Extended Family of Fullerenes

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Overview

A (geometric) fullerene F_n is a simple (i.e., 3-valent) polyhedron (putative carbon molecule) whose *n* vertices (carbon atoms) are arranged in 12 pentagons and $(\frac{n}{2} - 10)$ hexagons.

- F_n exist for all even $n \ge 20$ except n = 22.
- 1, 1, 1, 2, 5..., 1812, ..., 214127713, ... isomers F_n , for n = 20, 24, 26, 28, 30..., 60, ..., 200,
- Graphite lattice (6^3) as F_{∞} : the "largest fullerene"
- Thurston, 1998, implies: no. of F_n grows as n^9 .
- C₂₀(I_h), C₆₀(I_h), C₈₀(I_h) are only icosahedral (i.e., with highest symmetry I_h or I) fullerenes with n ≤ 80 vertices.
- preferable (or IP) fullerenes, C_n , satisfy isolated pentagon rule.

 I. 8 families of standard ({a, b}, k)-spheres

(R, k)-spheres: curvature $\kappa_i = 1 + \frac{i}{k} - \frac{i}{2}$ of *i*-gons

- Fix R ⊂ N, an (R, k)-sphere is a k-regular, k ≥ 3, map on S² whose faces are i-gons, i ∈ R. Let m=min and M=max_{i∈R} i.
- Let v, e and $f = \sum_{i} p_{i}$ be the numbers of vertices, edges and faces of S, where p_{i} is the number of *i*-gonal faces. Clearly, $kv=2e=\sum_{i} ip_{i}$ and Euler formula v e + f = 2 become $2=\sum_{i} p_{i}\kappa_{i}$, where $\kappa_{i}=1+\frac{i}{k}-\frac{i}{2}$ is the curvature of *i*-gons.
- So, m<^{2k}/_{k-2}. For m≥3, it implies 3 ≤ m, k ≤ 5, i.e. 5 Platonic pairs of parameters (m, k)=(3,3), (4,3), (3,4), (5,3), (3,5).
- If M<^{2k}/_{k-2} (min_{i∈R} κ_i>0), then either 1) k = 3, M ≤ 5, or 2) k ∈ {4,5}, M ≤ 3. So, for m ≥ 3, they are only Octahedron, Icosahedron and 11 ({3,4,5},3)-spheres: 8 dual *deltahedra*, Cube and its truncations on 1 or 2 opposite vertices (*Dürer octahedron*). In other words: five Platonic and eight ({3,4,5},3)-spheres.

Standard (R, k)-spheres

- An (R, k)-sphere is standard if M=^{2k}/_{k-2}, i.e. min_{i∈R} κ_i=0. So, (M, k)=(6,3), (4,4), (3,6) (Euclidean parameter pairs). Exclusion of *i*-faces with κ_i<0 simplifies enumeration, while number p_M of flat (κ_M=0) M-faces not being restricted, there is an infinity of such (R, k)-spheres.
- The number of such v-vertex (R, k)-spheres with |R|=2 increases polynomially with v.
 Such spheres admit parametrization and description in terms

of rings of (*Gaussian* if k=4 and *Eisenstein* if k=3, 6) *integers*. All eight series of such spheres will be considered in detail.

Remaining (R, k)-spheres (with M>^{2k}/_{k-2}, i.e. min_{i∈R} κ_i< 0) do not admit above, in general. We will consider only simplest case: ({3,4},5)-spheres. The number of such *v*-vertex spheres grows at least exponentially with *v*.

8 families of standard $(\{a, b\}, k)$ -spheres

- An $(\{a, b\}, k)$ -sphere is an (R, k)-sphere with $R = \{a, b\}$, $1 \le a < b$. It has $v = \frac{1}{k}(ap_a + bp_b)$ vertices.
- Such standard sphere has $b = \frac{2k}{k-2}$; so, (b,k) = (6,3), (4,4), (3,6) and Euler formula become $2 = \kappa_a p_a = (1 + \frac{a}{k} \frac{a}{2})p_a = (1 \frac{a}{b})p_a$.
- So, p_a = ^{2b}/_{b-a} and all possible (a, p_a) are: (5,12), (4,6), (3,4), (2,3) for (b, k)=(6,3); (3,8), (2,4) for (b, k)=(4,4); (2,6), (1,3) for (b, k)=(3,6).
- Those 8 families can be seen as spheric analogs of the regular plane partitions {6³}, {4⁴}, {3⁶} with p_a disclinations ("defects") κ_a added to get the curvature 2 of the sphere.

8 families: existence criterions

Grűnbaum-Motzkin, 1963: criterion for $k=3 \le a$; Grűnbaum, 1967: for ({3,4},4)-spheres; Grűnbaum-Zaks, 1974: for a = 1, 2.

k	(a, b)	smallest one	it exists if and only if	pa	V
3	(5,6)	Dodecahedron	$p_6 eq 1$	12	$20 + 2p_6$
3	(4,6)	Cube	$p_6 eq 1$	6	$8 + 2p_6$
4	(3,4)	Octahedron	$p_4 eq 1$	8	$6 + p_4$
6	(2,3)	$6 imes K_2$	p_3 is even	6	$2 + \frac{p_3}{2}$
3	(3,6)	Tetrahedron	p ₆ is even	4	$4 + 2p_{6}$
4	(2,4)	$4 imes K_2$	p ₄ is even	4	$2 + p_4$
3	(2,6)	$3 imes K_2$	$p_6 = (k^2 + kl + l^2) - 1$	3	$2 + 2p_{6}$
6	(1,3)	Trifolium	$p_3=2(k^2+kl+l^2)-1$	3	$\frac{1+p_3}{2}$
5	(3,4)	Icosahedron	$p_4 eq 1$	2 <i>p</i> ₄ +20	2 <i>p</i> ₄ +12

({3,6},3)- (Grűnbaum-Motzkin, 1963) and ({2,4},4)-spheres (Deza-Shtogrin, 2003) admit a simple 2-parametric description.

8 families of standard $(\{a, b\}, k)$ -spheres

- Let us denote $(\{a, b\}, k)$ -sphere with v vertices by $\{a, b\}_v$.
- ({5,6},3)- and ({4,6},3)-spheres are (geometric) fullerenes and boron nitrides. {5,6}₆₀(I_h): a new carbon allotrope C₆₀.
- ({*a*, *b*}, 4)-spheres are minimal projections of alternating links, whose components are their *central circuits* (those going only ahead) and crossings are the verices.
- By smallest member Dodecahedron {5,6}₂₀, Cube {4,6}₈, Tetrahedron {3,6}₄, Octahedron {3,4}₆ and 3×K₂ {2,6}₂, 4×K₂ {2,4}₂, 6×K₂ {2,3}₂, Trifolium {1,3}₁, we call eight families: dodecahedrites, cubites, tetrahedrites, octahedrites and 3-bundelites, 4-bundelites, 6-bundelites, trifoliumites.
- *b*-icosahedrites (({3, b}, 5)-spheres) are not standard if $b \ge 3$, $p_b \ge 0$, since $p_3 = p_b(3b-10)+20$ and $\kappa_b = \frac{10-3b}{10b} < 0$.

Generation of standard $(\{a, b\}, k)$ -spheres

- ({2,3},6)-spheres, except 2 × K₂ and 2 × K₃, are the duals of ({3,4,5,6},3)-spheres with six new vertices put on edge(s).
 Exp: ({5,6},3)-spheres with 5-gons organized in six pairs.
- ({1,3},6)-spheres, except {1,3}₁ and {1,3}₃, are as above but with 3 edges changed into 2-gons enclosing one 1-gon.
- ({2,6},3)-spheres are given by the Goldberg-Coxeter construction from Bundle₃ = 3 × K₂ {2,6}₂.
- ({1,3},6)-spheres come by the *Goldberg-Coxeter construction* (extended below on 6-regular spheres) from Trifolium {1,3}₁.

III. $(\{a, b\}, k)$ -spheres with small p_b : listings

$(\{a, b\}, k)$ -spheres with $p_b \leq 2 < a < b$

- Remind: (*a*, *k*)=(3, 3), (4, 3), (3, 4), (5, 3), (3, 5) if *k*, *a* ≥ 3.
- The only ({a, b}, k)-spheres with p_b ≤ 1 are 5 Platonic (a^k): Tetrahedron, Cube (Prism₄), Octahedron (APrism₃), Dodecahedron (snub Prism₅), Icosahedron (snub APrism₃).
- There exists unique trivial 3-connected ({a, b}, k)-sphere with p_b=2 for ({4, b}, 3)-, ({3, b}, 4)-, ({5, b}, 3)-, ({3, b}, 5)-: D_{bh} Prism_b and D_{bd} APrism_b, snub Prism_b, snub APrism_b: two b-gons separated by b-ring of 4-gons, 2b-ring of 3-gons, two b-rings of 5-gons, two 3b-rings of 3-gons.
- Also, for t≥2, 10 non-trivial ({a, at}, k)-spheres with p_{at}=2: 5 ({a, ta}, k)-spheres are (D_{th}) necklaces of polycycles {a^k}-e, 3 are (D_{th}) necklaces of t v-split {3⁴} and e-split {5³}, {3⁵}, ({3,3t}, 5)-spheres C_{th}, D_t are necklaces of t v-, f-split {3⁵}.

