

DENSE BALL PACKINGS BY TUBE MANIFOLDS AS NEW MODELS FOR HYPERBOLIC CRYSTALLOGRAPHY

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Abstract. We intend to continue our previous papers on dense ball packing hyperbolic space \mathbf{H}^3 by equal balls, but here with centres belonging to different orbits of the fundamental group $\mathbf{Cw}(2z, 3 \leq z \in \mathbf{N}, \text{ odd number})$, of our new series of *tube or cobweb manifolds* $Cw = \mathbf{H}^3/\mathbf{Cw}$ with z -rotational symmetry. As we know, \mathbf{Cw} is a fixed-point-free isometry group, acting on \mathbf{H}^3 discontinuously with appropriate tricky fundamental domain Cw , so that every point has a ball-like neighbourhood in the usual factor-topology.

Our every $\mathbf{Cw}(2z)$ is minimal, i.e. does not cover regularly a smaller manifold. It can be derived by its general symmetry group $\mathbf{W}(u; v; w = u)$ that is a complete Coxeter orthoscheme reflection group, extended by the half-turn \mathbf{h} ($0 \leftrightarrow 3, 1 \leftrightarrow 2$) of the complete orthoscheme $A_0A_1A_2A_3 \sim b_0b_1b_2b_3$ (see Figure 1). The vertices A_0 and A_3 are outer points of the (Beltrami-Cayley-Klein) *B-C-K model of \mathbf{H}^3* , as $1/u + 1/v \leq 1/2$ is required, $3 \leq u = w, v$ for the above orthoscheme parameters. For the above simple manifold-construction we specify $u = v = w = 2z$. Then the polar planes a_0 and a_3 of A_0 and A_3 , respectively, make complete with reflections \mathbf{a}_0 and \mathbf{a}_3 the Coxeter reflection group, where the other reflections are denoted by $\mathbf{b}^0, \mathbf{b}^1, \mathbf{b}^2, \mathbf{b}^3$ in the sides of the orthoscheme $b^0b^1b^2b^3$.

The situation is described first in Figure 1 of the half trunc-orthoscheme W and its usual extended Coxeter diagram, moreover, by the scalar product matrix $(b^{ij}) = (\langle \mathbf{b}^i, \mathbf{b}^j \rangle)$ in formula (1) and its inverse $(A_{jk}) = (\langle \mathbf{A}_j, \mathbf{A}_k \rangle)$ in (3). These will describe the hyperbolic angle and distance metric of the half trunc-orthoscheme W , then its ball packings, densities, then those of the manifolds $\mathbf{Cw}(2z)$.

As first results we concentrate only on particular constructions by computer for probable material model realizations, atoms or molecules by equal balls, for general $W(u; v; w = u)$ as well, summarized at the end of our paper.

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1. Introduction

1.1 Hyperbolic space \mathbf{H}^3 , as a projective metric space. Generalized Beltrami-Cayley-Klein (B-C-K) model

Our Bolyai-Lobachevsky hyperbolic space $\mathbf{H}^3 = \mathcal{P}^3\mathcal{M}(\mathbf{V}^4, \mathbf{V}_4, \mathbf{R}, \sim, \langle \cdot, \cdot \rangle)$ will be a projective-metric space over a real vector space \mathbf{V}^4 for points $X(X \sim cX, c \in \mathbf{R} \setminus \{0\})$; its dual (i.e. linear form space) \mathbf{V}_4 will describe planes (2-planes) $u(u \sim \mathbf{u}c, c \in \mathbf{R} \setminus \{0\})$. The scalar product $\langle \cdot, \cdot \rangle$ will be specified in (1), (3) by a so-called complete orthoscheme as a projective coordinate simplex $b^0b^1b^2b^3 = A_0A_1A_2A_3$ by $\mathbf{A}_i b^j = \delta_i^j$ (Kronecker delta), i.e. $b^i = A_j A_k A_l, \{i; j; k; l\} = \{0; 1; 2; 3\}$.

Furthermore, the starting Coxeter-Schläfli matrix (1) will be defined by three natural parameters $3 \leq u, v, w$; (think of $u = 5, v = 3, w = 5$ at the characteristic orthoscheme of our previous football manifold $\{5, 6, 6\}$ in [11, 13]);

$$(b^{ij}) := (\langle \mathbf{b}^i, \mathbf{b}^j \rangle) = (\cos(\pi - \beta^{ij})), \beta^{ii} = \pi;$$

$$(b^{ij}) = \begin{pmatrix} 1 & -\cos \frac{\pi}{u} & 0 & 0 \\ -\cos \frac{\pi}{u} & 1 & -\cos \frac{\pi}{v} & 0 \\ 0 & -\cos \frac{\pi}{v} & 1 & -\cos \frac{\pi}{w} \\ 0 & 0 & -\cos \frac{\pi}{w} & 1 \end{pmatrix}, \quad (1)$$

as scalar products of basis forms $\mathbf{b}^i \in \mathbf{V}_4$ ($i = 0, 1, 2, 3$) to the side faces of the coordinate simplex $b^0b^1b^2b^3 = A_0A_1A_2A_3$ as usual. Thus, the essential face angles $(\angle b^i b^j) = \beta^{ij}$ are $\beta^{01} = \pi/u = \pi/5, \beta^{12} = \pi/v = \pi/3, \beta^{23} = \pi/w = \pi/5$, the others are $\beta^{02} = \beta^{03} = \beta^{13} = \pi/2$ (rectangle).

The above scalar product by (1) is equivalent by giving a (polar) plane \rightarrow (pole) point $\mathbf{V}_4 \rightarrow \mathbf{V}^4$ (linear symmetric) polarity

$b \rightarrow B, \mathbf{b}^i \rightarrow \mathbf{B}^i := b^{ij} \mathbf{A}_j, i, j \in \{0; 1; 2; 3\}$, Einstein-Schouten convention;

i.e. by (1) : $\mathbf{b}^0 \rightarrow \mathbf{B}^0 = \mathbf{A}_0 - \cos \frac{\pi}{u} \mathbf{A}_1,$

$\mathbf{b}^1 \rightarrow \mathbf{B}^1 = -\cos \frac{\pi}{u} \mathbf{A}_0 + \mathbf{A}_1 - \cos \frac{\pi}{v} \mathbf{A}_2,$ (2)

$\mathbf{b}^2 \rightarrow \mathbf{B}^2 = -\cos \frac{\pi}{v} \mathbf{A}_1 + \mathbf{A}_2 - \cos \frac{\pi}{w} \mathbf{A}_3, \mathbf{b}^3 \rightarrow \mathbf{B}^3 = -\cos \frac{\pi}{w} \mathbf{A}_2 + \mathbf{A}_3.$

