XII BGL Conference Budapest, 2024 May 1-3

Non-Euclidean Geometry in Modern Physics and Mathematics

MTA Domus Collegium Hungaricum Vendégház

H-1146 Budapest, Abonyi utca 10.

NON - EUCLIDEAN GEOMETRY
IN MODERN PHYSICS AND MATHEMATICS

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Quantum "dots" and non-Euclidean crystallography
on the 200th anniversary of János Bolyai's absolute geometry

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Abstract

My ~40 years old paper [1] in **References** had got a surprising actuality in the Chemistry Nobel Prize 2023 awards for the three Laureates:

Alexey YEKIMOV, Luis E. BRUS and Moungi G. BAWENDI.

Of course, the present author of that paper could not guess that time the actuality and importance that was an incidental consequence of my erroneous paper [2], intended to construct an infinite series of non-orientable compact hyperbolic manifolds, as a polyhedral tiling series in the *Bolyai-Lobachevsky* hyperbolic space $\mathbf{H}^3$. Fortunately, I observed and improved the mistake soon. Namely, those constructions were not manifolds because the two fixed points as *punctures,* where point reflections (central inversions) occur in the symmetry group of the tricky polyhedral tilings.

But *these singular points, as* "quantum dots" e.g. for *copper and chlorine ions*, respectively, in *glass (silicon) fluid* cause *light effects* (by "electron jumping-leaping") *whose colours might depend on the sizes of crystal particles.* That means, the mistake was much more interesting than the original intention that can be reached easily later!

XII BGL Conference 2024, Budapest

References

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[4] *The Nobel Prize in Chemistry 2023. The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Chemistry 2023 to Moungi G. Bawendi, Louis E. Brus and Alexey Yekimov "for the discovery and synthesis of quantum dots", PRESS RELEASE, 4 October 2023.*

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COLLOQUIA MATHEMATICA SOCIETATIS JÁNOS BOLYAI

46. TOPICS IN DIFFERENTIAL GEOMETRY

DEBRECEN-HAJDÚSZOBOSZLÓ (HUNGARY), 1984.

TWICE PUNCTURED COMPACT EUCLIDEAN AND HYPERBOLIC MANIFOLDS AND THEIR TWOFOLD COVERINGS

E. MOLNÁR

A complete connected Riemannian n-dimensional manifold of constant sectional curvature is briefly called a space form. Intuitively, each space form is locally isometric to one of the classical n-spaces of constant curvature. It is well-known that each space form can be represented as an orbit space M/G.

Manifold (cont) and “twice punctured manifold”

Here M is one of simply connected n-spaces of curvature K, i.e. M is either a spherical ($K>0$) or the Euclidean ($K=0$) or a hyperbolic n-space ($K<0$). The isometry group G acts discontinuously and freely on M, i.e. there is a nonempty open set V in M so that no two distinct points of V are equivalent under G, moreover, the identity 1 is the only element of G which has fixed points. Then G can be considered as the fundamental group of the manifold M/G.

There are „manifolds” which have two exceptional *singular points* with „ball neighbourhood, but its centrally opposite points are glued together”. Such a fundamental group ***G*** *has two singular orbits, i.e. M/****G*** *is „twice punctured”.*

6. Euclidean example

Orientation preserving transforms:

1 (x^1, x^2, x^3); *identity*

s$_1$ $(½ + x^1, ½ - x^2, -x^3)$;

screw

s$_2$ $(-x^1, ½ + x^2, ½ - x^3)$;

motions

s$_3$ $(½ - x^1, -x^2, ½ + x^3)$;

Orientation reversing transforms:

-1 $(-x^1, -x^2, -x^3)$; *point reflection*

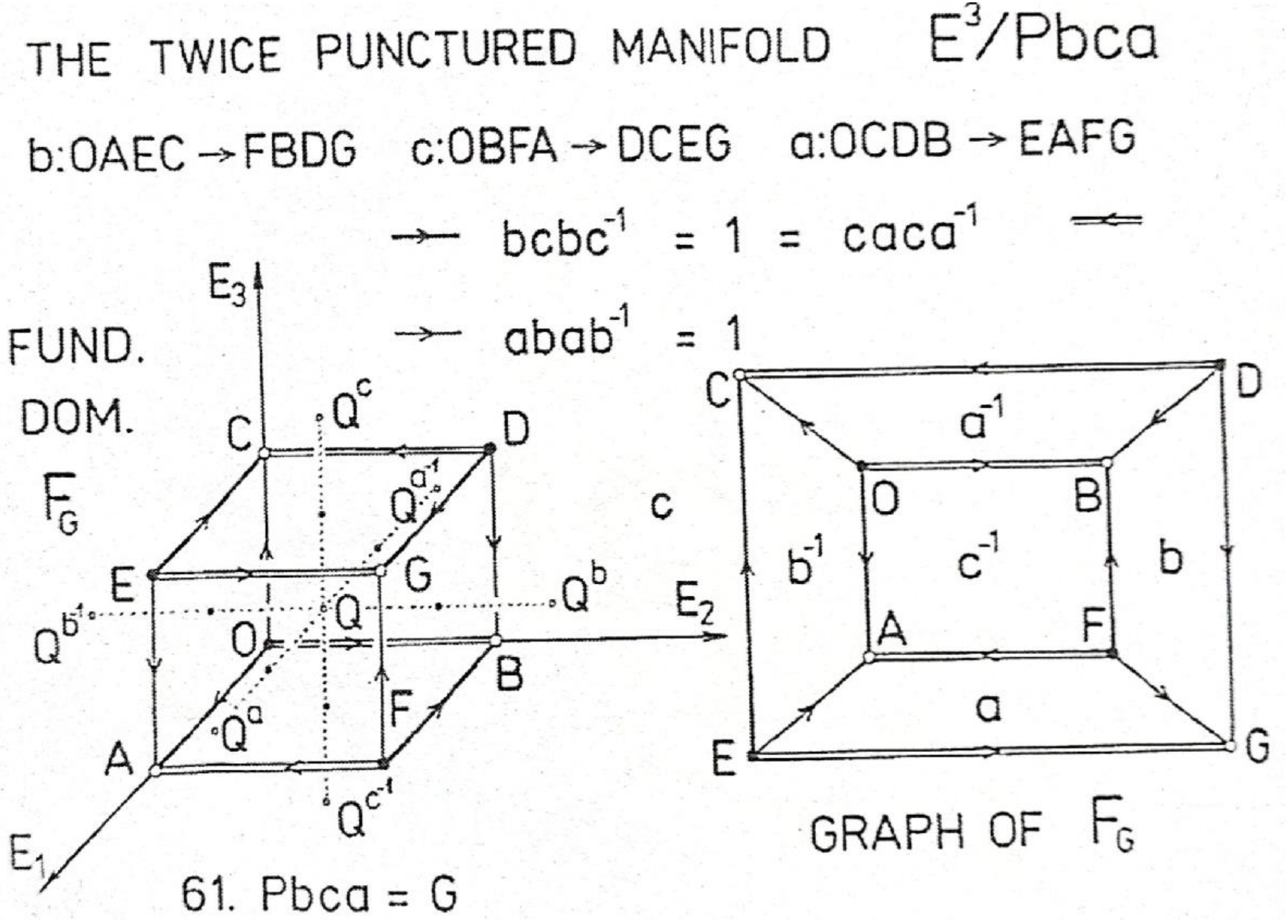
b $(½ - x^1, ½ + x^2, x^3)$; *OAEC =:* b^{-1} → *FBDG =: b*

glide

c $(x^1, ½ - x^2, ½ + x^3)$;

reflections

a $(½ + x^1, x^2, ½ - x^3)$



Super group occurs: 205. **Pa3⁻ =: *G*˜**, if **F$_G$** is a cube with 3-rotations**!?!**

To 61. Pbca = *G* in Figure of former dia 6

The *fundamental domain* (*asymmetric unit*) $\mathbf{F}_G$ of **61. Pbca = *G*** geometrically describes this group, in the *orthorhombic* coordinate system $OE_1E_2E_3$, where the *lengthes* of *basis vectors* $|OE_i := \boldsymbol{e}_i| = a_i$ (i = 1, 2, 3) are given parameters (by *measuring the material crystal*, to be determined). An *orthorhombic lattice* Λ_G of ***G*** are given by *integer coordinate triple* to the *identity transform* **1** (as *linear part*). As we know (in our conventions), each

$$\propto(\mathbf{A}, \mathbf{a}) \in \boldsymbol{G} \text{ can be given by a } \textit{mapping} \quad \propto: \boldsymbol{X} \mapsto \boldsymbol{X}\mathbf{A} + \mathbf{a} =: \boldsymbol{X}^{\propto}$$

with **A** **as *linear integer unimodular matrix*** to the basis ($\boldsymbol{e}_i = OE_i$) above, and the broken part **a**, as symbolically indicated in dia 6, the *position vector* is $OX = \boldsymbol{X} = x^i\boldsymbol{e}_i$ (*summing convention*).