$(\{a, ta\}, k)$ -spheres with $p_{ta} = 2$, k=3, 4, 5; case t=2











Proof method: elementary (a, k)-polycycles

- A (a, k)-polycycle is a 2-connected plane graph with faces partitioned in a-gonal proper faces and holes, exterior face among them, so that vertex degrees are in {2,...,k} and can be < k only for a vertex lying on the boundary of a hole.
- Any (*a*, *k*)-polycycle decomposes uniquely along its bridges (non-boundary going hole-to-hole, possibly, same, edges) into elementary ones. Cf. integer factorisation into primes.
- We listed them for $\kappa_a = 1 + \frac{a}{k} \frac{a}{2} \ge 0$. Othervise, continuum.



This $({5,15},3)$ -sphere with $p_{15}=3$ is a 3-holes $({5},3)$ -polycycle It decomposes into five 1-hole elementary $({5},k)$ -polycycles.

- ({a, b}, k)-sphere with p_b = 3 exists if and only if b ≡ 2, a, 2a - 2 (mod 2a) and b ≡ 4, 6 (mod 10) if a=5.
- Such sphere are unique if b is not ≡ a (mod 2a) and then their symmetry is D_{3h}, except when (a, k) = (3, 5) when the symmetry is D₃.
- There are 7 such spheres with $t = \lfloor \frac{b}{6} \rfloor = 0$ and 3+4+5+17 of them for any $t \ge 1$.

IV. 8 standard families:4 smallest members

First four $({4,6},3)$ - and $({5,6},3)$ -spheres



First four $(\{2,6\},3)$ - and $(\{3,6\},3)$ -spheres

Number of $(\{2,6\}_{v}$'s is nr. of representations $v=2(k^{2}+kl+l^{2})$, $0 \le l \le k$ $(GC_{k,l}(\{2,6\}_{2}))$. It become 2 for $v=7^{2}=5^{2}+15+3^{2}$.



First four $({2,4}, 4)$ - and $({3,4}, 4)$ -spheres



Above links/knots are given in Rolfsen, 1976 and 1990 notation. Herschel graph: the smallest non-Hamiltonian polyhedral graph.

First four $(\{2,3\},6)$ - and $(\{1,3\},6)$ -spheres



Grűnbaum-Zaks, 1974: $\{1,3\}_{\nu}$ exists iff $\nu = k^2 + kl + l^2$ for integers $0 \le l \le k$. We show that the number of $\{1,3\}_{\nu}$'s is the number of such representations of ν , i.e. found $GC_{k,l}(\{1,3\}_1)$.

V. Symmetry groups of $(\{a, b\}, k)$ -spheres

All finite groups of isometries of 3-space \mathbb{E}^3 are classified. In Schoenflies notations, they are:

- C₁ is the trivial group
- C_s is the group generated by a plane reflexion
- $C_i = \{I_3, -I_3\}$ is the inversion group
- C_m is the group generated by a rotation of order m of axis Δ
- C_{mv} (\simeq dihedral group) is the group generated by C_m and m reflexion containing Δ
- $C_{mh} = C_m \times C_s$ is the group generated by C_m and the symmetry by the plane orthogonal to Δ
- S_{2m} is the group of order 2m generated by an antirotation, i.e. commuting composition of a rotation and a plane symmetry

Finite isometry groups D_m , D_{mh} , D_{md}

- D_m (\simeq dihedral group) is the group generated of C_m and m rotations of order 2 with axis orthogonal to Δ
- D_{mh} is the group generated by D_m and a plane symmetry orthogonal to Δ
- D_{md} is the group generated by D_m and m symmetry planes containing Δ and which does not contain axis of order 2



Remaining 7 finite isometry groups

- $I_h = H_3$ is the group of isometries of Dodecahedron; $I_h \simeq A l t_5 \times C_2$
- $I \simeq A l t_5$ is the group of rotations of Dodecahedron
- $O_h = B_3$ is the group of isometries of Cube
- $O \simeq Sym(4)$ is the group of rotations of Cube
- $T_d = A_3 \simeq Sym(4)$ is the group of isometries of Tetrahedron
- $T \simeq A l t (4)$ is the group of rotations of Tetrahedron
- $T_h = T \cup -T$

While (point group) $Isom(P) \subset Aut(G(P))$ (combinatorial group), Mani, 1971: for any 3-polytope P, there is a map-isomorphic 3-polytope P' (so, with the same skeleton G(P') = G(P)), such that the group Isom(P') of its isometries is isomorphic to Aut(G).

8 families: symmetry groups

- **2**8 for $\{5,6\}_{\nu}$: C_1 , C_s , C_i ; C_2 , $C_{2\nu}$, C_{2h} , S_4 ; C_3 , $C_{3\nu}$, C_{3h} , S_6 ; D_2 , D_{2h} , D_{2d} ; D_3 , D_{3h} , D_{3d} ; D_5 , D_{5h} , D_{5d} ; D_6 , D_{6h} , D_{6d} ; T, T_d , T_h ; I, I_h (Fowler-Manolopoulos, 1995)
- **2** 16 for $\{4, 6\}_{v}$: C_1 , C_s , C_i ; C_2 , C_{2v} , C_{2h} ; D_2 , D_{2h} , D_{2d} ; D_3 , D_{3h} , D_{3d} ; D_6 , D_{6h} ; O, O_h (Deza-Dutour, 2005)
- **3** 5 for $\{3,6\}_{v}$: D_2 , D_{2h} , D_{2d} ; T, T_d (Fowler-Cremona,1997)
- I for {2,6}_v: D₃, D_{3h} (Grünbaum-Zaks, 1974)
- **(a)** 18 for $\{3, 4\}_{\nu}$: C_1 , C_s , C_i ; C_2 , $C_{2\nu}$, C_{2h} , S_4 ; D_2 , D_{2h} , D_{2d} ; D_3 , D_{3h} , D_{3d} ; D_4 , D_{4h} , D_{4d} ; O, O_h (Deza-Dutour-Shtogrin, 2003)
- **5** for $\{2,4\}_{v}$: D_2 , D_{2h} , D_{2d} ; D_4 , D_{4h} , all in $[D_2, D_{4h}]$ (same)
- **3** for $\{1,3\}_{v}$: C_{3} , C_{3v} , C_{3h} (Deza-Dutour, 2010)
- **3** 22 for $\{2,3\}_{\nu}$: C_1 , C_s , C_i ; C_2 , $C_{2\nu}$, C_{2h} , S_4 ; C_3 , $C_{3\nu}$, C_{3h} , S_6 ; D_2 , D_{2h} , D_{2d} ; D_3 , D_{3h} , D_{3d} ; D_6 , D_{6h} ; T, T_d , T_h (same)

38 for icosahedrites $({3,4}, 5)$ - (same, 2011).

8 families: Goldberg-Coxeter construction $GC_{k}(.)$ $C_m = \{C_m, C_{mv}, C_{mh}, S_{2m}\}, D_m = \{D_m, D_{mh}, D_{md}\}, \text{ we get }$ **1** for $(\{5, 6\}, 3)$ -: C₁, C₂, C₃, D₂, D₃, D₅, D₆, T, I 2 for $(\{2,3\},6)$ -: C₁, C₂, C₃, D₂, D₃, $\{D_6, D_{6h}\}$, T **(** $\{4, 6\}, 3$)-: **C**₁, **C**₂\S₄, **D**₂, **D**₃, { D_6, D_{6h} }, **O** • for $(\{3,4\},4)$ -: C₁, C₂, D₂, D₃, D₄, O **5** for $(\{3, 6\}, 3-: \mathbf{D}_2, \{T, T_d\}, \{D_3, D_{3h}\}$ **6** for $(\{2,4\},4)$ -: **D**₂, $\{D_4, D_{4h}\}$ • for $(\{2, 6\}, 3)$ -: $\{D_3, D_{3h}\}$ **8** for $(\{1,3\},6)$ -: **C**₃\ $S_6 = \{C_3, C_{3\nu}, C_{3h}\}$

if $(\{3,4\},5)$ -: C₁, C₂, C₃, C₄, C₅, D₂, D₃, D₄, D₅, T, O, I.

