Fullerenes
and
Polygonal Partitions of Surfaces

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The talk is devoted to classical and recent mathematical results, which had drawn attention of physicists and chemists in connection with problems of nanotechnology.

- **Fullerenes**
  Nobel Prize 1996 in Chemistry
  R. F. Kurl, H. Kroto, R. E. Smalley
  «for their discovery of fullerenes».

- **Graphene**
  Nobel Prize 2010 in Physics
  A. K. Geim and K. S. Novoselov
  «for groundbreaking experiments regarding the two-dimensional material graphene».
We will formulate combinatorial, geometrical, and topological tasks concerning molecular carbon structures in terms of convex polytopes, polygonal partitions of 2-surfaces.

The connection of these tasks with known and new problems in graph theory and toric topology will be discussed.

The talk is prepared jointly with N.Yu.Erokhovets.
A fullerene is a spherical-shaped molecule of carbon such that any atom belongs to exactly three carbon rings, which are pentagons or hexagons.

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.

Fullerene $C_{60}$
Fullerenes were named after Richard Buckminster Fuller – a noted American architectural modeler.

Are also called buckyballs
The plane $\mathbb{R}^2$ can be tiled by regular hexagons.

The schematic picture of the graphene. Nodes are atoms of carbon, edges – bonds that hold atoms in the graphene sheet.
Carbon nanotubes are obtained when the graphene sheet is rolled up into the infinite cylinder. They are characterized by the chiral vector \( c = na + mb \).

The shift by the vector \( c \) moves the lattice to itself. The nodes that differ by the shift are identified during the rolling up.

\[ c = na + mb \]
Carbon nanotubes

Because of the symmetry and unique electronic structure of graphene, the structure of a nanotube strongly affects its electrical properties.

For a given \((n, m)\)-nanotube,
- if \(n = m\), the nanotube is metallic;
- if \(n - m\) is a multiple of 3, then the nanotube is semiconducting with a very small band gap,
- otherwise the nanotube is a moderate semiconductor.

To obtain a finite nanotube one should cut off the infinite cylinder along two simple edge cycles. Any of the cycles should divide the cylinder into two infinite parts. The cycles should not intersect and not selfintersect.
(n, 0)-nanotubes are called zigzag nanotubes, while (n, n)-nanotubes are called armchair. These tubes have mirror symmetry. All other types are chiral, that is they do not coincide with the mirror image.
By a **capped nanotube** we mean a surface obtained by gluing up the ends of a finite nanotube by disks subdivided into pentagons and hexagons.
Carbon nanobuds

A **nanobud** is a concatenation of a fullerene with a nanotube. Nanotubes are chemically neutral, therefore it is difficult to combine them with other materials. Fullerenes are chemically active and give good conditions for this.
A convex polytope $P$ is a bounded set of the form

$$P = \{ x \in \mathbb{R}^n : a_i x + b_i \geq 0, i = 1, \ldots, m \}$$

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

Archimedean solid – snub dodecahedron
A Schlegel diagram (1886) of a convex polytope $P$ in $\mathbb{R}^3$ is a projection of $P$ from $\mathbb{R}^3$ into $\mathbb{R}^2$ through a point beyond one of its facets.

- A Schlegel diagram is a polygonal subdivision of the facet.
- The graph of edges drown on the diagram is a complete combinatorial invariant of 3-polytopes.

Schlegel diagram of the dodecahedron
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

$$f_0 - f_1 + f_2 = 2$$

<table>
<thead>
<tr>
<th>Polytope</th>
<th>$f_0$</th>
<th>$f_1$</th>
<th>$f_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tetrahedron</td>
<td>4</td>
<td>6</td>
<td>4</td>
</tr>
<tr>
<td>Cube</td>
<td>8</td>
<td>12</td>
<td>6</td>
</tr>
<tr>
<td>Octahedron</td>
<td>6</td>
<td>12</td>
<td>8</td>
</tr>
<tr>
<td>Dodecahedron</td>
<td>20</td>
<td>30</td>
<td>12</td>
</tr>
<tr>
<td>Icosahedron</td>
<td>12</td>
<td>30</td>
<td>20</td>
</tr>
</tbody>
</table>
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.

