, f_2) is a face vector of a 3-polytope if and only if

$$f_0 - f_1 + f_2 = 2, \quad f_2 \leqslant 2f_0 - 4, \quad f_0 \leqslant 2f_2 - 4$$

Corollary

$$f_2 + 4 \leqslant 2f_0 \leqslant 4f_2 - 8$$

Problem

For polytopes of dimension 4 the relations characterizing their face vectors (f_0, f_1, f_2, f_3) are still unknown.

Graphs of 3-polytopes

Definition

The 1-skeleton of a polytope is its edge graph.

Definition

A simple graph is a graph without loops and multiple edges.

The Steinitz theorem (1922)

A graph G is the edge graph of a 3-polytope if and only if G is a simple 3-connected planar graph i.e. with at least 4 vertices and the graph remains connected after deletion of any two of its vertices.

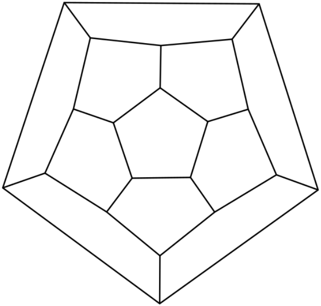
A Schlegel diagram gives a planar realization of an edge graph of a 3-polytope.

Schlegel diagrams (Victor Schlegel, 1843 – 1905)

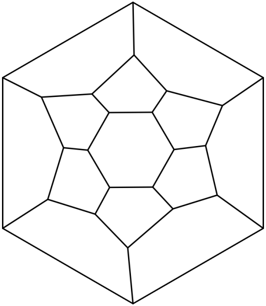
Definition

A Schlegel diagram (1886) of a convex 3-polytope P is a partition of its facet into polygons obtained by a projection of P from a point outside of the polytope close to this facet.

- The diagram depends on the choice of a facet.
- The edge graph on the diagram is a complete combinatorial invariant of a polytope P.

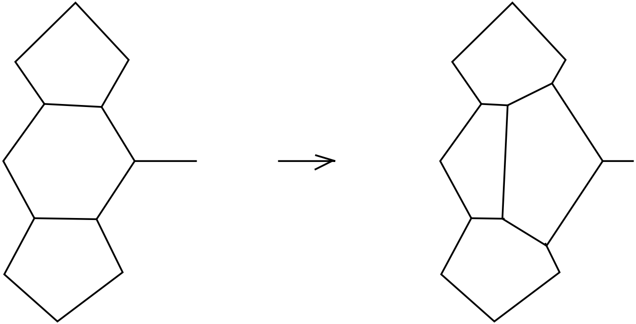


Dodecahedron, $p_6 = 0$
5-barrel B_5



Barrel, $p_6 = 2$
6-barrel B_6

For any $m > 5$ there is a convex 3-polytope B_m with $p_m(B_m) = 2$, $p_5(B_m) = 2m$, and $p_k = 0$ for $k \neq 5, m$.



By using the Endo–Kroto operation one can obtain fullerenes with any $p_6 = k$, $k > 2$ starting from the 6-barrel B_6, $p_6(B_6) = 2$.

Number of combinatorial types of fullerenes

Paul William Thurston (1946 – 2012, USA).
Fields medal (1982) for his contributions to the theory of 3-manifolds.

Theorem (P.W.Thurston, 1998)

The number $F(p_6)$ of combinatorial types (isomers) of fullerenes grows asymptotically as p_6^9.

For example, for C_{400} we have $F(202) = 132.247.999.328$.

C_n	C_{20}	C_{22}	C_{24}	C_{26}	C_{28}	C_{30}	...	C_{60}	...	C_{70}
p_6	0	1	2	3	4	5	...	20	...	25
$F(p_6)$	1	0	1	1	2	3	...	1812	...	8149

http://hog.grinvin.org

IPR-fullerenes

Definition

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

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

The number $F_{IPR}(p_6)$ of combinatorial isomers of IPR-fullerenes also grows fast as a function of p_6.
For example, for C_{400} we have $F_{IPR}(202) = 40.286.153.024$.

