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SOME OLD AND NEW ASPECTS ON THE CRYSTALLOGRAPHIC GROUPS

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Abstract

The derivation of crystallographic groups in the Euclidean n-space $\mathcal{E}^n$ (think of $n = 2, 3$) will be illustrated by the space groups **Pm, Pb** and **Bm, Bb** belonging to the geometric crystal class (point group) **m**. Some new directions of investigations will be indicated, e.g. the orbit for densest ball packing, minimally presenting fundamental polyhedron, data base and computer realization for each space group class amongst the 219 (230) ones. This paper is based on the lectures held several times by the author.

1. Introduction, Pm as a Typical Example

Figures like point systems, ideal crystals, etc. in the Euclidean n-space $\mathcal{E}^n$ can be characterized by those *geometric transformations* which carry a given figure $\mathcal{F}$ in itself. The set G of these one-to-one self-mappings of $\mathcal{F} \subset \mathcal{E}^n$ is equipped by the operation of composing a first mapping $\alpha \in G$ with a second one $\beta \in G$ to obtain the product $\gamma = \alpha\beta \in G$. The following notations indicate this for any point $X \in \mathcal{F}$

$$\alpha : X \mapsto X^{\alpha}; \quad \beta : X \mapsto X^{\beta}; \quad \gamma := \alpha\beta : X \mapsto X^{\gamma} := (X^{\alpha})^{\beta}. \tag{1.1}$$

Introducing an *origin* $O \in \mathcal{E}^n$ and a vector *basis*

$$\{\mathbf{e}_i\} := \{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\} \tag{1.2}$$

for the Euclidean real vector space $\mathbf{E}^n$, any point $X \in \mathcal{E}^n$ can be described by the position vector

$$\overrightarrow{OX} := \mathbf{x} = \sum_{i=1}^{n} x^i \mathbf{e}_i =: x^i \mathbf{e}_i \tag{1.3}$$

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(summing up for $i = 1, 2, \dots, n$ by *Einstein convention,* used also later on) with the *real coordinates* $x^1, x^2, \dots, x^n \in \mathbb{R}$. Then the *inner product* (of signature $(+, +, \dots, +)$)

$$\begin{aligned}\langle;\rangle : \mathbf{E}^n \times \mathbf{E}^n \to \mathbb{R}, \langle \mathbf{x}; \mathbf{y} \rangle = \langle x^i \mathbf{e}_i; y^i \mathbf{e}_j \rangle = \\ = x^i y^i \langle \mathbf{e}_i; \mathbf{e}_j \rangle =: x^i y^i g_{ij}\end{aligned} \tag{1.4}$$

is defined in $\mathbf{E}^n$ by the symmetric matrix $g_{ij} =: \langle \mathbf{e}_i; \mathbf{e}_j \rangle = \langle \mathbf{e}_j; \mathbf{e}_i \rangle = g_{ji}$. Thus, the *distance* for any two points and the *angle* $\in [0, \pi]$ of any two vectors can be usually introduced by

$$d(X, Y) := \sqrt{(x^i - y^i)(x^j - y^j) g_{ij}}$$

and

$$\cos a(\mathbf{x}, \mathbf{y}) := x^i y^i g_{ij} / \sqrt{(x^r x^s g_{rs})(y^u y^v g_{uv})}, \tag{1.5}$$

respectively. An *affine transformation* $\alpha = (\mathbf{A}, \mathbf{a})$ of $\mathcal{E}^n$ is defined by a *linear transformation* $\mathbf{A}$ of $\mathbf{E}^n$ and a vector $\mathbf{a} := \overrightarrow{OO^\alpha}$. Here

$$\begin{aligned}\mathbf{x}^\alpha := \mathbf{x}\mathbf{A} + \mathbf{a}; (x^i \mathbf{e}_i)^\alpha = (x^i \mathbf{e}_i)\mathbf{A} + a^j \mathbf{e}_j = \\ = x^i (\mathbf{e}_i \mathbf{A}) + a^j \mathbf{e}_j = x^i a_i^j \mathbf{e}_j + a^j \mathbf{e}_j = (x^i a_i^j + a^j) \mathbf{e}_j\end{aligned} \tag{1.6}$$

show how to get the image of a point $X(\mathbf{x} = x^i \mathbf{e}_i)$ by the matrix a_i^j of $\mathbf{A}$ and by the vector $\overrightarrow{OO^\alpha} =: \mathbf{a} = a^j \mathbf{e}_j$. The product of $\alpha(\mathbf{A}, \mathbf{a})$ and $\beta(\mathbf{B}, \mathbf{b})$ will be

$$\alpha\beta(\mathbf{AB}, \mathbf{aB} + \mathbf{b}). \tag{1.7}$$

With the *identity mapping* $1 = (\mathbf{1}, \mathbf{0})$ the *inverse* of α will be

$$\alpha^{-1} = (\mathbf{A}, \mathbf{a})^{-1} = (\mathbf{A}^{-1}, -\mathbf{a}\mathbf{A}^{-1}), \tag{1.8}$$

where $\mathbf{A}^{-1}$ denotes the inverse of $\mathbf{A}$. In particular, $\alpha = (\mathbf{A}, \mathbf{a})$ is said to be an *isometry* of $\mathcal{E}^n$, if $\mathbf{A}$ preserves the inner product, i.e. for any $\mathbf{x}, \mathbf{y} \in \mathbf{E}^n$

$$\langle \mathbf{xA}; \mathbf{yA} \rangle = \langle \mathbf{x}; \mathbf{y} \rangle. \tag{1.9}$$

For the matrix a_i^j of $\mathbf{A}$ this implies the matrix equation

$$a_i^r a_j^s g_{rs} = g_{ij}. \tag{1.10}$$

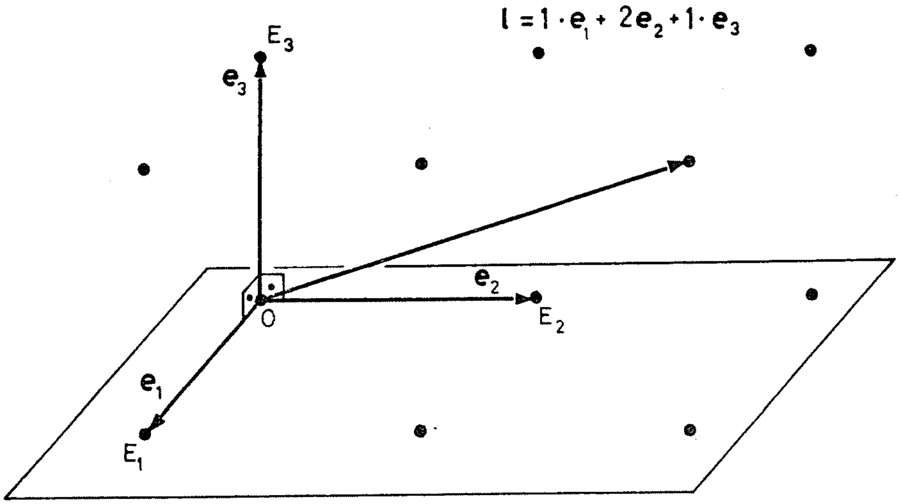


Fig. 1.1. A monoclinic primitive lattice mP with Gramian (1.11). Here $-\sqrt{2}/2 \leq g_{12}/\sqrt{g_{11}g_{22}} = \cos(\mathbf{e}_1, \mathbf{e}_2) \leq 0$ can be assumed

Summarizing, the affine transformations of $\mathcal{E}^n$ form a group Aff $\mathcal{E}^n$ with the composition as group operation. The isometries of $\mathcal{E}^n$ is a subgroup Isom $\mathcal{E}^n \subset$ Aff $\mathcal{E}^n$. The transformation group of a figure $\mathcal{F} \subset \mathcal{E}^n$ can be considered as a subgroup of Aff $\mathcal{E}^n$ or rather a subgroup of Isom $\mathcal{E}^n$.