For any simple 3-polytope \( f_0 = 2(f_2 - 2), f_1 = 3(f_2 - 2) \).
Consequence of Euler’s formula for simple 3-polytopes

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

For any simple 3-polytope $P$

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

Corollary

- If $p_k = 0$ for $k = 3, 4$, then $p_5 = 12 + \sum_{k\geq 7} (k - 6)p_k$.
- If $p_k = 0$ for $k \neq 5, 6$, then $p_5 = 12$.
- There is no simple 3-polytopes with all faces hexagons.
- $3p_3 + 2p_4 + p_5 \geq 12$. 
Theorem (Eberhard, 1891)

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

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

there exist a simple 3-polytope \(P^3\) with \(p_k = p_k(P^3), k \neq 6\).

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

- There are infinitely many realizable values of \(p_6\).
- There exists realizable \(p_6 \leq 3 \left( \sum_{k \neq 6} p_k \right)\) (J.C. Fisher, 1974)

- If \(p_3 = p_4 = 0\) then any \(p_6 \geq 8\) is realizable (B. Grunbaum, 1968).
A simple polytope is called flag if any set of pairwise intersecting facets $F_{i_1}, \ldots, F_{i_k}$: $F_{i_s} \cap F_{i_t} \neq \emptyset$, $s, t = 1, \ldots, k$, has a nonempty intersection $F_{i_1} \cap \cdots \cap F_{i_k} \neq \emptyset$.
A (mathematical) fullerene is a simple 3-polytope with all 2-facets pentagons and hexagons.

For any fullerene \( p_5 = 12 \),

\[
\begin{align*}
    f_0 &= 2(10 + p_6), \\
    f_1 &= 3(10 + p_6), \\
    f_2 &= (10 + p_6) + 2
\end{align*}
\]

There exist fullerenes with any \( p_6 \neq 1 \).
Schlegel diagrams of fullerenes

Fullerene barrel

Schlegel diagram of the barrel
The Endo-Kroto operation increases $p_6$ by 1.

Starting from the Barrel and applying a sequence of Endo-Kroto operations it is possible to obtain a fullerene with arbitrary $p_6 = k$, $k \geq 2$. 
Two combinatorially nonequivalent fullerenes with the same number $p_6$ are called **combinatorial isomers**.

Let $F(p_6)$ be the number of combinatorial isomers with given $p_6$. It is known that $F(p_6) = \mathcal{O}(p_6^g)$.

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

<table>
<thead>
<tr>
<th>$p_6$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>\ldots</th>
<th>75</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F(p_6)$</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>6</td>
<td>6</td>
<td>15</td>
<td>\ldots</td>
<td>46.088.157</td>
</tr>
</tbody>
</table>
The function $F(n - 10)$.

The sequence $A007894(n)$ see in on-line encyclopedia of integer sequences, founded in 1964 by N.J.A. Sloane.
The function \( \ln(F(n - 10)) \).

See in on-line encyclopedia of integer sequences, founded in 1964 by N.J.A. Sloane.
**IPR-fullerenes**

**Definition**

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

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

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

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

<table>
<thead>
<tr>
<th>$p_6$</th>
<th>20</th>
<th>21</th>
<th>22</th>
<th>23</th>
<th>24</th>
<th>25</th>
<th>26</th>
<th>27</th>
<th>28</th>
<th>...</th>
<th>97</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_{IPR}$</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>...</td>
<td>36.173.081</td>
</tr>
</tbody>
</table>
Conjecture (Brinkman, Dress)

The functions $F(p_6)$ and $F_{IPR}(p_6 + 24)$ are in some sense good approximations of each other asymptotically.

<table>
<thead>
<tr>
<th>$p_6$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>...</th>
<th>73</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F(p_6)$</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>6</td>
<td>6</td>
<td>15</td>
<td>...</td>
<td>36.798.433</td>
</tr>
<tr>
<td>$F_{IPR}(p_6 + 24)$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>5</td>
<td>7</td>
<td>9</td>
<td>24</td>
<td>...</td>
<td>36.173.081</td>
</tr>
</tbody>
</table>
Construction of simple 3-polytopes

Theorem (Eberhard (1891), Brückner (1900))

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.
(2, 7)-truncation
(2, 7)-truncation
(2, 7)-truncation
Combinatorially the edge-truncation is a local operation and affects only the facets $F_1$ and $F_3$, the edge $E$, and it’s vertices:

- the edge $E$ is transformed into the quadrangle $F$;
- the number of edges of $F_1$ and $F_3$ increases by 1.
Combinatorially the \((2, k)\)-truncation is a local operation and affects only the facets \(F, F_1,\) and \(F_4\), and the edges \(E_1 = F_1 \cap F\) and \(E_4 = F_4 \cap F\):