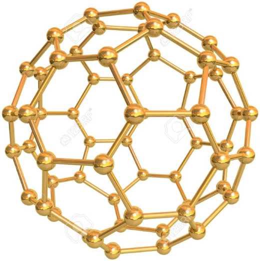
C_n	C_{60}	C_{62}	C_{64}	C_{66}	C_{68}	C_{70}	C_{72}	C_{74}	C_{76}
p_6	20	21	22	23	24	25	26	27	28
F_{IPR}	1	0	0	0	0	1	1	1	2

http://hog.grinvin.org

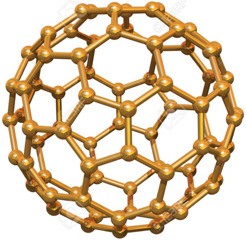
Icosahedral fullerenes

Definition

A fullerene whose group of combinatorial symmetries is the icosahedral group is called icosahedral.



C_{60}



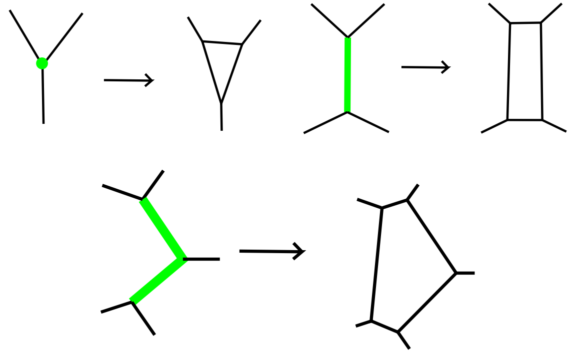
C_{80}

From $F(20) = 1812$ fullerenes, only C_{60} is icosahedral. From $F(30) = 31924$, only C_{80} is icosahedral.

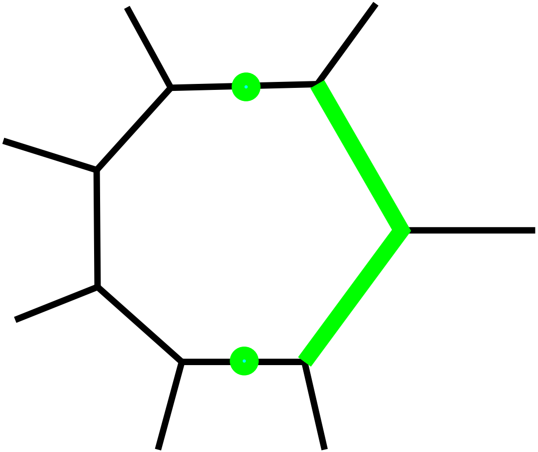
Constructions of simple 3-polytopes

Theorem (Eberhard, 1891)

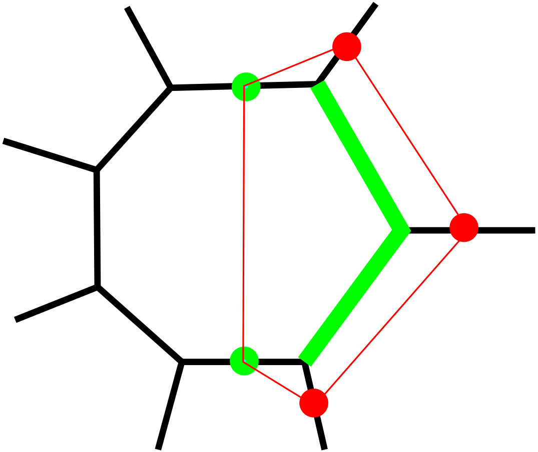
Each simple 3-polytope is combinatorially equivalent to a polytope obtained from a tetrahedron by a sequence of vertex cuts, edge cuts and $(2, k)$-truncations.