First for $\mathbf{u} = \mathbf{b}^i u_i, \mathbf{v} = \mathbf{b}^j v_j$ let $\langle \mathbf{u}, \mathbf{v} \rangle := (u_i \mathbf{B}^i, \mathbf{b}^j v_j) = (u_i b^{ik} \mathbf{A}_k, \mathbf{b}^j v_j) = u_i b^{ik} \delta_k^j v_j = u_i b^{ij} v_j$ be defined step by step, Then

$$\cos(\angle uv) = \frac{-\langle \mathbf{u}, \mathbf{v} \rangle}{\sqrt{\langle \mathbf{u}, \mathbf{u} \rangle \langle \mathbf{v}, \mathbf{v} \rangle}}$$

defines the ‘‘usual angle’’ according to (1), (2), indeed. Proper plane u means that $\langle \mathbf{u}, \mathbf{u} \rangle = (\mathbf{U}\mathbf{u}) > 0$. Then its pole $U(\mathbf{U})$ is (unproper) outer point in (B-C-K) model.

Its “inverse scalar product” is by

$$(A_{ij}) = (b^{ij})^{-1} = \langle \mathbf{A}_i, \mathbf{A}_j \rangle := \frac{1}{B} \begin{pmatrix} \sin^2 \frac{\pi}{w} - \cos^2 \frac{\pi}{v} & \cos \frac{\pi}{u} \sin^2 \frac{\pi}{w} & \cos \frac{\pi}{u} \cos \frac{\pi}{v} & \cos \frac{\pi}{u} \cos \frac{\pi}{v} \cos \frac{\pi}{w} \\ \cos \frac{\pi}{u} \sin^2 \frac{\pi}{w} & \sin^2 \frac{\pi}{w} & \cos \frac{\pi}{v} & \cos \frac{\pi}{w} \cos \frac{\pi}{v} \\ \cos \frac{\pi}{u} \cos \frac{\pi}{v} & \cos \frac{\pi}{v} & \sin^2 \frac{\pi}{u} & \cos \frac{\pi}{w} \sin^2 \frac{\pi}{v} \\ \cos \frac{\pi}{u} \cos \frac{\pi}{v} \cos \frac{\pi}{w} & \cos \frac{\pi}{w} \cos \frac{\pi}{v} & \cos \frac{\pi}{w} \sin^2 \frac{\pi}{u} & \sin^2 \frac{\pi}{u} - \cos^2 \frac{\pi}{v} \end{pmatrix}, \quad (3)$$

where $B = \det(b^{ij}) = \sin^2 \frac{\pi}{u} \sin^2 \frac{\pi}{w} - \cos^2 \frac{\pi}{v} < 0$, i.e. $\sin \frac{\pi}{u} \sin \frac{\pi}{w} - \cos \frac{\pi}{v} < 0$.

We assume, and this will be crucial in the following, that $u = w$, so our orthoscheme will be symmetric by a half-turn h : $0 \leftrightarrow 3, 1 \leftrightarrow 2$. The half-turn axis h joins the midpoints F_{03} of A_0, A_3 and F_{12} of A_1, A_2 (see also Figure 1).

Figure 1 shows our novelty at later cobweb (tube) manifolds: $\pi/u + \pi/v < \pi/2$. Thus, our scalar product (1) (and its inverse (3)) as well will be of signature $(+++)$, A_0 and A_3 will be outer vertices of the B-C-K-model, so we truncate the orthoscheme by their proper polar planes a_0 and a_3 (look also at the extended Coxeter-Schläfli diagram in Figure 1), respectively, to obtain a compact domain with proper (or interior) points, a so-called complete orthoscheme (trunc-orthoscheme). Algebraically, the upper minor determinant sequence in (1) guarantees the signature $(+++)$ of the scalar products (1), (3) to be hyperbolic indeed.

Extensions of angle and distance metrics are also standard by complex \cos and \cosh functions (through exponential one, of course), respectively: $\cosh x = \cos(x/i)$, i is the imaginary unit. We mention only that the matrix (3) defines the scalar product of basis vectors of \mathbf{V}^4 . These determine the XY distance in \mathbf{H}^3 through the scalar product $\langle \mathbf{X}, \mathbf{Y} \rangle = X^i A_{ij} Y^j$ of vectors $\mathbf{X} = X^i \mathbf{A}_i$ and $\mathbf{Y} = Y^j \mathbf{A}_j \in \mathbf{V}^4$ (Einstein-Schouten index conventions). Namely,

$$\cosh \frac{XY}{k} = \frac{-\langle \mathbf{X}, \mathbf{Y} \rangle}{\sqrt{\langle \mathbf{X}, \mathbf{X} \rangle \langle \mathbf{Y}, \mathbf{Y} \rangle}}, \quad (\langle \mathbf{X}, \mathbf{X} \rangle, \langle \mathbf{Y}, \mathbf{Y} \rangle < 0). \quad (4)$$

Here $k = \sqrt{-\frac{1}{K}}$ is the natural length unit, where K is the sectional curvature. K can be chosen to -1 , so $k = 1$ in the following. But other K can be important in the applications (in nano size)!

We recall the volume formula of complete orthoscheme $\mathcal{O}(\beta^{01}, \beta^{12}, \beta^{23})$ by R. Kellerhals to the Coxeter-Schläfli matrix (1) on the genial ideas of N. I. Lobachevsky.

THEOREM 1.1 ([2]). *The volume of a three-dimensional hyperbolic complete orthoscheme $\mathcal{O}(\beta^{01}, \beta^{12}, \beta^{23}) \subset \mathbf{H}^3$ is expressed with the essential angles $\beta^{01} = \frac{\pi}{u}$, $\beta^{12} = \frac{\pi}{v}$, $\beta^{23} = \frac{\pi}{w}$, ($0 \leq \alpha_{ij} \leq \frac{\pi}{2}$) in the following form:*

$$\begin{aligned} \text{Vol}(\mathcal{O}) = & \frac{1}{4} \{ \mathcal{L}(\beta^{01} + \theta) - \mathcal{L}(\beta^{01} - \theta) + \mathcal{L}(\frac{\pi}{2} + \beta^{12} - \theta) \\ & + \mathcal{L}(\frac{\pi}{2} - \beta^{12} - \theta) + \mathcal{L}(\beta^{23} + \theta) - \mathcal{L}(\beta^{23} - \theta) + 2\mathcal{L}(\frac{\pi}{2} - \theta) \}, \end{aligned}$$

where $\mathcal{L}(x) := -\int_0^x \log |2 \sin t| dt$ denotes the Lobachevsky function (introduced by J. Mil-

nor [4] in this form) and $\theta \in [0, \frac{\pi}{2})$ is defined by:

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

The volume $\text{Vol}(B(R))$ of a ball $B(R)$ of radius R can be computed by the classical formula of J. Bolyai:

$$\text{Vol}(B(R)) = 2\pi(\cosh(R) \sinh(R) - R) = \pi(\sinh(2R) - 2R) = \frac{4}{3}\pi R^3(1 + \frac{1}{5}R^2 + \frac{2}{105}R^4 + \dots).$$

The usual (plane) reflection $\sigma(u, U) : X(\mathbf{X}) \rightarrow Y(\mathbf{Y})$ in the plane $u(\mathbf{u})$ with pole $U(\mathbf{U})$ is for points:

$$\sigma(u, U) : \mathbf{X} \rightarrow \mathbf{Y} = \mathbf{X} - \frac{2(\mathbf{X}\mathbf{u})}{\langle \mathbf{u}, \mathbf{u} \rangle} \mathbf{U}, \text{ here } \langle \mathbf{u}, \mathbf{u} \rangle = (\mathbf{U}\mathbf{u}).$$

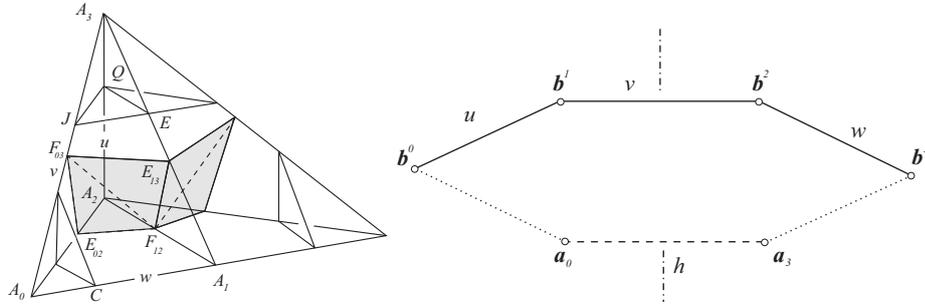


Figure 1: The half trunc-orthoscheme fundamental domain $W(u; v; w = u)$, i.e. that of the extended (by halfturn h) complete orthoscheme group and its extended Coxeter-Schläfli diagram.

Thus we could easily describe the extended complete orthoscheme reflection group $\mathbf{W}(u; v; w = u)$. A point $X(\mathbf{X})$ has an orthogonal projection $X_b(\mathbf{X}_b)$ on a plane b with pole B by

$$\mathbf{X}_b = \mathbf{X} - \frac{(\mathbf{X}\mathbf{b})}{\langle \mathbf{b}, \mathbf{b} \rangle} \mathbf{B}, \text{ by } \langle \mathbf{b}, \mathbf{b} \rangle = (\mathbf{B}\mathbf{b}). \tag{5}$$

So the distance of point X from plane b , denoted simply by Xb , can easily be expressed, etc.

1.2 The cobweb (tube) manifolds $Cw(2z, 2z, 2z) = Cw(2z)$

For our new cobweb manifolds we start with its previously mentioned symmetry group $\mathbf{W}(u; v; w = u)$ as complete extended reflection group. We shall apply $u = v = w = 2z, 3 \leq z$ is odd natural number, i.e. $b^0 b^1 b^2 b^3 = A_0 A_1 A_2 A_3$ is an orthoscheme; it will be complete, i.e. doubly truncated with polar planes a_3 and a_0 of A_3 and A_0 , respectively, called also half trunc-orthoscheme $W(2z)$.

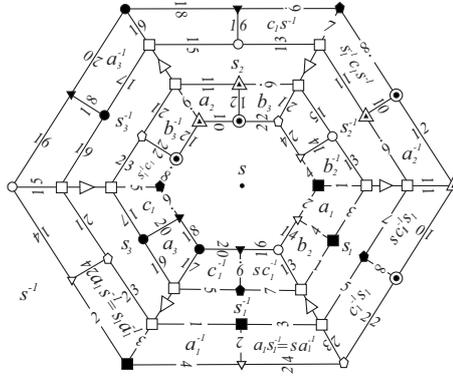


Figure 2: The starting cobweb (tube) manifold $Cw(6)$ with its symbolic face pairing isometries: e.g. $s^{-1} \rightarrow s$ by mapping (screw motion) s . Signed equivalent edge triples are equally numbered (from 1 to 24, odd and even edges play different roles). We obtain signed vertex classes (by various symbols), indicated here all together $1 + 3 \times 3 = 10$ ones. Any point has a ball-like neighbourhood (for later nanotube manifold by the above fundamental group $Cw(6)$, on the base of $W(6), z = 3$.

We consider this smaller asymmetric unit $W(2z = u = v = w)$ with the half-turn axis h and a variable halving plane through h . Then we choose the point $Q = a_3 \cap A_3 A_2$ with its stabilizer subgroup W_Q of order $4u = 8z$ in the extended reflection group $W(2z)$ to its fundamental domain $W(2z)$ (Figure 1). Then we reflect $W(2z)$ around Q to get the cobweb polyhedron $Cw(2z)$ (Figure 2 first for $z = 3$) as a fundamental domain of our new manifold with a new interesting fundamental group denoted by $Cw(2z)$.

Carbon atoms, or other ones (with valence 4, e.g. at F_{12} and its Cw -equivalent positions) can be placed very naturally in this tube-like structure.

It turns out that for $z = 4p - 1$ and for $z = 4q + 1$ ($1 \leq p, q \in \mathbf{N}$) we get two analogous series (Figure 6, 7), each of them is unique by z -rotational symmetry and manifold requirements.

Then come our new ball packing constructions as our new initiatives with more ball centre orbits by the above symmetry groups $W(u; v; w = u)$ but equal balls. There is only a part of a ball B_X in half orthoschem W of centre $X \in W$ just by the order $|W_X|$ of stabilizer subgroup W_X . Our goal, to find the densest ball packing on a natural average, is not completed yet. Our top density here is $0.68248 \dots ??$ This problem seems to be very hard, of course (maybe hopeless, in general?).

Our summaries follow in Theorems 4.1 and 4.2 in Section 4.

We intend to make our paper self-contained as possible. Our basic papers here are [11, 13] with further references. To the important simplex tiling theory we cite here [15, 16]. To the algorithmic polyhedral construction of tilings and manifolds see [6, 8, 12, 18, 19]. For the ball packing problems in other Turston geometries we refer to [10, 14, 21, 22]. For non-Euclidean crystallography see [6, 9, 14]. All these are

with partial results.