As an example, we introduce the crystallographic space group **Pm** consisting of two types of isometries of $\mathcal{E}^3$: The *monoclinic primitive lattice* $\mathbf{L}_{\mathbf{Pm}} =: mP$ is spanned by three *translations* (*Fig. 1.1*)

$$(\mathbf{1}, \mathbf{e}_1), (\mathbf{1}, \mathbf{e}_2), (\mathbf{1}, \mathbf{e}_3) \text{ with the } \textit{Gramian}$$
$$(g_{ij}) := (\langle \mathbf{e}_i; \mathbf{e}_j \rangle) := \begin{pmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix}, \tag{1.11}$$

and the other transformations (*reflections, glide reflections*) are of the form $(\mathbf{M}, \mathbf{l} := l^i \mathbf{e}_i)$ with integer triples (l^1, l^2, l^3) and with

$$\mathbf{e}_i \mathbf{M} = m_i^j \mathbf{e}_j, \quad (m_i^j) = \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}. \tag{1.12}$$

The space group **Pm** is no. 6 in the *International Tables* (1976, 1983). It is briefly given by the following notations

$$\begin{array}{llllll} 2 & c & \mathbf{1} & x,y,z & x,y,\bar{z} & (\bar{z} \text{ means } -z) \\ 1 & b & \mathrm{m} & x,y,\frac{1}{2} & & \\ 1 & a & \mathrm{m} & x,y,0. & & \end{array} \tag{1.13}$$

In dimension $n = 3$, $\mathbf{x} = x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3$ usually denotes a general position vector, and in the first row of (1.13) the row matrix $(x\,y\,z)$ is understood modulo an integer triple, characterizing the lattice mP in (1.11) implicitly. In the first row of (1.13)

$$(x\ y\ {-z}) = (x\ y\ z)\begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix} \text{ mod integer triple}$$

means just reflections and glide reflections at (1.12).

In the first row of (1.13) 2 means the number of the c-type (most general) Wyckoff positions (orbit type) in a *unit parallelepiped* (*unit cell*) with respect to the basis $\{\mathbf{e}_i\}$ at (1.11) (*Fig. 1.2*):

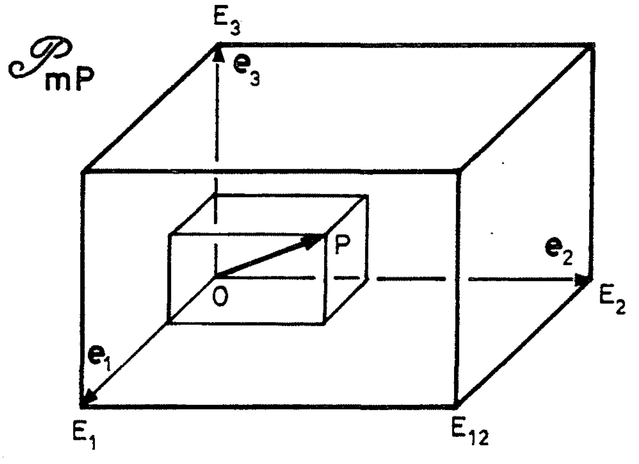


Fig. 1.2. A *unit parallelepiped (unit cell)* $\mathcal{P}_{\mathrm{mP}}$ for mP (see (1.14))

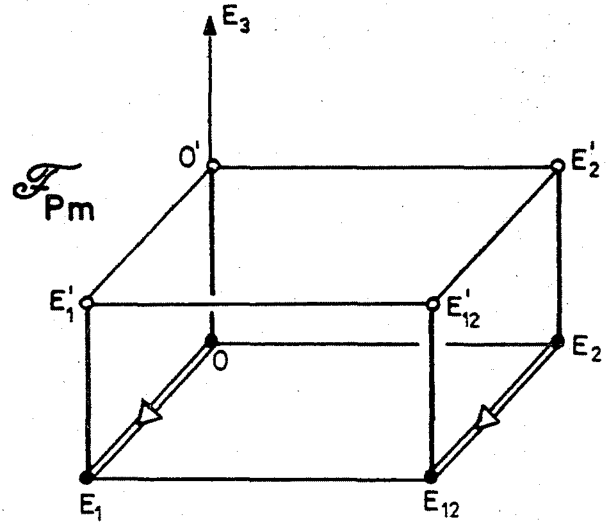


Fig. 1.3. A *fundamental domain* $\mathcal{F}_{\mathbf{Pm}}$ for the space group **Pm**, which serves a *minimal presentation* described at formulas (1.17–1.19)

$$\mathcal{P}_{mP} := \{P(p^1, p^2, p^3) : 0 \le p^1 < 1, \quad 0 \le p^2 < 1, \quad 0 \le p^3 < 1\}. \qquad (1.14)$$

To each point of this orbit the trivial *stabilizer subgroup* **1** (in **Pm**) is associated.

In the second row of (1.13) we find the *b*-type orbit with 1 point in the unit cell (1.14). From this orbit each point is fixed under certain reflection in **Pm**, e.g.

$$\left(x\ y\ \frac{1}{2}\right) = \left(x\ y\ \frac{1}{2}\right) \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix} + (0\ 0\ 1).$$

Now the stabilizer subgroup is denoted by $\mathbf{m} = \{\mathbf{1}, \mathbf{M}\}$ as a linear finite matrix group consisting of

$$(\mathbf{1}) = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}, \ (\mathrm{M}) = \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}. \qquad (1.15)$$

In the third row of (1.13) we find the *a*-type orbit analogously. From (1.13) we read off a *fundamental polyhedron* (*Fig. 1.3*) by halving the unit cell $\mathcal{P}_{mP}$:

$$\mathcal{F}_{\mathbf{Pm}} := \{F(f^1, f^2, f^3) : 0 \le f^1 \le 1, \quad 0 \le f^2 \le 1, \quad 0 \le f^3 \le \frac{1}{2}\}. \quad (1.16)$$

This is an *asymmetric unit* for the space group **Pm**. This marked parallelepiped $OE_1E_{12}E_2O'E_1'E_{12}'E_2'$ is equipped by *face pairing transformations (involutive face identifications)* as follows.

$$\begin{array}{llcll} \mu: & OE_1E_{12}E_2 & \longrightarrow & OE_1E_{12}E_2 & \text{reflection in a (mirror) plane,} \\ \mu': & O'E_1'E_{12}'E_2' & \longrightarrow & O'E_1'E_{12}'E_2' & \text{plane reflection again,} \\ \tau_1: & OE_2E_2'O' & \longrightarrow & E_1E_{12}E_{12}'E_1' & \text{translation by } \mathbf{e}_1, \\ \tau_2: & OE_1E_1'O' & \longrightarrow & E_2E_{12}E_{12}'E_2' & \text{translation by } \mathbf{e}_2. \end{array} \quad (1.17)$$

These face pairing isometries generate the space group **Pm**, and they induce the edge classes of $\mathcal{F}_{\mathbf{Pm}}$. Any edge class determines a relation for these generators. E.g. for the class $\Longrightarrow \{OE_1, E_2E_{12}\}$ we have the following *Poincaré algorithm:*

$$\begin{array}{lcl} (OE_1; OE_1E_{12}E_2) & \xrightarrow{\mu} & (OE_1; OE_1E_{12}E_2), \\ (OE_1; OE_1E_1'O') & \xrightarrow{\tau_2} & (E_2E_{12}; E_2E_{12}E_{12}'E_2'), \\ (E_2E_{12}; E_2E_{12}E_1O) & \xrightarrow{\mu} & (E_2E_{12}; E_2E_{12}E_1O), \\ (E_2E_{12}; E_2E_{12}E_{12}'E_2') & \xrightarrow{\tau_2^{-1}} & (OE_1; OE_1E_1'O'); \text{periodically,} \\ (OE_1; OE_1E_{12}E_2) & & \text{would be the next flag, again.} \end{array} \quad (1.18)$$

That means, we start with a *flag* of incident vertex O, edge OE_1 and face $OE_1E_{12}E_2$ of $\mathcal{F}_{\mathbf{Pm}}$ and consider the image flag under the face pairing (1.17). Then we keep the image edge (oriented) and link the second face incident to this edge at $\mathcal{F}_{\mathbf{Pm}}$, and so on (see MOLNÁR, E. (1992), MOLNÁR, E. – PROK, I. (1988)). Now, the *cycle transformation,* as a product, is

$$\mu\tau_2\mu\tau_2^{-1} = 1 \text{ the identity mapping.}$$

Because it fixes the edge OE_1 and – by the right angles at OE_1 and E_2E_{12} – it fixes also the starting flag.

In *Fig. 1.3* we did not indicate all the 5 edge classes induced by the generators on $\mathcal{F}_{\mathbf{Pm}}$. We have 5 *edge relations* for **Pm** and, with the 2 *reflection relations,* we finally obtain a *minimal geometric presentation* for the space group

$$\begin{aligned} \mathbf{Pm} := (\mu, \mu', \tau_1, \tau_2 - 1 = \mu^2 = \mu'^2 = \mu\tau_2\mu\tau_2^{-1} = \\ \mu\tau_1\mu\tau_1^{-1} = \mu'\tau_2\mu'\tau_2^{-1} = \mu'\tau_1\mu'\tau_1^{-1} = \tau_1\tau_2\tau_1^{-1}\tau_2^{-1}). \end{aligned} \quad (1.19)$$

Note that the translation $\tau_3(\mathbf{1}, \mathbf{e}_3)$ is a product $\mu\mu'$ of the generators. Thus, every transformation of **Pm** can be expressed as a *product* (word) of the above generators and their inverses, and every relation in **Pm** is an *algebraic consequence* of the above *defining relations.*

For instance, the relation $1 = \tau_1\tau_3\tau_1^{-1}\tau_3^{-1}$, expressing the commutativity of the translations τ_1 and $\tau_3 = \mu\mu'$, can be derived as

$$\tau_1\mu\mu'\tau_1^{-1}(\mu'^{-1}\mu^{-1}) = \tau_1\mu(\mu'\tau_1^{-1}\mu')\mu = \tau_1\mu\tau_1^{-1}\mu = 1.$$

Indeed, it is a consequence of the 1st, 2nd, 6th, 4th defining relations.

