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Combinatorial construction of tilings by barycentric simplex orbits (D symbols) and their realizations in Euclidean and other homogeneous spaces

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A new method, developed in previous works by the author (partly with co-authors), is presented which decides algorithmically, in principle by computer, whether a combinatorial space tiling $(\mathcal{T}, \Gamma)$ is realizable in the d-dimensional Euclidean space $\mathbf{E}^d$ (think of $d = 2, 3, 4$) or in other homogeneous spaces, *e.g.* in Thurston's 3-geometries:

$$\mathbf{E}^3,\ \mathbf{S}^3,\ \mathbf{H}^3,\ \mathbf{S}^2\times\mathbf{R},\ \mathbf{H}^2\times\mathbf{R},\ \widetilde{\mathbf{SL_2R}},\ \mathbf{Nil},\ \mathbf{Sol}.$$

Then our group Γ will be an isometry group of a projective metric 3-sphere $\mathcal{PS}^3(\mathbf{R}, \langle\ ,\ \rangle)$, acting discontinuously on its above tiling $\mathcal{T}$. The method is illustrated by a plane example and by the well known rhombohedron tiling $(\mathcal{T}, \Gamma)$, where $\Gamma = \mathbf{R\bar{3}m}$ is the Euclidean space group No. 166 in *International Tables for Crystallography*.

1. A plane example for motivation

Our machinery will be based on a symbolic theory of tiling, *i.e.* on the concept of the D symbol. Furthermore, we shall realize tilings in Euclidean and non-Euclidean spaces by projective metric geometries as well. Therefore, we shall motivate our topic in a plane, first, to save describing large and complicated theories, referring to arbitrary dimensional spaces, in general.

1.1. Consider the very popular tiling $\mathcal{T}$ in Fig. 1(a) with symmetry group $\mathbf{G} = \mathbf{p4mm}$. The fundamental domain $\mathcal{F}_\mathbf{G} = A_0A_1A_2$, with small parts of an octagon and a square, characterizes all the tiling by the generating line reflections

$$\mathbf{m}_0 \text{ (in side } A_1A_2 = m_0),$$
$$\mathbf{m}_1 \text{ (in } A_0A_2 = m_1),$$
$$\mathbf{m}_2 \text{ (in } A_0A_1 = m_2).$$

These are generators of $\mathbf{G}$ by a presentation

$$\begin{aligned}\mathbf{G} = \mathbf{p4mm} := \big(\mathbf{m}_0, \mathbf{m}_1, \mathbf{m}_2 — \mathbf{1}\\ = \mathbf{m}_0^2 = \mathbf{m}_1^2 = \mathbf{m}_2^2 = (\mathbf{m}_0\mathbf{m}_1)^4\\ = (\mathbf{m}_0\mathbf{m}_2)^2 = (\mathbf{m}_1\mathbf{m}_2)^4\big).\end{aligned} \quad (1)$$

The second part of this presentation expresses the so-called defining relations. Here $\mathbf{1}$ denotes the identity map and, for example, $\mathbf{m}_0\mathbf{m}_1$ denotes a product map of the two reflections (to read from left to right by our convention here), which is a rotation of order 4 about the point A_2, *i.e.* about 90° in the negative (clockwise) direction.

To describe the tiling $\mathcal{T}$ in a combinatorial way, we introduce its barycentric subdivision $\mathcal{C}$ invariant under $\mathbf{G}$, with $I = \{0, 1, 2\}$ labelled vertices and labelled sides according to the opposite vertices. Namely, an i-dimensional centre is labelled by i, $i \in I = \{0, 1, 2\}$. The symbols

$$\sigma_0 : \cdots\cdots, \quad \sigma_1 : ----, \quad \sigma_2 : —— \quad (2)$$

denote the sides of the barycentric triangles and the corresponding adjacency operations σ_i as well (Fig. 1b).

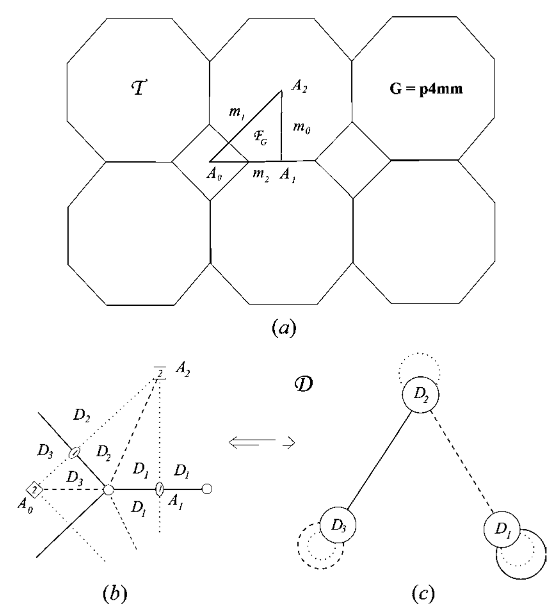

Figure 1
A well known Archimedean tiling in the Euclidean plane with its D diagram

Our notations

$$\sigma_i C^{\mathbf{g}} := \sigma_i(C^{\mathbf{g}}) = (\sigma_i C)^{\mathbf{g}},$$

moreover
$$(\sigma_j\sigma_i)C^{(\mathbf{g}_1\mathbf{g}_2)} = \sigma_j(\sigma_i C^{(\mathbf{g}_1\mathbf{g}_2)}) = ((\sigma_j\sigma_i)C^{\mathbf{g}_1})^{\mathbf{g}_2}; \quad (3)$$
$$C \in \mathcal{C}; \quad \mathbf{g}_1, \mathbf{g}_2 \in \mathbf{G}; \quad \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \in \boldsymbol{\Sigma}_I$$

indicate the $\mathbf{G}$ invariance of the barycentric adjacencies. Furthermore, if $\mathbf{G}$ acts (assumed) on the right, then the group $\boldsymbol{\Sigma}_I$ of adjacency operations acts on the left on the barycentric subdivision $\mathcal{C}$.

In Fig. 1(b), we denote by D_1 the $\mathbf{G}$ orbit of a barycentric triangle C_1 of $\mathcal{C}$ in $\mathcal{F}_{\mathbf{G}}$. Similarly, the $\mathbf{G}$ orbits D_2 and D_3 and their adjacencies (induced from $\mathcal{C}$) are introduced in the D diagram $\mathcal{D} = \{D_1, D_2, D_3\}$, where we have three vertices of $\mathcal{D}$ according to the three different $\mathbf{G}$ orbits of $\mathcal{C}$ (see Fig. 1c).

Now, up to symmetry-respecting deformations, the D diagram $\mathcal{D}$ together with the symmetric integral matrix function

$$M : \mathcal{D} \to \mathbb{N}_{I\times I}, \quad D \mapsto m_{ij}(D),$$

with
$$m_{ij}(D_1) = m_{ij}(D_2) = \begin{pmatrix} 1 & 8 & 2 \\ 8 & 1 & 3 \\ 2 & 3 & 1 \end{pmatrix}, \quad (4)$$
$$m_{ij}(D_3) = \begin{pmatrix} 1 & 4 & 2 \\ 4 & 1 & 3 \\ 2 & 3 & 1 \end{pmatrix},$$

completely specifies the tiling $(\mathcal{T}, \mathbf{G})$, with the group $\mathbf{G}$ in (1). Here and throughout, $\mathbb{N}$ denotes the set of natural numbers and the formal definition of M is, in general, as follows:

$$m_{ij}(D) = \min\Big\{m \in \mathbb{N} : \overbrace{(\sigma_j\sigma_i)\ldots(\sigma_j\sigma_i)(\sigma_j\sigma_i)}^{m \text{ times}}\, C = C \quad C \in D \in \mathcal{D}\Big\}. \quad (5)$$

Thus, $m_{01}(D_1) = m_{01}(D_2) = 8$ means in (4) that D_1, D_2 form an octagon by σ_0, σ_1 operations; $m_{01}(D_3) = 4$ describes our square tiles.

The entries $m_{12}(D_1) = m_{12}(D_2) = m_{12}(D_3) = 3$ just indicate that three polygons meet at a vertex. The connectedness of our D diagram minus σ_0 operation [by cancelling dotted $(\cdots\cdots)$ lines] means that we have exactly one $\mathbf{G}$-equivalence class of vertices. This is a criterion for Archimedean tilings.

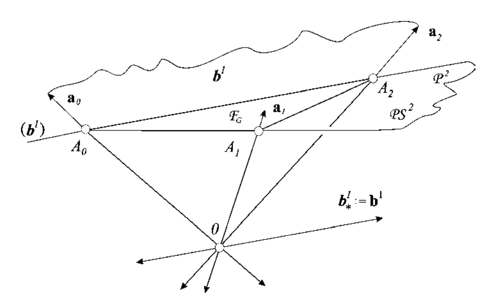

Figure 2
A projective coordinate triangle to our fundamental domain $\mathcal{F}_{\mathbf{G}}$ in $\mathcal{P}^2$ or in $\mathcal{PS}^2$. The plane by form class of $\boldsymbol{b}^1$ describes the line A_0A_2. The point by $\boldsymbol{b}^1_* =: \mathbf{b}^1$ is its pole.

Now we have a freedom: the octagons are not necessarily regular, the vertex can be varied in the interior of segment A_0A_1 (Figs. 1a, b).

By cancelling the σ_1 (- - - -) operation from $\mathcal{D}$, the two remaining components just indicate the two $\mathbf{G}$ classes of edges of $\mathcal{T}$. Similarly, by cancelling σ_2 (——) operation from $\mathcal{D}$, we get the two tile classes of $\mathcal{T}$ under $\mathbf{G}$.