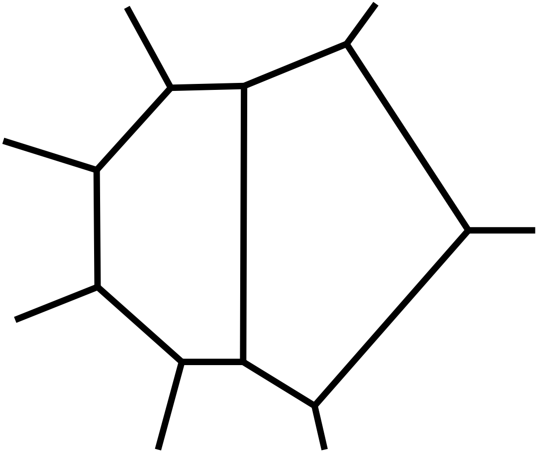
(2, 7)-truncation



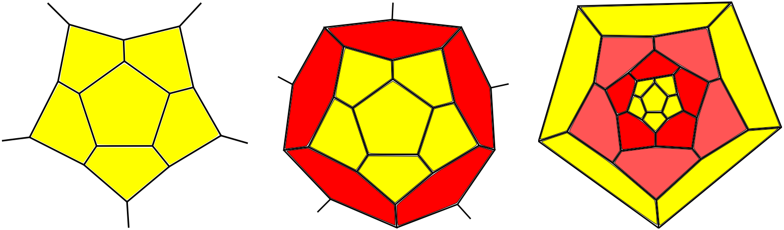
$(2,7)$-truncation



$(2,7)$-truncation



$(5,0)$-nanotubes



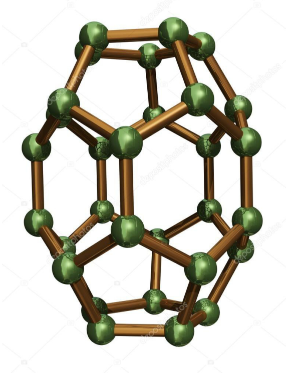
1. Take patch C of the dodecahedron drawn on the left;
2. add $k \geqslant 1$ five-belts of hexagons;
3. glue up by the patch C again to obtain the fullerene D_{5k}.

Proposition

A fullerene has the form D_{5k}, $k \geqslant 0$, iff it contains a patch C.

A (5, 0)-nanotube D_{5k} is a fullerene C_n for $n = 20 + 10k$, $k \geqslant 1$.

The first (5, 0)-nanotube C_{30}



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Constructions of combinatorial fullerenes

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

Each fullerene

- different from the dodecahedron and $(5,0)$-nanotubes

is combinatorially equivalent to a polytope obtained from

- the 6-barrel

by a sequence of

- $(2,6)$- and $(2,7)$-truncations

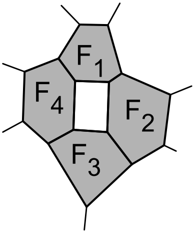
in such a way that each intermediate polytope is

- either a fullerene or a simple 3-polytope with facets pentagons, hexagons and at most one heptagon, which should be adjacent to a pentagon.

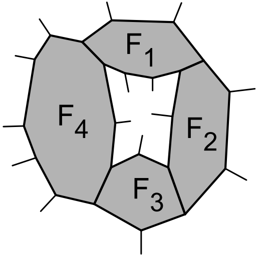
Let P be a simple convex 3-polytope.

Definition

A k-belt of a polytope P is a cyclic sequence of its facets $(F_{j_1}, \dots, F_{j_k})$ such that $F_{i_{j_1}} \cap \dots \cap F_{i_{j_r}} \neq \varnothing$ iff $\{i_1, \dots, i_r\} \in \{\{1,2\}, \dots, \{k-1, k\}, \{k, 1\}\}$.