Assume *that O, D, E, F are **G**-equivalent* point reflection centres, say with copper (**Cu**) ion parts, so are *G, A, B, C* with Chlorine (**Cl**) ion parts, so that the fundamental cube $\mathbf{F}_G$ contain also **central** silicon (**Si**) atoms and **2-2 ones at** the opposite face pairs of $\mathbf{F}_G$ equivalent by glide reflections **b**, **c**, **a**, respectively. Imagine that this 1:1:7 proportions of **Cu**, **Cl**, **Si** can form crystal particles with appropriate cube size, and this particles float in a silicon fluid that freezes. The singularities in near **Cu** and **Cl** ions cause electron **“jumping-leaping”** with light effects, i.e. ***quantum dots.***

Fundamental domain $\mathbf{F}^1_{tu}$ of $\boldsymbol{G}^1_{tu}$

Generators:

$\boldsymbol{a}_i$ $(-t \le i \le +t)$ *glide reflections*, $\boldsymbol{a}_i : a_i^{-1} \to a_i$

$\boldsymbol{p}_i$ $(-t \le i \le +t)$ *screw motions*, $\boldsymbol{p}_i : p_i^{-1} \to p_i$

$\boldsymbol{r}_i$ $(-t \le i \le +t)$ *screw motions*, $\boldsymbol{r}_i : r_i^{-1} \to r_i$

$\boldsymbol{s}_u$ $(0 \le u \le t)$ *screw motion*

Altogether: $3q + 1 = 6t + 3$ generators

Relations

To arrowed edges in Table 1

e.g. $\Rightarrow$ $\boldsymbol{a}_{-t}\boldsymbol{a}_{-t}\ldots\boldsymbol{a}_0\boldsymbol{a}_0\ldots\boldsymbol{a}_{+t}\boldsymbol{a}_{+t} = \mathbf{1}$ identity

e.g. ***ooo>*** $\boldsymbol{a}_0\boldsymbol{p}_0\boldsymbol{a}_{-u}^{-1}\boldsymbol{r}_t = \mathbf{1}$

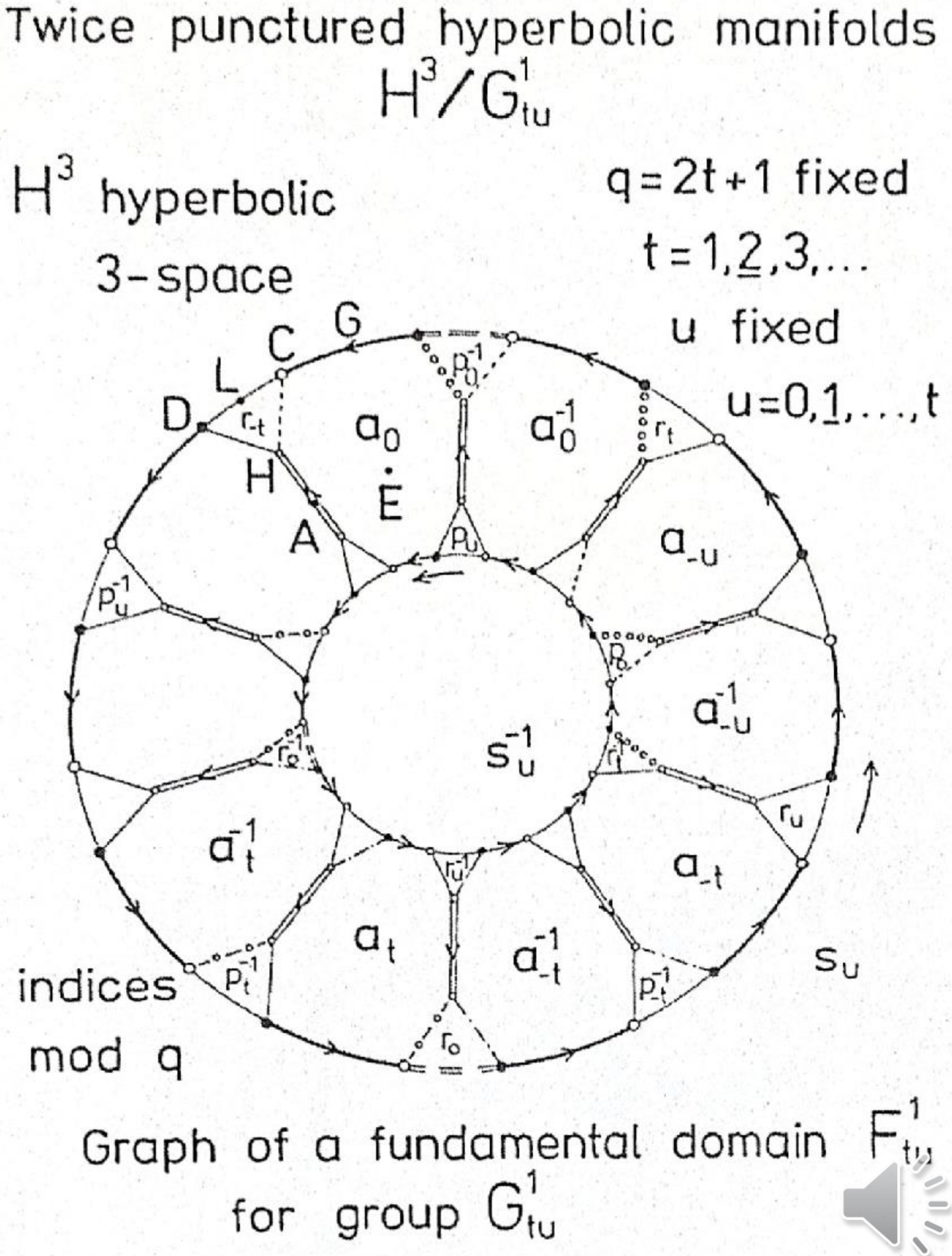
The equivalence classes *C* (**Cu**) and *D* (**Cl**) *are reflections centres* with *half ball neighbourhood,* i.e *punctures for quantum dots*..

The other point classes (orbits, e.g. for *G, E, A, H, L*, … for **Si** atoms) have ball neighbourhood, as at manifolds.

The *proportions* depends on parameter $q = 2t + 1$.

We have infinitely many hyperbolic possibilities.

The minimal one with $t = 1$, $q = 3$ is extremely interesting for realizations!?



