The parametrization of fullerenes

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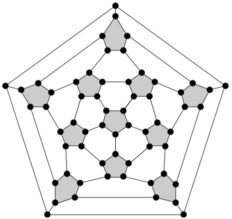
I. Fullerenes

Fullerenes

- A fullerene is a 3-valent plane graph, whose faces are 5 or 6-gonal.
- They exist for any even $n \geq 20$, $n \neq 22$.

- There exist extremely efficient programs to enumerate them (FullGen by G. Brinkman, CPF by T. Harmuth)
- Fullerenes with isolated pentagons have $n \geq 60$. The smallest one:



Truncated icosahedron,
soccer ball,
Buckminsterfullerene

Euler formula and positive curvature

- For a 3-valent plane graph Euler formula can be rewritten as
$$\sum_{i\geq 3}(6-i)p_i = 12$$
with p_i the number of i-gons.
- We restrict ourselves to graphs of positive curvature, i.e. those with $c_i = 6 - i \geq 0$.
- Thus we have the following possibilities for (p_3, p_4, p_5):

$(0,0,12)$	$(0,1,10)$	$(0,2,8)$	$(0,3,6)$	$(0,4,4)$
$(0,5,2)$	$(0,6,0)$	$(1,0,9)$	$(1,1,7)$	$(1,2,5)$
$(1,3,3)$	$(1,4,1)$	$(2,0,6)$	$(2,1,4)$	$(2,2,2)$
$(2,3,0)$	$(3,0,3)$	$(3,1,1)$	$(4,0,0)$	

- The goal is to try to understand how one can describe such graphs:
  - W.P. Thurston, *Shapes of polyhedra and triangulations of the sphere*, The Epstein birthday schrift, 511–549 (electronic), Geom. Topol. Monogr., 1, Geom. Topol. Publl., Coventry, 1998.

Symmetry groups and number of fullerenes

- The possible symmetry groups of fullerenes are

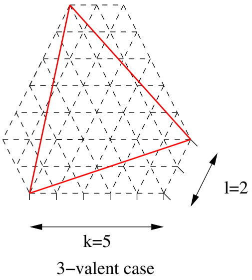
class	all group	# param
C_1	C_1, C_s, C_i	10
C_2	C_2, C_{2h}, C_{2v}	6
C_3	C_3, C_{3h}, C_{3v}	4
D_2	D_2, D_{2h}, D_{2d}	4
D_3	D_3, D_{3h}, D_{3d}	3
D_5	D_5, D_{5h}, D_{5d}	2
D_6	D_6, D_{6h}, D_{6d}	2
T	T, T_h, T_d	2
I	I, I_h	1

- The number of fullerene grows polynomially with the number of vertices.
- The goal is to describe the fullerenes by those parameters.

II. Simple parameterizations

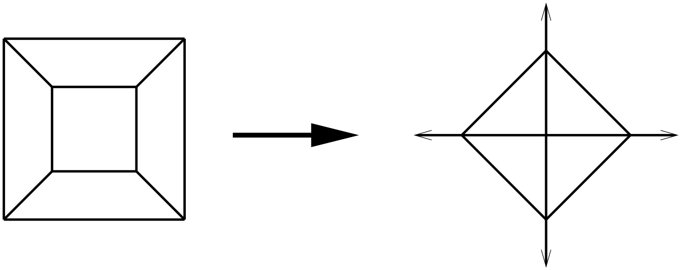
The case of 1 parameter: Goldberg-Coxeter construction

- Take a 3-valent plane graph G_0 and two parameters $k, l \geq 0$.
- The graph G_0^* is a triangulation.
- Break the triangles of G_0^* into smaller triangles:



- Glue all those pices together and get another triangulation
- Take the dual and get a 3-valent plane graph $GC_{k,l}(G_0)$.