We imagine that the group **Pm** transforms the fundamental polyhedron $\mathcal{F}_{\mathbf{Pm}}$ first onto its face neighbours. E.g. the image $\mathcal{F}^{\tau_1}$ is adjacent to $\mathcal{F}$ at the common face

$$E_1E_{12}E'_{12}E'_1 =: f_{\tau_1} = (OE_2E'_2O')^{\tau_1} =: (f_{\tau_1^{-1}})^{\tau_1}.$$

Then the second neighbours follow, e.g.

$$\mathcal{F}^{\tau_1} \text{ and } \mathcal{F}^{\mu\tau_1} \text{ are adjacent at the common face } (f_\mu)^{\tau_1} = (f_\mu)^{\mu\tau_1};$$

$$\mathcal{F}^{\tau_1} \text{ and } \mathcal{F}^{\tau_2\tau_1} \text{ are adjacent at } (f_{\tau_2})^{\tau_1} = (f_{\tau_2^{-1}})^{\tau_2\tau_1},$$

and so on. We obtain a *space tiling* by the **Pm**-images of $\mathcal{F}_{\mathbf{Pm}}$. $\mathcal{F}_{\mathbf{Pm}}$ itself represents the identity 1 of **Pm**, each other represents a word of the generators obtained by the path crossing the faces of image polyhedra, consecutively. Any *circle path* (i.e. *circuit)* in this *group graph* of **Pm**, above, means a relation amongst the generators. Without any more explanations we indicate the geometric proof that

any relation is an algebraic consequence of the defining relations.

Indeed, any circle path can be simplified around the edges of the tiling step-by-step to the trivial circuit.

We emphasize that **Pm** has also other fundamental polyhedra with other presentations, analogously as above. A typical one is the very important *Dirichlet polyhedron* belonging to a general orbit (c-type) of **Pm**. *Fig. 1.4* shows a *hexagonal prism* $\mathcal{D}_{\mathbf{Pm}}(D)$ to a kernel point $D(d^1, d^2, \frac{1}{4})$. The Dirichlet polyhedron itself is defined as

$$\mathcal{D}_{\mathbf{Pm}}(D) := \{X \in \mathcal{E}^3 : DX \leq XD^\alpha \text{ for any } \alpha \in \mathbf{Pm}\}. \qquad (1.20)$$

Only finitely many *half-spaces* occur at forming $\mathcal{D}_{\mathbf{Pm}}(D)$, in general. We have a presentation again for the space group

$$\begin{aligned}\mathbf{Pm} = (\mu, \mu', \tau_1, \tau_2, \tau_{12} - 1 = \mu^2 = \mu'^2 = \mu\tau_1\mu\tau_1^{-1} = \mu\tau_2\mu\tau_2^{-1} = \\ = \mu\tau_{12}\mu\tau_{12}^{-1} = \mu'\tau_1\mu'\tau_1^{-1} = \mu'\tau_2\mu'\tau_2^{-1} = \mu'\tau_{12}\mu'\tau_{12}^{-1} = \\ = \tau_1\tau_2\tau_{12}^{-1} = \tau_2\tau_1\tau_{12}^{-1}).\end{aligned} \qquad (1.21)$$

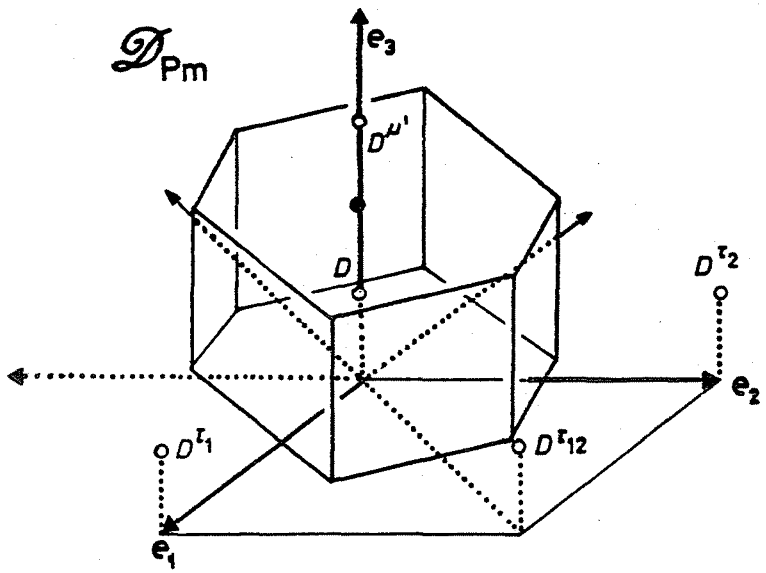


Fig. 1.4. The *Dirichlet polyhedron* $\mathcal{D}_{\mathbf{Pm}}$ for the orbit of a point D under the space group $\mathbf{Pm}$ (see (1.20))

For each general point $X(x^1, x^2, x^3)$ of c-type we can consider the orbit of X under $\mathbf{Pm}$ and the ball packing with centres at the orbit

$$X^{\mathbf{Pm}} := \{X^\alpha \in \mathcal{E}^3 : \alpha \in \mathbf{Pm}\} \tag{1.22}$$

and with radius

$$r(X, \mathbf{Pm}) = \min_{\alpha\in\mathbf{Pm}, X\neq X^\alpha} \{\frac{1}{2} d(X, X^\alpha)\}. \tag{1.23}$$

The *density* of the ball packing is defined now as

$$\delta(X, \mathbf{Pm}) = \frac{4}{3} r^3 \pi / \mathrm{vol}\, \mathcal{F}_{\mathbf{Pm}}, \tag{1.24}$$

where the volume of $\mathcal{F}_{\mathbf{Pm}}$ depends on the Gramian in (1.11)

$$\mathrm{vol}\, \mathcal{F}_{\mathbf{Pm}} = \frac{1}{2} \mathrm{vol}\, \mathcal{P} = \frac{1}{2}\sqrt{(g_{11}g_{22} - g_{12}g_{21})g_{33}}. \tag{1.25}$$

Thus, we can ask for the *densest ball packing* under the space group $\mathbf{Pm}$ up to a *similarity*, and for the maximal density depending on the isomorphism class of $\mathbf{Pm}$.

$$\delta(\mathbf{Pm}) := \max_{X, (g_{ij})} \{\delta(X, \mathbf{Pm})\}. \tag{1.26}$$

For the orbits of c-type the densest ball packing is attained with a point D and Dirichlet polyhedron $\mathcal{D}_{\mathbf{Pm}}(D)$ at formula (20), with Gramian, radius and density

$$(g_{ij}) = \begin{pmatrix} 4 & -2 & 0 \\ -2 & 4 & 0 \\ 0 & 0 & 16 \end{pmatrix}; \; r = 1, \; \delta(\mathbf{Pm}) = \frac{\pi \cdot \sqrt{3}}{9} \approx 0,6046, \qquad (1.27)$$

respectively. The same question for the orbits of a- or b-type is answered by Gramian, radius and the same density as

$$(\bar{g}_{ij}) = \begin{pmatrix} 4 & -2 & 0 \\ -2 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \; \bar{r} = 1, \; \bar{\delta}(\mathbf{Pm}) = \frac{\pi\sqrt{3}}{9}. \qquad (1.28)$$

We remark that an orbit and a ball packing under **Pm** has a larger self-symmetry group, in general. This is the space group **P2/m** no. 10 that will be described in Section 6.

2. About the History and the General Theory

It was a great discovery in the history of science that E. S. FEDOROV (1890), A. SCHOENFLIES (1891) and W. BARLOW (1894) completed the list of 219 isomorphism classes (or 230 oriented affine classes) of the crystallographic space groups in the Euclidean space $\mathcal{E}^3$. Thus, the initiatives of F. C. HESSEL (1830), A. BRAVAIS (1850), C. JORDAN (1867), L. SOHNCKE (1879) and others had been fulfilled before the discovery of material crystal structures by M. VON LAUE (1912).