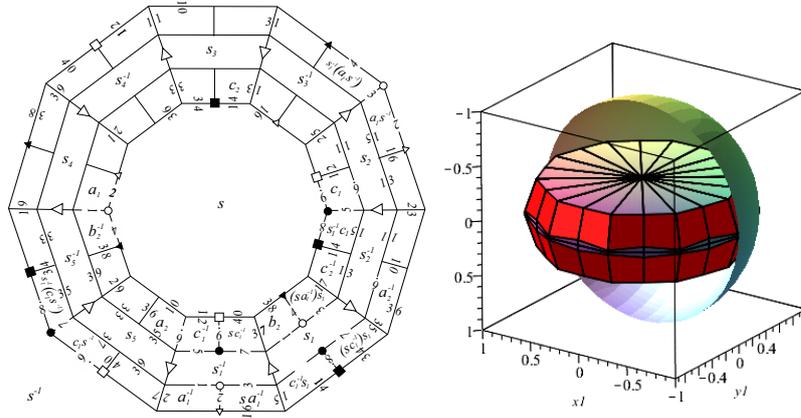


Figure 3: Our old cobweb (tube) manifolds $Cw(2z = 8q + 2)$, illustrated by $z = 5, q = 1$. A picture of its animation in Beltrami-Cayley-Klein model.

2. Manifold constructions in new versions, with new ball packing initiatives

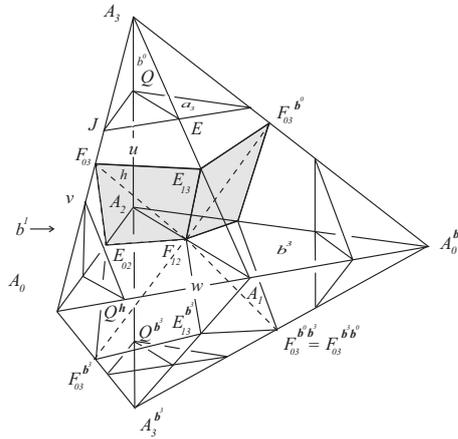


Figure 4: The b^3 -reflected part $W(u; v; w = u)$ and its b^0 mirror image W^{b^0} in the coordinate plane b^0 . So the new bent “quadrangle” face $F_{03}E_{13}F_{03}^{b^0}E_{02}F_{03}^{b^0}E_{13}^{b^3}F_{03}^{b^3}E_{02}$ will be a c_i -type side face of the new “cut-reglued” fundamental polyhedron Cw . The a_3 reflected part of b^2 -face (together with b^2) will be an s_j -type face of the new Cw (not indicated here).

2.1 Construction of cobweb (tube) manifold $Cw(6, 6, 6) = Cw(6)$ and the general two series $Cw(2z)$

For the theory of manifolds see [25] (cited also in works [1, 3, 18, 20, 23]); for its projective interpretation and visualization we refer to [5, 7, 24].

By the theory we have to construct a fixed point free group acting in hyperbolic space \mathbf{H}^3 with the above compact fundamental domain. In the Introduction to Figure 1 and analogously to Figure 2 we have repeatedly described from [13] the extended reflection group $\mathbf{W}(6; 6; 6) = \mathbf{W}(6)$ with fundamental domain $W(6)$, as a half complete Coxeter orthoscheme, and glued together to the cobweb polyhedron $Cw(6; 6; 6) = Cw(6)$ as Dirichlet-Voronoi (in short $D - V$) cell of the kernel point Q by its orbit under the group $\mathbf{W}(6)$. Now by Figure 2, 4, 5 we shall give a new simpler face identification of $Cw(6)$, so that it will be a cut-reglued fundamental polyhedron of the previous fixed-point-free group, denoted also by $\mathbf{Cw}(6)$, generated just by the new face identifying isometries (as hyperbolic screw motions).

By gluing $4u = 24$ domains (at A_2 and) at Q around (whose stabilizer subgroup \mathbf{W}_Q is just of order $|\mathbf{W}_Q| = 4u = 24$ as for A_2 as well), we simply “kill out” the fixed points of $\mathbf{W}(6)$, as we made in our former paper [13].

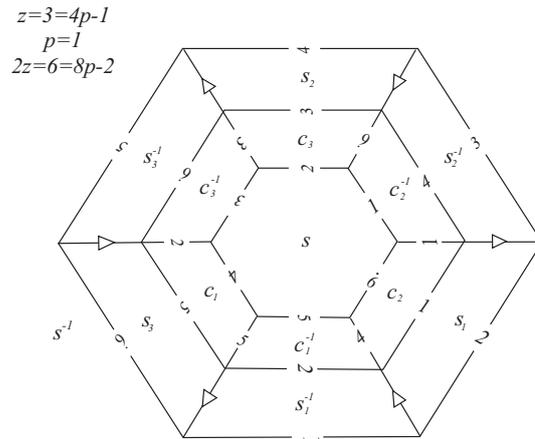


Figure 5: The new simplified $Cw(6 = 2z)$ manifold. Only with $7 = 2z + 1$ edge classes (4 edges in each of 6 classes, $6 = 2z$ edges in class $-\triangleright$.) The former odd classes 1, 3 will be the new class 1 here; former 5, 7 \rightarrow new edge class 2. The former even classes are glued together in the interior of c_i -type faces. We have only $14 = 4z + 2$ side faces, i.e. $7 = 2z + 1$ generators for the fundamental group \mathbf{Cw} .

We shortly repeat from [13] our new unified algorithmic presentation of fundamental group of the first series. At the beginning there stand the generator screw motions: \mathbf{s} for the tube form by rotational component $2\pi(z - 1)/2z$; $\mathbf{s}_1, \dots, \mathbf{s}_z$ are half screws around; $\mathbf{c}_1, \dots, \mathbf{c}_z$ come from specific rotation around the tube axis, combined with a halfturn (a conjugate of \mathbf{h}). Then come the relations to the numbered or signed

edges:

$$\begin{aligned}
 & \mathbf{Cw}(2z = 8p - 2) : (\mathbf{s}, \mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_z, \mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_z; - \\
 & \text{edge } 2i - 1 : \mathbf{s}_i \mathbf{c}_{i+p}^{-1} \mathbf{c}_{i-1+2p}^{-1} \mathbf{s}^{-1} = 1; \text{ edge } 2i : \mathbf{s}_i^{-1} \mathbf{c}_i \mathbf{c}_{i-p} \mathbf{s}^{-1} = 1; - \\
 & \text{edge } \rightarrow \leftarrow : 1 = \prod_i^i (\mathbf{c}_i \mathbf{c}_{i-p} \mathbf{c}_{i-1+2p} \mathbf{c}_{i+p}), \text{ for } i = 1, 2, \dots, z; \text{ indices are } \pmod{z}.
 \end{aligned} \tag{6}$$