8 families: Goldberg-Coxeter construction $GC_{k}(.)$ $C_m = \{C_m, C_{mv}, C_{mh}, S_{2m}\}, D_m = \{D_m, D_{mh}, D_{md}\}, \text{ we get }$ **1** for $(\{5, 6\}, 3)$ -: C₁, C₂, C₃, D₂, D₃, D₅, D₆, T, **1 2** for $(\{2,3\},6)$ -: C₁, C₂, C₃, D₂, D₃, $\{D_6, D_{6h}\}$, T **(** $\{4, 6\}, 3$)-: **C**₁, **C**₂\S₄, **D**₂, **D**₃, { D_6, D_{6h} }, **O** • for $(\{3,4\},4)$ -: C₁, C₂, D₂, D₃, D₄, O **5** for $(\{3, 6\}, 3-: \mathbf{D}_2, \{T, T_d\}, \{D_3, D_{3h}\}$ **6** for $(\{2,4\},4)$ -: **D**₂, $\{D_4, D_{4h}\}$

- for $(\{2,6\},3)$ -: $\{D_3, D_{3h}\}$
- **6** for $(\{1,3\},6)$ -: $C_3 \setminus S_6 = \{C_3, C_{3\nu}, C_{3h}\}$

if $(\{3,4\},5)$ -: **C**₁, **C**₂, **C**₃, **C**₄, **C**₅, **D**₂, **D**₃, **D**₄, **D**₅, **T**, **O**, **I**. Spheres of blue symmetry are $GC_{a,b}$ from 1st such; so, given by one complex (Gaussian for k=4, Eisenstein for k=3,6) parameter. Goldberg, 1937 and Coxeter, 1971: $\{5,6\}_{v}(I,I_{h}), \{4,6\}_{v}(O,O_{h}),$ $\{3,6\}_{v}(T,T_{d})$. Dutour-Deza, 2004 and 2010: for other cases. VI. Goldberg-Coxeter construction

Goldberg-Coxeter construction $GC_{k,l}(.)$

- Take a 3- or 4-regular plane graph *G*. The faces of dual graph *G*^{*} are triangles or squares, respectively.
- Break each face into pieces according to parameter (k, l).
 Master polygons below have area A(k²+kl+l²) or A(k²+l²), where A is the area of a small polygon.



Gluing the pieces together in a coherent way

 Gluing the pieces so that, say, 2 non-triangles, coming from subdivision of neighboring triangles, form a small triangle, we obtain another triangulation or quadrangulation of the plane.



- The dual is a 3- or 4-regular plane graph, denoted GC_{k,l}(G); we call it Goldberg-Coxeter construction.
- It works for any 3- or 4-regular map on oriented surface.

$GC_{k,l}(Cube)$ for (k, l) = (1, 0), (1, 1), (2, 0), (2, 1)



Goldberg-Coxeter construction from Octahedron









The case (k, l) = (1, 1)





3-regular case $GC_{1,1}$ is called leapfrog ($\frac{1}{3}$ -truncation of the dual) truncated Octahedron 4-regular case $GC_{1,1}$ is called medial $(\frac{1}{2}$ -truncation) Cuboctahedron

The case (k, l) = (k, 0) of $GC_{k,l}(G)$: k-inflation

Chamfering (quadrupling) $GC_{2,0}(G)$ of 8 1st $(\{a, b\}, k)$ -spheres, (a, b)=(2, 6), (3, 6), (4, 6), (5, 6) and (2, 4), (3, 4), (1, 3), (2, 3), are:



For 4-regular G, $GC_{2k^2,0}(G) = GC_{k,k}(GC_{k,k}(G))$ by $(k+ki)^2 = 2k^2i$.

First four $GC_{k,l}(3 \times K_2)$ and $GC_{k,l}(4 \times K_2)$

All ({2,6},3)-spheres are $G_{k,l}(3 \times K_2)$: D_{3h} , D_{3h} , D_3 if l=0, k, else.



First four $GC_{k,l}(6 \times K_2)$ and $GC_{k,l}(Trifolium)$



All ({2,3},6)-spheres are $G_{k,l}(6 \times K_2)$: C_{3v} , C_{3h} , C_3 if l=0, k, else.
Plane tilings $\{4^4\}$, $\{3^6\}$ and complex rings $\mathbb{Z}[i]$, $\mathbb{Z}[w]$

- The vertices of regular plane tilings {4⁴} and {3⁶} form each, convenient algebraic structures: lattice and ring. Path-metrics of those graphs are *I*₁- 4-*metric* and *hexagonal* 6-*metric*.
- {4⁴}: square lattice \mathbb{Z}^2 and ring $\mathbb{Z}[i] = \{z = k + li : k, l \in \mathbb{Z}\}$ of Gaussian integers with norm $N(z) = z\overline{z} = k^2 + l^2 = ||(k, l)||^2$.
- {3⁶}: hexagonal lattice $A^2 = \{x \in \mathbb{Z}^3 : x_0 + x_1 + x_2 = 0\}$ and ring $\mathbb{Z}[w] = \{z = k + lw : k, l \in \mathbb{Z}\}$, where $w = e^{i\frac{\pi}{3}} = \frac{1}{2}(1 + i\sqrt{3})$, of Eisenstein integers with norm $N(z) = z\overline{z} = k^2 kl + l^2$. We identify points $x = (x_0, x_1, x_2) \in A^2$ with $x_0 + x_1 w \in \mathbb{Z}[w]$.

Plane tilings $\{4^4\}$, $\{3^6\}$ and complex rings $\mathbb{Z}[i]$, $\mathbb{Z}[w]$

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- {4⁴}: square lattice Z² and ring Z[i]={z=k+li: k, l ∈ Z} of Gaussian integers with norm N(z)=zz=k²+l²=||(k, l)||².
- {3⁶}: hexagonal lattice $A^2 = \{x \in \mathbb{Z}^3 : x_0 + x_1 + x_2 = 0\}$ and ring $\mathbb{Z}[w] = \{z = k + lw : k, l \in \mathbb{Z}\}$, where $w = e^{i\frac{\pi}{3}} = \frac{1}{2}(1 + i\sqrt{3})$, of Eisenstein integers with norm $N(z) = z\overline{z} = k^2 kl + l^2$. We identify points $x = (x_0, x_1, x_2) \in A^2$ with $x_0 + x_1 w \in \mathbb{Z}[w]$.
- A natural number $n = \prod_i p_i^{\alpha_i}$ is of form $n = k^2 + l^2$ if and only if any α_i is even, whenever $p_i \equiv 3 \pmod{4}$ (Fermat Theorem). It is of form $n = k^2 + kl + l^2$ if and only if $p_i \equiv 2 \pmod{3}$.
- The first cases of non-unicity with $gcd(k, l)=gcd(k_1, l_1)=1$ are $91=9^2+9+1^2=6^2+30+5^2$ and $65=8^2+1^2=7^2+4^2$. The first cases with l=0 are $7^2=5^2+15+3^2$ and $5^2=4^2+3^2$.

The bilattice of vertices of hexagonal plane tiling $\{6^3\}$

- We identify the hexagonal lattice A² (or equilateral triangular lattice of the vertices of the regular plane tiling {3⁶}) with Eisenstein ring (of Eisenstein integers) Z[w].
- The hexagon centers of $\{6^3\}$ form $\{3^6\}$. Also, with vertices of $\{6^3\}$, they form $\{3^6\}$, rotated by 90° and scaled by $\frac{1}{3}\sqrt{3}$.
- The complex coordinates of vertices of {6³} are given by vectors v₁=1 and v₂=w. The lattice L=ℤv₁+ℤv₂ is ℤ[w].
- The vertices of {6³} form bilattice L₁ ∪ L₂, where the bipartite complements, L₁=(1+w)L and L₂=1+(1+w)L, are stable under multiplication. Using this,

 $GC_{k,l}(G)$ for 6-regular graph G can be defined similarly to 3- and 4-regular case, but only for $k + lw \in L_2$, i.e. $k \equiv l \pm 1 \pmod{3}$.

$\mathbb{Z}[i]$ (Gaussian integers) and $\mathbb{Z}[\omega]$ (Eisenstein integers) are unique factorization rings

Dictionary

	3-regular G	4-regular G	6-regular G
the ring	Eisenstein $\mathbb{Z}[\omega]$	Gaussian $\mathbb{Z}[i]$	Eisenstein $\mathbb{Z}[\omega]$
Euler formula	$\sum_i (6-i)p_i = 12$	$\sum_i (4-i)p_i = 8$	$\sum_i (3-i)p_i = 6$
curvature 0	hexagons	squares	triangles
ZC-circuits	zigzags	central circuits	both
$GC_{11}(G)$	leapfrog graph	medial graph	or. tripling

Goldberg-Coxeter operation in ring terms

- Associate z=k+lw (Eisenstein) or z=k+li (Gaussian integer) to the pair (k, l) in 3-,6- or 4-regular case. Operation $GC_z(G)$ correspond to scalar multiplication by z=k+lw or k+li.
- Writing $GC_z(G)$, instead of $GC_{k,l}(G)$, one has:

 $GC_z(GC_{z'}(G)) = GC_{zz'}(G)$

• If G has v vertices, then $GC_{k,l}(G)$ has vN(z) vertices, i.e., $v(k^2+l^2)$ in 4-regular and $v(k^2+kl+l^2)$ in 3- or 6-reg. case.