Famous mathematicians as H. MINKOWSKI (1905), G. FROBENIUS (1911), L. BIEBERBACH (1912), H. ZASSENHAUS (1948), A. C. HURLEY (1951, 67), E. C. DADE (1965), R. BÜLOW (1967), J. NEUBÜSER (1969), H. WONDRATSCHEK (1971) and many others worked on the n-dimensional theory, particularly for $n = 4$. Finally by 1973 the 4783 isomorphism classes (4895 oriented affine classes) had been listed by computer and published (1978) in the book of H. BROWN, R. BÜLOW, J. NEUBÜSER, H. WONDRATSCHEK, H. ZASSENHAUS.

There is a Soviet school, the students of B. N. DELONE (DELAUNAY) as S. S. RYSHKOV, E. P. BARANOVSKI, A. M. ZAMORZAEV; moreover, A. V. SHUBNIKOV, N. V. BELOV and their students and many others.

A living classic is H. S. M. COXETER. There is a Hungarian school of the discrete geometry around L. FEJES TÓTH (1965). He initiated the systematical investigations how to characterize a regular system of figures by extrema properties. Thus, he refreshed the classical ideas of J. KEPLER and G. LEIBNIZ.

New classification methods had been developed by B. GRÜNBAUM and G. C. SHEPHARD (1987), moreover by M. S. DELANEY (1980) and A. W. M. DRESS (1987). We mention a recent work of A. W. M. DRESS, D. HUSON, E. MOLNÁR (1991) where a classification problem in $\mathcal{E}^3$ has been solved by D-symbols (DELONE–DELANEY–DRESS-symbols) and by computer.

Of course, many physicists, crystallographers and other scientists elaborated the methods and the theory of crystallographic measurements.

We mention only the relations to the geometric number theory, to the algebra, topology, discrete and differential geometry.

Now we give a sketch on the general concepts and theorems which lead to the classification of the space groups in $\mathcal{E}^2$ and $\mathcal{E}^3$ or generally in $\mathcal{E}^n$, up to $n = 4$ nowadays.

A group $G \subset \text{Isom}\, \mathcal{E}^n$ of isometric transformations *acts* on $\mathcal{E}^n$ *discretely* or *discontinuously*, or G is called a *discrete group*, if any orbit $X^G := \{X^\alpha \in \mathcal{E}^n : \alpha \in G\}$ has the property: any compact point set in $\mathcal{E}^n$ meets only finitely many points from the orbit. By other words: *for any orbit X^G there exists a positive real radius $r(X,G)$ such that the balls of radius r, centred in the points of X^G, have disjoint interiors.*

Then we can define a *fundamental domain* $\mathcal{F}_G$ for the group G, a closed point set with face identifications on its boundary. Moreover, the *fundamental tiling*, as the G-images of $\mathcal{F}_G$, is required to cover the whole space $\mathcal{E}^n$ with disjoint interiors. This was illustrated for $G = \mathbf{Pm}$ in the introduction.

A discrete group G is called *crystallographic* or briefly a *space group* if it has a *bounded* fundamental domain $\mathcal{F}_G$. There is a deep result of A. SCHOENFLIES ($n = 2,3$) and L. BIEBERBACH (for $n \geq 3$):

Theorem 2.1. *Any space group G of $\mathcal{E}^n$ has n independent translations, generating a commutative invariant subgroup of G.*

Thus, we obtain the *lattice* of G denoted by $\mathbf{L}_G$. Then any space group G is a set of point transformations of the form

$$G := \{\alpha(\mathbf{A}, \mathbf{a})\}, \tag{2.1}$$

where $\mathbf{A}$ preserves the inner product of the Euclidean vector space $\mathbf{E}^n$ (see formula (1.9)) and the vector $\mathbf{a} := \overrightarrow{OO^\alpha}$ depends also on the origin O. As formulas (1.6) and (1.7) show, the mapping

$$\alpha \mapsto \mathbf{A} \tag{2.2}$$

keeps the corresponding multiplications, i.e. it is a *homomorphism*. Thus the set of linear parts

$$G_0 := \{\mathbf{A}\} \tag{2.3}$$

forms a group, the so-called *point group* of G, and the kernel of the above homomorphism is just the lattice

$$\mathbf{L}_G := \{\lambda(\mathbf{1},\mathbf{l})\} \text{ mapped onto } \mathbf{1}. \tag{2.4}$$

We simply say that the vector $\mathbf{l} \in \mathbf{E}^n$ belongs to the lattice $\mathbf{L}_G$. Any *coset* in the *factor group* $G/\mathbf{L}_G \cong G_0$:

$$\{(\mathbf{A}, \mathbf{a}+\mathbf{l}) : (\mathbf{1},\mathbf{l}) \in \mathbf{L}_G\} \tag{2.5}$$

is described by $\mathbf{A} \in G_0$ and a *vector (cohomology) class* $\mathbf{a} + \mathbf{L}_G$ as the formulas (1.7) and (2.7) characterize (later on). The Schoenflies–Bieberbach theorem has important consequences:

Con. 1. *G is a space group, iff the point group G_0 is finite.*

Con. 2. (Barlow theorem) *The orders of rotation subgroups in G_O can be* 1, 2, 3, 4, 6 (Barlow stated this for $n = 2, 3$).

Con. 3. (Bieberbach–Frobenius theorem). *Two space groups G and G' are isomorphic iff they are conjugate by an affine transformation* $\varphi(\mathbf{F},\mathbf{f})$ of $\mathcal{E}^n$, i.e.

$$G' = \varphi^{-1}G\varphi := \{\varphi^{-1}\alpha\varphi \in G' : \alpha \in G\}. \tag{2.6}$$

An important formula is for $\alpha(\mathbf{A},\mathbf{a})$ and $\varphi(\mathbf{F},\mathbf{f})$ as follows:

$$\begin{aligned}\varphi^{-1}\alpha\varphi &= (\mathbf{F},\mathbf{f})^{-1}(\mathbf{A},\mathbf{a})(\mathbf{F},\mathbf{f}) = (\mathbf{F}^{-1}, -\mathbf{f}\mathbf{F}^{-1})(\mathbf{A}\mathbf{F}, \mathbf{a}\mathbf{F}+\mathbf{f}) = \\ &= (\mathbf{F}^{-1}\mathbf{A}\mathbf{F}, -\mathbf{f}\mathbf{F}^{-1}\mathbf{A}\mathbf{F} + \mathbf{a}\mathbf{F} + \mathbf{f}) = (\mathbf{F}^{-1}\mathbf{A}\mathbf{F}, \mathbf{f}(\mathbf{1} - \mathbf{F}^{-1}\mathbf{A}\mathbf{F}) + \mathbf{a}\mathbf{F}).\end{aligned} \tag{2.7}$$

In particular:

If $\alpha(\mathbf{1},\mathbf{a})$ is a translation, then $\varphi^{-1}\alpha\varphi(\mathbf{1},\mathbf{a}\mathbf{F})$ is also a translation by the vector $\mathbf{a}\mathbf{F}$.

If $\varphi(\mathbf{1},\mathbf{f})$ is a translation, then $\varphi^{-1}\alpha\varphi(\mathbf{A}, \mathbf{f}(\mathbf{1}-\mathbf{A})+\mathbf{a})$. The position vector $-\mathbf{f}$ is just fixed at α, iff the null vector $\mathbf{0}$ is fixed at $\varphi^{-1}\alpha\varphi$, i.e. $\mathbf{f}(\mathbf{1}-\mathbf{A})+\mathbf{a} = \mathbf{0}$.

If $\varphi(\mathbf{F},\mathbf{0})$ fixes the origin, then $\varphi^{-1}\alpha\varphi(\mathbf{F}^{-1}\mathbf{A}\mathbf{F}, \mathbf{a}\mathbf{F})$.

Theorem 2.2. Classification of space groups in $\mathcal{E}^n$).
a) *There are* 17, 219, 4783 *isomorphism classes of space groups in* $\mathcal{E}^2, \mathcal{E}^3, \mathcal{E}^4$, *respectively.*
b) *The numbers of affine conjugacy classes* $\mathcal{E}^n$ *by positive affinities* $\varphi(\mathbf{F}, \mathbf{f})$ *with* $\det \mathbf{F} > 0$ *are* $17(n = 2)$, $230(n = 3)$, $4895(n = 4)$. *These are the numbers of proper classes under orientation preserving affinities, which are finite for any dimension* n.

The last assertion is the answer to the 18th Hilbert problem by L. BIEBERBACH (1912).

The formula (2.7) is the main tool of deriving the space groups in $\mathcal{E}^n$ for any n. Preparatory results are collected in

Theorem 2.3. *For* $n = 2, 3, 4$ *there are*

i) 10, 32, 227 (271) *point groups in the role of* G_0.
ii) 5, 14, 64 (74) *Bravais types of lattices* $\mathbf{L}_G$, *distributed into*
4, 7, 33 (40) *crystal systems and*
4, 6, 23 (29) *crystal families.*
iii) *On the base of* G_0 *and* $\mathbf{L}_G$ *we have* 13, 73, 710 (780) *arithmetic crystal classes.*

The number of proper classes (under orientation preserving affinities) *are given in parentheses, respectively.*

The *algebraic derivation* of space group classes in $\mathcal{E}^n$ is based on determining all the maximal finite subgroups of the full group $GL_n(\mathbb{Z})$ of *unimodular* $n - n$ *matrices*, i.e. with entries from the integer numbers $\mathbb{Z}$ and with determinants -1.