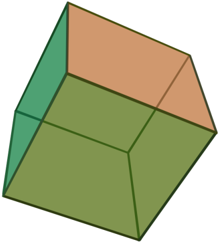


A 4-belt around the 4-gon

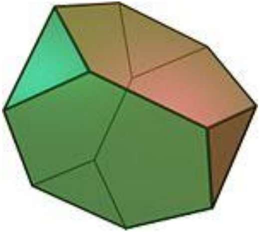


A general 4-belt

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



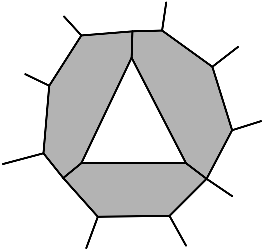
Flag polytope



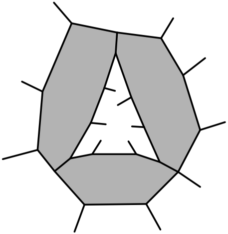
Nonflag polytope

Lemma

A simple 3-polytope P is flag polytope iff $P \neq \Delta^3$ and P does not have 3-belts.

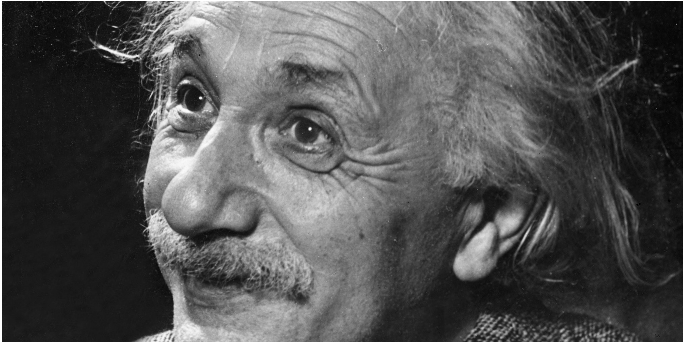


A 3-belt around the triangle



A general 3-belt

Albert Einstein (Ulm, 1879 – Princeton, 1955)



Two postulates of the special theory of relativity:

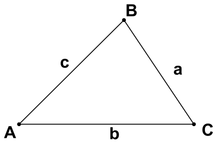
- The laws of physics are invariant in all inertial systems (i.e., non-accelerating frames of reference).
- The speed of light in a vacuum is the same for all observers, regardless of the motion of the light source.

Nikolai Lobachevsky (1792, N. Novgorod – 1856, Kazan)

"Lobachevsky is Copernicus of geometry".
William Clifford (1845–1879, UK).

One of the creators of non-euclidean geometry. In 1842, following recommendation of K.Gauss, he became the corresponding member of Göttingen scientific society with recognition as "one of the greatest mathematicians of Russian Empire".

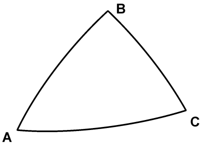
Triangles



Euclidean geometry

$\angle A + \angle B + \angle C = \pi$

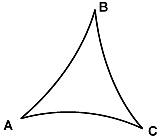
$S^2 = p(p-a)(p-b)(p-c)$



Elliptic geometry

$\angle A + \angle B + \angle C > \pi$

$S = \angle A + \angle B + \angle C - \pi$

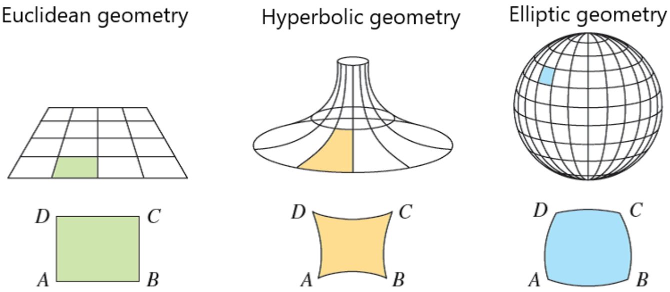


Hyperbolic geometry

$\angle A + \angle B + \angle C < \pi$

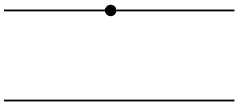
$S = \pi - \angle A - \angle B - \angle C$

Rectangles

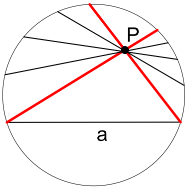


$\angle D = 90$ $\angle D < 90$ $\angle D > 90$

All angles of such 4-gons are equal.