Fundamental domain $\mathbf{F}^2{}_t$ of $\boldsymbol{G}^2{}_t$ (u = 0)

Generators:

$\boldsymbol{a}_i$ $(-t \le i \le +t)$ *glide reflections*, $\boldsymbol{a}_i : a_i^{-1} \rightarrow a_i$
$\boldsymbol{c}_i$ $(-t \le i \le +t)$ *glide reflections*, $\boldsymbol{c}_i : c_i^{-1} \rightarrow c_i$
$\boldsymbol{d}_i$ $(-t \le i \le +t)$ *glide reflections*, $\boldsymbol{d}_i : d_i^{-1} \rightarrow d_i$
$\boldsymbol{e}$ $(0 \le u \le t)$ *glide reflection*
Altogether: $3q + 1 = 6t + 3$ generators

Relations

To arrowed edges in Table 1

e.g. $\Rightarrow \boldsymbol{a}_{-t}\boldsymbol{a}_{-t}\ldots\boldsymbol{a}_0\boldsymbol{a}_0\ldots\boldsymbol{a}_{+t}\boldsymbol{a}_{+t}$ $=\mathbf{1}$ identity
e.g. ***ooo>*** $\boldsymbol{a}_0\boldsymbol{c}_0\boldsymbol{a}_0^{-1}\boldsymbol{d}_t = \mathbf{1}$

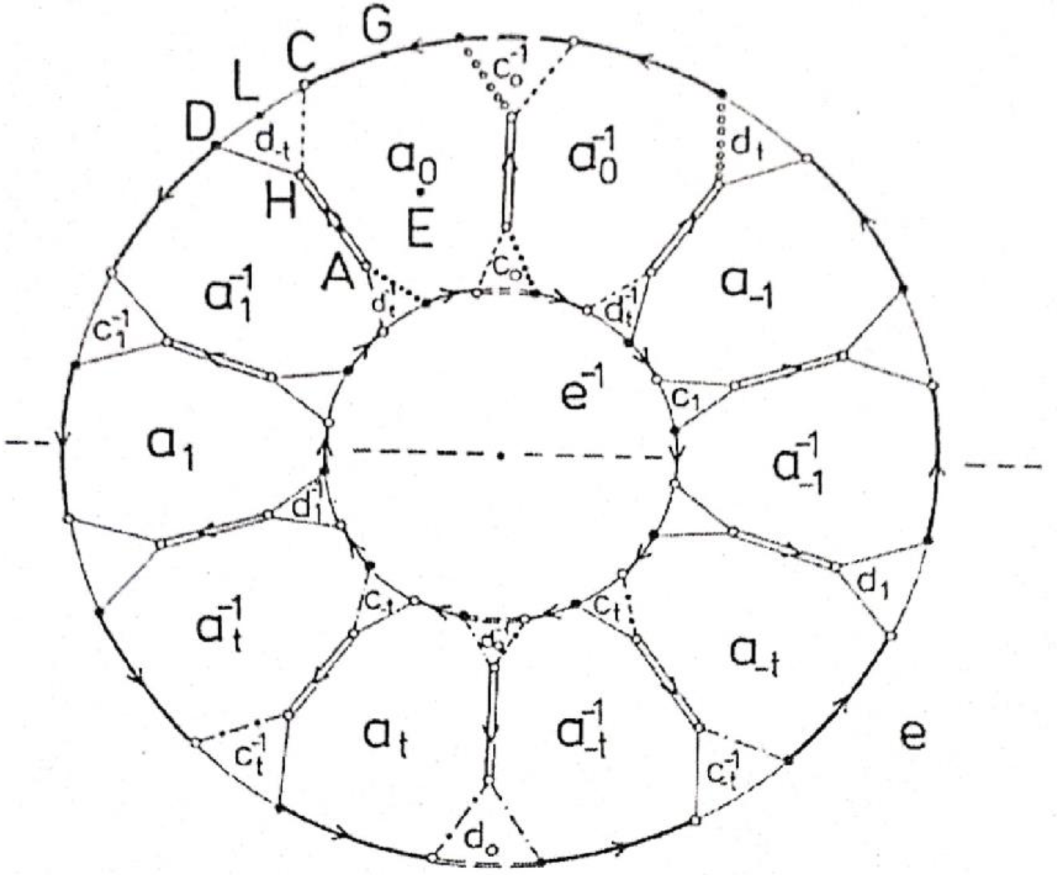
The equivalence classes *C* (**Cu**) and *D* (**Cl**) are *reflection centres* with *half ball neighbourhood,* i.e *punctures for quantum dots.*
An integer parameter u with 0 ≤ *u* ≤ *t* can be introduced for other (non-isometric) manifolds, similarly as before.

The (projective) metric comes later on Bolyai - Lobachevsky geometry!

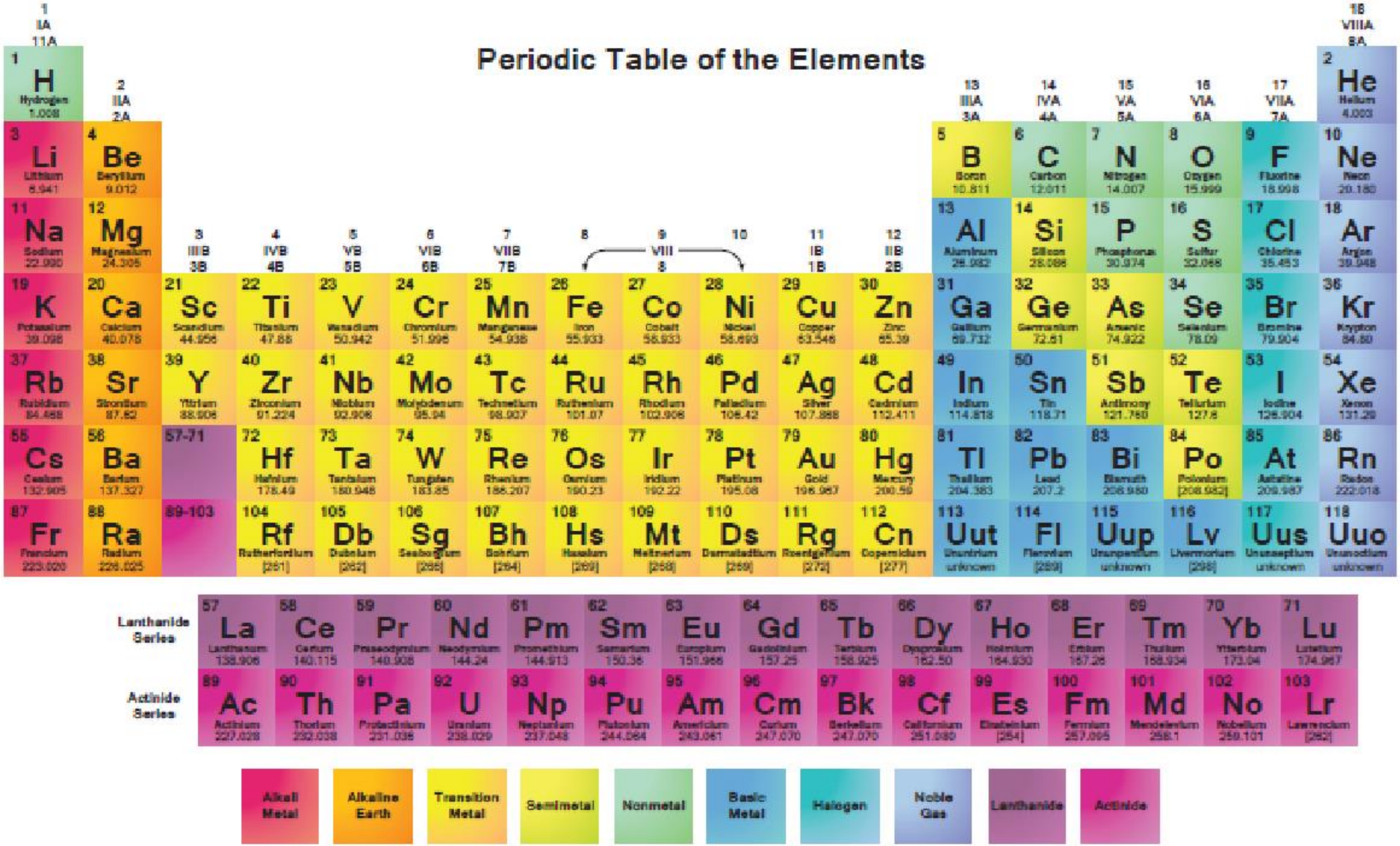
Twice punctured hyperbolic manifolds
H^3/G_t^2