Theorem 2.4. *Up to unimodular conjugacy there are finitely many maximal finite subgroups of* $GL_n(\mathbb{Z})$. *For* $n = 2, 3, 4$ *these numbers are* 2, 4, 9, *respectively. The representatives of these conjugacy classes characterize the most symmetric lattices in* $\mathcal{E}^n$ *by their full symmetry groups (each fixing a lattice point as origin).*

We remark that this problem is solved also for $n = 5$ by S. S. RYSKOV and Z. D. LOMAKINA (1972, 1980) and by W. PLESKEN and M. POHST (1977, 1980) for $5 - n - 10$. However, the derivation of other data, analogous as before, has not been completed yet for $n - 5$.

Before sketching the general procedure we turn to illustrate it with concrete examples in $\mathcal{E}^3$.

3. Derivation of the Arithmetic Crystal Classes mP and mB in the Geometric Crystal Class m

The geometric crystal class $G_0 = \mathbf{m}$ consists of two linear transformations of $\mathbf{E}^3$ with presentation

$$\mathbf{m} := (\mathbf{M} - \mathbf{M}^2 = \mathbf{1}). \tag{3.1}$$

M is an orthogonal reflection in a vector plane $\mathbf{E}^2 \subset \mathbf{E}^3$. We look for the 3-lattices $\mathbf{L}^3$ invariant under the point group $G_0 = \mathbf{m}$. First we prove the following:

Proposition 3.1. *For any* $\mathbf{m}$*-invariant lattice* $\mathbf{L}^3$ *there are three independent translation vectors* $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$*, such that* $\mathbf{e}_1, \mathbf{e}_2$ *span the sublattice* $\mathbf{L}^2(\subset \mathbf{L}^3)$ *in the vector plane* $\mathbf{E}^2$ *of reflection, and* $\mathbf{e}_3$ *spans sublattice* $\mathbf{L}^1(\subset \mathbf{L}^3)$ *orthogonal to* $\mathbf{L}_2$.

Proof: Let $\mathbf{l} \in \mathbf{L}^3$ a translation vector not lying in $\mathbf{E}^2$ and not orthogonal to $\mathbf{E}^2$. Then this is the case also for the image vector $\mathbf{lM}$. Moreover, $\mathbf{l} + \mathbf{lM} \in \mathbf{E}^2$ because it is fixed at $\mathbf{M}$:

$$(\mathbf{l} + \mathbf{lM})\mathbf{M} = \mathbf{lM} + \mathbf{lM}^2 = \mathbf{lM} + \mathbf{l1} = \mathbf{l} + \mathbf{lM}; \tag{3.2}$$

and $\mathbf{l} - \mathbf{lM} \perp \mathbf{E}^2$ because (*Fig. 3.1*)

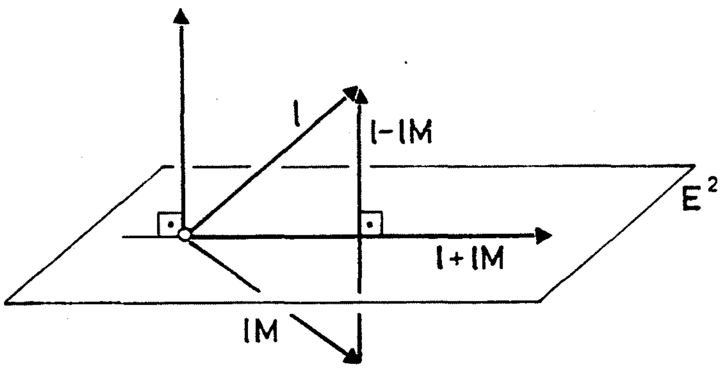


Fig. 3.1. Any vector $\mathbf{l}$ of general position to the vector plane $\mathbf{E}^2$ of reflection $\mathbf{M}$, induces $\mathbf{l} + \mathbf{lM} \in \mathbf{E}^2$ and $\mathbf{l} - \mathbf{lM} \perp \mathbf{E}^2$

$$(\mathbf{l} - \mathbf{lM})\mathbf{M} = \mathbf{lM} - \mathbf{lM}^2 = -(\mathbf{l} - \mathbf{lM}). \tag{3.3}$$

Take another lattice vector, not lying in the vector plane spanned by $\mathbf{l}$ and $\mathbf{l}\mathbf{M}$, then we obtain another lattice vector in $\mathbf{E}^2$. Thus, we guarantee a 2-lattice in $\mathbf{E}^2$ and a 1-lattice orthogonal to $\mathbf{E}^2$; so $\mathbf{e}_1, \mathbf{e}_2$ as a basis for $\mathbf{L}^2$, furthermore, $\mathbf{e}_3$ as a basis for $\mathbf{L}_1$ can be chosen. *Q. e. d.*

The primitive monoclinic lattice $mP =: \mathbf{L}^3$ is defined by any basis $\mathbf{e}_1, \mathbf{e}_2$ of $\mathbf{L}^2$ in the mirror plane $\mathbf{E}^2$ and by a shortest lattice vector $\mathbf{e}_3$ orthogonal to $\mathbf{L}^2$ (*Fig. 1.1*).

Any translation vector $\mathbf{l} \in \mathbf{L}^3$ may have a form (*Fig. 3.1*)

$$\begin{aligned} &\mathbf{l} = l^1\mathbf{e}_1 + l^2\mathbf{e}_2 + l^3\mathbf{e}_3 \text{ with components} \\ &l^i \equiv 0 \text{ or } \tfrac{1}{2} \bmod \mathbb{Z} \text{ (the set of integers).} \end{aligned} \tag{3.4}$$

From $\left(\frac{1}{2}, 0, \frac{1}{2}\right), \left(0, \frac{1}{2}, \frac{1}{2}\right), \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) \bmod \mathbb{Z}^3$ (triples of integers) any will be equivalent to the first choice $\left(\frac{1}{2}, 0, \frac{1}{2}\right)$. In the other cases we consider either

$$\begin{pmatrix} \mathbf{e}_1' \\ \mathbf{e}_2' \\ \mathbf{e}_3' \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{pmatrix} = \begin{pmatrix} \mathbf{e}_2 \\ \mathbf{e}_1 \\ \mathbf{e}_3 \end{pmatrix}$$

or

$$\begin{pmatrix} \bar{\mathbf{e}}_1 \\ \bar{\mathbf{e}}_2 \\ \bar{\mathbf{e}}_3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{pmatrix} = \begin{pmatrix} \mathbf{e}_1 + \mathbf{e}_2 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{pmatrix} \tag{3.5}$$

as new bases. Both are obtained by $GL_3(\mathbb{Z})$ matrices. Then, only $\left(\frac{1}{2}, 0, \frac{1}{2}\right)$ mod $\mathbb{Z}^3$ vectors occur in $\mathbf{L}^3$. If, say, $\left(0, \frac{1}{2}, \frac{1}{2}\right) \bmod \mathbb{Z}^3$ also appear in $\mathbf{L}^3$, then $\left(-\frac{1}{2}, \frac{1}{2}, 0\right)$ would be in $\mathbf{L}^2$, although $\mathbf{e}_1, \mathbf{e}_2$ was a basis in $\mathbf{L}^2$, a contradiction. That means, we have one possible *single face centred monoclinic lattice* $\mathbf{L}^3 = mS$ besides the primitive one, up to unimodular equivalence.

Let $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ be the *B-centred basis* with

$$\begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{pmatrix} \text{ or } \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{pmatrix} \tag{3.6}$$

as it is indicated in *Fig. 3.2*.