Euclidean plane



Beltrami–Klein model
of Lobachevsky plane

The replacement of Euclid's fifth postulate by Lobachevsky's postulate on parallel lines in the space of velocities of material point leads to the replacement of postulate of equal course of time by the postulate of equal speed of light in all inertial reference systems.

Right-angled polytopes

Definition

A simple 3-polytope P is called right-angled if it has a bounded realization in Lobachevsky space $\mathbb{L}^3$ such that all its dihedral angles are right angles.

Pogorelov polytopes

Definition

A Pogorelov polytope is a simple flag 3-polytope without 4-belts.

Theorem (A.Pogorelov, 1967; E.Andreev, 1970)

The class of Pogorelov polytopes coincides with the class of right-angled polytopes.

The realization of Pogorelov polytope in $\mathbb{L}^3$ is unique up to isometry.

Hyperbolic 2-manifolds

Any compact Riemannian 2-manifold $\mathcal{M}^2$

- different from a sphere, a torus, a Klein bottle or a projective plane

has a realisation as

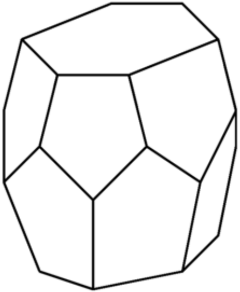
- a compact Riemannian manifold of constant negative curvature.

Hyperbolic 3-manifolds

In 1890 Felix Klein (1849 –1925) posed the problem:

Find a compact Riemannian 3-manifold
of constant negative curvature.

Following Killing–Hopf theorem, each manifold of this type is isometric to a quotient space $\mathbb{L}^3/G$, where $\mathbb{L}^3$ is the Lobachevsky 3-space, and G is a cocompact discrete group of isometries of $\mathbb{L}^3$ acting without fixed points.



In 1931 German mathematician F. Löbel constructed the first example of a closed orientable 3-manifold of constant negative curvature. It was obtained by gluing 8 copies of the 6-barrel B_6.

Right-angled Coxeter groups

Coxeter (1907, London – 2003, Toronto).

Let P be a right-angled polytope with m facets.
Let G(P) be the group generated by reflections of the space $\mathbb{L}^3$ in the facets $\{F_1, \ldots, F_m\}$ of the polytope P.

The group G(P) is the right-angled Coxeter group, given by the presentation:

$$\mathcal{R}C(P) = \langle g_1, \ldots, g_m | g_i^2 = 1,\ g_i g_j = g_j g_i \text{ if } F_i \cap F_j \neq \emptyset \rangle,$$

where g_i corresponds to the reflection in respect to the facet F_i.

The group G(P) acts on $\mathbb{L}^3$ discretely with finite isotropy subgroups and fundamental domain P.

Lemma

Let $\phi : \mathrm{G(P)} \to \mathbb{Z}_2^3$ be an epimorphism. The subgroup $\mathrm{Ker}\phi \subset \mathrm{G(P)}$ does not contain elements of finite order iff the vectors $\phi(\mathrm{g}_{\mathrm{i}_1}), \phi(\mathrm{g}_{\mathrm{i}_2}), \phi(\mathrm{g}_{\mathrm{i}_3})$ are linearly independent in $\mathbb{Z}_2^3$ for each triple of intersecting facets $\mathrm{F}_{\mathrm{i}_1}, \mathrm{F}_{\mathrm{i}_2}, \mathrm{F}_{\mathrm{i}_3}$ of P.