Example of $GC_{2,1}(Cube)$



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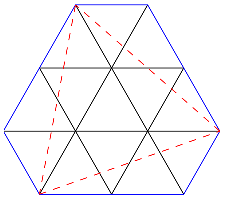

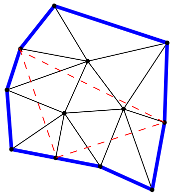

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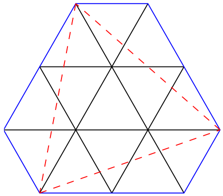

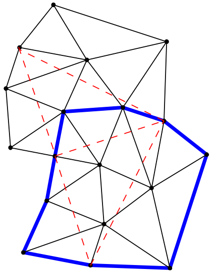

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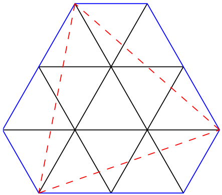

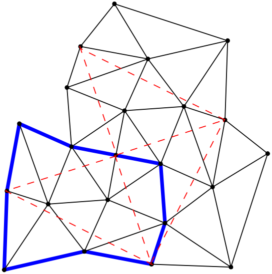

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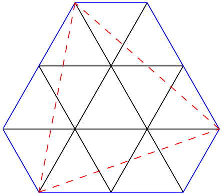

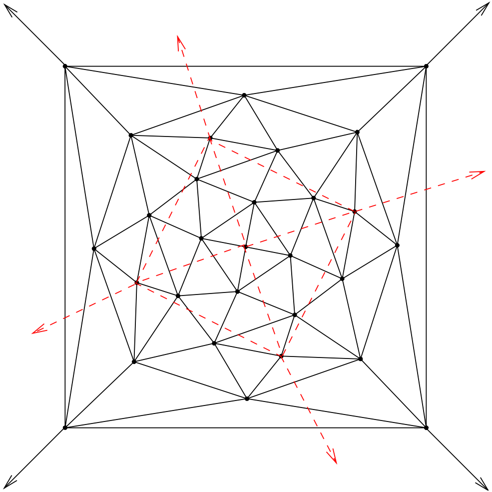

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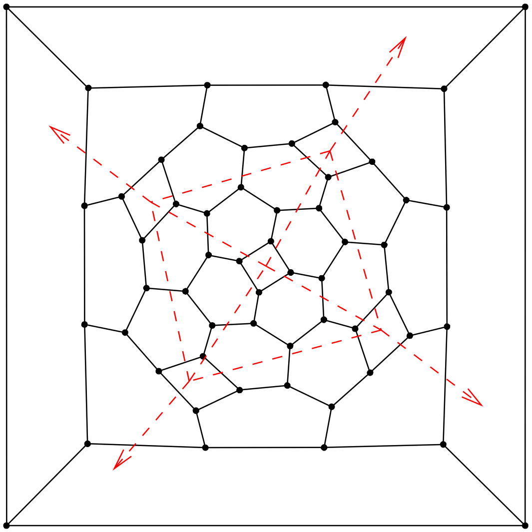
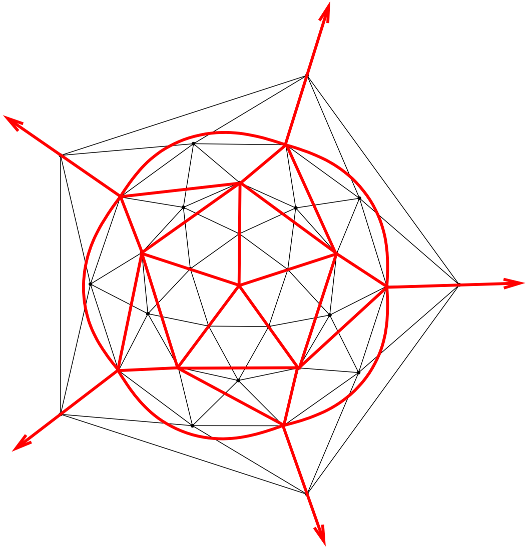


Properties of Goldberg Coxeter construction

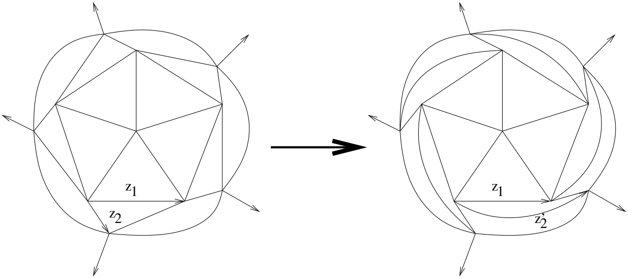
- It is more convenient to work with the dual.
- If a fullerene is of symmetry (I, I_h) then it is of the form $GC_{k,l}(Dodecahedron)$ for some k, l.
  Similarly, if a $(0,6,0)$-, $(4,0,0)$ is of symmetry (O, O_h), (T, T_d) then it is $GC_{k,l}(Cube)$, $GC_{k,l}(Tetrahedron)$.
  - M. Goldberg, *A class of multi-symmetric polyhedra*, Tohoku Mathematical Journal **43** (1937) 104–108.
- It is useful to embed k, l as an Eisenstein integer, i.e. $z = k + l\omega$ with $\omega = e^{i\pi/3}$.
- $GC_{k,l}(G_0)$ has $(k^2 + kl + l^2)|G_0| = |z|^2|G_0|$ vertices.
- The parameter symmetry $z \mapsto z\omega^r$ does not change the graph.