Then the linear reflection $\mathbf{M}$ can be expressed in the primitive lattice mP as in formulas (1.12), (1.15) and in the B-centred lattice (from the lattice class mS) as well.

$$\mathbf{M} : \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{pmatrix} \mapsto \begin{pmatrix} \mathbf{b}_1\mathbf{M} \\ \mathbf{b}_2\mathbf{M} \\ \mathbf{b}_3\mathbf{M} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{pmatrix}. \tag{3.7}$$

It is a basic fact that this formula can be obtained from (1.12) by conjugacy under (3.6). Indeed by (1.12):

$$\begin{pmatrix}\mathbf{e}_1\\ \mathbf{e}_2\\ \mathbf{e}_3\end{pmatrix} \overset{\mathbf{M}}{\mapsto} \begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}\begin{pmatrix}\mathbf{e}_1\\ \mathbf{e}_2\\ \mathbf{e}_3\end{pmatrix} \Rightarrow$$

$$\begin{pmatrix}1&0&-1\\0&1&0\\1&0&1\end{pmatrix}\begin{pmatrix}\mathbf{b}_1\\ \mathbf{b}_2\\ \mathbf{b}_3\end{pmatrix} \overset{\mathbf{M}}{\mapsto} \begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}\begin{pmatrix}1&0&-1\\0&1&0\\1&0&1\end{pmatrix}\begin{pmatrix}\mathbf{b}_1\\ \mathbf{b}_2\\ \mathbf{b}_3\end{pmatrix}$$

hold. Multiplying from left by the inverse, as (3.6) shows,

$$\begin{pmatrix}\mathbf{b}_1\\ \mathbf{b}_2\\ \mathbf{b}_3\end{pmatrix} \overset{\mathbf{M}}{\mapsto} \begin{pmatrix}\frac{1}{2}&0&\frac{1}{2}\\0&1&0\\-\frac{1}{2}&0&\frac{1}{2}\end{pmatrix}\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}\begin{pmatrix}1&0&-1\\0&1&0\\1&0&1\end{pmatrix}\begin{pmatrix}\mathbf{b}_1\\ \mathbf{b}_2\\ \mathbf{b}_3\end{pmatrix} =$$

$$\begin{pmatrix}0&0&-1\\0&1&0\\-1&0&0\end{pmatrix}\begin{pmatrix}\mathbf{b}_1\\ \mathbf{b}_2\\ \mathbf{b}_3\end{pmatrix}, \tag{3.8}$$

i.e. the conjugacy yields the reflection formula (3.7) in the B-centered lattice. As we see, this conjugacy is no more unimodular but rational, i.e. $\mathbf{Q}$-conjugacy. Another way, the basis transformation $\mathbf{b}_i = b_i^j \mathbf{e}_j$ or the matrix equation

$$\begin{pmatrix}b_1^1&b_1^2&b_1^3\\b_2^1&b_2^2&b_2^3\\b_3^1&b_3^2&b_3^3\end{pmatrix}\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix} = \begin{pmatrix}0&0&-1\\0&1&0\\-1&0&0\end{pmatrix}\begin{pmatrix}b_1^1&b_1^2&b_1^3\\b_2^1&b_2^2&b_2^3\\b_3^1&b_3^2&b_3^3\end{pmatrix}, \tag{3.9}$$

equivalent to the affine conjugacy, would imply the equations

$$b_1^1 = -b_3^1,\quad b_1^2 = -b_3^2,\quad -b_1^3 = -b_3^3;\quad b_2^1 = b_2^1,\quad b_2^2 = b_2^2,\quad -b_2^3 = b_2^3;$$
$$b_3^1 = -b_1^1,\quad b_3^2 = -b_1^2,\quad -b_3^3 = -b_1^3;\ \text{i.e.}$$

$$(b_i^j) = \begin{pmatrix}b_1^1&b_1^2&b_1^3\\b_2^1&b_2^2&0\\-b_1^1&-b_1^2&b_1^3\end{pmatrix},\quad \det b_i^j = 2b_1^3(b_1^1b_2^2 - b_1^2b_2^1). \tag{3.10}$$

This means, the affine conjugacy (3.9), expressing geometrically the same reflection, is no more unimodular with a $\mathbf{Z}$-matrix.

We say that we have *two arithmetic classes*, denoted by **mP** and **mB**, *in the same geometric class* **m**:

$$\mathbf{mP}:\left\{\mathbf{1} = \begin{pmatrix}1&&\\&1&\\&&1\end{pmatrix};\mathbf{M} = \begin{pmatrix}1&&\\&1&\\&&-1\end{pmatrix}\right\};$$
$$\mathbf{mB}:\left\{\mathbf{1} = \begin{pmatrix}1&&\\&1&\\&&1\end{pmatrix};\mathbf{M} = \begin{pmatrix}&&-1\\&1&\\-1&&\end{pmatrix}\right\}. \tag{3.11}$$

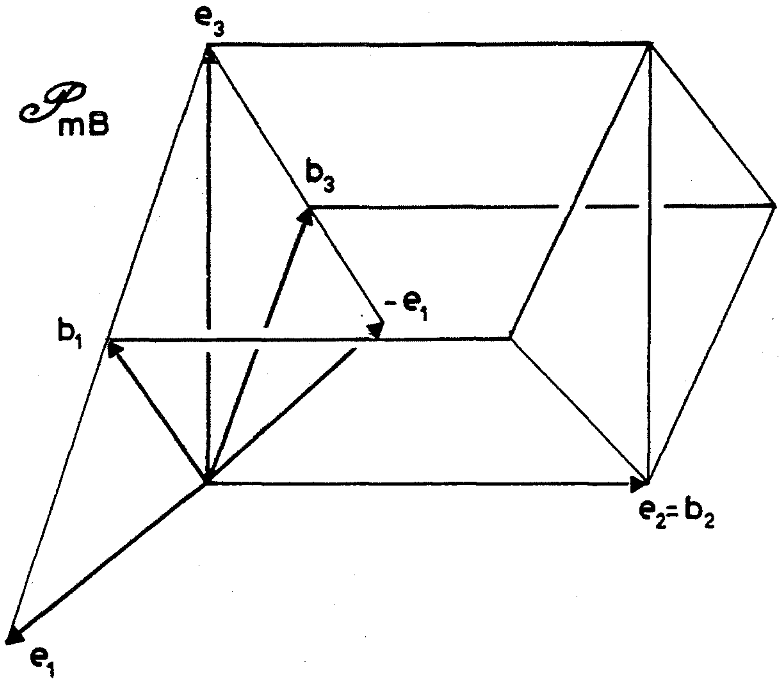


Fig. 3.2. The basis $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ of the *monoclinic B-centred lattice mB* and the unit parallelepiped $\mathcal{P}_{mB}$

4. The Two Space Groups Pm and Pb in the Arithmetic Crystal Class mP

Any space group G in the arithmetic class **mP** consists of transformations like

$$\lambda : (x,y,z) \mapsto (x,y,z) + \text{ integer triples} \tag{1.4}$$
$$\mu : (x,y,z) \mapsto (x,y,z) \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix} + (m^1, m^2, m^3) + \text{ integer triples,}$$

expressed in the P-lattice basis (*Fig. 1.1*).

Then any transformation $\mu\mu$ will be a translation, because $\mathbf{MM} = \mathbf{1}$ is the linear identity:

$$\begin{aligned}(x,y,z) &\overset{\mu}{\mapsto} (x,y,z)\begin{pmatrix}1 & & \\ & 1 & \\ & & -1\end{pmatrix} + (m^1,m^2,m^3) \overset{\mu}{\mapsto} \\ &\overset{\mu}{\mapsto} (x,y,z) + (m^1,m^2,m^3)\begin{pmatrix}1 & & \\ & 1 & \\ & & -1\end{pmatrix} + \begin{matrix}(m^1,m^2,m^3) \\ +\text{integer triples}\end{matrix}\end{aligned} \tag{4.2}$$

leads to a congruence, called *Frobenius congruence*,

$$\begin{gathered}2m^1 \equiv 0 \mod \mathbb{Z},\quad 2m^2 \equiv 0 \mod \mathbb{Z}, \text{ and} \\ \text{no restriction for } m^3.\end{gathered} \tag{4.3}$$

We shall prove the following

Proposition 4.1. *Any solution of* (4.3) *will be affinely equivalent either to*

$$(m^1,m^2,m^3) \equiv (0,0,0) \mod \mathbb{Z}^3, \text{ then } G = \mathbf{Pm}, \tag{4.4}$$

or to

$$(m^1,m^2,m^3) \equiv (0,\frac{1}{2},0) \mod \mathbb{Z}^3, \text{ then } G = \mathbf{Pb} \tag{4.5}$$

is a new space group in the arithmetic class **mP**.