Subgroups acting freely on $\mathbb{L}^3$

Suppose an epimorphism ϕ satisfies the condition of lemma. Then

- The subgroup Kerϕ acts freely on $\mathbb{L}^3$.
- (A.Vesnin, 1987) The orbit space $\mathcal{H}(\mathrm{P};\phi) = \mathbb{L}^3/\mathrm{Ker}\phi$ is a compact hyperbolic 3-manifold.
  The manifold $\mathcal{H}(\mathrm{P};\phi)$ is obtained by gluing $|\mathbb{Z}_2^3| = 8$ copies of the polytope P and has the Riemannian metric of constant negative curvature.
- A compact manifold $\mathcal{H}(\mathrm{P};\phi)$ is aspherical, since its universal cover $\mathbb{L}^3$ is contractible.

Let P be a simple 3-polytope.
The boundary ∂P partitioned into facets $F_1, \ldots, F_m$ can be considered as a map on a sphere S^2.
According to the solution of The Four Color Theorem (K. Appel, W. Haken, 1976)

the boundary ∂P admits a regular 4-coloring, i.e. each two facets sharing a common edge are colored differently.

Since P is simple, we have $F_i \cap F_j \neq \emptyset$ iff $F_i \cap F_j$ is an edge.

Corollary

For each regular 4-coloring of ∂P and each vertex $v_k = F_{i_1} \cap F_{i_2} \cap F_{i_3}$, the facets $F_{i_1}, F_{i_2}, F_{i_3}$ have pairwise different colours.

A regular 4-coloring of a polytope P is a function

$$\chi\colon \{F_1, \dots, F_m\} \to \{1, 2, 3, 4\},$$

where $\chi(F_i) = k$.

Consider the set $E = \{e_k \mid k = 1, ..., 4\}$ of elements in $\mathbb{Z}_2$-vector space $\mathbb{Z}_2^3$, where e_k, $k = 1, 2, 3$, form a basis and $e_4 = e_1 + e_2 + e_3$.

Each 3 vectors of E form a basis of $\mathbb{Z}_2^3$.

Let P be a right-angled polytope. Consider the homomorphism $\phi : \mathrm{G(P)} \to \mathbb{Z}_2^3$ defined by the coloring χ of polytope P such that $\phi(\mathrm{g_i}) = \chi(\mathrm{F_i})$.

Theorem

The group Kerϕ acts freely on $\mathbb{L}^3$.

Corollary

For each right-angled polytope P with a regular 4-coloring χ, there exist a compact hyperbolic manifold $\mathcal{H}(\mathrm{P};\chi)$.

Results by T. Došlić (1998, 2003) imply

Theorem

Each fullerene is a Pogorelov polytope.

Corollary

For each regular 4-coloring χ of a fullerene P we have a hyperbolic manifold $\mathcal{H}(\mathrm{P};\chi)$.

A Hamiltonian cycle in a graph is a cycle passing through each vertex exactly once.

Mathematical physicist Peter G. Tait (1831-1901) is known in graph theory mainly for Tait's conjecture.

Conjecture (P. G. Tait, 1884)

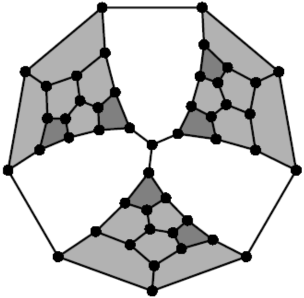
Every 3-connected planar cubic graph has a Hamiltonian cycle.

According to the Steinitz theorem (1922) this conjecture is equivalent to

Conjecture

Graph of any simple 3-polytope has a Hamiltonian cycle.

The Tait's conjecture was disproved by W. T. Tutte (1946).



The Tutte's graph – 3-connected planar cubic graph without Hamiltonian cycle.

Hamiltonian cycles in fullerenes

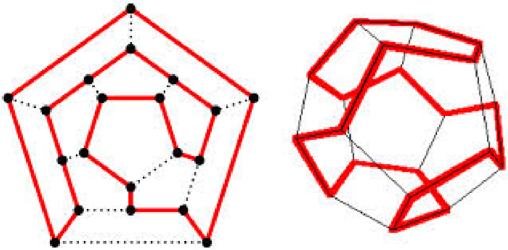
Conjecture (D. W. Barnette, 1969)

Graph of any simple 3-polytope with at most hexagonal facets has a Hamiltonian cycle.