One case of 2 parameters: symmetry D_5

- The 5-fold axis has to pass through a vertices of degree 5. There are 5 vertices of degree 5 around it.

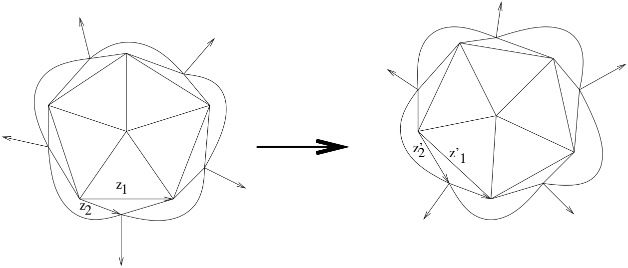


Parameter symmetries in D_5 case



- Operation 1: $(z_1, z_2) \mapsto (z_1, z_1 + z_2)$

Parameter symmetries in D_5 case



- Operation 2: $(z_1, z_2) \mapsto (z_1 + \omega^2 z_2, z_1 - z_2)$
- Operation 3: $(z_1, z_2) \mapsto (z_1, z_2)\omega^r$
- For a given parameter (z_1, z_2) a graph may not exist.
- $n_{triangle}(z_1, z_2) = 10\{z_1\overline{z_1} - (z_1\overline{z_2} - \overline{z_1}z_2)(\omega - \overline{\omega})/3\}$.

III. General Thurston theory

Parameterization of (p_3, p_4, p_5)-graphs

- For a class of 3-valent plane graph (p_3, p_4, p_5) the number of complex parameters needed to describe it is

$$m = p_3 + p_4 + p_5 - 2$$

  We denote by $z_1, \dots, z_m$ the set of parameters.
- The number of vertices is expressed as a Hermitian form q in the parameters $(z_1, \dots, z_m)$
- The signature of q is $(1, m-1)$.
- Denote by $\mathbb{H}^m$ the cone of $(z_1, \dots, z_m) \in \mathbb{C}^m$ such that $q(z_1, \dots, z_m) > 0$.

Monodromy group

- The set of parameters describing the group is not unique, some operations generalizing the previous ones occur.
- The Hermitian form is invariant under those transformations
- The group defined by them is a monodromy group $M(p_3, p_4, p_5)$:
  - P. Deligne, G.D. Mostow, *Monodromy of hypergeometric functions and nonlattice integral monodromy*, Inst. Hautes tudes Sci. Publ. Math. **63** (1986) 5–89.
  - G.D. Mostow, *Generalized Picard lattices arising from half-integral conditions*, Inst. Hautes tudes Sci. Publ. Math. **63** (1986) 91–106.

  (The groups $M(p_3, p_4, p_5)$ form 18 of the 94 discrete such groups)
- Those monodromy groups are image of the braid group B_m and the invariant form q corresponds to the intersection form on $H^1(S^2 - \{p_1, \ldots, p_{m+2}\}, L)$ with L a line bundle.
- As a consequence $M(p_3, p_4, p_5)$ acts discretely over $\mathbb{H}^m$.

Representability and covolume

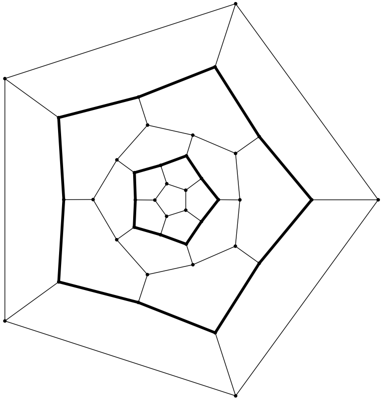
- Thurston states that if $z \in \mathbb{Z}[\omega]^m$ and $q(z) > 0$ then there exists $g \in M(p_4, p_4, p_5)$ such that $g(z_1, \ldots, z_m)$ is realizable as a (p_3, p_4, p_5)-graph.
- Thus $\mathbb{H}^m \cap \mathbb{Z}[\omega]^m$ up to the action of the monodromy group $M(p_3, p_4, p_5)$ is a parameter space for the (p_3, p_4, p_5)-graphs.
- The quotient

$$\mathbb{H}^m / (\mathbb{R}_{>0} \times M(p_3, p_4, p_5))$$

  is of finite covolume.
- The number of (p_3, p_4, p_5)-graphs with n vertices grows like $O(n^{m-1})$.
  - C.H. Sah, *A generalized leapfrog for fullerene structures*, Fullerenes Science and Technology **2-4** (1994) 445–458.