H^3 hyperbolic 3-space

$q = 2t+1$ fixed
$t = 1, \underline{2}, 3, \ldots$



Graph of a fundamental domain F_t^2 for group G_t^2


Periodic Table of the Elements
1 H 2 He
3 Li 4 Be 5 B 6 C 7 N 8 O 9 F 10 Ne
11 Na 12 Mg 13 Al 14 Si 15 P 16 S 17 Cl 18 Ar
19 K 20 Ca 21 Sc 22 Ti 23 V 24 Cr 25 Mn 26 Fe 27 Co 28 Ni 29 Cu 30 Zn 31 Ga 32 Ge 33 As 34 Se 35 Br 36 Kr
37 Rb 38 Sr 39 Y 40 Zr 41 Nb 42 Mo 43 Tc 44 Ru 45 Rh 46 Pd 47 Ag 48 Cd 49 In 50 Sn 51 Sb 52 Te 53 I 54 Xe
55 Cs 56 Ba 57-71 72 Hf 73 Ta 74 W 75 Re 76 Os 77 Ir 78 Pt 79 Au 80 Hg 81 Tl 82 Pb 83 Bi 84 Po 85 At 86 Rn
87 Fr 88 Ra 89-103 104 Rf 105 Db 106 Sg 107 Bh 108 Hs 109 Mt 110 Ds 111 Rg 112 Cn 113 Uut 114 Fl 115 Uup 116 Lv 117 Uus 118 Uuo
Lanthanide Series
57 La 58 Ce 59 Pr 60 Nd 61 Pm 62 Sm 63 Eu 64 Gd 65 Tb 66 Dy 67 Ho 68 Er 69 Tm 70 Yb 71 Lu
Actinide Series
89 Ac 90 Th 91 Pa 92 U 93 Np 94 Pu 95 Am 96 Cm 97 Bk 98 Cf 99 Es 100 Fm 101 Md 102 No 103 Lr
Alkali Metal
Alkaline Earth
Transition Metal
Semimetal
Nonmetal
Basic Metal
Halogen
Noble Gas
Lanthanide
Actinide

Reflection group C_t and its fundamental domain as truncated orthoscheme, generators for G^1_{tu} and G^2_t; some distances for *Coxeter* diagram

The *orthoscheme projective coordinate simplex* $A_0A_1A_2A_3 \sim b^0b^1b^2b^3$ will be described in the real (left) vector 4-space $\mathbf{V}^4$ (for points $X(\boldsymbol{X} = X^i\boldsymbol{A}_i \sim c\boldsymbol{X})$ and its dual (right) form space $\boldsymbol{V}_4$ (for planes $u(\boldsymbol{u} = \boldsymbol{b}^j u_j \sim \boldsymbol{u}c)$, by the *symmetric*

Coxeter – Schläfli matrix $(b^{ij}) = \langle \boldsymbol{b}^i, \boldsymbol{b}^j \rangle = (\cos(\pi - \beta^{ij}))$,

first for *angles* $\beta^{ij} = (\angle \boldsymbol{b}^i\boldsymbol{b}^j)$ with $(\angle \boldsymbol{b}^i\boldsymbol{b}^i) = \pi$,

then for *distances by* the inverse $(b^{ij})^{-1} =: (A_{ij}) =: \langle \boldsymbol{A}_i, \boldsymbol{A}_j \rangle$ and

$$\cosh(XY/k) = -\langle \boldsymbol{X}, \boldsymbol{Y} \rangle / (\langle \boldsymbol{X}, \boldsymbol{X} \rangle \langle \boldsymbol{Y}, \boldsymbol{Y} \rangle)^{1/2}$$

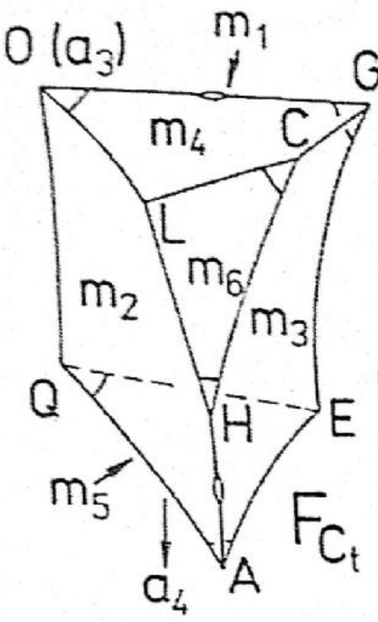
is the distance of points X and Y. Here $k = (-1/K)$ is the universal unit distance of the hyperbolic space $\mathbf{H}^3$, K is the *constant negative sectional curvature.* In nano size k has to be “measured” (determined).

The Periodic Table of the Elements gives important information!

The mathematical details can be found in the References, e.g. [1, 8].

In our Figure the doubly truncated orthoscheme comes from the nowadays coordinate simplex above from [8], but here we used the previous notations of paper [1]: $\boldsymbol{A}_2 \rightarrow \boldsymbol{a}_3$ for point O, $\boldsymbol{A}_1 \rightarrow \boldsymbol{a}_2$ for point G, $\boldsymbol{A}_3 \rightarrow \boldsymbol{a}_4$ for outer point A_3, whose polar plane a_3 is m_5 here, A_0 is outer point whose polar plane a_0 is denoted by m_6 here. The simplex planes b^0, b^1, b^2, b^3 are denoted by m_1, m_2, m_3, m_4 now.

G^j_t as subgroups of Coxeter groups C_t



$a_0 = m_1 m_2 m_3$

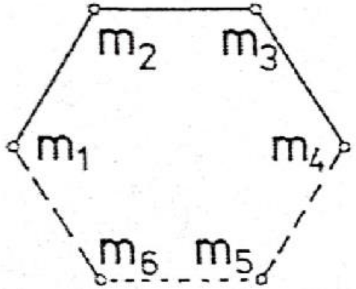
$a_i = (m_1 m_2)^{-2i} a_0 (m_1 m_2)^{2i}$

$s_u = (m_1 m_2)^{q+2u} (m_5 m_4)$

$e = (m_1 m_2)^{-t} m_1 (m_1 m_2)^{t} (m_5 m_4)$

$p_i = (m_1 m_2)^{-(2i-1)} (m_6 m_5) \cdot (m_1 m_2)^{2i-1} (m_2 m_1)^{2u}$

$r_i = s_u p_i s_u$



$c_0 = m_1 (m_2 m_6 m_5) m_1$

$c_i = (m_2 m_1)^{2i} c_0 (m_2 m_1)^{2i}$

$d_i = e c_i e$

indices mod q

—— $-\cos\frac{\pi}{2q}$ - - - $-\mathrm{ch}\,\frac{OQ}{k} = -\sqrt{1 + \frac{\sin^2\frac{\pi}{q}}{4\cos\frac{\pi}{q}}}$

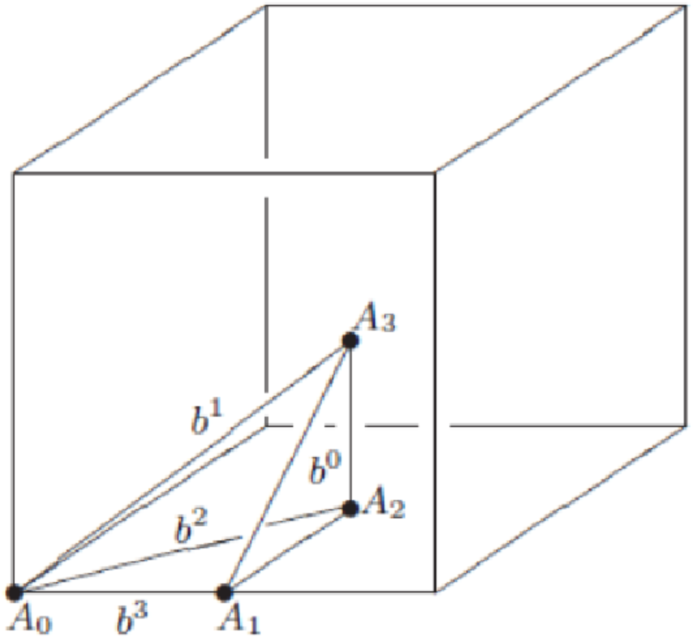
······ $-\mathrm{ch}\,\frac{AH}{k} = -\frac{\cos^3\frac{\pi}{2q}}{\cos\frac{\pi}{q}}$