1.2. Now imagine generalizations $\mathcal{T}(2a; b)$ of our tiling with the same D diagram as in Fig. 1(c), but with matrix function

$$m_{ij}(D_1) = m_{ij}(D_2) = \begin{pmatrix} 1 & 2a & 2 \\ 2a & 1 & 3 \\ 2 & 3 & 1 \end{pmatrix},$$
$$m_{ij}(D_3) = \begin{pmatrix} 1 & b & 2 \\ b & 1 & 3 \\ 2 & 3 & 1 \end{pmatrix}, \quad 2 \le a \in \mathbb{N},\ 3 \le b \in \mathbb{N}. \quad (6)$$

This means we choose our tiling group instead of (1) by the following presentation:

$$\mathbf{G}(2a; b) := \big(\mathbf{m}_0, \mathbf{m}_1, \mathbf{m}_2 — \mathbf{1} = \mathbf{m}_0^2 = \mathbf{m}_1^2 = \mathbf{m}_2^2 = (\mathbf{m}_0\mathbf{m}_1)^a = (\mathbf{m}_0\mathbf{m}_2)^2 = (\mathbf{m}_1\mathbf{m}_2)^b\big). \quad (7)$$

Imagine the reflection triangle $\mathcal{F}_{\mathbf{G}}$ in Fig. 1(a) with angles $\pi/b, \pi/2, \pi/a$ at A_0, A_1, A_2, respectively, for an Archimedean tiling by one b-gon and two $2a$-gons about any vertex. We know that the angular assumptions

$$\frac{\pi}{b} + \frac{\pi}{2} + \frac{\pi}{a} \begin{matrix} > \\ = \\ < \end{matrix} \pi \quad \begin{matrix} -\mathbf{S}^2 \\ -\mathbf{E}^2 \\ -\mathbf{H}^2 \end{matrix} \quad (8)$$

provide us with spherical ($\mathbf{S}^2$, $e.g.$ $b = 4, a = 3$), Euclidean [$\mathbf{E}^2$: $(b = 4, a = 4)$ or $(b = 3, a = 6)$ or $(b = 6, a = 3)$] or hyperbolic [$\mathbf{H}^2$, $e.g.$ $(b = 4, 5 \le a \in \mathbb{N})$] tilings. Since the situation is much more complicated in three-dimensional spaces later on, we shall indicate the projective metric method to the above plane cases (Fig. 2).

1.3. We consider for our fundamental triangle $\mathcal{F}_{\mathbf{G}} = A_0A_1A_2$ the real vector space $\mathbf{V}^3(\mathbb{R})$ spanned by a basis $\overrightarrow{OA_0} \sim \mathbf{a}_0, \overrightarrow{OA_1} \sim \mathbf{a}_1, \overrightarrow{OA_2} \sim \mathbf{a}_2$ (Fig. 2). Here the equivalence $\sim$ means

$$\mathbf{x} \sim \mathbf{y} \Longleftrightarrow \mathbf{y} = c\mathbf{x} \quad \text{with} \quad 0 < c \in \mathbb{R}, \quad \mathbf{x}, \mathbf{y} \in \mathbf{V}^3 \setminus \{\mathbf{0}\}. \quad (9)$$

Thus we define a point $(\mathbf{x}) = (\mathbf{y})$ of the projective metric sphere $\mathcal{PS}^2$ over $\mathbf{V}^3(\mathbb{R})$. Unifying opposite points (rays) $(\mathbf{x})$ and $(-\mathbf{x})$, we get the projective plane $\mathcal{P}^2$ from $\mathcal{PS}^2$. Dually, we define the two-dimensional subspaces of $\mathbf{V}^3$, or the 1-rays of the form space $\boldsymbol{V}_3$ by

$$\boldsymbol{u} \sim \boldsymbol{v} \Longleftrightarrow \boldsymbol{v} = \boldsymbol{u}\tfrac{1}{c}$$
$$\text{with } 0 < c \in \mathbb{R}, \Longleftrightarrow (\boldsymbol{u}) = (\boldsymbol{v}), \quad (10)$$
$$(\mathbf{x}\boldsymbol{u}) = 0 \text{ means that } (\mathbf{x})\,\mathrm{I}\,(\boldsymbol{u}).$$

These describe that two lines (oriented circles) of $\mathcal{PS}^2$ are coincident, and express the incidence $\mathbf{I}$ above of a point $(\mathbf{x})$ to a line $(\boldsymbol{u})$. This means each line (in space: plane, in general: hyperplane) is characterized by a linear form class $(\boldsymbol{u})$ (with boldface italic letter) over the vector space $\mathbf{V}^3$. This means:

$$\mathbf{x}\boldsymbol{u} \in \mathbb{R}\,\text{(real numbers)}, \quad (c^1\mathbf{x}_1 + c^2\mathbf{x}_2)\boldsymbol{u} = c^1(\mathbf{x}_1\boldsymbol{u}) + c^2(\mathbf{x}_2\boldsymbol{u})$$

are required for any $c^1, c^2 \in \mathbb{R}$ and $\mathbf{x}_1, \mathbf{x}_2 \in \mathbf{V}^3$ (vectors).

These forms $\boldsymbol{u}, \boldsymbol{v}, \ldots$ constitute the dual space $\boldsymbol{V}_3$ with a built-in linear structure defined by

$$\mathbf{x}(\boldsymbol{u}^1c^1 + \boldsymbol{u}^2c^2) := (\mathbf{x}\boldsymbol{u}^1)c_1 + (\mathbf{x}\boldsymbol{u}^2)c_2$$
$$\text{for any} \quad \mathbf{x} \in \mathbf{V}^3; \quad c^1, c^2 \in \mathbb{R}; \quad \boldsymbol{u}^1, \boldsymbol{u}^2 \in \boldsymbol{V}_3;$$

as is well known from the linear algebra courses.

In Fig. 2, we have indicated that the side A_0A_2 of our $\mathcal{F}_\mathbf{G}$ is described by the form $\boldsymbol{b}^1$ of $\boldsymbol{V}_3$. Thus the dual basis $\{\boldsymbol{b}^0, \boldsymbol{b}^1, \boldsymbol{b}^2\}$ for $\boldsymbol{V}_3$ can be introduced by the 'incidence relations'

$$(\mathbf{a}_i\boldsymbol{b}^j) = \delta_i^j \quad \text{(the Kronecker symbol).} \tag{11}$$

Now, we introduce projective collineations of $\mathcal{PS}^2$ by linear transforms of $\mathbf{V}^3$ or dually of $\boldsymbol{V}_3$, up to constant factors as projective freedom. For example, our reflections $\mathbf{m}_0, \mathbf{m}_1, \mathbf{m}_2$ can be described by

$$\mathbf{m}_0 : \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{a}_1 \\ \mathbf{a}_2 \end{pmatrix} \to \begin{pmatrix} -1 & n & p \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{a}_1 \\ \mathbf{a}_2 \end{pmatrix}$$

$$\text{or} \qquad \begin{pmatrix} \boldsymbol{b}^0 & \boldsymbol{b}^1 & \boldsymbol{b}^2 \end{pmatrix} \to \begin{pmatrix} \boldsymbol{b}^0 & \boldsymbol{b}^1 & \boldsymbol{b}^2 \end{pmatrix} \begin{pmatrix} -1 & n & p \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{12}$$

$$\mathbf{m}_1 : \begin{pmatrix} 1 & 0 & 0 \\ q & -1 & r \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{m}_2 : \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ s & t & -1 \end{pmatrix}$$

as involutive transforms with free parameters for a while. This means in our conventions that we apply row–column multiplication for matrices; in the i'th row of $\mathbf{m}_0$ stand the coordinates of the $\mathbf{m}_0$ image of basis vector $\mathbf{a}_i$; in the j'th column of $\mathbf{m}_0$ are the coordinates of the $\mathbf{m}_0$ image of basis form $\boldsymbol{b}^j$. Thus, the transform $\mathbf{m}_0$ acts on the vectors (points) and on the forms (lines) as well.

The coordinate transforms are induced, for example, as

$$\mathbf{m}_0 : \begin{pmatrix} x^0 & x^1 & x^2 \end{pmatrix} \to \begin{pmatrix} x^0 & x^1 & x^2 \end{pmatrix} \begin{pmatrix} -1 & n & p \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

for $\mathbf{x} = x^i\mathbf{a}_i \in \mathbf{V}^3$ (Einstein convention),

$$\mathbf{m}_0 : \begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix} \to \begin{pmatrix} -1 & n & p \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix} \quad \text{for} \quad \boldsymbol{u} = \boldsymbol{b}^j\boldsymbol{u}_j \in \boldsymbol{V}_3.$$

In general, we apply matrix pairs, inverse to each other, with determinants -1 (or $+1$, later for orientation-preserving transforms) in a natural manner.