Non-compacity

- The quotient $\mathbb{H}^m/(\mathbb{R}_{>0} \times M(p_3, p_4, p_5))$ is non-compact.
- But the direction of non-compacity are well understood.
- They correspond to partition of (p_3, p_4, p_5) faces into two (p_3^i, p_4^i, p_5^i) with $i = 1$, 2 and $3p_3^i + 2p_4^i + p_5^i = 6$.
- Geometrically those are nanotubes



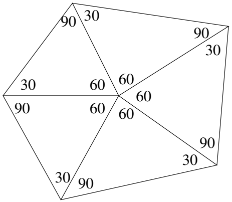
Possible generalizations?

- We can consider 4-valent plane graphs. Euler formula for them is
$$\sum_{i\geq 3}(4-i)p_i = 8$$
with p_i the number of i-gons. A priori those correspond to some Deligne-Mostow orbifolds.
- What is not clear is how the theory depends on
    - The positive curvature. What can go wrong if $p_7 = 1$?
    - Parameterization of orientable surfaces. There Euler formula is
$$\sum_{i\geq 3}(6-i)p_i = 6(2-2g)$$
There is no doubt that such parameterization are possible. But what is the geometric structure of the quotient?

IV. Angle description

Alternative parameterization: by angles

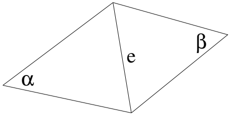
- Suppose we have a triangulation of a 2-dimensional manifold with t triangles.
- If we assign the angles of a triangle then the length of the edges is specified up to some multiple. So, we can describe a structure by its angles.
- The problem is with cycles:



since going over the cycle we see that only length 0 is coherent.

Dihedral angles

- For an edge e between two triangles:



the dihedral angle is $\pi(e) = \pi - \alpha - \beta$. We can assume $\pi(e) \geq 0$ since otherwise we can switch the edge e.

- For a triangle t of angle α, β, γ the hyperbolic volume is:

$$L(t) = L(\alpha, \beta, \gamma) = L(\alpha) + L(\beta) + L(\gamma)$$

with

$$L(x) = -\int_0^x \log(2\sin\ t)dt$$

a strictly concave function.

Rivin's theory

- For a triangulation $t_1, \ldots, t_N$ with a set of dihedral angles $\Pi = \{\pi(e)\}$ we minimize over the set of all possible angles the sum
$$\sum_i L(t_i)$$
subject to the constraint that its set of dihedral angles is Π
- Necessarily the minimum is unique and is attained by a set of angles all positive.
- The derivative with respect to angle being 0 are equivalent to the coherency of the length.
- So, dihedral angles form a set of parameters. For fullerene this is 18 parameters.
- I. Rivin, *Euclidean structure on simplicial surfaces and hyperbolic volume*, The Annals of mathematics **139** (1994) 553–580.

V. Spectrum

Eigenvalues of graphs

- For a 3-valent plane graph G the adjacency matrix A is a symmetric matrix with

$$A(i,j) = \begin{cases} 1 & \text{if } (i,j) \text{ is an edge} \\ 0 & \text{otherwise} \end{cases}$$

- 3 is always an eigenvalue while -3 is an eigenvalue if and only if G is bipartite that is has faces of only even size.
- The infinite plane tiling by hexagon has spectrum $[-3, 3]$.
  - P. E. John and H. Sachs, *Spectra of toroidal graphs*, Discrete Mathematics **309** (2009) 2663.
- This is also the case of infinite nanotubes:
  - L. F. Chibotaru, D. Compernolle and A. Ceulemans, *Electron transmission through atom-contacted carbon nanotubes*, Physical Review B **68** (2003) 125412 (31 pp).