In case $p = 1$ we obtain the presentation of $\mathbf{Cw}(6)$ by Figure 5. We analogously obtain the algorithmic presentation of our second series

$$\begin{aligned}
 & \mathbf{Cw}(2z = 8q + 2) : (\mathbf{s}, \mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_z, \mathbf{c}, \mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_z; - \\
 & \text{edge } 2i - 1 : \mathbf{s}_i \mathbf{c}_{i-q}^{-1} \mathbf{c}_{i+2q}^{-1} \mathbf{s}^{-1} = 1; \text{ edge } 2i : \mathbf{s}_i^{-1} \mathbf{c}_i \mathbf{c}_{i+q} \mathbf{s}^{-1} = 1; - \\
 & \text{edge } \rightarrow \leftarrow : 1 = \prod_i^i (\mathbf{c}_i \mathbf{c}_{i+q} \mathbf{c}_{i+2q} \mathbf{c}_{i-q}), \text{ for } i = 1, \dots, z; \text{ indices are } \pmod{z}.
 \end{aligned} \tag{7}$$

In case $q = 1$ we obtain the presentation of $\mathbf{Cw}(10)$ by Figure 3, here in new interpretation.

In both cases we have some consequences, e.g. in first case $\mathbf{s}_i = \mathbf{s} \mathbf{c}_{i-1+2p} \mathbf{c}_{i+p} = \mathbf{c}_i \mathbf{c}_{i-p} \mathbf{s}^{-1}$ that was utilized in the last product relation.

The face pairing structure of these manifolds can be derived generally in Figure 6, 7 (see also Figure 3). The above tube screw motion \mathbf{s} has rotation component $2\pi(z - 1)/2z$, throughout in the following. The crucial difference between the two series is that the third edge in class 1 in the triple will be placed opposite to each other on the cobweb (tube) polyhedron, as (6) and (7) express as well. Geometrically each manifold $Cw(2z)$ and also $W(2z)$ appears in two mirror forms (in our figures as well), equivalent mathematically, maybe not so in the occasional applications (similarly as in the Euclidean crystallography).

Very probably (!?), these manifolds realize nanotubes in small (nanometer= 10^{-9} m) size. And of course, there arise new open questions.

For completeness we recall the presentation of the symmetry group of our cobweb (tube) manifolds $Cw(2z)$ in more general (a most economical) version. Thus we have for the extended complete half-orthoscheme reflection group with parameters $3 \leq u = w, v \in \mathbf{N}$ by the Coxeter-Schläfli diagram in Figure 1, as follows:

$$\begin{aligned}
 \mathbf{W}(u; v; w = u) &= (\mathbf{a}_3, \mathbf{b}^0, \mathbf{b}^1, \mathbf{h} \quad -1 = \mathbf{a}_3 \mathbf{a}_3 = \mathbf{b}^0 \mathbf{b}^0 = \mathbf{b}^1 \mathbf{b}^1 = \mathbf{h} \mathbf{h} = \\
 &= (\mathbf{a}_3 \mathbf{b}^0)^2 = (\mathbf{a}_3 \mathbf{b}^1)^2 = (\mathbf{a}_3 \mathbf{h} \mathbf{b}^1 \mathbf{h})^2 = (\mathbf{b}^0 \mathbf{b}^1)^u = \\
 &= (\mathbf{h} \mathbf{b}^0 \mathbf{h} \mathbf{b}^0)^2 = (\mathbf{h} \mathbf{b}^0 \mathbf{h} \mathbf{b}^1)^2 = (\mathbf{h} \mathbf{b}^1 \mathbf{h} \mathbf{b}^1)^v).
 \end{aligned} \tag{8}$$

Of course, we can express the generators of the above $\mathbf{Cw}(2z = 8p - 2)$ and $\mathbf{Cw}(2z = 8q + 2)$, respectively, with generators of \mathbf{W} , and check the corresponding relations by those of \mathbf{W} in (8). Here the rotation $(\mathbf{b}^0 \mathbf{b}^1)$ of order $u (= 2z)$ plays important role.

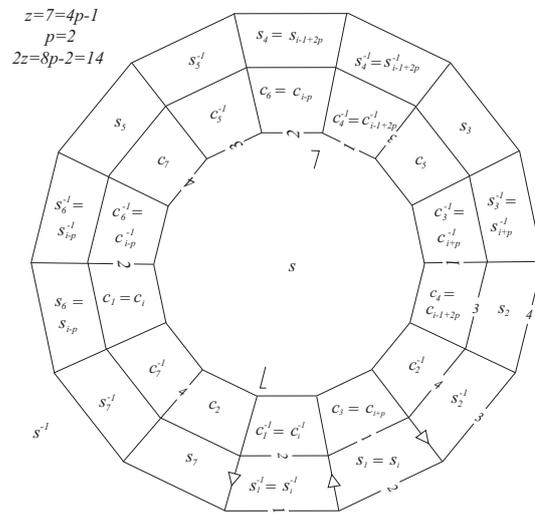


Figure 6: The general new $Cw(2z)$ manifold scheme for $z = 4p-1$, illustrated by $p = 2, z = 7$. See also formula (6) for algorithmic presentation

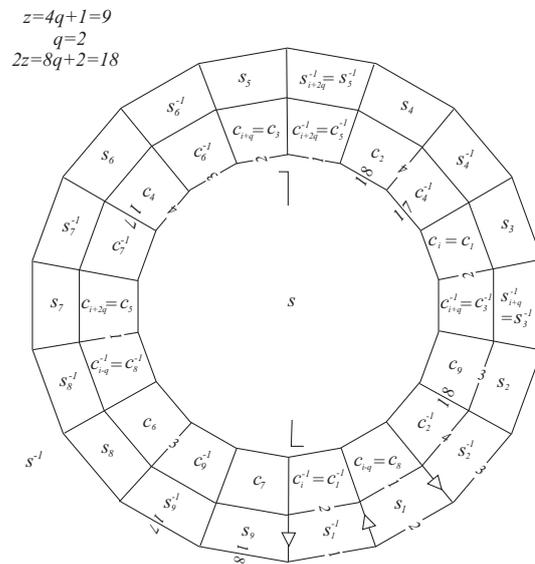


Figure 7: General new manifold scheme for $z = 4q + 1$, illustrated by $q = 2$, i.e. $z = 9$. See also formula (7) for algorithmic presentation