To satisfy all the relations of (7), we take first the products

$$\mathbf{m}_0\mathbf{m}_2 : \begin{pmatrix} -1+ps & n+pt & -p \\ 0 & 1 & 0 \\ s & t & -1 \end{pmatrix},$$
$$\mathbf{m}_0\mathbf{m}_1 : \begin{pmatrix} -1+nq & -n & nr+p \\ q & -1 & r \\ 0 & 0 & 1 \end{pmatrix}, \tag{13}$$
$$\mathbf{m}_1\mathbf{m}_2 : \begin{pmatrix} 1 & 0 & 0 \\ q+rs & -1+rt & -r \\ 0 & 0 & -1 \end{pmatrix}.$$

These have to be of order 2, a, b, respectively. Thus,

$$p = s = 0, -2 + nq = \cos\frac{2\pi}{a}, \quad -2 + rt = 2\cos\frac{2\pi}{b},$$
$$\textit{i.e.} \quad nq = 4\cos^2\frac{\pi}{a}, \quad rt = 4\cos^2\frac{\pi}{b};$$
$$\text{and} \quad n = q = 2\cos\frac{\pi}{a}, \quad r = t = 2\cos\frac{\pi}{b}$$

can be assumed by the projective freedom, as shown by the type of basis change $\mathbf{a}_{i'} = c\mathbf{a}_i$, $\boldsymbol{b}^{i'} = \boldsymbol{b}^i\frac{1}{c}$. Indeed, the matrices

$$\mathbf{m}_0, : \begin{pmatrix} -1 & 2\cos\frac{\pi}{a} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$
$$\mathbf{m}_1 : \begin{pmatrix} 1 & 0 & 0 \\ 2\cos\frac{\pi}{a} & -1 & 2\cos\frac{\pi}{b} \\ 0 & 0 & 1 \end{pmatrix} \tag{14}$$
$$\mathbf{m}_2 : \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 2\cos\frac{\pi}{b} & -1 \end{pmatrix}.$$

satisfy the relations (7). For example, the $2a$ images of triangle $\mathcal{F}_\mathbf{G}$ simply (without gap and overlap) surround the starting vertex A_2.

1.4. To characterize the realizing projective metric plane for $\mathbf{S}^2$, $\mathbf{E}^2$ or $\mathbf{H}^2$ tilings, we look for a symmetric linear polarity

$$({}_*) : \boldsymbol{V}_3 \to \mathbf{V}^3, \; \boldsymbol{b}^i \to \boldsymbol{b}^i_* := b^{ij}\mathbf{a}_j \quad \text{with } b^{ij} = b^{ji},$$

which is invariant under $\mathbf{m}_0, \mathbf{m}_1, \mathbf{m}_2$ above.

Here and later on, we apply the Einstein sum convention for indices $i, j = 0, 1, 2$. Fig. 2 also shows how to assign a pole vector $\boldsymbol{b}^1_* := \mathbf{b}^1 = b^{1j}\mathbf{a}_j$ to the polar form $\boldsymbol{b}^1$, thus the pole point $(\mathbf{b}^1)$ to the polar line $(\boldsymbol{b}^1)$. By this we shall first have a symmetric scalar product in $\boldsymbol{V}_3$:

$$\begin{aligned} \langle\,,\,\rangle : \boldsymbol{V}_3 \times \boldsymbol{V}_3 \to \mathbf{R}, \quad \langle \boldsymbol{u}, \boldsymbol{v}\rangle &= (\boldsymbol{u}_*\boldsymbol{v}) \\ = \langle \boldsymbol{b}^i u_i, \boldsymbol{b}^j v_j\rangle = \langle u_i\mathbf{b}^i, \boldsymbol{b}^j v_j\rangle &= \langle u_i b^{ir}\mathbf{a}_r, \boldsymbol{b}^j v_j\rangle \\ = u_i b^{ir}\delta^j_r v_j &= u_i b^{ij} v_j \end{aligned} \tag{15}$$

(with Kronecker's δ^j_r), *i.e.* by coordinates, then comes orthogonality of lines *etc.*, as usual. For example, the lines $(\boldsymbol{u})$ and $(\boldsymbol{v})$ are orthogonal, *i.e.* $(\boldsymbol{v})$ is incident to the pole $(\boldsymbol{u}_*)$ of line $(\boldsymbol{u})$, iff $\langle \boldsymbol{u}, \boldsymbol{v}\rangle = 0$.

The signature of $\langle\ \rangle$, *i.e.* the signs in its diagonal form, will be determined later:

(a) spherical ($\mathbf{S}^2$) metric with signature $(+++)$,

(b) Euclidean ($\mathbf{E}^2$) metric with signature $(0++)$,

(c) hyperbolic ($\mathbf{H}^2$) metric with signature $(-++)$.

Now the image coordinates of basis forms stand in the matrix columns of $\mathbf{m}_i'$s, respectively. The invariance of the polarity above under $\mathbf{m}_0$ (for example) means that a line and its $\mathbf{m}_0$ image have poles that are also $\mathbf{m}_0$ images to each other. Thus we obtain linear equations for the above polarity matrix (b^{ij}). For example, from $\mathbf{m}_0$ by (14) we get

$$\begin{aligned} c_0 b^{00} &= (-1)(-1)b^{00}, \\ c_0 b^{01} &= (-1)2\cos\frac{\pi}{a}b^{00} + (-1)(1)b^{01}, \\ c_0 b^{02} &= (-1)(1)b^{02}, \\ c_0 b^{11} &= 4\cos^2\frac{\pi}{a}b^{00} + 4\cos\frac{\pi}{a}b^{01} + b^{11}, \\ c_0 b^{12} &= 2\cos\frac{\pi}{a}b^{02} + b^{12} \\ c_0 b^{22} &= b^{22}, \quad 0 < c_0 \in \mathbb{R}. \end{aligned} \tag{16}$$

Similarly, from $\mathbf{m}_1$ and $\mathbf{m}_2$, we shall have the (non-zero) matrix of the invariant symmetric polarity (scalar product) by

$$b^{ij} = \begin{pmatrix} 1 & -\cos\frac{\pi}{a} & 0 \\ -\cos\frac{\pi}{a} & 1 & -\cos\frac{\pi}{b} \\ 0 & -\cos\frac{\pi}{b} & 1 \end{pmatrix},$$

i.e. the quadratic form

$$\begin{aligned} \langle \boldsymbol{u}, \boldsymbol{u} \rangle &= u_i b^{ij} u_j = u_0 u_0 - 2\cos\frac{\pi}{a}u_0 u_1 \\ &\quad + u_1 u_1 - 2\cos\frac{\pi}{b}u_1 u_2 + u_2 u_2 \\ &= \left(u_2 - \cos\frac{\pi}{b}u_1\right)^2 + \left(\sin\frac{\pi}{b}u_1 - \frac{\cos\frac{\pi}{a}}{\sin\frac{\pi}{b}}u_0\right)^2 \\ &\quad + \frac{\cos\left(\frac{\pi}{a} - \frac{\pi}{b}\right)}{\sin^2\frac{\pi}{b}}\sin\left(\frac{\pi}{a} + \frac{\pi}{b} - \frac{\pi}{2}\right)u_0 u_0 \end{aligned} \tag{17}$$

invariant under $\mathbf{m}_0, \mathbf{m}_1, \mathbf{m}_2$. Indeed, we have obtained the signature, *i.e.* the signs of square terms as desired, see formula (8). Moreover, a coordinate transform (by corresponding basis transform, according to the index position, Schouten's primed index convention)

$$\begin{pmatrix} u_{0'} \\ u_{1'} \\ u_{2'} \end{pmatrix} = \begin{pmatrix} \pm|K|^{1/2}/\sin\frac{\pi}{b} & 0 & 0 \\ -\cos\frac{\pi}{a}/\sin\frac{\pi}{b} & \sin\frac{\pi}{b} & 0 \\ 0 & -\cos\frac{\pi}{b} & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix}$$

or by the inverse matrix

$$\begin{aligned} &\begin{pmatrix} x^{0'} & x^{1'} & x^{2'} \end{pmatrix} \\ &= \begin{pmatrix} x^0 & x^1 & x^2 \end{pmatrix} \begin{pmatrix} \sin\frac{\pi}{b}/\pm|K|^{1/2} & 0 & 0 \\ \cos\frac{\pi}{a}/\pm|K|^{1/2}\sin\frac{\pi}{b} & 1/\sin\frac{\pi}{b} & 0 \\ \cos\frac{\pi}{a}\cot\frac{\pi}{b}/\pm|K|^{1/2} & \cot\frac{\pi}{b} & 1 \end{pmatrix} \end{aligned} \tag{18}$$

helps us to turn to a Cartesian (homogeneous) projective coordinate system if

$$K = \cos\left(\frac{\pi}{a} - \frac{\pi}{b}\right)\sin\left(\frac{\pi}{a} + \frac{\pi}{b} - \frac{\pi}{2}\right) \begin{matrix} > \\ < \end{matrix}\ 0 \quad \begin{matrix} -\mathbf{S}^2 \\ -\mathbf{H}^2 \end{matrix} \tag{19}$$

for non-Euclidean planes $\mathbf{S}^2(>, +)$ and $\mathbf{H}^2(<, -)$, respectively. The cases where $K = 0$ yield Euclidean tilings, and then (*e.g.*)

$$\begin{pmatrix} u_{0'} \\ u_{1'} \\ u_{2'} \end{pmatrix} = \begin{pmatrix} 1/\sin\frac{\pi}{b} & 0 & 0 \\ -\cos\frac{\pi}{a}/\sin\frac{\pi}{b} & \sin\frac{\pi}{b} & 0 \\ 0 & -\cos\frac{\pi}{b} & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix}$$

and

$$\begin{pmatrix} x^{0'} & x^{1'} & x^{2'} \end{pmatrix} = \begin{pmatrix} x^0 & x^1 & x^2 \end{pmatrix} \begin{pmatrix} \sin\frac{\pi}{b} & 0 & 0 \\ \cos\frac{\pi}{a}\sin\frac{\pi}{b} & 1/\sin\frac{\pi}{b} & 0 \\ \cos\frac{\pi}{a}\cot\frac{\pi}{b} & \cot\frac{\pi}{b} & 1 \end{pmatrix},$$

$$\text{moreover } x^{1'}/x^{0'} =: x \text{ and } x^{2'}/x^{0'} =: y, \text{ if } x^{0'} \neq 0, \tag{20}$$

provide also a usual rectangular Cartesian system $\{\boldsymbol{b}^{j'}\}$, $\{\mathbf{a}_{i'}\}$ as dual basis pair, according to the index positions and to the analogous formulas above.