Goldberg-Coxeter operation in ring terms

- Associate z=k+lw (Eisenstein) or z=k+li (Gaussian integer) to the pair (k, l) in 3-,6- or 4-regular case. Operation GC_z(G) correspond to scalar multiplication by z=k+lw or k+li.
- Writing $GC_z(G)$, instead of $GC_{k,l}(G)$, one has:

$GC_z(GC_{z'}(G)) = GC_{zz'}(G)$

- If G has v vertices, then $GC_{k,l}(G)$ has vN(z) vertices, i.e., $v(k^2+l^2)$ in 4-regular and $v(k^2+kl+l^2)$ in 3- or 6-reg. case.
- GC_z(G) has all rotational symmetries of G in 3- and 4-regular case, and all symmetries if *I*=0, *k* in general case.
- $GC_z(G) = GC_{\overline{z}}(\overline{G})$ where \overline{G} differs by a plane symmetry only from G. So, if G has a symmetry plane, we reduce to $0 \le l \le k$; otherwise, graphs $GC_{k,l}(G)$ and $GC_{l,k}(G)$ are not isomorphic.

$GC_{k,l}(G)$ for 6-regular plane graph G and any k, l

- Bipartition of G^* gives vertex 2-coloring, say, red/blue of G.
- Truncation Tr(G) of $\{1, 2, 3\}_v$ is a 3-regular $\{2, 4, 6\}_{6v}$.
- Coloring white vertices of G gives face 3-coloring of Tr(G). White faces in Tr(G) correspond to such in $GC_{k,l}(Tr(G))$.
- For $k \equiv l \pm 1 \pmod{3}$, i.e. $k + lw \in L_2$, define $GC_{k,l}(G)$ as $GC_{k,l}(Tr(G))$ with all white faces shrinked.
- If k ≡ l((mod 3), faces of Tr(G) are white in GC_{k,l}(Tr(G)). Among 3 faces around each vertex, one is white. Coloring other red gives unique 3-coloring of GC_{k,l}(Tr(G)). Define GC_{k,l}(G) as pair G₁, G₂ with Tr(G₁)=Tr(G₂)=GC_{k,l}(Tr(G)) obtained from it by shrinking all red or blue faces.
- $GC_{1,0}(G) = G$ and $GC_{1,1}(G)$ is oriented tripling.

Oriented tripling $GC_{1,1}(G)$ of 6-regular plane graph G

- Let C_1, C_2 be bipartite classes of G^* . For each C_i , oriented tripling $GC_{1,1}(G)$ is 6-regular plane graph $Or_{C_i}(G)$ coming by each vertex of $G \rightarrow 3$ vertices and 4 3-gonal faces of $Or_{C_i}(G)$. Symmetries of $Or_{C_i}(G)$ are symmetries of G preserving C_i .
- Orient edges of C_i clockwise. Select 3 of 6 neighbors of each vertex v: {2,4,6} are those with directed edge going to v; for {1,5,5}, edges go to them.



• Any $z=k+lw\neq 0$ with $k\equiv l \pmod{3}$ can be written as $(1+w)^{s}(k'+l'w)w$, where $s\geq 0$ and $k'\equiv l'\pm 1 \pmod{3}$. So, it holds reduction $GC_{k,l}(G)=G_{k',l'}(Or^{s}(G))$.

Examples of oriented tripling $GC_{1,1}(G)$

Below: $\{2,3\}_2$ and $\{2,3\}_4$ have *unique* oriented tripling.



Examples of oriented tripling $GC_{1,1}(G)$

Below: $\{2,3\}_2$ and $\{2,3\}_4$ have *unique* oriented tripling.



Above: first 4 consecutive oriented triplings of the Trifolium.

VII. Parameterizing $(\{a, b\}, k)$ -spheres

Example: construction of the $({3,6},3)$ -spheres in $Z[\omega]$



In the central triangle ABC, let A be the origin of the complex plane



The corresponding triangulation



All $(\{3, 6\}, 3)$ -spheres come this way; two complex parameters in $Z[\omega]$ defined by the points B and C

Parameterizing standard $(C_b = 0)$ $(\{a, b\}, k)$ -spheres

Thurston, 1998 implies: $(\{a, b\}, k)$ -spheres have p_a -2 parameters and the number of *v*-vertex ones is $O(v^{m-1})$ if $m=p_a$ -2 > 2. Idea: since *b*-gons are of zero curvature, it suffices to give relative positions of *a*-gons having curvature 2k - a(k-2) > 0. At most $p_a - 1$ vectors will do, since one position can be taken 0. But once $p_a - 1$ a-gons are specified, the last one is constrained. The number of *m*-parametrized spheres with at most *v* vertices is $O(v^m)$ by direct integration. The number of such *v*-vertex spheres is $O(v^{m-1})$ if m > 1, by a Tauberian theorem.

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- Goldberg, 1937: $\{a, 6\}_{v}$ (highest 2 symmetries): 1 parameter
- Fowler and al., 1988: $\{5,6\}_{\nu}$ (D_5 , D_6 or T): 2 parameters.
- Grűnbaum-Motzkin, 1963: $\{3,6\}_{\nu}$: 2 parameters.
- Deza-Shtogrin, 2003: $\{2,4\}_{v}$; 2 parameters.
- Thurston, 1998: {5,6}_v: 10 (again complex) parameters.
 Graver, 1999: {5,6}_v: 20 integer parameters.
- Rivin, 1994: parameter desciption by dihedral angles.

Thurston, 1998 parametrized (dually, as triangulations) such (R, 3)-spheres, i.e. 19 series of $(\{3, 4, 5, 6\}, 3)$ -spheres. In general, such (R, k)-spheres are given by $m = \sum_{3 \le i < \frac{2k}{k-2}} p_i - 2$ complex parameters z_1, \ldots, z_m . The number of vertices is expressed as a non-degenerate Hermitian form $q=q(z_1,\ldots,z_m)$ of signature (1,m-1). Let H^m be the cone of $z=(z_1,\ldots,z_m)\in\mathbb{C}^m$ with q(z)>0. Given (R, k)-sphere is described by different parameter sets; let $M = M(\{p_3, \ldots, p_m\}, k)$ be the discrete linear group preserving q. For k=3, the quotient $H^m/(\mathbb{R}_{>0} \times M)$ is of finite covolume (Thurston, 1998, actually, 1993). Sah, 1994 deduced from it that the number of corresponding spheres grows as $O(v^{m-1})$. Dutour partially generalized above for other k and surface maps.

8 families: number of complex parameters by groups

- **•** $\{5,6\}_{\nu}$ C₁(10), C₂(6), C₃(4), D₂(4), D₃(3), D₅(2), D₆(2), T(2), $\{I, I_h\}(1)$
- **2** $\{4,6\}_{v}$ **C**₁(4), **C**₂\S₄(3), **D**₂(2), **D**₃(2), $\{D_6, D_{6h}\}(1)$, $\{O, O_h\}(1)$
- **3** $\{3,4\}_{v}$ C₁(6), C₂(4), D₂(3), D₃(2), D₄(2), $\{O, O_h\}(1)$
- **a** $\{2,3\}_{v}$ **C**₁(4), **C**₂(3?), **C**₃(3?), **D**₂(2?), **D**₃(2?), **T**(1), $\{D_6, D_{6h}\}(1)$
- **5** $\{3,6\}_{v}$ **D**₂(2), $\{T, T_{d}\}(1)$
- **6** $\{2,4\}_{\nu}$ **D**₂(2), $\{D_4, D_{4h}\}(1)$
- **(2,6)**_v $\{D_3, D_{3h}\}(1)$
- **3** $\{1,3\}_{\nu}$ $\{C_3, C_{3\nu}, C_{3h}\}(1)$

Thurston, 1998 implies: $(\{a, b\}, k)$ -spheres have p_a -2 parameters and the number of *v*-vertex ones is $O(v^{m-1})$ if $m=p_a$ -2 > 1.

Number of complex parameters



 $\{3,6\}_{\nu}$ and $\{2,4\}_{\nu}$: 2 complex parameters but 3 natural ones will do: *pseudoroad* length, number of circumscribing *railroads*, *shift*.

VIII. Railroads and tight ({a, b}, k)-spheres

ZC-circuits

- The edges of any plane graph are doubly covered by zigzags (Petri or left-right paths), i.e., circuits such that any two but not three consecutive edges bound the same face.
- The edges of any *Eulerian* (i.e., even-valent) plane graph are partitioned by its central circuits (those going straight ahead).
- A ZC-circuit means *zigzag* or *central circuit* as needed. CC- or Z-vector enumerate lengths of above circuits.

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- The edges of any *Eulerian* (i.e., even-valent) plane graph are partitioned by its central circuits (those going straight ahead).
- A ZC-circuit means *zigzag* or *central circuit* as needed. CC- or Z-vector enumerate lengths of above circuits.
- A railroad in a 3-, 4- or 6-regular plane graph is a circuit of 6-, 4- or 3-gons, each adjacent to neighbors on opposite edges. Any railroad is bound by two "parallel" ZC-circuits. It (any if 4-, simple if 3- or 6-regular) can be collapsed into 1 ZC-circuit.