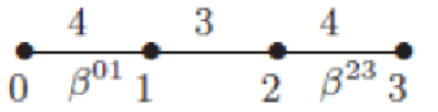
Presentations of fundamental groups $\boldsymbol{G}^1_{tu}$ and $\boldsymbol{G}^2_t$ by generators and defining relations to figures

Table 1

Group	Generators: Glide reflections	Generators: Screw motions	Relations (indices mod q)
G^1_{tu} $q=2t+1$ fixed $(t=1,2,3,\dots)$ u fixed $(u=0,1,\dots,t)$	a_i $(i=-t,\dots,0,\dots,t)$	$s_u,\ p_i,\ r_i$	$1=a_{-t}^2\dots a_0^2\dots a_t^2=(a_{-t}s_u a_{u+1}s_u^{-1})$ $(a_{-t+1}s_u a_{u+2}s_u^{-1})\dots(a_t s_u a_u s_u^{-1})=$ $=p_i s_u r_i^{-1} s_u=$ $=a_i p_i a_{i-u}^{-1} r_{i+t}=\quad i=-t,\dots,0,\dots,t$ $=a_i r_{i-t}^{-1} a_{i-u}^{-1} p_i^{-1}$
G^2_t $q=2t+1$ fixed $(t=1,2,3,\dots)$	$e,\ a_i,\ c_i,\ d_i$ $(i=-t,\dots,0,\dots,t)$		$1=a_{-t}^2\dots a_0^2\dots a_t^2=(a_0 e a_t^{-1} e^{-1})$ $(a_1 e a_{t-1}^{-1} e^{-1})\dots(a_{-1} e a_{-t}^{-1} e^{-1})=$ $=c_i e d_i^{-1} e=$ $=a_i c_i a_{-i} d_{t+i}=\quad i=-t,\dots,0,\dots,t$ $=a_i d_{-t+i}^{-1} a_{-i} c_i^{-1}$

The Euclidean cube tiling and its characteristic orthoscheme (4, 3, 4), *Coxeter-Schläfli* diagram, matrix (for later projective metric)





$$\begin{pmatrix} 1 & -\frac{\sqrt{2}}{2} & 0 & 0 \\ -\frac{\sqrt{2}}{2} & 1 & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{\sqrt{2}}{2} \\ 0 & 0 & -\frac{\sqrt{2}}{2} & 1 \end{pmatrix} = (b^{ij})$$

Figure 3: Cube tiling in $\mathbf{E}^3$ and symbols for it. Coxeter-Schläfli diagram for the $\mathbf{E}^4$ cube tiling.

Coxeter-Schläfli matrix and its inverse for orthoscheme ($u, v, w(=u)$) and for "trunc-simplices". Scalar products for forms (planes) and vectors (points)

$$(b^{ij}) = \langle \boldsymbol{b}^i, \boldsymbol{b}^j \rangle := \begin{pmatrix} 1 & -\cos\frac{\pi}{u} & 0 & 0 \\ -\cos\frac{\pi}{u} & 1 & -\cos\frac{\pi}{v} & 0 \\ 0 & -\cos\frac{\pi}{v} & 1 & -\cos\frac{\pi}{w} \\ 0 & 0 & -\cos\frac{\pi}{w} & 1 \end{pmatrix}.$$

$$(a_{ij}) = (b^{ij})^{-1} = \langle \mathbf{a}_i, \mathbf{a}_j \rangle :=$$

$$= \frac{1}{B} \begin{pmatrix} \sin^2\frac{\pi}{w} - \cos^2\frac{\pi}{v} & \cos\frac{\pi}{u}\sin^2\frac{\pi}{w} & \cos\frac{\pi}{u}\cos\frac{\pi}{v} & \cos\frac{\pi}{u}\cos\frac{\pi}{v}\cos\frac{\pi}{w} \\ \cos\frac{\pi}{u}\sin^2\frac{\pi}{w} & \sin^2\frac{\pi}{w} & \cos\frac{\pi}{v} & \cos\frac{\pi}{w}\cos\frac{\pi}{v} \\ \cos\frac{\pi}{u}\cos\frac{\pi}{v} & \cos\frac{\pi}{v} & \sin^2\frac{\pi}{u} & \cos\frac{\pi}{w}\sin^2\frac{\pi}{u} \\ \cos\frac{\pi}{u}\cos\frac{\pi}{v}\cos\frac{\pi}{w} & \cos\frac{\pi}{w}\cos\frac{\pi}{v} & \cos\frac{\pi}{w}\sin^2\frac{\pi}{u} & \sin^2\frac{\pi}{u} - \cos^2\frac{\pi}{v} \end{pmatrix}, \quad (2.2)$$

where

$$B = \det(b^{ij}) = \sin^2\frac{\pi}{u}\sin^2\frac{\pi}{w} - \cos^2\frac{\pi}{v} < 0 \quad \text{or} \quad \sin\frac{\pi}{u}\sin\frac{\pi}{w} - \cos\frac{\pi}{v} < 0.$$

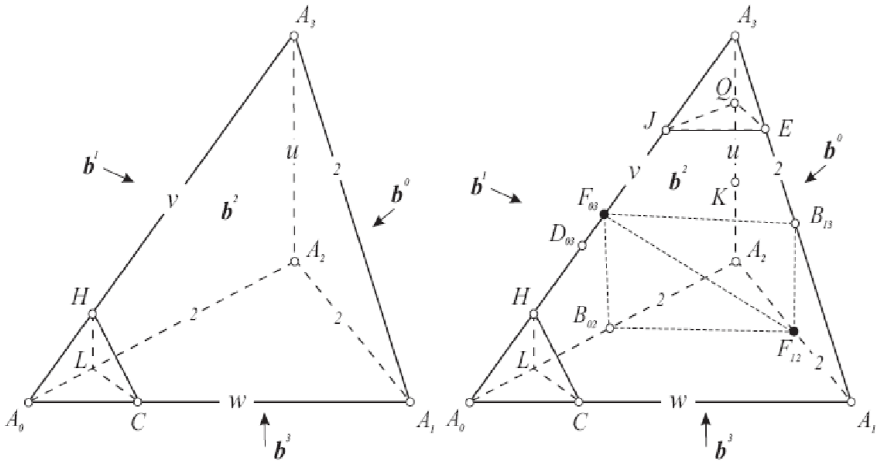
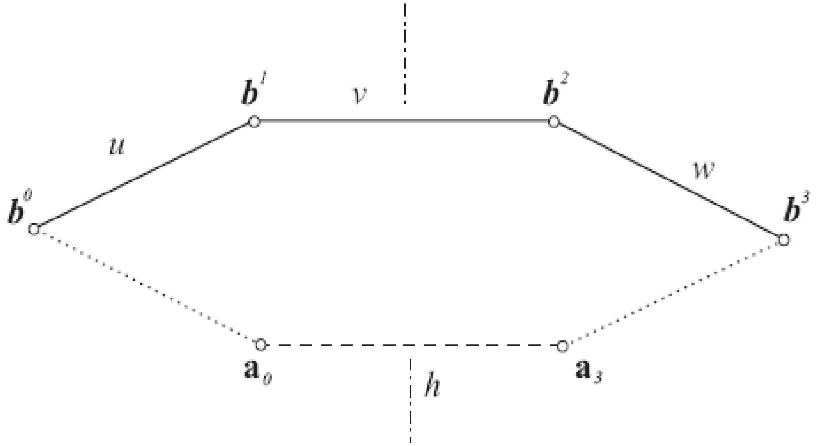