All these formulas, implemented on a computer, produce the tilings on the screen. For example, with $K < 0$, the formulas (17)–(19) produce the Cayley–Klein model of a Bolyai–Lobachevskian hyperbolic plane $\mathbf{H}^2$ in a circle disc (Fig. 3) of radius

$$\sin\frac{\pi}{b}\Big/|K|^{1/2} := \rho, \tag{21}$$

see *e.g.* Bölcskei & Molnár (1999) and Bölcskei (2003).

All these arguments will be much more complicated in the 3-space where the two-dimensional ($\mathbf{S}^2$, $\mathbf{E}^2$ and $\mathbf{H}^2$) situations will also be applied for some stabilizers. But, in principle, we shall follow the same strategy. I ask for patience of the interested reader. The topic is far from easily understandable, but it may help in better imagination of non-Euclidean geometries in describing real crystals. The author and other colleagues think that non-Euclidean geometries might play a similar role in contemporary crystallography (*e.g.* in better understanding quasicrystals and fullerenes), as quantum physics did in the last century. The mathematical difficulties might be similar(?!).

We mention only an initiative of Alan L. Mackay: how to apply hyperbolic plane geometry $\mathbf{H}^2$ to describing triply periodic minimal surfaces (TPMS) in Euclidean space $\mathbf{E}^3$

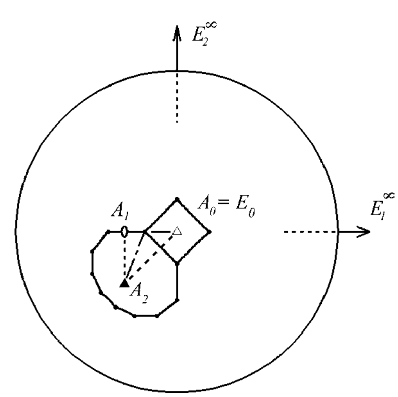

Figure 3
A symbolic picture on the Archimedean tiling $\mathcal{T}(2a; b)$ with $a = 5$, $b = 4$ in the hyperbolic plane $\mathbf{H}^2$

(Molnár, 2001, 2002; Hyde & Ramsden, 2003; Robins *et al.*, 2004).

2. The rhombohedron tiling as an introductory example

We consider a rhombohedron T, *i.e.* a parallelepiped with equal length spanning edge vectors (Fig. 4), and its tiling $\mathcal{T}$ under the symmetry group Γ, generated by two plane reflections $\mathbf{m}_0$, $\mathbf{m}_1$ and two half-turns $\mathbf{r}_2$, $\mathbf{r}_3$ as follows:

$$\begin{aligned} \mathbf{m}_0 &: A_1A_2A_3 \rightarrow A_1A_2A_3, \\ \mathbf{m}_1 &: A_0A_2A_3 \rightarrow A_0A_2A_3, \\ \mathbf{r}_2 &: A_0A_1A_3 \rightarrow A_0A_3A_1, \\ \mathbf{r}_3 &: A_0A_1A_2 \rightarrow A_1A_0A_2. \end{aligned} \tag{22}$$

Thus, our Γ will act transitively on the faces of the rhombohedron tiling $\mathcal{T}$ (Dress *et al.*, 1993). To illustrate this, we consider the barycentric subdivision of $\mathcal{T}$ (Fig. 4). Each barycentric simplex C has 3, 2, 1, 0 labelled vertices as centres of three-, two-, one-, zero-dimensional faces of $\mathcal{T}$. Γ acts also on the barycentric simplices. Thus we get four simplex orbits. For example, $C_1 = 0_1 1_1 2_1 3_1 = A_3A_{03}A_{13}A_2$ represents an orbit denoted by D_1. The i face of any C is opposite to its i vertex, $i \in \{0, 1, 2, 3 = d\} = I$ as index set. Thus, the adjacency relations σ_i,

$$\sigma_0 : \cdots\cdots, \quad \sigma_1 : ----, \quad \sigma_2 : \text{——}, \quad \sigma_3 : \sim\sim,$$

and the so-called D diagram $\mathcal{D}$ (Fig. 5), as well as the D-matrix function (Dress *et al.*,1993) will be introduced by

$$M(k) = m_{ij}(k) = \begin{pmatrix} 1 & 4 & 2 & 2 \\ 4 & 1 & 3 & 2 \\ 2 & 3 & 1 & 4 \\ 2 & 2 & 4 & 1 \end{pmatrix}, \tag{23}$$
$$k \in \{D_1, D_2, D_3, D_4\} = \mathcal{D}; \quad i, j \in I = \{0, 1, 2, 3\}.$$

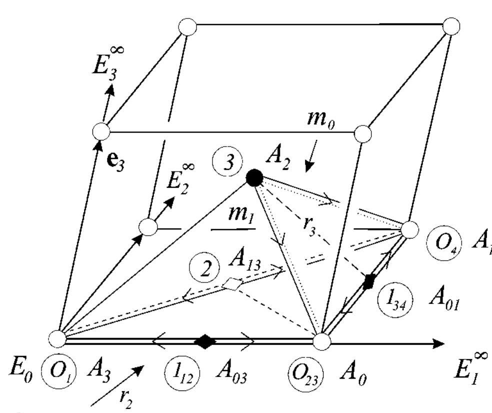

Figure 4
The rhombohedron tiling under space group No. 166 $\mathbf{R\bar{3}m}$. Encircled 0_1, 0_{23}, 0_4, 1_{12}, 1_{34}, 2, 3 indicate the zero-, one-, two-, three-dimensional centres of our rhombohedron, respectively, as vertices of the barycentric simplices $C_1 = 0_1 1_1 2_1 3_1$, then of C_2, C_3, C_4. The union of these simplices is $A_0A_1A_2A_3$, forming the fundamental simplex of space group $\Gamma = \mathbf{R\bar{3}m}$. E_0, E_1^∞, E_2^∞, $E_3^\infty = (\mathbf{e}_3)$ denote the usual coordinate simplex to the rhombohedron.

For example, $m_{23}(k) = 4$ means how many rhombohedra (topologically, as cubes) surround any edge in the tiling $\mathcal{T}$.

Definition 1. A D diagram $\mathcal{D}$ with a D-matrix function M, with certain requirements as given below (Dress, 1987; Dress *et al.*, 1993), is called a D symbol $(\mathcal{D}, M)$ (in honour of B. N. Delone, M. S. Delaney and A. W. M. Dress).

(i) $m_{ii}(D) = 1$ for each $D \in \mathcal{D}$ and $i \in I = \{0, 1, 2, 3\}$;
(ii) $m_{ij}(D) = m_{ij}(\sigma_i D) = m_{ji}(D) \geq 2; \quad i > j \in I; \quad D \in \mathcal{D}$;
(iii) $m_{ij}(D) = 2$ if $|j - i| \geq 2$; $D \in \mathcal{D}$;
(iv) $(\sigma_j\sigma_i)^{m_{ij}(D)}(D) = D; \quad D \in \mathcal{D}; \; i, j \in I.$

As we can see, the requirements just guarantee (see *e.g.* Molnár, 1996) that a D symbol now codes an orbifold by a triangulated fundamental domain.

Orbifold is the concept that generalizes the structure of orbits under a space group. Below we shall give [after formula (27)] also a more formal definition but the examples will be satisfactory and more important for us now (Delgado-Friedrichs & Huson, 1997; Johnson *et al.*, undated).

We remark that the face transitivity of the Γ action on our rhombohedron tiling $\mathcal{T}$ can be checked only on the D diagram (Fig. 5). If we cancel the two-dimensional adjacencies σ_2, *i.e.* the continuous (——) edges from the D diagram, then there remains one connected component. In the same way, our $(\mathcal{T}, \Gamma)$ is transitive on the solids, edges, vertices of $\mathcal{T}$ as well (see Fig. 4). Our simplex $A_0A_1A_2A_3$ is just a fundamental domain $\mathcal{F}$ for the $\mathbf{E}^3$ space group No. 166, $\mathbf{R\bar{3}m} = \Gamma$. Note that our rhombohedron is just the unit lattice cell for the translation lattice of $\mathbf{R\bar{3}m}$ and we have a free affine parameter for our rhombohedron, stretching it along its solid diagonal (A_3A_2).

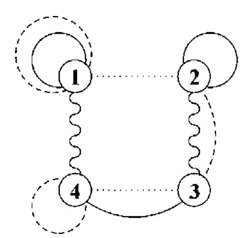

Figure 5
D diagram for the rhombohedron tiling.

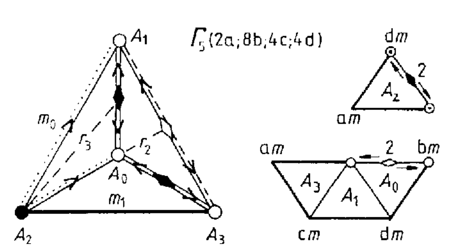

Figure 6
Schlegel diagram and vertex domains.