- \(k\)-gon \(F\) is divided into \((k - 1)\)-gon \(F'\) and 5-gon \(F''\);
- \(E_1\) and \(E_4\) are divided into two edges;
- the number of edges of \(F_1\) and \(F_4\) increases by 1.
The Endo-Kroto operation as a $(2, 6)$-truncation

The Endo-Kroto operation is the only $(2, k)$-truncation that transforms a fullerene into a fullerene. In this case $k = 6$ and $F_1$ and $F_4$ are pentagons.
Construction of combinatorial fullerenes

Theorem (Buchstaber-Erokhovets, 2015)

- Any fullerene is combinatorially equivalent to a polytope obtained from the cube by a sequence of edge-truncations and (2, 6)- and (2, 7)-truncations, such that at each step the polytope has facets only 4-, 5-, 6-gons and no more than one 7-gon, and this 7-gon is incident to 4- or 5-gon.

- Any operation increases the number of facets by one, therefore the number of operations in a sequence is $6 + p_6$. 
Realization of the dodecahedron

\[(p_4, p_5, p_6) = (3, 6, 0) \quad (p_4, p_5, p_6) = (2, 8, 1) \quad (p_4, p_5, p_6) = (0, 12, 0)\]

- 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.
Theorem (Buchstaber-Erokhovets, 2015)

Consider a sequence of edge-, (2, 6)- and (2, 7)- truncations that give a combinatorial fullerene $P$ from the cube. Then

- The first and the second operations are edge-truncations;
- The first 5 operations can be chosen to be edge-truncations;
- If $P$ is not a dodecahedron, then the first 7 operations can be chosen to be edge-truncations;
- The last operation is a (2, 6)- or a (2, 7)-truncation, and $F_1$ and $F_4$ – quadrangle or pentagon. This gives two incident facets: a $(k - 1)$-gon $F'$ and a pentagon $F''$.
- The sequence of operations is not unique. Moreover, any pentagon $F''$ and incident facet $F'$ of a given fullerene appear as a pair $(F', F'')$ at the last step of some sequence of operations.
A polygonal partition of a compact 2-surface $M^2$ (closed or with boundary) is called \textit{simple}, if the intersection of any two polygons is either empty or their common edge.
Simple partitions 2-surfaces

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
- $p_k$ be a number of $k$-gons in a simple partition,
- $\mu_i$ be the number of boundary vertices of valency $i = 2, 3$.

\[ p_4 = 3 \]
\[ \mu_2 - \mu_3 = 0, \quad \chi(M) = 1 \]
\[ 2 \cdot 3 = 6 \cdot 1 + 0 \]

\[ p_3 = 1, p_4 = 2 \]
\[ \mu_2 - \mu_3 = -1, \quad \chi(M) = 1 \]
\[ 3 \cdot 1 + 2 \cdot 2 = 6 \cdot 1 + 1 \]
Simple partitions of 2-surfaces

For any simple partition of $M^2$

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

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

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

$$p_5 = 6 - \delta \implies -\infty < \delta \leq 6$$

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

\[ p_5 = 1, p_6 = 5, \delta = 5; \quad p_5 = 0, p_6 = 7, \delta = 6; \quad p_5 = 7, p_6 = 2, \delta = -1 \]
Simple partitions of the cylinder into 5- and 6-gons

For the cylinder $\chi(M^2) = 0$ and $p_5 = -\delta \implies \delta \leq 0$.

There are simple partitions of the cylinder for any

$$p_5 + p_6 \geq 3 \implies p_6 \geq 3 + \delta.$$ 

$p_5 = 0, p_6 = 5, \delta = 0$; $p_5 = 0, p_6 = 6, \delta = 0$; $p_5 = 5, p_6 = 2, \delta = -5$

For simple partition of the cylinder into hexagons:

- $\mu_2 = \mu_3$;
- $f_0 = \mu_2 + 2p_6$, $f_1 = \mu_2 + 3p_6$, $f_2 = p_6$. 
Applications to nanotubes

On each component of the boundary the number of 2-valent vertices is equal to the number of 3-valent.

