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Short Communication

Fullerene and nanotube models in Bolyai – Lobachevsky hyperbolic geometry H^3 on the 200th anniversary of its discovery

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The Archimedean solid (5, 6, 6), where regular pentagon, hexagon and hexagon surround each vertex, so altogether 60 vertices (with carbon atoms for C_{60} fullerene). 12 pentagons and 20 hexagons bound this football polyhedron, as a regular (say white) icosahedron truncated by 12 (black) pentagons at its 12 vertices. But now (Figure 1) we consider this as a *fundamental polyhedron F with paired side faces for a hypothetic (for a while) future space tiling* F^G *under a space group G, generated by the face pairing mappings* ([1,2] for analogous constructions).

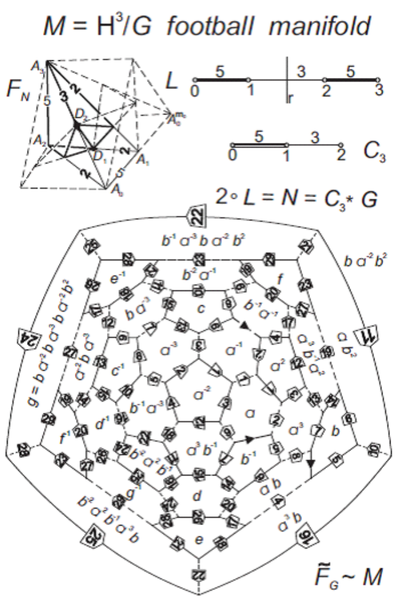

Figure 1: The football manifold as fullerene model in hyperbolic space H3 with possible carbon atoms in the vertices.

In the following necessary technical explanation (which can be skipped at first glance, see only the summarizing diagram (1)), first we start with this face pairing at the 3 → (arrow) edges: **a**: a^{-1} --> a means that the motion maps the hexagon face a^{-1} (with 1st →) onto hexagon face a (with 2nd →) and polyhedron F onto its **a**-image $F^{\mathbf{a}}$ in the other half-space of a; $\mathbf{a}^{-1}$: a --> a^{-1}, F --> $F^{\mathbf{a}^{-1}}$ define inverse generator. Then take the other face on F at this 2nd → as pentagon b^{-1} and its image pentagon face b at the third → and the motion **b**: b^{-1} --> b as before, also with $F^{\mathbf{b}}$. As a result, we obtain at the 3rd → the face ab, then at the 1st →, face $b^{-1}a^{-1}$, thus **ab**: $b^{-1}a^{-1}$ --> ab and $F^{\mathbf{ab}}$ can also be obtained by our convention. This also means that the edge → are surrounded by 3 polyhedra in the fundamental space tiling F^G.

$$\begin{array}{ccc} F & \xrightarrow{\ \mathbf{g}\ } & F^{\mathbf{g}} \\ \mathbf{a}\downarrow & & \downarrow \mathbf{g}^{-1}\mathbf{a}\,\mathbf{g} = \mathbf{a}^{\mathbf{g}} \\ F^{\mathbf{a}} & \xrightarrow{\ \mathbf{g}\ } & F^{\mathbf{ag}} \end{array} \qquad (1)$$

$G \ni \mathbf{g}$ is a product of generators **a**, **b** (and or their inverses). $F^{\mathbf{ag}}$ is adjacent to $F^{\mathbf{g}}$ at the image face $a^{\mathbf{g}}$, as a general rule.

Look at our Figure 1, where we see our lucky situation: after having assigned the 3 → edges and generator motions **a** and **b**, we can finish the side face pairing on the fundamental polyhedron F as *identity domain* F^1, by introducing new and new

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edge tripples and getting either new face pairing expressed by **a** and **b,** or we get trivial relation, or non-trivial, so-called *defining relation* for the future fundamental group *G*. The first new edge tripple is denoted by 1 also as a type of arrow between faces a^{-1} and a, introducing a^2 and its inverse a^{-2}. In the end, we have obtained 30 edge tripples (the last one is 29) with two essential defining relations to the two generators **a** and **b**. For details, [1,2]. It turns out that we have 15 *G*-equivalence classes of the 60 vertices, 4 vertices in each class. From any vertex 4 edge classes start or end as at carbon atoms. It seems that C_{15} would be a better notation instead of C_{60}.

This construction was published first in [3] in 1988, **a**s a hyperbolic football manifold (without any fullerene reference). For our other results, partly joint with István PROK, e.g. [1,2] and our didactical introductory paper [4] is extremely advised. The existence in hyperbolic space H^3 is based on the generalized projective *Beltrami-Cayley-Klein model of* $\mathbf{H}^3$ also described in [1,2] and summarized below.

The left upper part of Figure 1 shows the so-called characteristic simplex $A_0A_1A_2A_3$, spanned by basis vectors $\mathbf{a}_0$, $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ of a real 4-dimensional (left) vector space $\mathbf{V}^4$. A usual vector $\mathbf{x} = x^i\mathbf{a}_i$ (with Einstein-Schouten index conventions) and its real multiple $c\mathbf{x} \sim \mathbf{x}$ express the same point, X. The side face b^i, opposite to A_i, is expressed by the linear form $\boldsymbol{b}^i$ of the (right) dual form space $\boldsymbol{V}_4$ by $\mathbf{a}_i\boldsymbol{b}^j = \delta_i^j$ (Kronecker delta symbol), as usual.