General finiteness theorem

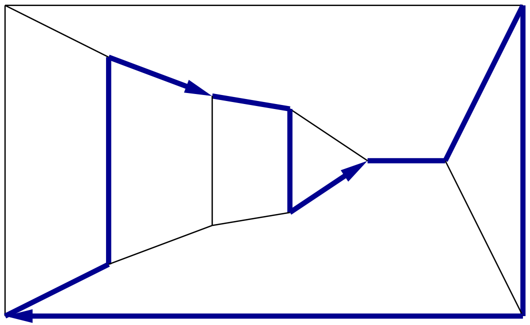
Consider a class of (p_3, p_4, p_5)-graphs

- Lemma: If the number n is large enough then a (p_3, p_4, p_5)-graph contains
  - a large enough patch of hexagons or
  - a long enough nanotube.
- Two proof methods:
  - One is based on a simple covering argument (by J. Graver).
  - Another on Thuston's parameterizations and the fact that the compactifications of the parameter space are indexed by the partititions of the 5-gons into two sets of six 5-gons.
- Theorem: For any interval $I = [a, b] \subset [-3, 3]$ with $a < b$ the set of (p_3, p_4, p_5)-graphs having no eigenvalue in I is finite.
  - M. Dutour Sikirić and P. Fowler, *Cubic ramapolyhedra with face size no larger than* 6, Journal of Mathematical Chemistry **49** (2011) 843–858.

VI. Zigzags

Definition

- In a plane graph a zigzag is a circuit of edges such that two consecutive share a face and vertex but three do not share a face.



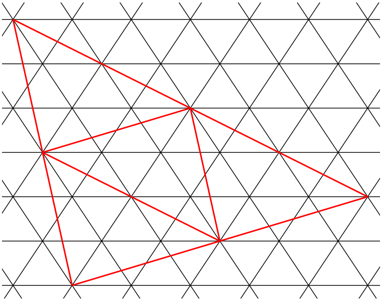
Zigzag structure of Goldberg Coxeter construction

- For a 3-valent plane graph G_0 we define a permutation group $Mov(G_0)$ and two elements L and R.
- The length of zigzags of $GC_{k,l}(G_0)$ is computed from the cycle structure of $L \odot_{k,l} R$:
  - $L \odot_{1,0} R = L$ and $L \odot_{0,1} R = R$.
  - If $gcd(k,l) = 1$ then we have

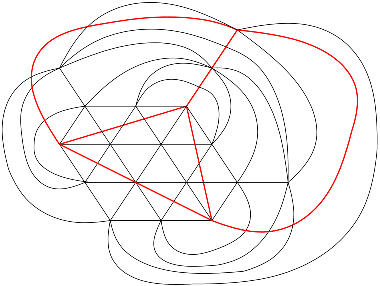
$$\begin{cases} L \odot_{k,l} R = L \odot_{k-ql\ ,\ l} RL^q & \text{if } k - ql \geq 0 \\ L \odot_{k,l} R = R^q L \odot_{k\ ,\ l-qk} R & \text{if } l - qk \geq 0 \end{cases}$$

    The product is defined only up to conjugacy.
- If $gcd(k,l) = m > 1$ then we simply multiply the length of zigzags by m:
  - M. Dutour and M. Deza, *Goldberg-Coxeter construction for* 3- *and* 4-*valent plane graphs*, Electronic Journal of Combinatorics **11-1** (2004) R20.

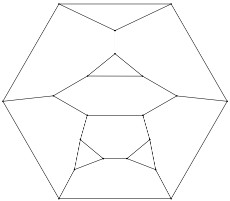
The structure of $(4, 0, 0)$-graphs



4 triangles in $\mathbb{Z}[\omega]$



The corresponding triangulation



A $(4, 0, 0)$-graph of symmetry D_{2d}

Zigzags in $(4,0,0)$- and $(0,6,0)$-graphs

- All zigzags of $(4,0,0)$-graphs are simple.
- The vector enumerating length of zigzags of $(4,0,0)$-graphs is

$$(4s_1)^{m_1}, (4s_2)^{m_2}, (4s_3)^{m_3} \quad \text{with} \quad s_i m_i = \frac{n}{4}.$$

- Conjecture: All $(0,6,0)$-graphs with only simple zigzags are:
  - $GC_{k,0}(Cube)$, $GC_{k,k}(Cube)$ and
  - the family of graphs with parameters (m,i) with $n = 4m(2m-3i)$ vertices and a vector of zigzags

$$z = (6m-6i)^{3m-3i}, (6m)^{m-2i}, (12m-18i)^{i}$$

They have symmetry D_{3d} or O_h or D_{6h}

THANK

YOU