For instance the half screw $s_1 : s_1^{-1} \rightarrow s_1$ for $Cw(2z = 8p - 2)$ with a fixed

fundamental domain W to faces s_1^{-1} and c_1^{-1} (see Figure 4 and 6 together in “mirror eyes”) will be $\mathbf{s}_1 = \mathbf{a}_3(\mathbf{h}\mathbf{b}^1\mathbf{h})\mathbf{b}^1\mathbf{b}^0$ (see this also by the image of first edge 1) on s_1^{-1} . The screw motion $\mathbf{c}_1 : c_1^{-1} \rightarrow c_1$ will be $\mathbf{c}_1 = \mathbf{h}(\mathbf{b}^0\mathbf{b}^1)^{1+p}$, as you see by the edge 2 on s_1^{-1} . The tube screw $\mathbf{s} : s^{-1} \rightarrow s$ will be $\mathbf{s} = \mathbf{a}_3(\mathbf{h}\mathbf{b}^0\mathbf{h})(\mathbf{b}^1\mathbf{b}^0)^{z-1}$ by the image of edge 1 on s_1^{-1} again.

THEOREM 2.1. *The above cobweb (tube) manifold $Cw(2z)$ are minimal, i.e. none of them covers regularly another (smaller) manifold.*

Proof. The proof is a consequence of the Mostow rigidity theorem [17] (see also Margulis [3]). Namely, The fundamental group of a compact hyperbolic manifold (as in our case as well) can be realized by a fixed-point-free isometry group of \mathbf{H}^3 with compact fundamental domain. The fundamental group of a regular covering manifold is an invariant subgroup of the fundamental group of the covered manifold. The factor group is called *covering group*. Any symmetry map of $Cw(2z)$ is conjugated by an isometry that carries any orbit of $Cw(2z)$, onto an orbit of it. So this holds for the generators of our half trunc-orthoscheme $W(2z)$, we can imagine it that tiles the fundamental domain $Cw(2z)$, as our manifold. That means, we would imagine two tilings of $Cw(2z)$: first, that with the fundamental domains of the covered manifolds under fixed-point-free isometries; second, with the half trunc-orthoscheme under plane reflections and halfturns. But this is not possible. The reflection domains cannot be divided into smaller parts, as well known for our orthoscheme. Other case cannot occur by the fixed point free actions of the covered manifold. Contradiction! \square

2.2 The strategy of our new dense ball packing construction

Let $w = u$ and later $u = v = 2z$, $JQEE_{13}F_{12}E_{02}F_{03}A_2$ be the vertices of the half truncated orthoscheme $W(u; v; w = u)$ in Figure 4.

Each essential typical point of W can be expressed by its vector. The types are the above vertices of W , a representing interior point of any edges, included that of axis h , a representing point of any reflection face, a representing point of the interior of W can also be characterized by vectors, as we indicated in the Introduction (see also [11,13]). We do not repeat these here, since the computations will be implemented to computer.

E.g. point A_2 will be by the coordinate simplex vector \mathbf{A}_2 , and point Q

$$Q(\mathbf{Q}) = a_3 \cap A_3A_2; \quad \mathbf{Q} = \mathbf{A}_2 - \frac{A_{23}}{A_{33}}\mathbf{A}_3, \text{ with}$$

$$\langle \mathbf{Q}, \mathbf{Q} \rangle = \frac{(A_{22}A_{33} - A_{23}^2)}{A_{33}} = \langle \mathbf{Q}, \mathbf{A}_2 \rangle = \frac{\sin^2 \frac{\pi}{u}}{\sin^2 \frac{\pi}{u} - \cos^2 \frac{\pi}{v}} = \frac{A_{22}}{A_{33}}$$

by matrix (3).

Point $E(\mathbf{E}) = a_3 \cap A_1A_3$ will be

$$\mathbf{E} = \mathbf{A}_1 - \frac{A_{13}}{A_{33}}\mathbf{A}_3, \text{ with}$$

$$\langle \mathbf{E}, \mathbf{E} \rangle = \frac{(A_{11}A_{33} - A_{13}^2)}{A_{33}} = \langle \mathbf{E}, \mathbf{A}_1 \rangle = \frac{1}{\sin^2 \frac{\pi}{u} - \cos^2 \frac{\pi}{v}} = \frac{1}{BA_{33}}.$$

In the considered cases $u = w$, therefore, the midpoints F_{03} of A_0A_3 and F_{12} of A_1A_2 , respectively, can play important roles (?), since $F_{03}F_{12} = h$ will be the axis of halfturn h ,

$$\begin{aligned}\mathbf{F}_{03} &= \mathbf{A}_0 + \mathbf{A}_3, \quad \langle \mathbf{F}_{03}, \mathbf{F}_{03} \rangle = 2(A_{00} + A_{03}) < 0, \\ \mathbf{F}_{12} &= \mathbf{A}_1 + \mathbf{A}_2, \quad \langle \mathbf{F}_{12}, \mathbf{F}_{12} \rangle = 2(A_{11} + A_{12}) < 0.\end{aligned}$$

So an interior point H of axis h can be $\mathbf{H} = \mathbf{F}_{03} + h\mathbf{F}_{12}$ (with $0 < h$ real number). Also the other vertices, edge points, interior points of reflection faces or interior points of the body W can be described by 0, 1, 2, 3 real parameters, respectively. For their known distance formulas, e.g. (4), (5) can be used for radii of packing balls, etc. For the contribution $\delta(B_O)$ of an O -centred ball B_O to packing density we shall use only $W(u; v; w = u)$ by formula

$$\delta(B_O) = \frac{\text{Vol}(B_O(r))}{|\mathbf{W}_O| \text{Vol}(W)}, \quad (9)$$

where the maximal unified radius r is restricted by the other balls, h and the walls of half trunc-orthoscheme W . The sum of the ball contributions yield *the packing density in W as our (new!?) definition for packing with equal balls by different group orbits*. For one ball orbit this agree with the general density definition of packing not assumed to be regular but with equal balls (by D-V-cells, as in the introduction of our paper [11]). But these are not valid for packings with equal balls of more orbits (when the computation of the general density seems to be almost hopeless!?). We recall some typical stabilizer orders (Figure 1, 4):

1. A_2 is the ball centre, $|\mathbf{W}_{A_2}| = 4u = |\mathbf{W}_Q|$ for $O = Q$;
2. F_{03} is the ball centre, $|\mathbf{W}_{F_{03}}| = 4v = |\mathbf{W}_J|$ for $O = J$;
3. F_{12} is the ball centre, $|\mathbf{W}_{F_{12}}| = 8 = |\mathbf{W}_E|$ for $O = E$.