3. A parametrized orbifold as generalization

The fundamental simplex tiling $(\mathcal{T}, \Gamma)$, now by the simplex $T := A_0A_1A_2A_3$ and $\Gamma = \mathbf{R\bar{3}m}$, generated in equation (22) and described in Fig. 5 and in formula (23) above, can be generalized to a parametrized orbifold $\mathcal{O}(a; b; c; d)$. Its group will be denoted by

$$\Gamma_5(2a; 8b; 4c; 4d), \tag{24}$$

see Fig. 6 (from Molnár *et al.*, 1997, 2005) as a Schlegel diagram of our simplex in Fig. 4. Here

$$a : \text{——}, \quad b : \text{═══}, \quad c : \text{-----}, \quad d : \text{·········} \tag{25}$$

denotes the rotational orders about the corresponding (half) edges. Any (half) edge of an equivalence class under Γ_5 will be surrounded by

$$2a;\ \ 8b;\ \ 4c;\ \ 4d \quad (\geq 3,\ \text{in general}) \tag{26}$$

Γ_5-image simplices, respectively, in the fundamental tiling $(\mathcal{T}, \Gamma_5)$. This just forms the so-called universal covering space of our generalized orbifold under the fundamental covering group Γ_5 above (Molnár, 1996; Molnár *et al.*, 1997) with presentation

$$\begin{aligned}\Gamma_5(2a; 8b; 4c; 4d) &:= \big(\mathbf{m}_0, \mathbf{m}_1, \mathbf{r}_2, \mathbf{r}_3 — \mathbf{1}\\ &= \mathbf{m}_0^2 = \mathbf{m}_1^2 = \mathbf{r}_2^2 = \mathbf{r}_3^2 = (\mathbf{m}_0\mathbf{m}_1)^a\\ &= (\mathbf{m}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_2\mathbf{m}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_2)^b = (\mathbf{m}_0\mathbf{r}_2\mathbf{m}_0\mathbf{r}_2)^c\\ &= (\mathbf{m}_0\mathbf{r}_3\mathbf{m}_1\mathbf{r}_3)^d\big).\end{aligned} \tag{27}$$

Our generalization means: $\mathcal{O}(a; b; c; d)$ is a compactified topological space where each point has a neighbourhood homeomorphic to a ball factorized either by a *spherical* ($\mathbf{S}^2$) finite group or by a Euclidean ($\mathbf{E}^2$) plane (crystallographic) *group* or by a hyperbolic ($\mathbf{H}^2$) plane (cocompact) group. Our illustration (Fig. 6) shows these phenomena for the (symbolic) neighbourhoods of vertices with stabilizer groups

$$\Gamma^0(A_2) = 2{*}ad, \quad \text{with} \quad 1 \underset{>}{\overset{<}{=}} \frac{1}{a} + \frac{1}{d}, \quad \text{and}$$

$$\Gamma^0(A_0, A_1, A_3) = 2{*}acdb, \quad \text{with} \quad 3 \underset{>}{\overset{<}{=}} \frac{1}{a} + \frac{1}{c} + \frac{1}{d} + \frac{1}{b}. \tag{28}$$

We have applied Macbeath–Conway's notations for plane (cocompact, *i.e.* with compact fundamental domain) groups with $\mathbf{S}^2$ ($<$), $\mathbf{E}^2$ ($=$), $\mathbf{H}^2$ ($>$) conditions, respectively.

These notations are based on Poincaré's classification of compact surfaces [either with orientable genus o^g, g handles, or with non-orientable genus $\otimes^g$, g cross-caps (circles with identified opposite points), and with boundary components indicated and separated by $*$ stars]. Macbeath in the late sixties refined this to the classification of plane orbifolds, where rotation centres (as singular points) of some orders are listed (if any occur, up to their permutations). Moreover, dihedral reflection corners may occur at the boundary components (between the stars): either in cyclic order if the surface is orientable, or 'reverse cyclically' if the surface is non-orientable. The boundary components (if they occur) are given up to their permutations, again (*e.g.* Molnár *et al.*, 2005).

For example, $2{*}ad$ above means a sphere (of genus zero) with one boundary component. Moreover, there occur a two-centre of angular neighbourhood $2\pi/2$ and two dihedral corners: one of angle π/a and another of angle π/d on the boundary component.

In our plane example in §1, $\mathbf{G} = \mathbf{p4mm} = {*}\mathbf{244}$, and the orbifold $\mathbf{E}^2/\mathbf{G}$ is the triangle disc with angles $\pi/2, \pi/4, \pi/4$. In the generalization, we introduced $\mathbf{G} = {*}\mathbf{2ab}$ and the disc of angles $\pi/2, \pi/a, \pi/b$ in the corresponding plane by formula (8).

For example, $(a; b; c; d) = (3; 1; 1; 1)$ provides our starting example where $\Gamma^0(A_2) = 2{*}3 = \bar{\mathbf{3}}\mathbf{m}$, $\Gamma^0(A_0, A_1, A_3) = 2{*}3 = \bar{\mathbf{3}}\mathbf{m}$, both are the well known point group of order 12. But $(2; 1; 1; 1)$ and $(a; 1; 1; 1)$ for $3 < a \in \mathbb{N}$ also provide us orbifolds of non-Euclidean realizations (in $\mathbf{S}^2 \times \mathbf{R}$ and in $\mathbf{H}^2 \times \mathbf{R}$, respectively, see Fig. 7).

Our aim is to construct metric realizations for our orbifolds $\mathcal{O}(a; b; c; d)$ for those parameters that yield spherical ($\mathbf{S}^2$) or Euclidean ($\mathbf{E}^2$) (cocompact) plane groups as stabilizers for the vertices of our fundamental simplex. Then Γ_5 will be an isometry group, acting discontinuously on the tiling $\mathcal{T}$ with metric presentation (27).

4. Constructing projective metric 3 sphere $\mathcal{PS}^3(\mathbf{R}, \langle\, ,\, \rangle)$

The construction will be sketched in three main steps (Molnár, 1997), according to plane situations.

4.1. We introduce a projective coordinate simplex (Fig. 4) just by $A_0(\mathbf{a}_0)$, $A_1(\mathbf{a}_1)$, $A_2(\mathbf{a}_2)$, $A_3(\mathbf{a}_3)$, where the vector basis $\{\mathbf{a}_i\}$ spans a real vector space $\mathbf{V}^4(\mathbf{R})$. This is in analogy to Fig. 2. Then the dual form basis $\{\boldsymbol{b}^j\}$ with $(\mathbf{a}_i\boldsymbol{b}^j) = \delta_i^j$ (the Kronecker symbol) describes any simplex plane $b^j = A_iA_kA_\ell$ $(\{i, j, k, \ell\} = \{0, 1, 2, 3\})$ and spans the dual form space $\mathbf{V}_*^4 = \boldsymbol{V}_4$.

Thus, the plane reflection $\mathbf{m}_0$ in $b^0 = A_1A_2A_3$ is given by [our convention (!)] row–column multiplication

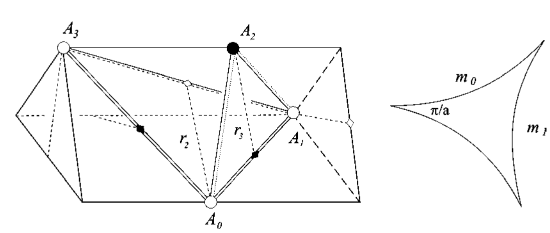

Figure 7
$\Gamma_5(2a; 8b; 4c; 4d)$, $(a; b; c; d) = (a; 1; 1; 1)$, $2 \leq a \in \mathbb{N}$. Euclidean ($a = 3$), $\mathbf{H}^2 \times \mathbf{R}$ tilings and an $\mathbf{S}^2 \times \mathbf{R}$ tiling for $a = 2$ are indicated.

$$\mathbf{m}_0 : \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} \to \begin{pmatrix} -1 & n & p & q \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}$$

for points (vectors), or

$$\begin{pmatrix} \boldsymbol{b}^0 & \boldsymbol{b}^1 & \boldsymbol{b}^2 & \boldsymbol{b}^3 \end{pmatrix} \to \begin{pmatrix} \boldsymbol{b}^0 & \boldsymbol{b}^1 & \boldsymbol{b}^2 & \boldsymbol{b}^3 \end{pmatrix} \begin{pmatrix} -1 & n & p & q \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

for planes (forms). (29)

These define the involutive (now) projective collineation fixing pointwise the above plane. We have a projective freedom as 'non-usual' now. Namely, any vectors $\mathbf{x}$ and $\mathbf{y} = c\mathbf{x}$ for $0 < c \in \mathbf{R}$ determine the same point $(\mathbf{x}) = (\mathbf{y})$ of the projective 3 sphere $\mathcal{PS}^3(\mathbf{R})$. Similarly, the forms $(\boldsymbol{u})$ and $\boldsymbol{u}(1/c) = \boldsymbol{v}$ define the same (oriented) plane (2 sphere) $(\boldsymbol{u}) = (\boldsymbol{v})$ in $\mathcal{PS}^3$. The real parameters n, p, q will be fixed later. Analogously, the further involutive generators will be described with some parameters:

$$\mathbf{m}_1 : \begin{pmatrix} 1 & 0 & 0 & 0 \\ t & -1 & r & s \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\mathbf{r}_2 : \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & u \\ w & v & -1 & uv \\ 0 & \frac{1}{u} & 0 & 0 \end{pmatrix}, \quad \mathbf{r}_3 : \begin{pmatrix} 0 & x & 0 & 0 \\ \frac{1}{x} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ y & xy & z & -1 \end{pmatrix},$$

where $0 < u$ and $0 < x$. (30)