Railroad in a 6-regular sphere: examples

*APrism*₃ with 2 base 3-gons doubled is the $\{2,3\}_6$ (D_{3d}) with CC-vector ($3^2, 4^3$), all five central circuits are simple. Base 3-gons are separated by a simple railroad *R* of six 3-gons, bounded by two parallel central 3-circuits around them. Collapsing *R* into one 3-circuit gives the $\{2,3\}_3$ (D_{3h}) with CC-vector (3; 6).



Above $\{2,3\}_4$ (T_d) has no railroads but it is not strictly tight, i.e. no any central circut is adjacent to a non-3-gon *on each side*.

Railroads can be simple or self-intersect, including triply if k = 3. First such Dutour ($\{a, b\}, k$)-spheres for (a, b) = (4, 6), (5, 6) are:



Which plane curves with at most triple self-intersectionss come so?

Number of ZC-circuits in tight $(\{a, b\}, k)$ -sphere

Call an $(\{a, b\}, k)$ -sphere tight if it has no railroads.

- ≤ 15 for $\{5, 6\}_{\nu}$ Shtogrin-Deza-Dutour, 2011
- $\bullet \leq 9$ for $\{4,6\}_{\nu}$ and $\{2,3\}_{\nu}$ Deza-Dutour, 2005 and 2010
- $\bullet\ \leq 3$ for $\{2,6\}_{\nu}$ and $\{1,3\}_{\nu}$ same
- \leq 6 for $\{3,4\}_v$ Deza-Shtogrin, 2003
- Any $\{3,6\}_{\nu}$ has ≥ 3 zigzags with equality iff it is tight. All $\{3,6\}_{\nu}$ are tight iff $\frac{\nu}{4}$ is prime > 2 and none iff it is even
- Any {2,4}_ν has ≥ 2 central circuits with equality iff it is tight. There is a tight one for any even ν.

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Call an $(\{a, b\}, k)$ -sphere tight if it has no railroads.

- $\bullet\ \leq 15$ for $\{5,6\}_{\nu}$ Shtogrin-Deza-Dutour, 2011
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- Any $\{3,6\}_{\nu}$ has ≥ 3 zigzags with equality iff it is tight. All $\{3,6\}_{\nu}$ are tight iff $\frac{\nu}{4}$ is prime > 2 and none iff it is even
- Any {2,4}_ν has ≥ 2 central circuits with equality iff it is tight. There is a tight one for any even ν.

First tight ones with max. of ZC-circuits are $GC_{21}(\{a, b\}_{min})$: {5,6}₁₄₀(*I*), {2,6}₁₄(*D*₃), {3,4}₃₀(0); and {*a*, *b*}_{min}: {3,6}₄(*T*_d), {2,4}₂(*D*_{4h}) with ZC=(28¹⁵), (14³), (10⁶), (4³), (2²), all simple. {4,6}₈₈(*D*_{2h}) and {2,3}₄₄(*D*_{3h}) are smallest with 8 zigzags.

Maximal number M_v of central circuits in any $\{2,3\}_v$

- $M_v = \frac{v}{2} + 1$, $\frac{v}{2} + 2$ for $v \equiv 0, 2 \pmod{4}$. It is realized by the series of symmetry D_{2d} with CC-vector $2^{\frac{v}{2}}, 2v_{0,v}$ and of symmetry D_{2h} with CC-vector $2^{\frac{v}{2}}, v_{0}^2 \frac{v-2}{2}$ if $v \equiv 0, 2 \pmod{4}$.
- For odd v, M_v is $\lfloor \frac{v}{3} \rfloor + 3$ if $v \equiv 2, 4, 6 \pmod{9}$ and $\lfloor \frac{v}{3} \rfloor + 1$, otherwise. Define t_v by $\frac{v-t_v}{3} = \lfloor \frac{v}{3} \rfloor$. M_v is realized by the series of symmetry C_{3v} if $v \equiv 1 \pmod{3}$ and D_{3h} , otherwise. CC-vector is $3^{\lfloor \frac{v}{3} \rfloor}, (2 \lfloor \frac{v}{3} \rfloor + t_v)_{0, \lfloor \frac{v-2t_v}{9} \rfloor}^3$ if $v \equiv 2, 4, 6 \pmod{9}$ and $3^{\lfloor \frac{v}{3} \rfloor}, (2v + t_v)_{0, v+2t_v}$, otherwise.

Smallest CC-knotted or Z-knotted $\{2,3\}_{v}$

- The minimal number of central circuits or zigzags, 1, have CC-knotted and Z-knotted {2,3}_v. They correspond to plane curves with only triple self-intersection points. For v≤16, there are 1, 2, 4, 7, 9, 12 Z-knotted if v=3, 7, 9, 11, 13, 15 and 1, 2, 2, 4, 11, 9, 1, 19 CC-knotted if v=4, 6, 8, 10, 12, 14, 15, 16.
- Conjecture (holds if v≤54): any Z-knotted {2,3}_v has odd v and a CC-knotted {2,3}_v is Z-knotted if and only if v is odd.



IX. Tight pure $(\{a, b\}, k)$ -spheres

Tight $(\{a, b\}, k)$ -spheres with only simple ZC-circuits

- Call ({*a*, *b*}, *k*)-sphere pure if any of its ZC-circuits is *simple*, i.e. has no self-intersections.
- Any ({3,6},3)- or ({2,4},4)-sphere is pure. They are tight if and only if have three or, respectively, two ZC-circuits.
- Any ZC-circuit of $\{2,6\}_{\nu}$ or $\{1,3\}_{\nu}$ self-intersects.

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- Any ({3,6},3)- or ({2,4},4)-sphere is pure. They are tight if and only if have three or, respectively, two ZC-circuits.
- Any ZC-circuit of $\{2,6\}_{\nu}$ or $\{1,3\}_{\nu}$ self-intersects.
- The number of tight pure $(\{a, b\}, k)$ -spheres is:
 - **9**? for $\{5, 6\}_v$ computer-checked for $v \leq 200$
 - 2 for $\{4, 6\}_v$
 - **3** 8 for $\{3, 4\}_{v}$
 - 5 for $\{2,3\}_v$
 - for $\{2,4\}_{v}$: ≥ 1 for any possible (i.e. even) v
 - So for {3,6}_ν: ≥ 1 for any odd ^ν/₄ (all if it is prime > 2 and none if it is even)
 - \bigcirc 0 for $\{2,6\}_{v}$ and $\{1,3\}_{v}$

All tight $(\{4, 6\}, 3)$ -spheres with only simple zigzags

There are exactly two such spheres: Cube and its leapfrog $GC_{11}(Cube)$, truncated Octahedron.



All tight $(\{4, 6\}, 3)$ -spheres with only simple zigzags

There are exactly two such spheres: Cube and its leapfrog $GC_{11}(Cube)$, truncated Octahedron.



Proof is based on a) The size of intersection of two simple zigzags in any ({4,6},3)-sphere is 0,2,4 or 6 and
b) Tight ({4,6},3)-sphere has at most 9 zigzags.
For ({2,3},6)-spheres, a) holds also, implying a similar result.

All tight $(\{3,4\},4)$ -spheres with only simple central circuits

The medial of a connected plane graph G = (X, E) is the graph Med(G) of edges of G with two being adjacent if they have a common vertex and bound the same face. Med(G) is a 4-regular plane graph; its central circuits correspond to zizags of G. 1st and 2nd below are the medials of Tetrahedron and Cube.



8 tight $({5,6},3)$ -spheres with only simple zigzags



The medials of 1 - 4, 6, 8-th above and of next one form complete arrangements of pseudocircles (CAP), i.e. any two intersect twice. Among 9, only 1, 4, 6, 8-th above are zigzag-transitive.

Other such 60-vertex $({5, 6}, 3)$ -sphere



This pair was first answer on a question in Grűnbaum, 1967, 2003 Convex Polytopes about existence of different simple polyhedra with the same p-vector and Z-vector.

Both have 60 vertices of degree 3; 12 5- and 20 6-gonal faces; and 10 (simple) zigzags of length 18 each. But they are different and their groups have, 1 and 3 orbits, respectively, on zigzags.

Pseudocircles arrangements from tight pure spheres

- A simple central circuit can be seen as a Jordan curve, i.e. a simple and closed plane curve.
- A (k, t)-AP (arrangements of pseudocircles) is a set of k Jordan curves where any two intersect (triple or tangent points excluded) exactly in t points; so, there are t(k-1) points. It is a tight pure 4-regular graph with k central circuits of length t(k-1) intersecting pairwise in t points. It is a projection of a link; Borromean rings is (3, 2)-AP.
- For $F_{20}(I_h)$, $F_{28}(T_d)$, $F_{48}(D_3)$, $F_{60}(I_h)$, $F_{60}D_3$, $F_{88}(T)$, $F_{140(I)}$, their medials form (k, 2)-APs with k = 6, 7, 9, 10, 10, 12, 15.
- The medials of truncated Tetrahedron, Cube, Icosahedron, Dodecahedron form (3, 6)-,(4, 6)-,(10, 2)-,(6, 6)-APs.
- For Oc₆(O_h), Oc₁₂(O_h), Oc₁₂(D_{3h}), Oc₂₀(D_{2d}), Oc₃₀(0), their central circuits form (k, 2)-APs with k = 3, 4, 4, 5, 6.