Proof: We apply the formula (2.7) with $\varphi(\mathbf{1},\mathbf{f}), \mathbf{f} = (f^1,f^2,f^3)$ for μ in (4.1). Then, the affine conjugacy leads to

$$\varphi^{-1}\mu\varphi = (\mathbf{M}, -\mathbf{fM}+\mathbf{f}+\mathbf{m}) = \left(\begin{pmatrix}1 & & \\ & 1 & \\ & & -1\end{pmatrix}, (m^1,m^2,m^3+2f^3)\right). \tag{4.6}$$

Thus, we may assume in (4.1) that $m^3 \equiv 0 \mod \mathbb{Z}$, because of taking $f^3 = -\frac{1}{2}m^3$ in (4.6) otherwise. The solution triples are:

$$(m^1,m^2,m^3) \equiv (0,0,0) \mod \mathbb{Z}^3, \tag{4.7}$$

$$(m^1,m^2,m^3) \equiv (0,\frac{1}{2},0); (\frac{1}{2},0,0); (\frac{1}{2},\frac{1}{2},0) \mod \mathbb{Z}^3. \tag{4.8}$$

The solution (4.7) just leads to $G = \mathbf{Pm}$, discussed in the Introduction. The other solutions in (4.8) will be affinely equivalent to the first one. Indeed,

$$\varphi_1\left(\begin{pmatrix}0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1\end{pmatrix}, (0,0,0)\right) \text{ resp. } \varphi_2\left(\begin{pmatrix}1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1\end{pmatrix}; (0,0,0)\right) \tag{4.9}$$

realize the corresponding affine equivalences. For instance, with the third vector class in (4.8) and with φ_2 we have

$$\varphi_2^{-1}\mu\varphi_2 =$$

$$\left(\begin{pmatrix}1&0&0\\1&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&&\\&1&\\&&-1\end{pmatrix}\begin{pmatrix}1&0&0\\-1&1&0\\0&0&1\end{pmatrix};\left(\frac{1}{2},\frac{1}{2},0\right)\begin{pmatrix}1&0&0\\-1&1&0\\0&0&1\end{pmatrix}\right)=$$

$$=\left(\begin{pmatrix}1&&\\&1&\\&&-1\end{pmatrix},(0,\frac{1}{2},0)\right), \tag{4.10}$$

as desired. However, there is no affine equivalence between the vector classes $(0,0,0)$ and $(0,\frac{1}{2},0)$, as we easily see. *Q. e. d.*

This new space group **Pb** appears under no. 7 in the *International Tables* (1976, 1983) analogously like **6.Pm** at (1.13)

$$2 \quad a \quad \mathbf{1} \quad x,y,z; \quad x,y+\frac{1}{2},\bar{z}; \quad (\bar{z}:=-z). \tag{4.11}$$

Again, we can form a fundamental domain $\mathcal{F}_{\mathbf{Pb}}$ by halving a unit cell $\mathcal{F}_{mP}$ (translated with resp. to *Fig. 1. 4*). $\mathcal{F}_{\mathbf{Pb}}$ is equipped by face pairing isometries and the presentation (a minimal, again, see E. MOLNÁR (1987))

$$\mathbf{Pb} := (\mu_1,\tau_1,\tau_3 - 1 = \mu\tau_1\mu^{-1}\tau_1^{-1} = \mu\tau_3\mu^{-1}\tau_3 = \tau_1\tau_3\tau_1^{-1}\tau_3^{-1}). \tag{4.12}$$

Here the generators are (*Fig. 4.1*):

$$\begin{aligned}\mu &: ABCD \to HGFE \text{ glide reflection,}\\ \tau_1 &: AEHD \to BFGC \text{ translation by } \mathbf{e}_1,\\ \tau_3 &: ABFE \to DCGH \text{ translation by } \mathbf{e}_3.\end{aligned} \tag{4.13}$$

As we see, **Pb** is a fixed point free space group. As a consequence, $\mathcal{F}_{\mathbf{Pb}}$ geometrically realizes the *space form* $\mathcal{E}^3/\mathbf{Pb}$, i.e. the set of **Pb**-orbits in $\mathcal{E}^3$. This means that the orbits have a natural locally Euclidean metric, and any orbit has an orbit-neighbourhood isometric to a Euclidean ball. The gluing procedure, induced by the face pairings, gives us pictures of ball-like neighbourhoods for boundary points of $\mathcal{F}_{\mathbf{Pb}}$. E.g. the eight corners of $\mathcal{F}_{\mathbf{Pb}}$, glued together, serve a full ball for the orbit containing the vertices. We see a compact (topological) space with locally Euclidean metric. In general, the 10 *fixed point free Euclidean space groups* provide us all the compact space forms with metric of zero (sectional) curvature. This fact only refers to the aspects in the topology and differential geometry.

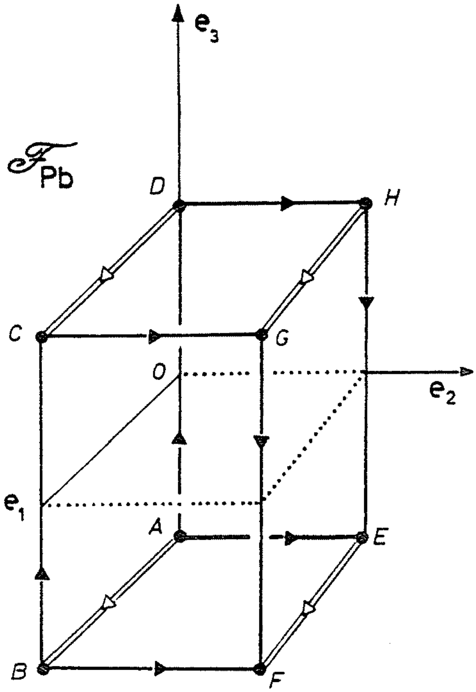


Fig. 4.1. A fundamental domain $\mathscr{F}_{\mathbf{Pb}}$ giving a minimal geometric presentation for the non-orientable Euclidean space form $\mathscr{E}^3/\mathbf{Pb}$ (see formulas (4.12–4.13)). The 8 corners amount a ball-like neighbourhood for the **Pb**-orbit of vertices

We can ask for the densest ball packing by the orbits of **Pb**, as we made for **Pm** at (1.26). The result is surprising. If the primitive lattice mP is given by the Gramian

$$(g_{ij}) = (\langle \mathbf{e}_i ; \mathbf{e}_j \rangle) = \begin{pmatrix} 4 & -4 & 0 \\ -4 & 8 & 0 \\ 0 & 0 & 8 \end{pmatrix}, \tag{4.14}$$

and the point X has the coordinates $(x, y, -\frac{1}{4})$ or $(x, y, \frac{1}{4})$, then the density of the unit ball packing under **Pb** by (4.11) equals

$$\delta(X, \mathbf{Pb}) = \frac{4\pi}{3} \Big/ \frac{1}{2}\sqrt{8(8 \cdot 4 - 4 \cdot 4)} = \pi \Big/ \sqrt{18} \approx 0.7405. \tag{4.15}$$

This is just the densest lattice-like ball packing in $\mathscr{E}^3$. Now the orbit $X^{\mathbf{Pb}}$ itself is a face centred cubic point-lattice with self-symmetry group $\mathbf{Fm\bar{3}m}$, larger than **Pb**. The Dirichlet-polyhedron is just the well-known *rhombododecahedron.*

5. The Space Groups Bm and Bb in the Arithmetic Crystal Class mB

We proceed analogously as before. Any space group G in the arithmetic class **mB** consists of transformations like

$$\begin{aligned} \lambda:\ (x,y,z) &\mapsto (x,y,z) + \text{ integer triples} \\ \mu:\ (x,y,z) &\mapsto (x,y,z)\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \begin{matrix} +(m^1,m^2,m^3) \\ +\textit{integer triples} \\ \ \end{matrix} \end{aligned} \tag{5.1}$$

expressed in the B-lattice basis by (3.6).

Again, $\mu\mu$ is a translation in the lattice mB (see (4.2))

$$(m^1,m^2,m^3)\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} + (m^1,m^2,m^3) \equiv (0,0,0) \bmod \mathbb{Z}^3,$$

i.e.

$$-m^3+m^1 \equiv 0,\ 2m^2 \equiv 0,\ -m^1+m^3 \equiv 0 \bmod \mathbb{Z}. \tag{5.2}$$

Proposition 5.1. *Any solution of (5.2) will be affinely equivalent either to*

$$(m^1,m^2,m^3) \equiv (0,0,0) \bmod \mathbb{Z}^3,\ \textit{then } G = \mathbf{Bm} \tag{5.3}$$

$$\textit{or to } (m^1,m^2,m^3) \equiv (0,\tfrac{1}{2},0) \bmod \mathbb{Z}^3,\ \textit{then } G = \mathbf{Bb}. \tag{5.4}$$

These two space groups **Bm** *and* **Bb** *are in the arithmetic crystal class* **mB**.