Of course, centre on h or on reflection faces involves half ball, centre in the interior of W involves a full ball. It is easy to see, that our manifold $Cw(2z)$, with $u = v = w = 2z$, $3 \leq z$, by its “ $2z$ -gonal fundamental polyhedron” can be packed with full equal balls, whose number of centre orbits is in accordance with that in $W(2z)$, so that the above density in $W(2z)$ will be equal to the sum of ball volumes divided by the volume of $Cw(2z)$, just by symmetry argument.

Strategies: *The ball packing construction into a general but fixed $W(u; v; w = u)$ for large density is a typical experimental interactive computer problem, e.g. by two possible strategies:*

- (i) The first one is as follows: We compute the distances of vertices, edges, faces from each other for overview. Then we place a centre into a vertex (or edge point, or face point) with a corresponding ball part of radius as big as possible, then try to place a full ball of radius as big as possible into the interior. Then equalize the two radii, and compute the packing density (by (9)) with two summands. Then we take two ball parts of optimal equal radii, then try a full ball into the interior, etc. . . . , this is a finite procedure. $W(2z)$ is extremely interesting for small z , say 3, 5, 7.

(ii) The second one is, after distance overview: We place the first ball into the interior of $W(u; v; w = u)$, then we take the ball parts, radius equalization, densities, etc. \square This is a tedious work. A good program would be actual, and it seems to be important.

3. Preliminary computation results

We present here only our seemingly relevant results for later computations by Strategy (i). Boldface printed δ^{opt} density data and some less ones deserve further approximations!?. Thus, one ball part orbits seem to be not relevant, compared with our former paper [11] adapted here.

3.1 Two ball part orbits

Ball centres	r^{opt}	$2 \cdot Vol(W_{uvw})$	$Vol(B(r^{opt}))$	δ^{opt}
F_{12}, E	0.27140	0.27899	0.08498	0.15230
F_{12}, Q	0.27140	0.27899	0.08498	0.12692
A_2, E	0.31215	0.27899	0.12991	0.19402

Table 1: Packings with 2 balls, $(u; v; w) = (3; 7; 3)$

Q, F_{03}	0.53064	0.43062	0.66207	0.34594
A_2, F_{03}	0.53064	0.43062	0.66207	0.34594
A_2, E	0.51921	0.43062	0.61872	0.53880
A_2, J	0.53064	0.43062	0.66207	0.34594

Table 2: Packings with 2 balls, $(u; v; w) = (4; 5; 4)$

Q, F_{03}	0.62687	0.46190	1.11606	0.54365
A_2, F_{03}	0.61123	0.46190	1.03061	0.50203
F_{12}, E	0.41334	0.46190	0.30609	0.33134
A_2, E	0.52717	0.46190	0.64869	0.49154

Table 3: Packings with 2 balls, $(u; v; w) = (5; 4; 5)$

Q, F_{03}	0.56651	0.57271	0.81195	0.283558
F_{12}, E	0.46453	0.57271	0.43838	0.38273
A_2, E	0.60020	0.57271	0.97324	0.59477

Table 4: Packings with 2 balls, $(u; v; w) = (5; 5; 5)$

Q, F_{03}	0.70337	0.55557	1.60883	0.60329
A_2, F_{03}	0.69217	0.55557	1.52838	0.57313
A_2, E	0.61947	0.55557	1.07504	0.64500
A_2, J	0.65848	0.55557	1.30405	0.48901

Table 5: Packings with 2 balls, $(u, v; w) = (6; 4; 6)$

A_2, E	0.65278	0.60917	1.26859	0.66938
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Table 6: Packings with 2 balls, $(u, v, w) = (7, 4, 7)$

Q, F_{03}	0.53278	0.38325	0.67042	0.41650
A_2, F_{03}	0.53278	0.38325	0.67042	0.41650
F_{12}, F_{03}	0.36227	0.38325	0.20444	0.22227
F_{12}, E	0.34463	0.38325	0.17557	0.22905

Table 7: Packings with 2 balls, $(u, v, w) = (7, 3, 7)$

F_{12}, E	0.46503	0.69130	0.43984	0.31812
F_{12}, Q	0.52985	0.69130	0.65901	0.31776
A_2, E	0.57941	0.69130	0.87126	0.42010

Table 8: Packings with 2 balls, $(u, v, w) = (6, 6, 6)$

F_{12}, E	0.44294	0.83993	0.37858	0.22536
F_{12}, Q	0.32119	0.83993	0.14169	0.05061
A_2, E	0.32119	0.83993	0.14169	0.05061

Table 9: Packings with 2 balls, $(u; v; w) = (10; 10; 10)$

F_{12}, E	0.44123	0.87770	0.37409	0.21311
F_{12}, Q	0.22661	0.87770	0.04925	0.01603
A_2, E	0.22661	0.87770	0.04925	0.01603

Table 10: Packings with 2 balls, $(u; v; w) = (14; 14; 14)$

3.2 Three ball part orbits

A_2, F_{03}, E	0.31215	0.27899	0.12991	0.22729
Q, F_{12}, F_{03}	0.27140	0.27899	0.08498	0.14867

Table 11: Packings with 3 balls, $(u; v; w) = (3; 7; 3)$

A_2, F_{03}, E	0.51921	0.43062	0.61872	0.68248
Q, F_{12}, E	0.38360	0.43062	0.24350	0.35341
Q, F_{12}, F_{03}	0.38360	0.43062	0.24350	0.26859

Table 12: Packings with 3 balls, $(u; v; w) = (4; 5; 4)$

A_2, F_{03}, E	0.52717	0.46190	0.64869	0.66709
A_2, F_{12}, E	0.33587	0.46190	0.16233	0.21087
Q, F_{12}, F_{03}	0.41334	0.46190	0.30609	0.31477

Table 13: Packings with 3 balls, $(u; v; w) = (5; 4; 5)$

A_2, F_{03}, E	0.52477	0.57271	0.63955	0.50252
A_2, F_{12}, E	0.46453	0.57271	0.43838	0.45927
Q, F_{12}, F_{03}	0.46453	0.57271	0.43838	0.34445

Table 14: Packings with 3 balls, $(u; v; w) = (5; 5; 5)$

A_2, F_{03}, E	0.49441	0.55557	0.53155	0.43852
Q, F_{12}, E	0.44069	0.55557	0.37268	0.39130
A_2, F_{12}, E	0.42501	0.55557	0.33340	0.35006
Q, F_{12}, F_{03}	0.46151	0.55557	0.42966	0.35446