Tight $(\{2,3\},6)$ -spheres with only simple ZC-circuits



All CC-pure, tight: Nrs. 1,2,4,5,6 (Nrs. 3,7 are not CC-pure). All Z-pure, tight: Nrs. 1,2,3,6,7 (4 is not Z-pure, 5 is not Z-tight). 1st, 3rd are strictly CC-, Z-tight: all ZC-circuits sides touch 2-gons
X. Other fullerene analogs: $({a, b, c}, k)$ -disks $(p_c=1)$

Other fullerene-like non-standard (min_{*i*∈*R*} κ_i < 0) spheres

Related non-standard (*R*, *k*)-spheres with $\kappa_{\max\{i \in R\}} < 0$, are:

- G-fulleroids (Deza-Delgado, 2000; Jendrol-Trenkler, 2001 and Kardos, 2007): ({5, b}, 3)-spheres with b≥7 and symmetry G.
- *b*-lcosahedrites: $(\{3, b\}, 5)$ -spheres with $b \ge 4$. They have $p_3=(3b-10)p_b+20$ 3-gons and $v=2(b-3)p_b+12$ vertices. Snub Cube and Snub Dodecahedron are the cases (b, v; group)=(4, 24; O) and (5, 60; I).
- Haeckel, 1887: ({5,6, c}, 3)-spheres with c = 7,8 representing skeletons of radiolarian zooplankton Aulonia hexagona.
- ({a, b, c}, k)-disk is an ({a, b, c}, k)-sphere with p_c = 1; so, its v=²/_{k-2}(p_a-1+p_b)=²/_{2k-a(k-2)}(a+c+p_b(b-a)) and (setting b'=^{2k}/_{k-2}) p_a=^{b'+c}/_{b'-a}+p_b^{b-b'}/_{b'-a}. So, p_a=^{b+c}/_{b-a} if b=b' (8 families). An ({a, b, c}, k)-disk is non-standard iff max{a, b, c} > ^{2k}/_{k-2}.
 Fullerene *c*-disk is the case (a, b, c; k) = (5, 6, c; 3) of above. So, they have p₅ = c + 6 and v = 2(p₆ + c + 5) vertices.

Fullerene *c*-disks: big picture

- Fullerene *c*-polycycle: an *c*-gon partitioned into 5- and 6-gons with vertices of degree 3 inside and 3 or 2 on the *c*-gon.
- Fullerene *c*-disk: full. *c*-polycycle without vertices of degree 2; so, *p*₅ = *p*₆ + 6. If *c* ∈ {5,6}, it is a fullerene without a face.
- Fullerene c-patch: full. c-polycycle which is a fullerene's part; so, p₅ ≤ 12. It is a fullerene c-disk if and only if c ∈ {5,6}.
- Theorem: full. c-disk with a face having ≥2 common edges with c-gon (so, non-3-connected) exists if and only if c ≥ 8. So, any fullerene c-disk with 3 ≤ c ≤ 7 is polyhedral. Conjecture (checked for c ≤ 20):
 - 1) minimal fullerene *c*-disk has 2(c + 11) vertices if $c \ge 13$.
 - 2) Only 3 gap full. c-disks: (c, v) = (5, 22), (3, 24), (1, 42).
- Fullerene *c*-thimble: a full. *c*-disk with only 5-gons adjacent to the *c*-gon. It exists if and only if $c \ge 5$, always polyhedral. Conjecture: minimal fullerene *c*-thimble has 5c 5 or 5c 6 vertices for odd or even, respectively, $c \ge 5$.

Reducibility of fullerene *c*-disks

- In a full. *c*-disk, a zigzag is an edge-circuit alternating left and right turns. The zigzags doubly cover the edges.
- A belt is simple circuit of 6-gons, adjacent to their neighbors on opposite faces. It is bounded by 2 disjoint simple zigzags. Call a fullerene *c*-disk is reducible if it has a belt.
- The belts of a full. *c*-thimble form a cylinder. So, *c*-thimbles are cuts of full. nanotubes: *c*-belt → two *c*-rings of 5-gons.
- Any simple zigzag in an irreducible full. *c*-disk has adjacent
 5-gon on each side and intersects any other simple zigzag.
 So, the number of simple zigzags is at most ^{5(c+6)}/₂.
- Each zigzag of an irreducible pure (all zigzags are simple) fullerene, is adjacent to at least two 5-gons on each side. So, their number is ≤ ⁵⁽⁶⁺⁶⁾/₄=15. F₁₄₀(I) has Z-vector 28¹⁵.
- Conjecture: pure irreducible fullerenes are only 9 fullerenes $F_v(G)$ with $(v, G) = (20, I_h), (28, T_d), (48, D_3), (60, I_h)$ and $(60, D_3), (76, D_{2d}), (88, T), (92, T_h), (140, I).$

Minimal fullerene *c*-disks for $1 \le c \le 8$

It is 1-vertex-, 1-edge-truncated, usual F_{20} , F_{24} for c=3, 4, 5, 6. It comes from minimal 4-disk for c=2: add edge with 2-gon on it. Checked for $c\leq20$: it has $p_6=14, 6, 3, 2, 0, 1, 3, 4, 6, 7, 8, 5$ and =6 if $1\leq c\leq12$ and $c\geq13$. Unique unless 2, 3, 10 for c=9, 10, 11.



 $1 \ 40 \ C_s \qquad 2 \ 26 \ C_{2v} \qquad 3 \ 22 \ C_{3v} \qquad 4 \ 22 \ C_{2v}$



5 20 I_h

6 24 D_{6d}

7 30 Cs



Minimal fullerene *c*-disks for $c \ge 9$



Conjecture: for $c \ge 13$, the only minimal *c*-disk is *c*-pentatube

 $B+Hex_3+Pen_{c-12}+Hex_3+B$ (symmetry C_s/C_2 for odd/even c).

Symmetries of fullerene c-disks

- Their groups: C_m, C_{mv} with m ≡ 0(mod c) (since any symmetry should stabilize unique c-gonal face) and m ∈ {1, 2, 3, 5, 6} since the axis pass by a vertex, edge or face.
- The minimal such 8- and 9-disks are given below.





9 40 C_{3v}



9 40 Cs



9 42 C₁

9 52 C_3

XI. Icosahedrites: $({3, 4}, 5)$ -spheres

Icosahedrites, i.e., $({3,4}, 5)$ -spheres

- They have $p_3 = 2p_b + 20$ and $v = 2p_b + 12$ vertices.
- Their number is 1, 0, 1, 1, 5, 12, 63, 246, 1395, 7668, 45460 for v = 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32. It grows at least exponentially with v.
- p_a is fixed in for standard ({a, b}, k)-spheres permitting Goldberg-Coxeter construction and parametrization of graphs which imply the polynomial growth of their number. It does not happen for icosahedrites; no parametrization for them.



A-operation keeps symmetries; B-operation: only rotational ones.

Proof for the number of icosahedrites

A weak zigzag ia a left/right, but never extreme, edge-circuit. If a *v*-vertex icosahedrite has a simple weak zigzag of length 6, a (v+6)-vertex one come by inserting a corona (6-ring of three 4-gons alternated by three pairs of adjacent 3-gons) instead of it. But such spheres exist for v=18, 20, 22; so, for $v\equiv0,2,4(mod 6)$. There are two options of inserting corona; so, the number of *v*-vertex icosahedrites grows at least exponentially.



An usual (strong) zigzag is a left/right, both extreme, edge-circuit.

38 symmetry groups of icosahedrites

- Agregating $C_1 = \{C_1, C_s, C_i\}$, $C_m = \{C_m, C_{mv}, C_{mh}, S_{2m}\}$, $D_m = \{D_m, D_{mh}, D_{md}\}$, $T = \{T, T_d, T_h\}$, $O = \{O, O_h\}$, $I = \{I, I_h\}$, all 38 symmetries of $(\{3, 4\}, 5)$ -spheres are: C_1 , C_m , D_m for $2 \le m \le 5$ and T, O, I.
- Any group appear an infinite number of times since one gets an infinity by applying *A*-operation iteratively.
- Group limitations came from *k*-fold axis only. Is it occurs for all ({*a*, *b*}, *k*)-spheres with *b*-faces of negative curvature?
- Examples (minimal whenever $v \leq 32$) are given below:













32 C_i

72 O_h

Minimal $(\{3,4\},5)$ -spheres of 5-fold symmetry

It exists iff $p_4 \equiv 0 \pmod{5}$, i.e., $v = 2p_4 + 12 \equiv 2 \pmod{10}$.