4.2. The relations in the presentation (27) will fix certain parameters by matrix equations. For instance, the product matrix is

$$(\mathbf{m}_0\mathbf{m}_1) : \begin{pmatrix} -1 & n & p & q \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ t & -1 & r & s \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} -1+nt & -n & nr+p & ns+q \\ t & -1 & r & s \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{31}$$

This has to be a rotation of order a, fixing pointwise the axis A_2A_3. From the matrix theory (trace formula), we know that

$$(\mathbf{m}_0\mathbf{m}_1)^a = \mathbf{1} \quad \text{allows one to choose}$$
$$n = t = 2\cos\frac{\pi}{a}, \quad \text{now } 2 \le a \in \mathbb{N}. \tag{32}$$

Similarly, the relations $(\mathbf{m}_0\mathbf{r}_2\mathbf{m}_0\mathbf{r}_2)^c = \mathbf{1} = (\mathbf{m}_0\mathbf{r}_3\mathbf{m}_1\mathbf{r}_3)^d$ imply polynomial equations for unknown parameters:

$$(pw-2)^2 = 4\cos^2\frac{\pi}{c} \quad \text{for } 2 \le c;$$
$$\text{and} \quad p = w = 0, \quad q = nu \quad \text{if } c = 1;$$
$$(qy-2)(sxy-2) = 4\cos^2\frac{\pi}{d} \quad \text{for } 3 \le d;$$
$$sxy = 2, \quad q = sx \quad \text{for } 2 = d;$$
$$\text{and} \quad y = 0, \quad q = -xs, \quad p = x(r+sz),$$
$$n = xxt \quad \text{for } 1 = d. \tag{33}$$

The most complicated $(\mathbf{m}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_2\mathbf{m}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_2)^b = \mathbf{1}$ implies

$$uvz = 2, \quad r = uz, \quad s = u(xt + xrw - 2) \quad \text{for } 1 = b$$
$$\text{and} \quad 4\cos^2\frac{\pi}{2b} = (uvz-2)(rv-2) \quad \text{for } 2 \le b \tag{34}$$

by careful computations and projective freedom as indicated later.

4.3. We determine a symmetric linear polarity (Einstein's index convention!)

$$({}_*) : \boldsymbol{b}^i \to \boldsymbol{b}^i_* := b^{ij}\mathbf{a}_j \quad (\text{with } b^{ij} = b^{ji}), \text{ and so by}$$
$$\langle\, , \,\rangle : \boldsymbol{V}_4 \times \boldsymbol{V}_4 \to \mathbf{R},$$
$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle = (\boldsymbol{u}_* \boldsymbol{v}) = u_r b^{rj}(\mathbf{a}_j \boldsymbol{b}^s) v_s = u_r b^{rj}\delta_j^s v_s = u_r b^{rs} v_s \tag{35}$$

a symmetric scalar product of forms $\boldsymbol{u} = \boldsymbol{b}^r u_r$ and $\boldsymbol{v} = \boldsymbol{b}^s v_s$ will be introduced, so that they will be invariant under the generator matrices (29) and (30), completely analogous to the plane cases but with more computations and complications. Such 'eigenvalue–eigenvector' problems

$$(a_i^r)(b^{ij})(a_j^s) = c(b^{rs})$$
$$\text{for every generator } (a_i^r) \text{ in equations (29), (30)} \tag{36}$$

and possibly different eigenvalues c's provide us with the symmetric matrix (b^{ij}), iff a non-trivial solution exists. If not, then we may face difficult problems as we see in Molnár (1997) and Molnár *et al.* (1997, 2005) and later in this paper. With a non-trivial (b^{ij}), its signature (*i.e.* the signs of its eigenvalues) and other invariant elements (fixed points and planes, for example) will determine a possible metric realization in (29), (30) and (36) by the table (given in Fig. 8) from Molnár (1997) and Molnár *et al.* (2005).

5. Our solution for orbifold $\mathcal{O}(3; 1; 1; 1)$

For instance, $(a; b; c; d) = (3; 1; 1; 1)$, our starting example, by the relations (27) yields the generators in equation (37) below. The solution of equations (32), (33) and (34) allows a projective basis change $\boldsymbol{b}^3\frac{1}{u} =: \boldsymbol{b}^{3'}$, then $u\mathbf{a}_3 =: \mathbf{a}_{3'}$; $\boldsymbol{b}^2 v =: \boldsymbol{b}^{2'}$, $\frac{1}{v}\mathbf{a}_2 =: \mathbf{a}_{2'}$, and we get

$$\mathbf{m}_0:\begin{pmatrix}-1&1&0&1\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\quad \mathbf{m}_1:\begin{pmatrix}1&0&0&0\\1&-1&2&-1\\0&0&1&0\\0&0&0&1\end{pmatrix},$$

$$\mathbf{r}_2:\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&1&-1&1\\0&1&0&0\end{pmatrix},\quad \mathbf{r}_3:\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&1&0\\0&0&2&-1\end{pmatrix},$$

moreover, the polarity matrix with parameter η:

$$(b^{ij})=\begin{pmatrix}1&-\frac{1}{2}&0&-\frac{1}{2}\\-\frac{1}{2}&1&-1&\frac{1}{2}\\0&-1&1+\eta&-\eta\\-\frac{1}{2}&\frac{1}{2}&-\eta&\eta\end{pmatrix}. \tag{37}$$

Thus, our Γ_5-invariant (scalar product and) quadratic form will be $\langle \boldsymbol{b}^r\xi_r, \boldsymbol{b}^s\xi_s\rangle$, *i.e.*

$$\begin{aligned}\xi_i b^{ij}\xi_j &= \xi_0\xi_0-\xi_0\xi_1-\xi_0\xi_3+\xi_1\xi_1-2\xi_1\xi_2\\ &\quad +\xi_1\xi_3+(1+\eta)\xi_2\xi_2-2\eta\xi_2\xi_3+\eta\xi_3\xi_3\\ &=(\xi_0-\tfrac{1}{2}\xi_1-\tfrac{1}{2}\xi_3)^2+\tfrac{3}{4}(\xi_1-\tfrac{4}{3}\xi_2+\tfrac{1}{3}\xi_3)^2\\ &\quad +(\eta-\tfrac{1}{3})(\xi_2-\xi_3)^2 \end{aligned} \tag{38}$$

of signature $(0\,+\,+\,+)$ iff $\eta > \frac{1}{3}$. Then we shall have a Euclidean metric. The plane $\boldsymbol{e}^0 := \boldsymbol{b}^0 1+\boldsymbol{b}^1 1+\boldsymbol{b}^2 1+\boldsymbol{b}^3 1$ is the common invariant plane of the generators; it will be chosen as the ideal plane $\omega_\infty(\boldsymbol{e}^0)$ at infinity. $A_3(\mathbf{a}_3) =: E_0(\mathbf{e}_0)$, $A_0(\mathbf{a}_0) =: (\mathbf{e}_0+\mathbf{e}_1)$, $A_1(\mathbf{a}_1) =: (\mathbf{e}_0+\mathbf{e}_1+\mathbf{e}_2)$, $A_2(\mathbf{a}_2) =: (\mathbf{e}_0+\frac{1}{2}\mathbf{e}_1+\frac{1}{2}\mathbf{e}_2+\frac{1}{2}\mathbf{e}_3)$ will define the traditional rhombohedral coordinate system (Fig. 4): $E_0(\mathbf{e}_0)$, $E_1^\infty(\mathbf{e}_1)$, $E_2^\infty(\mathbf{e}_2)$, $E_3^\infty(\mathbf{e}_3)$, with the origin E_0 and the ideal points E_1^∞, E_2^∞, E_3^∞ of the coordinate axes, respectively.

In this coordinate system, we finally get $\mathbf{m}_0$, $\mathbf{m}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$ as in *International Tables for Crystallography* (Hahn, 2002), space group No. 166 $\mathbf{R\bar{3}m}$:

$$\begin{gathered}\mathbf{m}_0:(x;\,y;\,z)\longmapsto(y;\,x;\,z),\quad \textit{i.e.}\text{ with } x^0=1\\ (x^1;\,x^2,x^3)\to(x^1;\,x^2;\,x^3)\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}=(x^2;\,x^1;\,x^3)\\ \text{and}\quad \mathbf{m}_1:(x;\,y;\,z)\longmapsto(x;\,z;\,y),\\ \mathbf{r}_2:(x;\,y;\,z)\longmapsto(-y+1;\ -x+1;\ -z),\\ \mathbf{r}_3:(x;\,y;\,z)\longmapsto(-z+1;\ -y+1;\ -x+1).\end{gathered} \tag{39}$$

Furthermore, the polarity $(_*)$ will be given by $u_i e^{ij} u_j$ where

$$(e^{ij})=\frac{1}{4}\begin{pmatrix}0&0&0&0\\0&1+\eta&-1+\eta&-1+\eta\\0&-1+\eta&1+\eta&-1+\eta\\0&-1+\eta&-1+\eta&1+\eta\end{pmatrix};$$

$$\begin{gathered}\text{thus }\cos(\boldsymbol{e}^i)(\boldsymbol{e}^j)=\frac{-e^{ij}}{(e^{ii}e^{jj})^{1/2}}=\frac{\eta-1}{\eta+1}>\tfrac{1}{2},\\ \text{because }\tfrac{1}{3}<\eta;\ \text{ and }\cos(\mathbf{e}_i)(\mathbf{e}_j)=\tfrac{1}{2}(1-\eta)<\tfrac{1}{3}\end{gathered} \tag{40}$$

can also be derived. Hence we see a geometric meaning for the (stretching) parameter η as well. It characterizes the rhombohedral lattice in the space group $\mathbf{R\bar{3}m}$. If $\eta \le \frac{1}{3}$, the metric is no longer convenient. There will be exceptional elements in the tilings of the corresponding $(0\,0\,+\,+)$ or $(0\,-\,+\,+)$ geometries which are now out of our scope.