Table 15: Packings with 3 balls, $(u; v; w) = (6; 4; 6)$

Q, F_{12}, E	0.48955	0.60917	0.51555	0.48361
A_2, F_{12}, E	0.48955	0.60917	0.51555	0.48361
Q, F_{12}, F_{03}	0.48955	0.60917	0.51555	0.37782

Table 16: Packings with 3 balls, $(u; v; w) = (7; 4; 7)$

A_2, F_{12}, E	0.38521	0.38325	0.24664	0.36774
Q, F_{12}, F_{03}	0.36227	0.38325	0.20444	0.26038

Table 17: Packings with 3 balls, $(u; v; w) = (7; 3; 7)$

Q, F_{12}, E	0.46503	0.69130	0.43984	0.37114
A_2, F_{12}, E	0.46503	0.69130	0.43984	0.37114

Table 18: Packings with 3 balls, $(u; v; w) = (6; 6; 6)$

Q, F_{12}, E	0.32119	0.83993	0.14169	0.09278
A_2, F_{12}, E	0.32119	0.83993	0.14169	0.09278

Table 19: Packings with 3 balls, $(u; v; w) = (10; 10; 10)$

Q, F_{12}, E	0.22661	0.87770	0.04925	0.03006
A_2, F_{12}, E	0.22661	0.87770	0.04925	0.03006

Table 20: Packings with 3 balls, $(u; v; w) = (14; 14; 14)$

3.3 Four ball part orbits

A_2, F_{03}, E, F_{12}	0.15608	0.27899	0.01600	0.04234
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Table 21: Packings with 4 balls, $(u; v; w) = (3; 7; 3)$

A_2, F_{03}, E, F_{12}	0.26532	0.43062	0.07934	0.13358
Q, F_{12}, E, F_{03}	0.26532	0.43062	0.07934	0.13358

Table 22: Packings with 4 balls, $(u; v; w) = (4; 5; 4)$

A_2, F_{03}, E, F_{12}	0.33587	0.46190	0.16233	0.25480
Q, F_{12}, E, F_{03}	0.31344	0.46190	0.13154	0.20647

Table 23: Packings with 4 balls, $(u; v; w) = (5; 4; 5)$

A_2, F_{03}, E, F_{12}	0.37373	0.57271	0.22485	0.27483
Q, F_{12}, E, F_{03}	0.42124	0.57271	0.32440	0.39650

Table 24: Packings with 4 balls, $(u; v; w) = (5; 5; 5)$

A_2, F_{03}, E, F_{12}	0.42501	0.55557	0.33340	0.42507
Q, F_{12}, E, F_{03}	0.44069	0.55557	0.37268	0.47515

Table 25: Packings with 4 balls, $(u; v; w) = (6; 4; 6)$

A_2, F_{03}, E, F_{12}	0.48947	0.60917	0.51528	0.58910
Q, F_{12}, E, F_{03}	0.48947	0.60917	0.51528	0.58910

Table 26: Packings with 4 balls, $(u; v; w) = (7; 4; 7)$

A_2, F_{03}, E, F_{12}	0.34463	0.38325	0.17557	0.33812
Q, F_{12}, E, F_{03}	0.34463	0.38325	0.17557	0.33812
J, Q, F_{12}, A_2	0.28313	0.38325	0.09661	0.14104

Table 27: Packings with 4 balls, $(u; v; w) = (7; 3; 7)$

A_2, F_{03}, E, F_{12}	0.37764	0.691309	0.23211	0.22384
Q, F_{12}, E, F_{03}	0.37764	0.691309	0.23211	0.22384

Table 28: Packings with 4 balls, $(u; v; w) = (6; 6; 6)$

A_2, F_{03}, E, F_{12}	0.17700	0.83993	0.023373	0.01670
Q, F_{12}, E, F_{03}	0.17700	0.83993	0.023373	0.01670

Table 29: Packings with 4 balls, $(u; v; w) = (10; 10; 10)$

A_2, F_{03}, E, F_{12}	0.11911	0.87770	0.00710	0.00462
Q, F_{12}, E, F_{03}	0.11911	0.87770	0.00710	0.00462

Table 30: Packings with 4 balls, $(u; v; w) = (14; 14; 14)$

4. Summary

We briefly collect our new main results in two summarizing theorems.

THEOREM 4.1. *The cobweb (tube) manifolds $Cw(2z)$ to fundamental cobweb (tube) polyhedra as fundamental domains have been constructed by two series of simplified face pairing identifications in Figures 4, 5, 6, 7, described above in Section 2. Any fundamental group $Cw(2z = 8p - 2)$ of first series and $Cw(2z = 8q + 2)$ of second series can be given by the algorithmic presentation in formulas (6) and (7), to Figures 6 and 7, respectively, on the base of their symmetry group $W(2z)$ with half trunc-orthoscheme fundamental domain $W(2z)$ in Figure 4.*

All necessary metric data of $Cw(2z)$ can be computed on the base of this half trunc-orthoscheme and its projective-metric coordinate simplex $b^0b^1b^2b^3 = A_0A_1A_2A_3$ by scalar products in (1), (3), respectively, or their (polar) plane \rightarrow (pole) point polarity in Section 1.

THEOREM 4.2. *The above cobweb (tube) manifolds $Cw(2z)$ are minimal, i.e. none of them covers regularly another (smaller) manifold. This assertion is based on the symmetry group $W(2z)$ that is an extended complete Coxeter reflection group with the half trunc-orthoscheme $W(2z = u = v = w)$ as fundamental domain in Figures 1, 4. So we also recall a most economical presentation of the general extended complete reflection group $W(u; v; w = u)$ in (8).*

We have given strategies in Section 2.2 for dense ball packing constructions with equal balls belonging to more ball centre orbits by $Cw(2z)$, or in more general by $W(u; v; w = u)$. As first results, we give dense enough constructions by the first strategy in Section 3.

For instance, in Table 12 at $(u; v; w = u) = (4; 5; 4)$ we look our top optimum $\delta^{opt} \approx 0.68248$ for the 3 orbits of A_2, F_{03}, E in the half trunc-orthoscheme W with $1/16, 1/20, 1/8$ ball parts, respectively of optimal radius ≈ 0.51921 , etc, that yield this preliminary optimum. This can be increased if an appropriate full ball can be placed into an interior point I of W .

In Table 8 of $(6; 6; 6)$ we similarly look $\delta^{opt} \approx 0.42010$ for 2 orbits of A_2, E in W with $1/24, 1/8$ ball parts, respectively with optimal radius ≈ 0.57941 , etc. Thus we get a preliminary optimum, that increases if we would place an appropriate full ball

into W . Then we can exactly tell, how many equal balls are placed into the above tube manifold $Cw(6)$.

We intend to continue these investigations, also for promising probable material applications.

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