Minimal $(\{3,4\},5)$ -spheres of 4-fold symmetry

It exists iff $p_4 \equiv 2 \pmod{4}$, i.e., $v = 2p_4 + 12 \equiv 0 \pmod{8}$.









32 D₄

 $16 D_{4d}$

40 D_{4h}











40 C₄

32 C_{4h}

32 S_8

Icosahedron, Snub Cube and, with (b, v; G) = (5, 60; I), Snub Dodecahedron are the only vertex-transitive $(\{3, b\}, 5)$ -spheres.

Minimal $(\{3,4\},5)$ -spheres of 3-fold symmetry

It exists iff $p_4 \equiv 0 \pmod{3}$, i.e., $v = 2p_4 + 12 \equiv 0 \pmod{6}$.



Minimal $(\{3,4\},5)$ -spheres of 2-fold symmetry









 $20 D_2$



24 D_{2h}











20 C₂

22 C_{2v}

28 C_{2h}

28 S₄

Face-regular $(\{3, b\}, 5)$ -spheres

- A 3-connected map (on sphere or torus) is pR_i face-regular if any p-gonal face is adjacent to exactly i p-gons.
- No ($\{3, b\}, 5$)-sphere, besides Icosahedron $3R_3$, is $3R_i$.
- Clearly, bR_j ({3, b}, 5)-sphere has j^{p_b}/₂ (b b)-edges. So, bR_j with odd j implies that 4 divides v = 2p_b(b - 3) + 12.
- There is infinity of bR_j ({3, b}, 5)-spheres for j = 0, 1, 2.



b-gon-transitive of $(\{3, b\}, 5)$ -spheres

- Icosahedron (snub *APrism*₃) is regular. So, let $p_b > 0$.
- Snub APrism_b has v = 4b vertices (2 orbits of size 2b), 2 b-gons (1 orbit) and 6b 3-gons (2 orbits of size 3b). Its group G is D_{bd} for b ≥ 4.
- With (b, v; G) = (4, 24; O), (5, 60; I), Snub Cube and Snub Dodecahedron are only vertex-transitive ({3, b}, 5)-spheres. They are also b-gon-transitive and have 2 orbits of triangles.
- Do other *b*-gon-transitive ({3, *b*}, 5)-spheres or ({3, *b*}, 5)-spheres with at most 3 orbits of faces exist?

XII. Standard ({*a*, *b*}, *k*)-maps on surfaces

Standard (R, k)-maps

- Given R ⊂ N and a surface F², an (R, k)-F² is a k-regular map M on surface F² whose faces have gonalities i ∈ R.
- Euler characteristic $\chi(M)$ is v e + f, where v, e and
 - $f = \sum_{i} p_{i}$ are the numbers of vertices, edges and faces of M.
- Since $kv=2e=\sum_{i}ip_{i}$, Euler formula $\chi = v e + f$ becomes Gauss-Bonnet-like one $\chi(M) = \sum_{i} p_{i}\kappa_{i}$.
- Again, let our maps be standard, i.e., $\min_{i \in R} (1 + \frac{i}{k} \frac{i}{2}) = 0$. So, $M = \max\{i \in R\} = \frac{2k}{k-2}$ and (M, k) = (6, 3), (4, 4), (3, 6).
- There are infnity of standard maps (R, k)-F², since the number p_M of flat (κ_M=0) faces is not restricted.
- Also, $\chi \ge 0$ with $\chi = 0$ if and only if $R = \{m\}$. So, \mathbb{F}^2 is \mathbb{S}^2 , \mathbb{T}^2 , \mathbb{P}^2 , \mathbb{K}^2 with $\chi = 2, 0, 1, 0$, respectively.
- Such $(\{a, b\}, k)$ - \mathbb{F}^2 map has $b = \frac{2k}{k-2}$, $p_a = \frac{\chi b}{b-a}$, $v = \frac{1}{k}(ap_a + bp_b)$ So, (a=b, k) = (6,3), (3,6), (4,4) if \mathbb{F}^2 is \mathbb{T}^2 or \mathbb{K}^2 .
- But $\chi = \frac{p_3 2p_4}{10}$ for icosahedrite maps ({3, 4}, 5) (non-standard) So, $\chi < 0$ is possible and $\chi = 0$ (i.e., $\mathbb{F}^2 = \mathbb{T}^2, \mathbb{K}^2$) iff $p_3 = 2p_4$.

Digression on interesting non-standard $({5, 6, c}, 3)$ -maps

Such maps, generalizing fullerenes, have $c \ge 7$. Examples are:

- Haeckel, 1887: ({5,6, c}, 3)-spheres with c = 7,8 representing skeletons of radiolarian zooplankton Aulonia hexagona
- Fullerene c-disks (($\{5, 6, c\}, 3$)-spheres with $p_c = 1$) if $c \ge 7$ (Deza-Dutour-Shtogrin, 2011-2012)
- G-fulleroids (Deza-Delgado, 2000; Jendrol-Trenkler, 2001 and Kardos, 2007): ({5, b}, 3)-spheres with b≥7 and symmetry G
- Azulenoids: ({5,6,7},3)-tori; so, $g = 1, p_5 = p_7$ (Kirby-Diudea, 2003, et al.)
- Schwartzits: ({5,6, c}, 3)-maps on minimal surfaces of constant negative curvature (g ≥ 2) with c = 7,8 (Terrones-MacKay, 1997, et al.) Knor-Potocnik-Siran-Skrekovski, 2010: such ({6, c}, 3)-maps exist for any g ≥ 2, p₆ ≥ 0 and c = 7,8,9,10,12. For c = 7,8 such polyhedral maps exist.

The $(\{a, b\}, k)$ -maps on torus and Klein bottle

The connected *closed* (compact and without boundary) irreducible surfaces are: sphere \mathbb{S}^2 , torus \mathbb{T}^2 (two orientable), real projective plane \mathbb{P}^2 and Klein bottle \mathbb{K}^2 with $\chi = 2, 0, 1, 0$, respectively.

The maps $(\{a, b\}, k)$ - \mathbb{T}^2 and $(\{a, b\}, k)$ - \mathbb{K}^2 have $a = b = \frac{2k}{k-2}$; so, (a = b, k) should be (6, 3), (3, 6) or (4, 4).

We consider only polyhedral maps, i.e. no loops or multiple edges (1- or 2-gons), and any two faces intersect in edge, point or \emptyset only.

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Smallest \mathbb{T}^2 and \mathbb{K}^2 -embeddings for (a=b, k)=(6,3), (3,6), (4,4): as 6-regular triangulations: K_7 and $K_{3,3,3}$ $(p_3 = 14, 18)$; as 3-regular polyhexes: Heawood graph (dual K_7) and dual $K_{3,3,3}$; as 4-regular quadrangulations: K_5 and $K_{2,2,2}$ $(p_4 = 5, 6)$. K_5 and $K_{2,2,2}$ are also smallest $(\{3,4\},4)$ - \mathbb{P}^2 and $(\{3,4\},4)$ - \mathbb{S}^2 , while K_4 is the smallest $(\{4,6\},3)$ - \mathbb{P}^2 and $(\{3,6\},3)$ - \mathbb{S}^2 .

Smallest 3-regular maps on \mathbb{T}^2 and \mathbb{K}^2 : duals K_7 , $K_{3,3,3}$













Smallest 3-regular maps on \mathbb{T}^2 and \mathbb{K}^2 : duals K_7 , $K_{3,3,3}$



3-regular polyhexes on \mathbb{T}^2 , cylinder, Möbius surface, \mathbb{K}^2 are $\{6^3\}$'s quotients by fixed-point-free group of isometries, generated by: two translations, a transl., a glide reflection, transl. *and* glide reflection.

8 families: symmetry groups with inversion

The point symmetry groups with inversion operation are: T_h , O_h , I_h , C_{mh} , D_{mh} with even m and D_{md} , S_{2m} with odd m. So, they are

- **9** for $\{5, 6\}_{v}$: C_{i} , C_{2h} , D_{2h} , D_{3d} , D_{6h} , S_{6} , T_{h} , D_{5d} , I_{h}
- **2** 7 for $\{2,3\}_{v}$: C_{i} , C_{2h} , D_{2h} , D_{3d} , D_{6h} , S_{6} , T_{h}
- **6** for $\{4, 6\}_{v}$: C_i , C_{2h} , D_{2h} , D_{3d} , D_{6h} , O_h
- **6** for $\{3,4\}_{v}$: C_{i} , C_{2h} , D_{2h} , D_{3d} , D_{4h} , O_{h}
- **5** 2 for $\{2,4\}_{v}$: D_{2h} , D_{4h}
- **1** for $\{3, 6\}_{v}$: D_{2h}
- **0** for $\{2, 6\}_{v}$ and $\{1, 3\}_{v}$
- Cf. 12 for icosahedrites (({3,4},5)-spheres):
 C_i, C_{2h}, C_{4h}, D_{2h}, D_{4h}, D_{3d}, D_{5d}, S₆, S₁₀, T_h, O_h, I_h

(R, k)-maps on the projective plane are the antipodal quotients of centrosymmetric (R, k)-spheres; so, halving their *p*-vector and *v*.