Now for our football manifold, the face angles of the characteristic simplex C (5, 3, 5) are specified by formal symmetric bilinear scalar product (of future signature **(+, +, +, −))** as follows (by the so-called Coxeter (ortho-scheme) diagram upper right of Figure 1):

$\langle \boldsymbol{b}^i, \boldsymbol{b}^j \rangle = -\cos(b^ib^j)$, with convention angle (b^ib^i), where $\langle \boldsymbol{b}^0, \boldsymbol{b}^1 \rangle = \langle \boldsymbol{b}^2, \boldsymbol{b}^3 \rangle = -\cos \mathrm{pi}/5$, $\langle \boldsymbol{b}^1, \boldsymbol{b}^2 \rangle = -\cos \mathrm{pi}/3$, $\langle \boldsymbol{b}^0, \boldsymbol{b}^2 \rangle = \langle \boldsymbol{b}^0, \boldsymbol{b}^3 \rangle = \langle \boldsymbol{b}^1, \boldsymbol{b}^3 \rangle = 0$.

Here the half-turn symmetry r *(0 ↔3, 1↔2), the reflections* $\boldsymbol{m}_i$ *in side face* b^i *(i = 0, 1, 2, 3)* of the characteristic simplex also play important roles. The signature of this scalar product is (+, +, +, −), indeed [1,2]! This involves the general angle metric. Its inverse scalar product (with the same signature) involves the general distance metric. Then inscribed ball, circumscribed ball, and densities of ball packing and covering can be computed, with better values than in Euclidean cases. The "only" task is to fill out the football tiling with materials under the "football group" G given above by generators and defining relations [1,3].

Our other initiative is the infinite series of nanotube models that are completely analogous. Only the characteristic simplex C (2z, 2z, 2z, 3 ≤ z odd) (in Figure 2, 4 z = 3 in two equivalent interpretations), but z = 5 (Figure 3), 7 are also simple) will be doubly truncated (by polar planes of A_0 and A_3) in the hyperbolic sense and its half part will be taken as in our recent paper [2] (to be continued). The prism-like fundamental polyhedron has two base planes paired by an appropriate z-screw motion, so we obtain an infinite tube. The side faces cause a screw structure

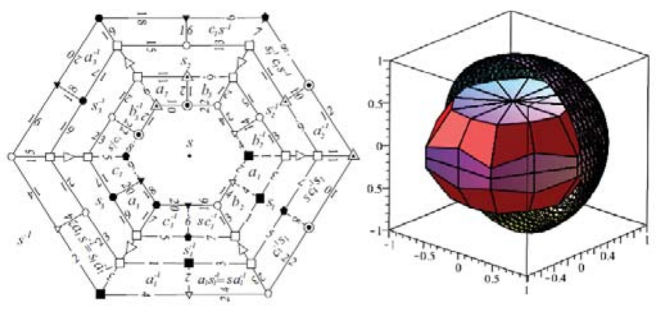

Figure 2: The "nano" domain from above *C* (2*z*, 2*z*, 2*z*, 3 = *z*) with face pairing (e.g. s^{-1} --> *s*), as H^3 manifold with possible "signed atoms" in its vertices and centre, then its animation.

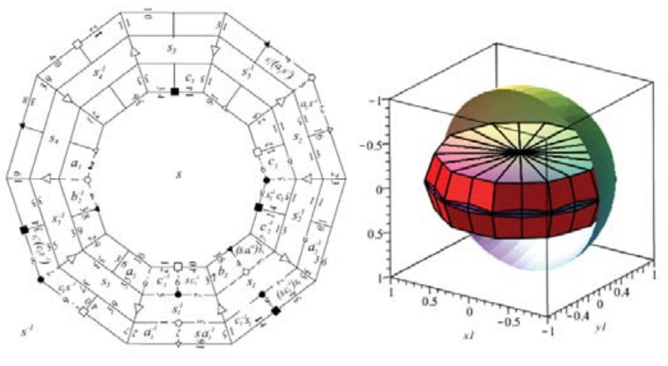

Figure 3: A tube manifold with z = 5 and so 5-rotational symmetry, then its animation.

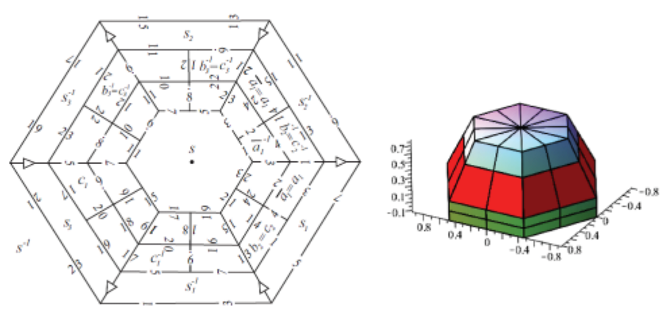

Figure 4: The second interpretation of the above 3-rotational nanotube with less generators.

of tubes with z-rotational symmetry. Our investigations with this tube manifold structures are going on.

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