Space $\mathbf{X}$	Signature of polarity $\Pi(.)$ or scalar product $\langle\ ,\ \rangle$ in V_4	Domain of proper points of $\mathbf{X}$ in $\mathcal{PS}^3$ $(\mathbf{V}^4(\mathbf{R}), V_4)$	The group $G=\mathrm{Isom}\,\mathbf{X}$ as a special transformation group of $\mathcal{PS}^3$
$\mathbf{S}^3$	$(++++)$	$\mathcal{PS}^3$	Coll. $\mathcal{PS}^3$ preserving $\Pi(.)$
$\mathbf{H}^3$	$(-+++)$	$\{(\mathbf{x})\in\mathcal{P}^3:\langle\mathbf{x},\mathbf{x}\rangle<0\}$	Coll. $\mathcal{P}^3$ preserving $\Pi(.)$
$\widetilde{\mathbf{SL_2R}}$	$(--++)$ with skew line fibering	Universal covering of $\mathcal{H}:=\{[x]\in\mathcal{PS}^3:\langle\mathbf{x},\mathbf{x}\rangle<0\}$ by fibering transformations	Coll. $\mathcal{PS}^3$ preserving $\Pi(.)$ and fibres
$\mathbf{E}^3$	$(0+++)$	$\mathcal{A}^3=\mathcal{P}^3\setminus\{\omega^\infty\}$ where $\omega^\infty:=(\boldsymbol{b}^0)$, $\boldsymbol{b}^0_\cdot=\mathbf{0}$	Coll. $\mathcal{P}^3$ preserving $\Pi(.)$ generated by plane reflections
$\mathbf{S}^2\!\times\!\mathbf{R}$	$(0+++)$ with O-line bundle fibering	$\mathcal{A}^3\setminus\{O\}$ O is a fixed origin	G is generated by plane reflections and sphere inversions, leaving invariant the O-concentric 2-spheres of $\Pi(.)$
$\mathbf{H}^2\!\times\!\mathbf{R}$	$(0-++)$ with O-line bundle fibering	$\mathcal{C}^+=\{X\in\mathcal{A}^3:$ $\langle\overrightarrow{OX},\overrightarrow{OX}\rangle<0$, half cone$\}$ by fibering	G is generated by plane reflections and hyperboloid inversions, leaving invariant the O concentric half-hyperboloids in the half cone $\mathcal{C}^+$ by $\Pi(.)$
Sol	$(0-++)$ with parallel plane fibering	$\mathcal{A}^3$ with parallel plane fibering	Coll. $\mathcal{P}^3$ preserving $\Pi(.)$ and the parallel plane fibering
Nil	$(0\,0\,0\,+)$ with parallel line bundle fibering	$\mathcal{A}^3$ with a distinguished parallel plane pencil along each line	Quadr. maps of $\mathcal{P}^3$ preserving $\Pi(.)$ and the line bundle with the plane pencil along each line

Figure 8
Table for the eight homogeneous geometries.

6. Further discussion

Now we consider Figs. 7, 9, 10 and 11 and report the further cases (Molnár *et al.*, 1997, 2005).

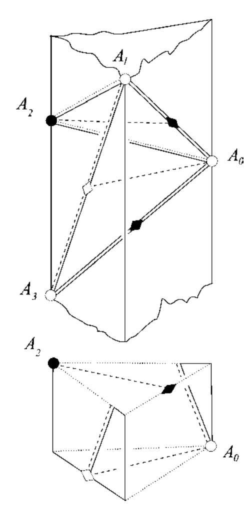

Figure 9
$(a;\,b;\,c;\,d)=(2;\,1;\,2;\,1)$, $\mathbf{H}^3$ tiling, A_0, A_1, A_3 ideal vertices, A_2 is proper.

$(a; b; c; d) = (2; 1; 2; 1)$ leads to a tiling in the Bolyai–Lobachevskian space $\mathbf{H}^3$. Our computations yield the invariant quadratic form

$$\begin{aligned} &\xi_0\xi_0 - \xi_0\xi_2 + \xi_1\xi_1 - \xi_1\xi_2 + \tfrac{1}{2}\xi_2\xi_2 - \xi_2\xi_3 + \xi_3\xi_3 \\ &\quad = \left(\xi_0 - \tfrac{1}{2}\xi_2\right)^2 + \left(\xi_1 - \tfrac{1}{2}\xi_2\right)^2 + \left(\xi_3 - \tfrac{1}{2}\xi_2\right)^2 - \tfrac{1}{4}\xi_2\xi_2 \\ &\qquad \text{of signature} \quad (- + + +). \end{aligned} \tag{41}$$

Thus we get a hyperbolic simplex: A_0, A_1, A_3 are ideal vertices at the absolute, A_2 is proper in $\mathbf{H}^3$. The face angles of our simplex will be

$$\beta^{01} = \beta^{03} = \beta^{13} = \frac{\pi}{2}, \quad \beta^{02} = \beta^{12} = \beta^{23} = \frac{\pi}{4}, \tag{42}$$

as can be calculated by (41). For example,

$$\cos\beta^{02} = \frac{-b^{02}}{(b^{00}b^{22})^{1/2}} = \frac{\frac{1}{2}}{(1 \times \frac{1}{2})^{1/2}} = \frac{2^{1/2}}{2} \tag{43}$$

shows the angle β^{02} between the faces m_0, r_2 at the edge - - - - - in Fig. 6, as the parameter $c = 2$ also involves this fact.

We only mention that $(a; b; c; d) = (2; 2; 1; 1)$ and $(2; 1; 1; 2)$ both lead to metrically non-realizable tilings by a splitting effect along an occurring Euclidean 2-orbifold $\mathbf{E}^2/\mathbf{pmm}$ (Figs. 10–11). The two parts are an $\mathbf{E}^3$ orbifold and an $\mathbf{H}^2 \times \mathbf{R}$ orbifold in the first case and two $\mathbf{H}^2 \times \mathbf{R}$ orbifolds in the second case.

Finally, $(a; 1; 1; 1)$ leads to an $\mathbf{S}^2 \times \mathbf{R}$ tiling, iff $a = 2$; and to infinitely many $\mathbf{H}^2 \times \mathbf{R}$ tilings, iff $4 \le a \in \mathbb{N}$. These 'intuitively easy' cases need some extra machinery, the so-called projective–inversive models of these geometries, indicated in Molnár (1997), not detailed more here (Fig. 7).

Our method seems to be new as providing effective Euclidicity criteria for combinatorially given tilings modelling possible real crystal structures (Johnson *et al.*, undated).

Moreover, the method can be used for other geometries using the table given in Fig. 8 and by an 'interactive algorithm' as follows in the next section. The barriers of the algorithm are obvious, in general, but it can work for any concrete finite D symbol (small enough) or orbifold as our results show.

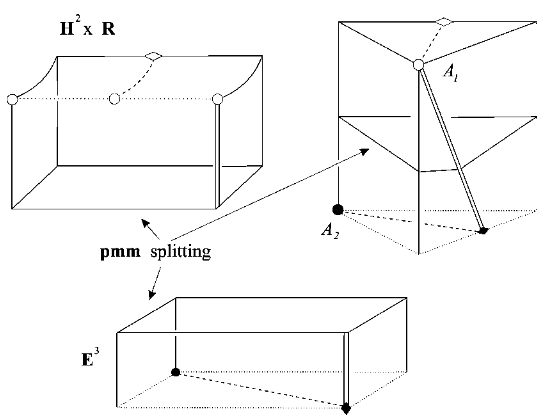

Figure 10
$(a; b; c; d) = (2; 2; 1; 1)$, splitting to $\mathbf{E}^3 + \mathbf{H}^2 \times \mathbf{R}$ case.

All these are related to the Thurston conjecture. The Poincaré conjecture is a special case (Molnár *et al.*, 2005), see also §7.

7. A strategy for finding Euclidean 3-tiling (sketch)

The previous Euclidicity criteria occur at the following steps.

7.1. Crystal problems will be formulated as tiling problems and as barycentric subdivisions, and hence as D symbols in some model chosen adequately (?). For example, we look for tilings with 1–1–1–1 equivalence classes of vertices, edges, faces, solids, respectively. The computer program lists *e.g.* the D diagram in Fig. 5 as we mentioned (Dress *et al.*, 1993; Molnár, 1996).

7.2. The σ_i, σ_j operations for any $i, j \in I = \{0, 1, 2, 3\}$ allow us to choose a convenient matrix function $m_{ij}(D)$, $D \in \mathcal{D}$, on the D set $\mathcal{D}$ (vertices of the D diagram). Any subdiagram component ${}^c\mathcal{D}_{ij}$ describes then a rotation about an ij edge (class) at the meeting of i and j faces, respectively, of a barycentric simplex (class). The corresponding rotational order has to be 1, 2, 3, 4, 6 by the Barlow condition.