F.Kardoš (2014) gave a computer-assisted proof of Barnette's conjecture.

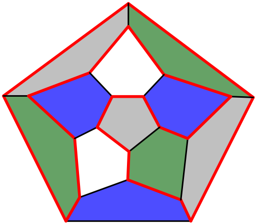
Corollary

The edge graph of any fullerene has a hamiltonian cycle.



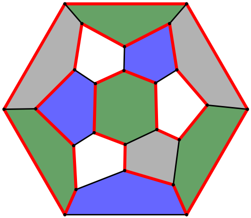
Lemma

A hamiltonian cycle on the edge graph of 3-polytope determines a regular 4-coloring of its facets.



4-coloring of a dodecahedron

12 facets: 4×3



4-coloring of a 6-barrel

14 facets: $2 \times 3 + 2 \times 4$

Using the notion of Pogorelov polytopes the following results can be formulated as

Theorem (G.D. Birkhoff (1884-1944), 1913)

The Four Color Problem for all maps can be reduced to coloring of facets of Pogorelov polytopes.

Conjecture (H.F. Hunter, 1962)

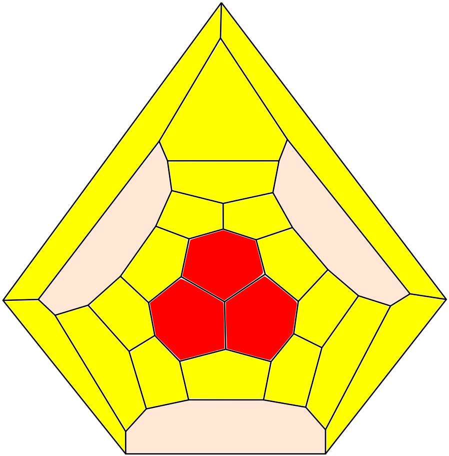
Any Pogorelov polytope admits a Hamiltonian cycle.

Theorem (H. Walther, 1965)

There are Pogorelov polytopes without Hamiltonian cycles.

Grinbergs's counterexample

A simple counterexample to Hunter's conjecture was found in 1968 by E.J. Grinbergs



Grinbergs's polytope

Problem

Prove The Four Color Theorem for fullerenes, using their specific combinatorial properties.

Definition

Two 4-colorings of a map are equivalent if they differ only by a permutation of colors.

Problem

Using the constructions of fullerenes mentioned earlier, find the number of non-equivalent regular colorings of their boundaries.

Theorem (V.Buchstaber, N.Erokhovets, M.Masuda, T.Panov and S.Park, 2016)

Let P and P' be simple polytopes with epimorphisms $\phi\colon \mathrm{G}(\mathrm{P}) \to \mathbb{Z}_2^3$ and $\phi'\colon \mathrm{G}(\mathrm{P}') \to \mathbb{Z}_2^3$ such that images of any three facets with common vertex are linearly independent. Assume P is a Pogorelov polytope. Then

- the hyperbolic manifolds $\mathcal{H}(\mathrm{P}, \phi)$ and $\mathcal{H}(\mathrm{P}', \phi')$ are diffeomorphic (isometric) if and only if $\mathrm{P} \sim \mathrm{P}'$ and ϕ, ϕ' differ by linear change of coordinates in $\mathbb{Z}_2^3$.

Corollary (V. Buchstaber, T. Panov, 2016)

Let P and P' be simple polytopes with 4-colorings χ and χ', and assume P is a Pogorelov polytope. Then

- the hyperbolic manifolds $\mathcal{H}(\mathrm{P}, \chi)$ and $\mathcal{H}(\mathrm{P}', \chi')$ are diffeomorphic (isometric) if and only if $\mathrm{P} \sim \mathrm{P}'$ and $\chi \sim \chi'$.

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Thank you for your attention!