Corollary

Each disk on the end of a capped nanotube has exactly 6 pentagons.
Construction of a nanobud

a) – the Buckminsterfullerene $C_{60}$
b) – a disk on a) partitioned into 3 pentagons and 4 hexagons.
c) – excision.
Construction of a nanobud

- **d)** – the graphene sheet;
- **e)** – a disk on **d)** partitioned into 7 hexagons.
- **f)** – excision.
Construction of a nanobud

- **g)** – $C_{60}$ and graphene sheet with holes;
- **h)** – a cylinder partitioned into 3 heptagons and 3 octagons with boundary components equal to those on **g)**.
- **i)** – a nanobud.
We constructed a nanobud $N$ with

- 9 pentagons;
- 3 heptagons;
- 3 octagons;
- $\chi(N) = 0$.

The numbers satisfy the equation

$$p_5 = p_7 + 2p_8$$
One of the main objects of the toric topology is the moment-angle functor $K \to Z_K$. It assigns to each simplicial complex $K$ with $m$ vertices a space $Z_K$ with an action of a compact torus $T^m$, whose orbit space $Z_K/T^m$ can be identified with the cone $CK$ over $K$.

To any simple partition $P$ of a closed 2-surface into polygons we can associate the nerve-complex $K_P$. Vertices of $K_P$ are facets of $P$. Vertices of $K_P$ form a simplex if and only if the corresponding facets have nonempty common intersection.

Thus to partition $P$ we associate the space $Z_P := Z_{K_P}$. 
Boundary of a simple polytope $P$ with $m$ facets is a polygonal partition of the sphere $S^2$.

In this case $\mathcal{K}_P$ is the boundary of the dual simplicial polytope $P^*$. 

The moment-angle complex $\mathcal{Z}_P$ has the structure of a smooth manifold with a smooth action of $T^m$. It is called a moment-angle manifold.

The orbit space $\mathcal{Z}_P/T^m$ can be identified with $P$ itself.

Thus to any fullerene $P$ we associate a smooth manifold $\mathcal{Z}_P$ with a smooth actions of the torus $T^m$, $m = 12 + p_6$. 
Let \( \{v_1, \ldots, v_m\} \) be the set of vertices of a simplicial complex \( K \). Then a **Stanley-Reisner ring** over \( \mathbb{Z} \) is defined as

\[
\mathbb{Z}[K] = \mathbb{Z}[v_1, \ldots, v_m]/(v_{i_1} \ldots v_{i_k} = 0, \text{ if } \{v_{i_1}, \ldots, v_{i_k}\} \not\in K).
\]

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

**Corollary**

The Stanley-Reisner ring of a fullerene is quadratic.
Let

\[ R^*(K) = \wedge[u_1, \ldots, u_m] \otimes \mathbb{Z}[K]/(u_iv_i, v_i^2), \]
\[ \text{mdeg}u_i = (-1, 2\{i\}), \text{mdeg}v_i = (0, 2\{i\}), du_i = v_i, dv_i = 0 \]

be a multigraded differential algebra.

**Theorem (Buchstaber-Panov)**

We have an isomorphism

\[ H[R^*(K), d] \simeq \text{Tor}_{\mathbb{Z}[v_1, \ldots, v_m]}^{*, *}(\mathbb{Z}[K], \mathbb{Z}) \simeq H^*(\mathbb{Z}_K, \mathbb{Z}) \]

Moreover, this isomorphism defines the structure of a multigraded algebras in Tor and \( H^*(\mathbb{Z}_K, \mathbb{Z}) \).
Main problems of toric topology of fullerenes:

- To build combinatorial invariants of fullerenes using methods of toric topology.
- To find such invariants that distinguish fullerenes from other simple 3-polytopes.

The talk of N. Erokhovets, *Fullerenes and combinatorics of 3-dimensional flag polytopes* is devoted to the results concerning this problems.
V.M. Buchstaber, T.E. Panov,
*Toric Topology*

V.M. Buchstaber, N. Erokhovets,
*Truncations of simple polytopes and applications*

X. Lu, Z. Chen,
Curved Pi-Conjugtion, Aromaticity, and the Related Chemistry of Small Fullerenes ($C_{60}$) and Single-Walled Carbon Nanotubes.
Chemical Reviews 105:10(2005), 3643-3696.

M. Deza, M. Dutour Sikiric, M.I. Shtogrin,
*Fullerenes and disk-fullerenes*

V.D. Volodin,
*Combinatorics of flag simplicial 3-polytopes*

B. Grünbaum,
*Convex polytopes*
Thank You for the Attention!