Figure 1: Simple and double truncated complete orthoschemes



The Volume of the orthoscheme by N. I. Lobachevsky ideas with generalization of R. Kellerhals

Theorem 2.2 (R. Kellerhals) *The volume of a three-dimensional hyperbolic complete orthoscheme* $\mathcal{O} = W_{uvw} \subset \mathbf{H}^3$ *is expressed with the essential angles* $\alpha_{01} = \frac{\pi}{u}$, $\alpha_{12} = \frac{\pi}{v}$, $\alpha_{23} = \frac{\pi}{w}$, $(0 \le \alpha_{ij} \le \frac{\pi}{2})$ *(Fig. 1.a, b) in the following form:*

$$\mathrm{Vol}(\mathcal{O}) = \frac{1}{4}\{\mathcal{L}(\alpha_{01}+\theta) - \mathcal{L}(\alpha_{01}-\theta) + \mathcal{L}(\frac{\pi}{2}+\alpha_{12}-\theta) + \\ + \mathcal{L}(\frac{\pi}{2}-\alpha_{12}-\theta) + \mathcal{L}(\alpha_{23}+\theta) - \mathcal{L}(\alpha_{23}-\theta) + 2\mathcal{L}(\frac{\pi}{2}-\theta)\},$$

where $\theta \in [0, \frac{\pi}{2})$ *is defined by:*

$$\tan(\theta) = \frac{\sqrt{\cos^2\alpha_{12} - \sin^2\alpha_{01}\sin^2\alpha_{23}}}{\cos\alpha_{01}\cos\alpha_{23}},$$

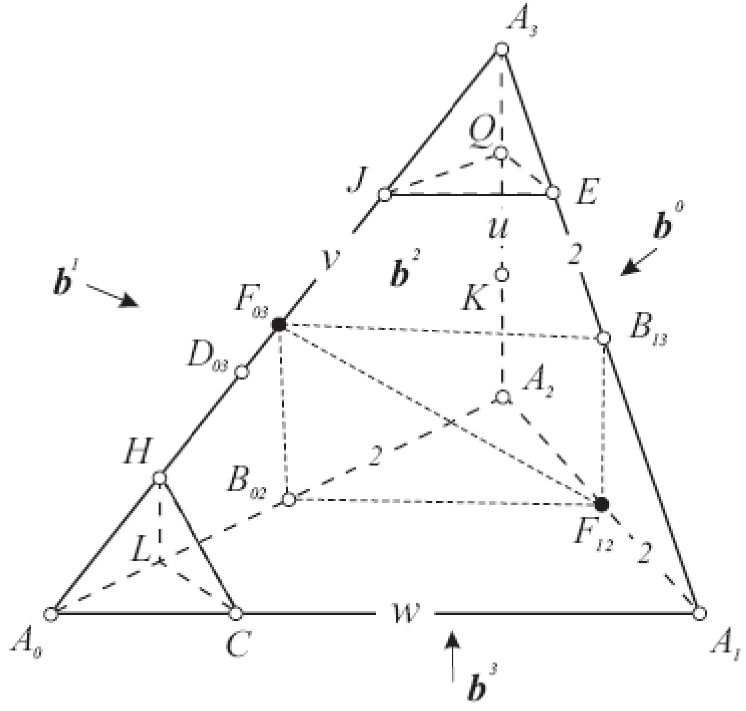
and where $\mathcal{L}(x) := -\int\limits_0^x \log|2\sin t|\,dt$ *denotes the Lobachevsky function.*

The football polyhedron {5, 6, 6} from the half orthoscheme (5, 3, 5)

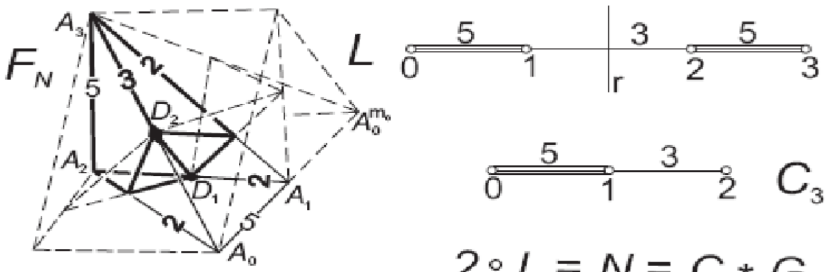
Trunc-simplex (u, v, $w = u$) with

$(1/u) + (1/v) < ½$; then

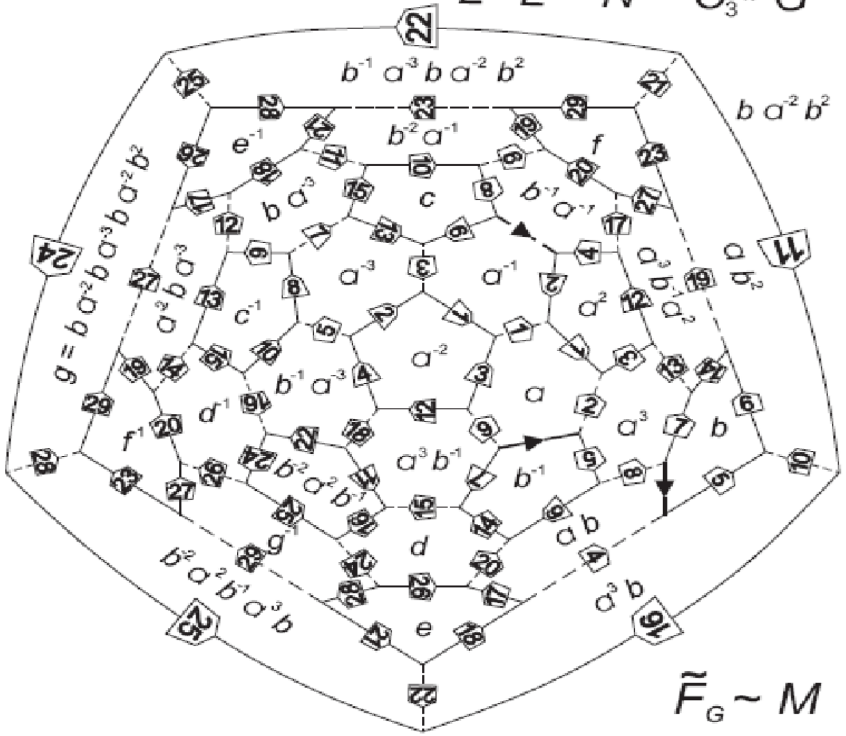
A_0 and A_3 are outer vertices with truncating polar planes a_0 resp. a_3