7.3. The σ_i, σ_j, σ_k operations, *i.e.* cancelling the σ_ℓ operation $\{i, j, k, \ell\} = \{0, 1, 2, 3\}$, describe any connected subdiagram component ${}^c\mathcal{D}_{ijk} =: {}^c\mathcal{D}^\ell$ with the matrix function ${}^c\mathcal{M}^\ell$, and hence the stabilizer subgroup of the corresponding ℓ centre (class). This stabilizer has to be a (finite) crystallographic point group by the corresponding two-dimensional D symbol $({}^c\mathcal{D}^\ell; {}^c\mathcal{M}^\ell)$.

7.4. The above steps lead from a D symbol to a simplicial (triangulated) fundamental domain $\mathcal{F}$ with pairing of the remaining (still free) triangle faces of $\mathcal{F}$, *i.e.* to an orbifold with its possible singular points where the stabilizers are (not trivial here, in general) finite point groups.

For the 219 non-isomorphic Euclidean space groups, the orbifold pictures of the direct space groups (orientable orbifolds) have already been determined by Dunbar (1988). Moreover, for any space group, the orbifold 'skeleton' (without indicating knots and links on it) can be read off the Wyckoff positions from *International Tables for Crystallography* (Henry & Lonsdale, 1969; Hahn, 2002). We mention here that this last problem was solved and computerized when the author visited Bielefeld University (1989–1991) and worked in the team of A. W. M. Dress. Let only Dress *et al.*

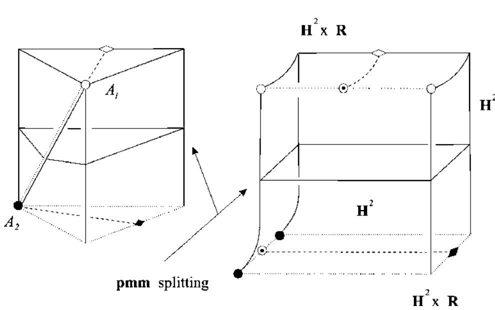

Figure 11
$(a; b; c; d) = (2; 1; 1; 2)$, splitting to $\mathbf{H}^2 \times \mathbf{R} + \mathbf{H}^2 \times \mathbf{R}$ case.

(1993), Delgado-Friedrichs (1994, 2003), Delgado-Friedrichs & Huson (1997) be mentioned here.

These preliminary steps may help in the following computational procedure which is of very high complexity because of the nature of the problem and it can directly be applied in each case. Thus some uncertainties, mentioned in Delgado-Friedrichs (1994) can also be excluded.

7.5. Taking the triangulated canonical (Molnár, 1996) fundamental domain $\mathcal{F}$ to our orbifold $\mathcal{O}$ by the D symbol $(\mathcal{D}, M)$ above, we start with embedding $\mathcal{F}$ into a real projective metric sphere $\mathcal{PS}^3(\mathbf{R}, \langle\, , \,\rangle)$.

Now, if it is possible, the scalar product $\langle\, , \,\rangle$ will be of signature $(0 + + +)$ for the form space $\boldsymbol{V}_4$, describing the 2 planes of $\mathbf{E}^3 \subset \mathcal{PS}^3$. A form $\boldsymbol{e}^0$ to the above 0 in the signature will be orthogonal to all forms of $\boldsymbol{V}_4$, and hence it characterizes the ideal plane ω_∞ of $\mathbf{E}^3$ to be constructed.

This is analogous to §5. But now, in general, the projective coordinate simplex, denoted *e.g.* by $C_0(\mathbf{c}_0)C_1(\mathbf{c}_1)C_2(\mathbf{c}_2)C_3(\mathbf{c}_3)$, will be chosen to be a first barycentric simplex ${}^1C \in {}^1D \in \mathcal{D}$ of the D symbol in a canonical way (Molnár, 1996). (This is ${}^1C = A_3A_{03}A_{13}A_2$ in Fig. 4.) The canonical gluing procedure, of other barycentric simplices to form $\mathcal{F}$, implies the face-pairing mappings as projective collineations of $\mathcal{PS}^3$. These collineations can be expressed (by matrices) for points, as in $\mathbf{V}^4$ spanned by the basis $\{\mathbf{c}_i\}$ of the coordinate simplex and for planes in its dual space $\boldsymbol{V}_4$ spanned by the dual basis $\{\boldsymbol{d}^j\}$ with $(\mathbf{c}_i\boldsymbol{d}^j) = \delta_i^j$ (Kronecker symbol).

These generating collineations will be given by 4×4 matrices up to projective freedom and with unknown parameters as in §4. Projective freedom brings a lot of simplification. For example, the determinants of generating matrices can be taken ± 1. In the dual-basis pair $\{\mathbf{c}_i\}$, $\{\mathbf{d}^j\}$, we may change $\mathbf{c}_{k'} := \alpha\mathbf{c}_k$, $\boldsymbol{d}^{k'} = \boldsymbol{d}^k\frac{1}{\alpha}$, $0 < \alpha \in \mathbf{R}$ for any $k = k' \in \{0, 1, 2, 3\}$.

7.6. The generating matrices make it possible to express any vertex and any (triangle) face plane of $\mathcal{F}$ in the dual basis pair $\{\mathbf{c}_i\}$, $\{\boldsymbol{d}^j\}$, possibly in a complicated but straightforward way, by computer. Moreover, the defining relations for the unknown space group Γ, chosen for the edge classes of $\mathcal{F}$ in **7.2** with corresponding rotational orders [as $(a; b; c; d)$ in §4], provide us matrix equations for determining the parameters in the generating matrices. Such an equation expresses that a product of generators is a rotation of given order about an edge of $\mathcal{F}$ which is expressible in the coordinate simplex ${}^1C = C_0C_1C_2C_3$. This is a standard method, yielding (possibly) complicated polynomial equations, by the nature of the problem, in general. See **4.2**. These polynomial equations may involve accurate fine numerical solutions, but symbolic computations can be satisfactory as well.

7.7. Now comes the linear equation system for the coefficients of the scalar product $\langle\, , \,\rangle$ defined by $(\langle \boldsymbol{d}^i, \boldsymbol{d}^j\rangle) =: (d^{ij})$ [as in **4.3** for (b^{ij})]. This $\langle\, , \,\rangle$ has to be invariant under any generating matrix (a_i^j) with $\det(a_i^j) = \pm 1$ iff $(a_i^r)(d^{ij})(a_j^s) = (d^{rs})$. This non-trivial symmetric matrix (d^{ij}) has to be of signature $(0 + + +)$ as indicated at the beginning of **7.5**. The symbolic computation may help, again. Free parameters can occur. Only trivial solution $(d^{ij}) = (0)$ may refer to splitting phenomena as our Fig. 10 shows. Then a connected sum (denoted by + here) of different geometric pieces may occur, surprisingly. This splitting recognition has not been computerized yet and it seems to be very difficult.

We can roughly formulate Thurston's geometrization conjecture that every orbifold (manifold) – after occasional splitting procedure along some spherical ($\mathbf{S}^2$) and Euclidean ($\mathbf{E}^2$) 2-orbifolds, and after some two- or one-dimensional changing, if necessary – can be equipped with a homogeneous Riemannian metric of the eight Thurston geometries in our table (Fig. 8). Thus our method is applicable modulo Thurston conjecture. It is not excluded yet that an orbifold by D symbol will represent a counter-example. In our papers (Molnár *et al.*, 1997, 2005), we mentioned also other phenomena to be examined by our method which also promise success (see Molnár, 1993; Molnár & Prok, 1994; Molnár *et al.*, 1998). We emphasize that it is enough – if the Thurston conjecture is true – to deal with a so-called minimal D symbol or, equivalently, with maximal group $\Gamma = \mathrm{Aut}\,\mathcal{T}$ whose metric realization above surely involves the realization of its 'symmetry breakings' where $\Gamma < \mathrm{Aut}\,\mathcal{T}$. Such a smaller group can be assigned with an asymmetric mark in its fundamental domain and in its images or, if possible, by deforming some faces or edges to be curved, conveniently according to Γ.

Assume that:

1. a non-trivial (d^{ij}) above exists;
2. the generating matrices can be metrically adjusted and they do not have any common fixed point, to exclude $\mathbf{S}^2 \times \mathbf{R}$ geometry by our table (Fig. 8);
3. these generators metrically tile the neighbourhood of any edge of $\mathcal{F}$ with the images of $\mathcal{F}$ (without gaps and overlaps) as the corresponding relation dictates.

Then our generators will be isometries for a group Γ acting on the Euclidean space $\mathbf{E}^3 := \mathcal{P}^3 \setminus (\boldsymbol{e}^0)$.

Here the projective space $\mathcal{P}^3$ is obtained from $\mathcal{PS}^3$ by unifying the opposite rays $(\mathbf{x})$ and $(-\mathbf{x})$, $\mathbf{x} \in \mathbf{V}^4$, and by unifying the 'opposite' planes $(\boldsymbol{u})$ and $(-\boldsymbol{u})$ $\boldsymbol{u} \in \boldsymbol{V}_4$. (Zero vector and zero form have been excluded, of course.) The ideal plane $(\boldsymbol{e}^0)$ (to 0 in the signature) and its ideal points $(\mathbf{z})$ with $(\mathbf{z}\boldsymbol{e}^0) =: z^0 = 0$ will be excluded from $\mathcal{P}^3$ as usual. This was followed in our example in §5.

Our algorithm was especially applied for the complete classification of simplex tilings in Molnár *et al.* (1997) and Molnár *et al.* (2005). Let us only extract here that there are 26 (non-equivariant) fundamental tilings in $\mathbf{E}^3$ by compact simplices under 20 space groups. This result was obtained in 1988 in a joint work with István Prok (Molnár & Prok, 1988). Of course, computer implementations would be very useful. We are working on these problems with colleagues.

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