Smallest $(\{a, b\}, k)$ -maps on the projective plane

- The smallest ones for (a, b) = (4, 6), (3, 4), (3, 6), (5, 6) are: K_4 (smallest \mathbb{P}^2 -quadrangulation), K_5 , 2-truncated K_4 , dual K_6 (Petersen graph), i.e., the antipodal quotients of Cube $\{4, 6\}_8, \{3, 4\}_{10}(D_{4h}), \{3, 6\}_{16}(D_{2h})$, Dodecahedron $\{5, 6\}_{20}$.
- The smallest ones for (a, b) = (2, 4), (2, 3) are points with 2, 3 loops; smallest without loops are 4×K₂, 6×K₂ but on P².



Smallest ($\{5, 6\}, 3$)- \mathbb{P}^2 and ($\{3, 4\}, 5$)- \mathbb{P}^2

The Petersen graph (in positive role) is the smallest \mathbb{P}^2 -fullerene. Its \mathbb{P}^2 -dual, K_6 , is the smallest \mathbb{P}^2 -icosahedrite (half-lcosahedron). K_6 is also the smallest (with 10 triangles) triangulation of \mathbb{P}^2 .



6 families on projective plane: parameterizing

- $\{2,3\}_{v}$: C_{i} , C_{2h} , D_{2h} , S_{6} , D_{3d} , D_{6h} , T_{h}
- **3** $\{4, 6\}_{v}$: C_{i} , C_{2h} , D_{2h} , D_{3d} , D_{6h} , O_{h}
- $(3,4)_{\nu}: C_i, C_{2h}, D_{2h}, D_{3d}, D_{4h}, O_h$
- **5** $\{2,4\}_{v}$: D_{2h} , D_{4h}
- **(3,6)**_v: D_{2h}

6 families on projective plane: parameterizing

- **2** $\{2,3\}_{v}$: C_{i} , C_{2h} , D_{2h} , S_{6} , D_{3d} , D_{6h} , T_{h}
- **3** $\{4,6\}_{\nu}$: C_i , C_{2h} , D_{2h} , D_{3d} , D_{6h} , O_h
- $(3,4)_{\nu}: C_i, C_{2h}, D_{2h}, D_{3d}, D_{4h}, O_h$
- **5** $\{2,4\}_{v}$: D_{2h} , D_{4h}
- **(3,6)**_v: D_{2h}

 $(\{2,3\}, 6)$ -spheres T_h and D_{6h} are $GC_{k,k}(2 \times Tetrahedron)$ and, for $k \equiv 1, 2 \pmod{3}$, $GC_{k,0}(6 \times K_2)$, respectively. Other spheres of blue symmetry are $GC_{k,l}$ with l = 0, k from the first such sphere. So, each of 7 blue-symmetric families is described by one natural parameter k and contains $O(\sqrt{v})$ spheres with at most v vertices.

$(\{a, b\}, k)$ -maps on Euclidean plane and 3-space

- An $(\{a, b\}, k)$ - \mathbb{E}^2 is a k-regular tiling of \mathbb{E}^2 by a- and b-gons.
- ({a, b}, k)-E² have p_a ≤ b/b-a and p_b = ∞. It follows from Alexandrov, 1958: any metric on E² of non-negative curvature can be realized as a metric of convex surface on E³. In fact, consider plane metric such that all faces became regular in it. Its curvature is 0 on all interior points (faces, edges) and ≥ 0 on vertices. A convex surface is at most half-S².
- There are ∞ of $(\{a, b\}, k)$ - \mathbb{E}^2 if $2 \le p_a \le \frac{b}{b-a}$ and 1 if $p_a = 0, 1$.
- The plane fullerenes (or nanocones) ({5,6}, k)-E² are classified by Klein and Balaban, 2007: the number of equivalence (isomorphism up to a finite induced subgraph) classes is 2,2,2,1 for p₅ = 2,3,4,5, respectively.

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- An ({a, b}, k)-ℝ³ is a 3-periodic k'-regular face-to-face tiling of the Euclidean 3-space ℝ³ by ({a, b}, k)-spheres.
- Next, we will mention such tilings by 4 special fullerenes, which are important in Chemistry and Crystallography. Then we consider extension of ({*a*, *b*}, *k*)-maps on manifolds.

XIII. Beyond surfaces

Frank-Kasper $(\{a, b\}, k)$ -spheres and tilings

- A ({*a*, *b*}, *k*)-sphere is Frank-Kasper if no *b*-gons are adjacent.
- All cases are: smallest ones in 8 families, 3 ({5,6},3)-spheres (24-, 26-, 28-vertex fullerenes), ({4,6},3)-sphere Prism₆, 3 ({3,4},4)-spheres (APrism₄, APrism₃², Cuboctahedron), ({2,4},4)-sphere doubled square and two ({2,3},6)-spheres (tripled triangle and doubled Tetrahedron).



FK space fullerenes

A FK space fullerene is a 3-periodic 4-regular face-to-face tiling of 3-space \mathbb{E}^3 by four Frank-Kasper fullerenes $\{5,6\}_v$.

They appear in crystallography of alloys, clathrate hydrates,

zeolites and bubble structures. The most important, A_{15} , is below.



Weaire-Phelan, 1994: best known solution of weak Kelvin problem

An $(\{a, b\}, k)$ - \mathbb{E}^3 is a 3-periodic k'-regular face-to-face \mathbb{E}^3 -tiling by $(\{a, b\}, k)$ -spheres. Deza-Shtogrin, 1999: first known non-FK space fullerene $(\{5, 6\}, 3)$ - \mathbb{E}^3 : 4-regular \mathbb{E}^3 -tiling by $\{5, 6\}_{20}$, $\{5, 6\}_{24}$ and its elongation $\simeq \{5, 6\}_{36}$ (D_{6h}) in proportion 7:2:1.

Fullerene manifolds

- Given 3 ≤ a < b ≤ 6, {a, b}-manifold is a (d-1)-dimensional d-valent compact connected manifold (locally homeomorphic to ℝ^{d-1}) whose 2-faces are only a- or b-gonal.
- So, any *i*-face, $3 \le i \le d$, is a polytopal *i*-{*a*, *b*}-manifold.
- Most interesting case is (a, b) = (5, 6) (fullerene manifold), when d = 2, 3, 4, 5 only since (Kalai, 1990) any 5-polytope has a 3- or 4-gonal 2-face.

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- The smallest polyhex is 6-gon on T². The "greatest": {633}, the convex hull of vertices of {63}, realized on a horosphere.
- Prominent 4-fullerene (600-vertex on S³) is 120-cell ({533}). The "greatest" polypent: {5333}, tiling of H⁴ by 120-cells.

Projection of 120-cell in 3-space



 $\{533\}$: 600 vertices, 120 dodecahedral facets, |Aut| = 14,400

- All known finite 4-fullerenes are "mutations" of 120-cell by interfering in one of ways to construct it: tubes of 120-cells, coronas, inflation-decoration method, etc.
 Some putative facets: F_n(G) with (n, G)=(20, I_h), (24, D_{6h}), (26, D₃), (28, T_d), (30, D_{5h}), (32, D_{3h}), (36, D_{6h}).
- Space fullerenes ({5,6},3)-ℝ³: example of infinite 4-fullerenes.

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- Space fullerenes ({5,6},3)-ℝ³: example of infinite 4-fullerenes.
- All known 5-fullerenes come from {5333}'s by following ways. With 6-gons also: glue two {5333}'s on some 120-cells and delete their interiors. If it is done on only one 120-cell, it is $\mathbb{R} \times \mathbb{S}^3$ (so, simply-connected).

Finite compact ones: the quotients of {5333} by its symmetry group (partitioned into 120-cells) and gluings of them.

Quotient *d*-fullerenes

- Selberg, 1960, Borel, 1963: if a discrete group of motions of a symmetric space has a compact fundamental domain, then it has a torsion-free normal subgroup of finite index.
- So, the *quotient* of a *d*-fullerene by such symmetry group (its points are group orbits) is a finite *d*-fullerene.

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- Exp. 1: Polyhexes on T², cylinder, Möbius surface and K² are the quotients of {6³} by discontinuous fixed-point-free group of isometries, generated by: 2 translations, a translation, a glide reflection, translation *and* glide reflection, respectively.

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- Exp 2: Poincaré dodecahedral space: the quotient of 120-cell by *l_h*; so, its *f*-vector is (5, 10, 6, 1) = ¹/₁₂₀ f(120-cell).
- Cf. 6-, 12-regular H³-tilings {5,3,4}, {5,3,5} by {5,6}₂₀ and 6-regular H³-tiling by (right-angled) {5,6}₂₄.
 Seifert-Weber, 1933 and Löbell, 1931 spaces are quotients of last 2 with *f*-vectors (1,6, *p*₅=6, 1), (24,72,48+8=*p*₅+*p*₆,8).