$M = H^3/G$ football manifold



$2 \circ L = N = C_3 * G$

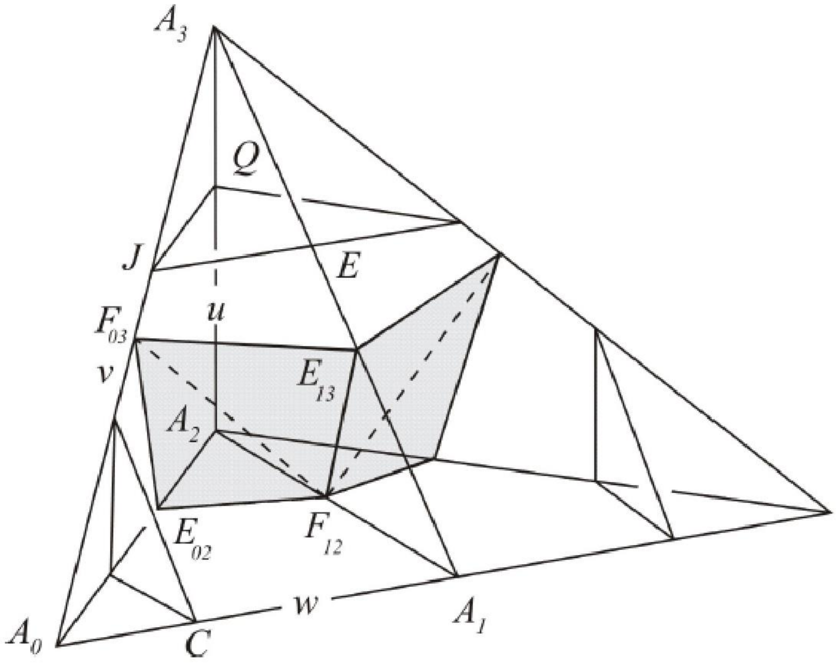


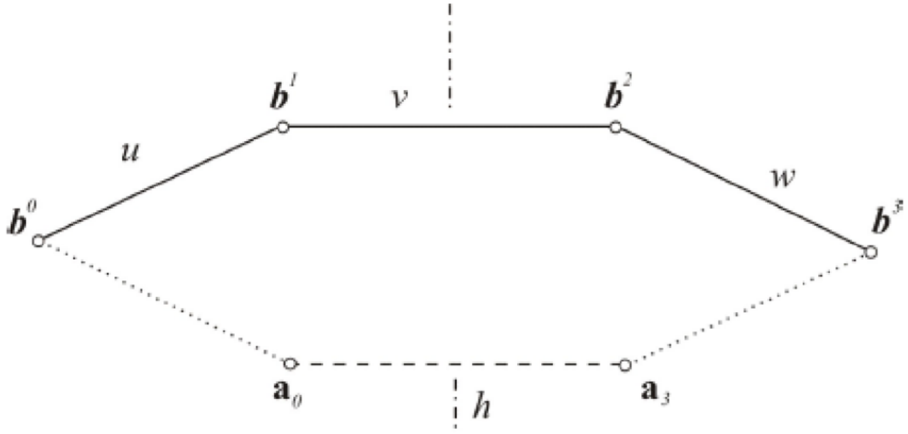
$\widetilde{F}_G \sim M$

E. Molnár, Two hyperbolic football manifolds. In: Proceedings of International Conference on Differential Geometry and Its Applications, Dubrovnik Yugoslavia, 1988. 217–241.

E. Molnár, On non-Euclidean crystallography, some football manifolds, Struct Chem (2012) 23:1057–1069

Construction of *cobweb* (or *tube*) manifolds from half trunc-orthoscheme, by $2z = u = v = w \geqq 6$



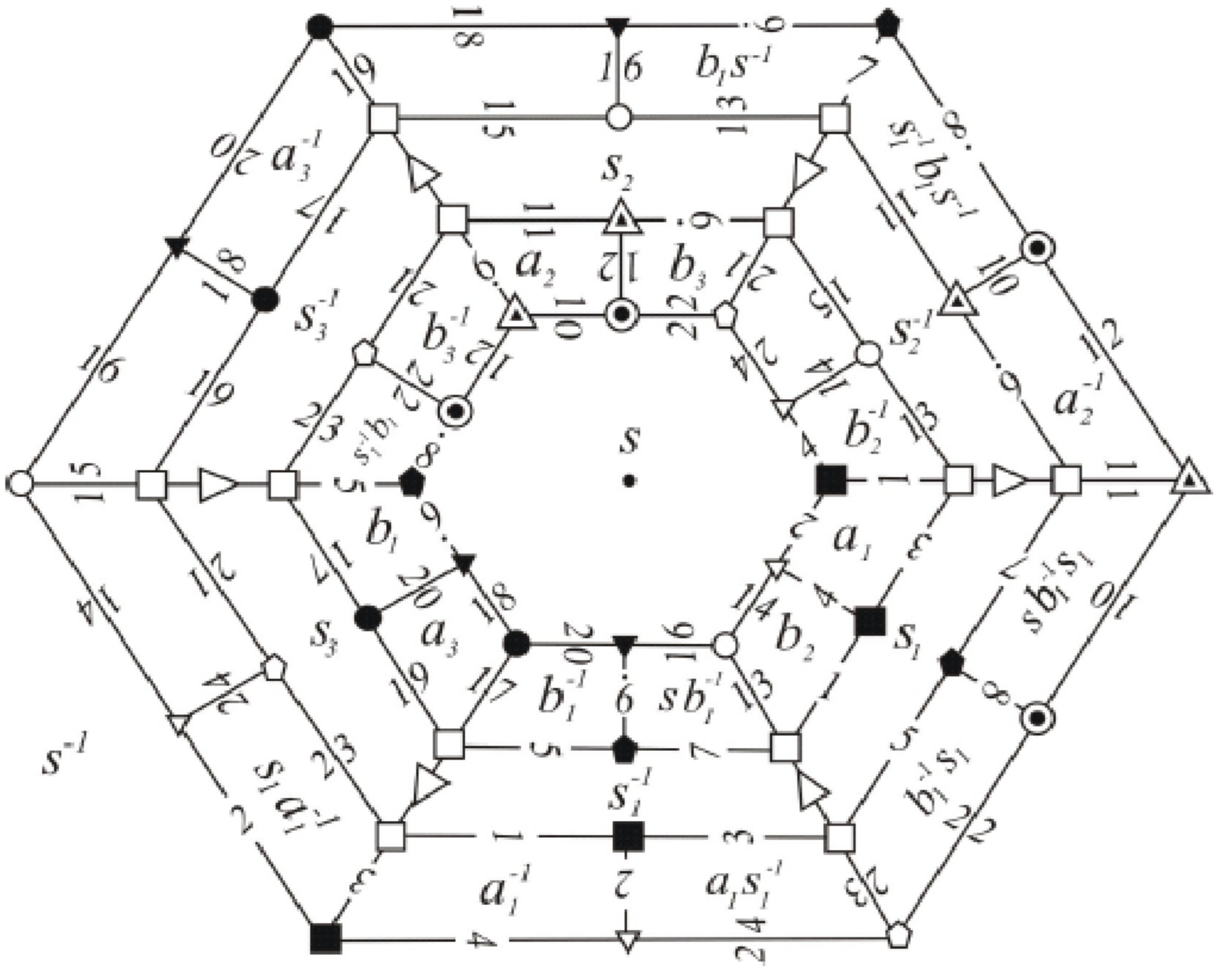


Theorem 1.1 *The cobweb manifold $Cw(6,6,6)$ to Fig.1,2 has been constructed by face identification in Fig. 4,5.*

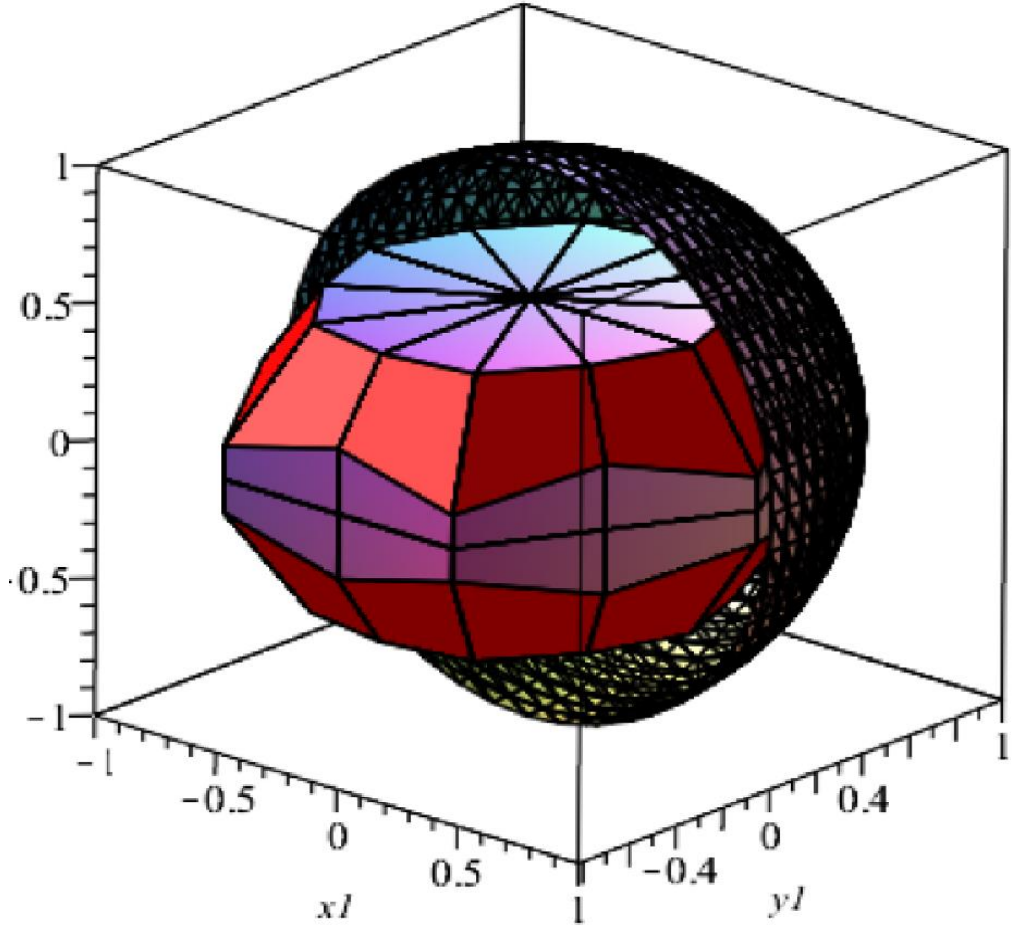
The fundamental group $\mathbf{Cw}(6,6,6)$ *can be described by 3-generators and three relations in formulas (2.13-15).*

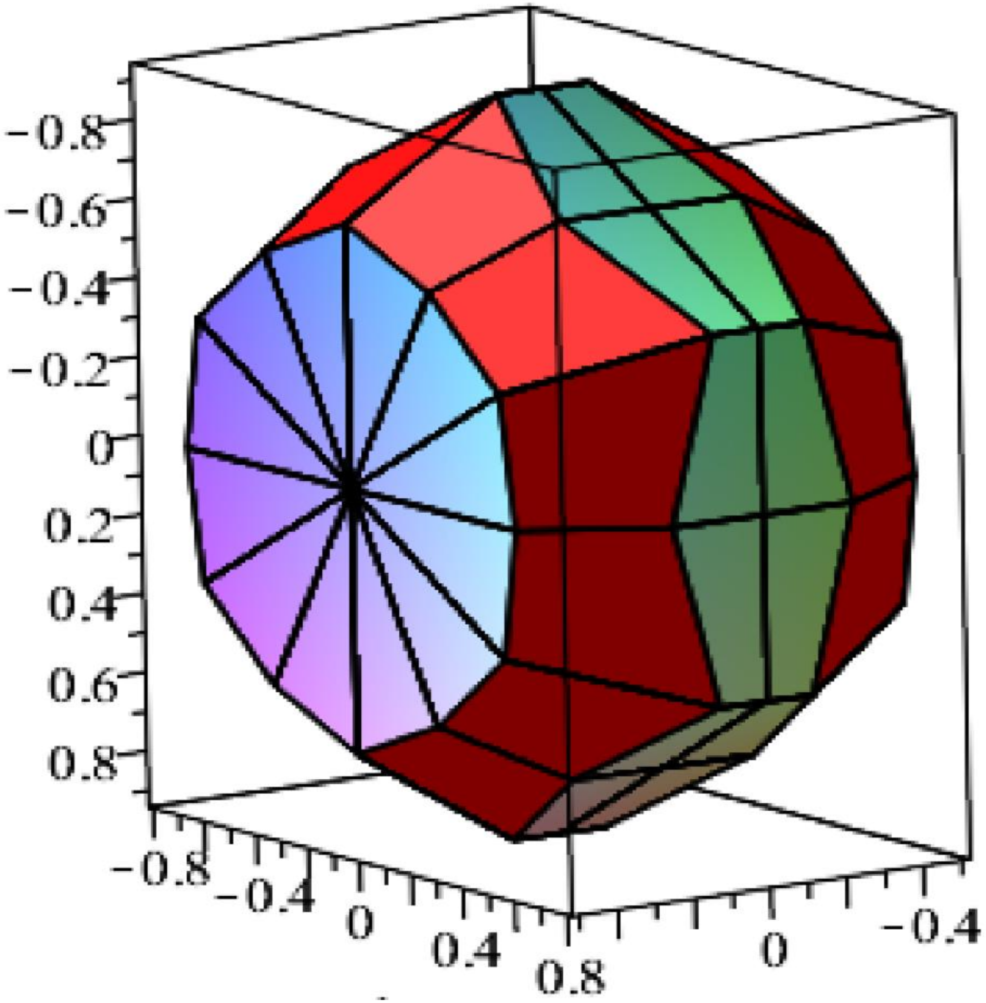
The volume of $Cw(6,6,6)$ is ≈ 8.29565 in (3.7). The largest ball contained in $Cw(6,6,6)$ is of radius $r \approx 0.57941$. The diameter of $Cw(6,6,6)$ is $2R \approx 3.67268$ by (3.4-5).

Construction of cobweb (tube) manifold Cw(6) by tricky face pairing identifications from *D-V* cell of previous point *Q*

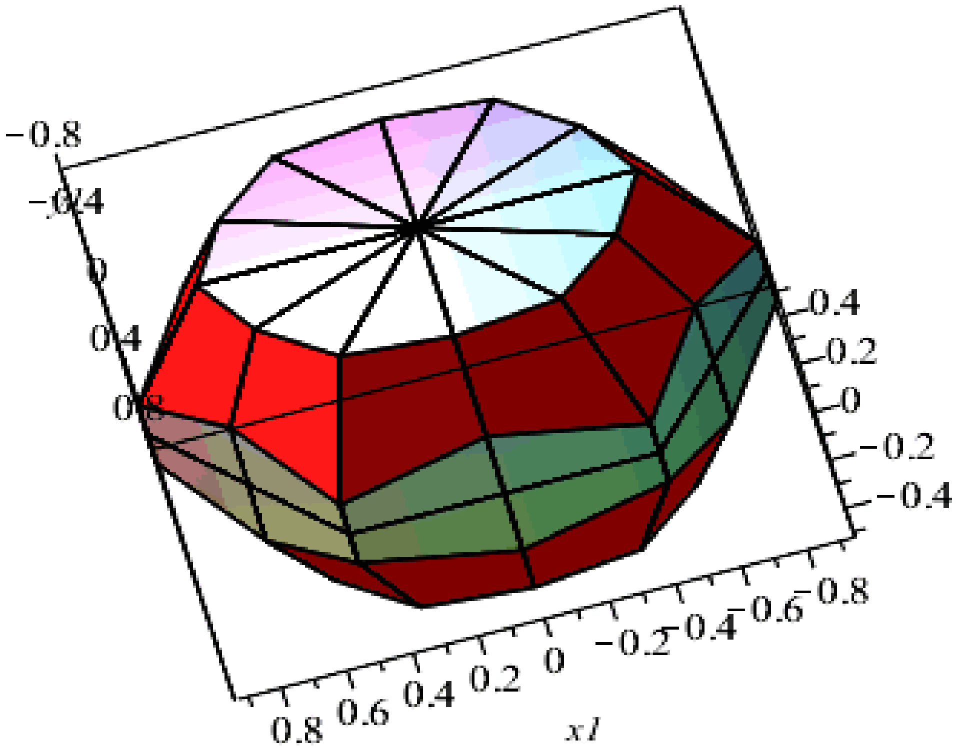


Animation of cobweb manifolds *Cw*(6) in *B-C-K model* of **H³**





Animation of *Cw*(6) manifold



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Thank you for kind Attention!

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