Proof: By (2.7), with $\varphi(\mathbf{1},\mathbf{f})$, $\mathbf{f} = (f^1,f^2,f^3)$ we obtain

$$\varphi^{-1}\mu\varphi = (\mathbf{M}, \mathbf{f}(\mathbf{1}-\mathbf{M})+\mathbf{m}) =$$

$$= \left(\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, (f^1+f^3+m^1, m^2, f^3+f^1+m^3)\right). \tag{5.5}$$

Thus, we may assume in (5.1) that $m^1 = 0$, otherwise we choose $f^1+f^3 = -m^1$ in formula (5.5). Then, from (5.2), we have $m^3 \equiv 0$ and $m^2 = 0$ or $\frac{1}{2} \bmod \mathbb{Z}$. *Q. e. d.*

The space group **Bm** appears under no. 8 in the *International Tables* (1976, 1983):

$$\textit{Coordinates of equivalent positions (i.e. centerings)}(0,0,0),(\frac{1}{2},0,\frac{1}{2})+$$

$$\begin{array}{llll} 4 & b & \mathbf{1} & x,y,z;\ x,y,\bar{z} \quad (\bar{z} \text{ means } -z) \\ 2 & a & \mathbf{m} & x,y,0. \end{array} \tag{5.6}$$

This means, the coordinates are understood in the primitive lattice mP, but the B-centering translations $\frac{1}{2}\mathbf{e}_1 + \frac{1}{2}\mathbf{e}_3 + mP$ are included in this information. Then we have 4 Wyckoff positions of (general) type b with trivial stabilizer **1**, and 2 positions of type a with stabilizer **m**. In *Fig 5.1* we have pictured the fundamental domain $\mathcal{F}_{\mathbf{Bm}}$, where the face pairing generators are

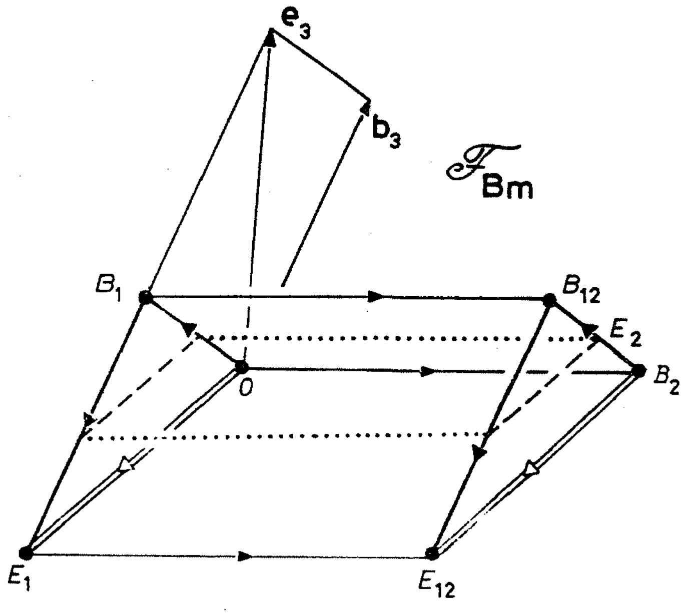


Fig. 5.1. A minimally presenting fundamental domain $\mathcal{F}_{\mathbf{Bm}}$ for the space group **Bm** (5.7–5.8). The 6 corners together form a neighbourhood as a half-ball in accordance with the fact that the stabilizer subgroup of each vertex is a reflection group of order 2.

$$\begin{aligned} \mu &: OE_1E_{12}E_2 \to OE_1E_{12}E_2 \text{ plane reflection}, \\ \beta &: OE_2B_{12}B_1 \to B_1B_{12}E_{12}E_1 \text{ glide reflection}, \\ \tau_2 &: OE_1B_1 \to E_2E_{12}B_{12} \text{ translation by } \mathbf{e}_2 = \mathbf{b}_2. \end{aligned} \tag{5.7}$$

Thus we obtain the minimal presentation

$$\mathbf{Bm} := (\mu, \beta, \tau_2 - 1 = \mu^2 = \mu\beta^2\mu\beta^{-2} = \mu\tau_2\mu\tau_2^{-1} = \beta\tau_2\beta^{-1}\tau_2^{-1}). \quad (5.8)$$

The densest unit ball packing under the space group **Bm** can be taken either for (general) b-type orbits or for a-type orbits. For b-type orbits we obtain the maximal density

$$\delta = \pi\sqrt{3}/9 \approx 0.6046 \quad (5.9)$$

with Gramians

$$(\langle \mathbf{e}_i; \mathbf{e}_j \rangle) = \begin{pmatrix} 16 & -4 & 0 \\ -4 & 4 & 0 \\ 0 & 0 & 16 \end{pmatrix} \quad \text{or} \quad (\langle \mathbf{b}_i; \mathbf{b}_j \rangle) = \begin{pmatrix} 8 & -2 & 0 \\ -2 & 4 & 2 \\ 0 & 2 & 8 \end{pmatrix} \quad (5.10)$$

expressed by the primitive basis or the B-centered one, respectively, and with a centre $X(x\mathbf{e}_1 + y\mathbf{e}_2 + \frac{1}{4}\mathbf{e}_3)$. For a-type orbits we obtain the absolute maximal density

$$\delta = \pi/\sqrt{18} \approx 0.7405 \quad (5.11)$$

with Gramian

$$(\langle \mathbf{b}_i; \mathbf{b}_j \rangle) = \begin{pmatrix} 4 & -2 & -2 \\ -2 & 4 & 2 \\ -2 & 2 & 4 \end{pmatrix}. \quad (5.12)$$

This is the densest lattice-like packing again with self-symmetry group $\mathbf{Fm\bar{3}m}$.

The space group **Bb** is no. 9 in the *International Tables* (1976, 1983).

Coordinates of equivalent positions (centerings): $(0,0,0), (\frac{1}{2}, 0, \frac{1}{2})+$

$$4 \quad a \quad \mathbf{1} \qquad x, y, z; \quad x, y, \tfrac{1}{2}, \bar{z} \quad (\bar{z} = -z). \quad (5.13)$$

A fundamental domain $\mathcal{F}_{\mathbf{Bb}}$ is pictured in *Fig. 5.2* with face pairing generators

$$\begin{aligned} &\mu : OB_1B_{13}B_3 \to B_2'B_3'B_{13}'B_1' \text{ glide reflection,} \\ &\tau_1 : OB_3B_3'B_2' \to B_1B_{13}B_{13}'B_1' \text{ translation by } \mathbf{b}_1, \\ &\tau_3 : B_{13}B_{13}'B_3'B_3 \to B_1B_1'B_2'O \text{ translation by } \mathbf{b}_3 \end{aligned} \quad (5.14)$$

and presentation

$$\mathbf{Bb} := (\mu, \tau_1, \tau_3 - 1 = \mu\tau_1\mu^{-1}\tau_3 = \mu\tau_3\mu^{-1}\tau_1 = \tau_1\tau_3\tau_1^{-1}\tau_3^{-1}). \quad (5.15)$$

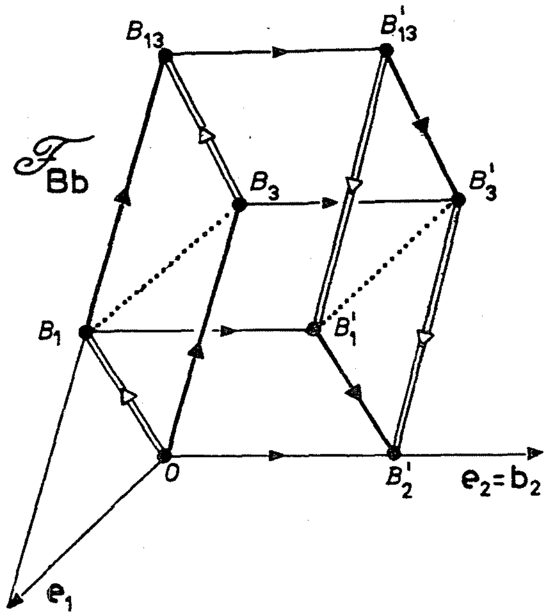


Fig. 5.2. A fundamental domain $\mathscr{F}_{\mathbf{Bb}}$, providing the 3-generator presentation (5.14–5.15). This represents the non-orientable Euclidean space form $\mathscr{E}^3/\mathbf{Bb}$

This presentation is not a minimal one. Indeed, the translation, say,

$$\tau_3 = \mu\tau_1^{-1}\mu^{-1} = \mu^{-1}\tau_1^{-1}\mu$$

can be expressed by the other two generators and first we get

$$\mathbf{Bb} := (\mu, \tau_1 - 1 = \mu^2\tau_1\mu^{-2}\tau_1^{-1} = \tau_1\mu\tau_1^{-1}\mu^{-1}\tau_1^{-1}\mu^{-1}\tau_1\mu). \tag{5.16}$$

Now, we introduce the glide reflection $\nu = \mu\tau_1$ with

$$\begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}, \begin{pmatrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\end{pmatrix} \text{ in } (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \quad \text{or} \quad \begin{pmatrix} & & -1 \\ & 1 & \\ -1 & & \end{pmatrix}, \begin{pmatrix}1, \frac{1}{2}, 0\end{pmatrix} \text{ in } (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3). \tag{5.17}$$

Thus from (5.16), we get the minimal presentation

$$\mathbf{Bb} := (\mu, \nu - 1 = \mu^2\nu\mu^{-2}\nu^{-1} = \nu^2\mu\nu^{-2}\mu^{-1}) \tag{5.18}$$

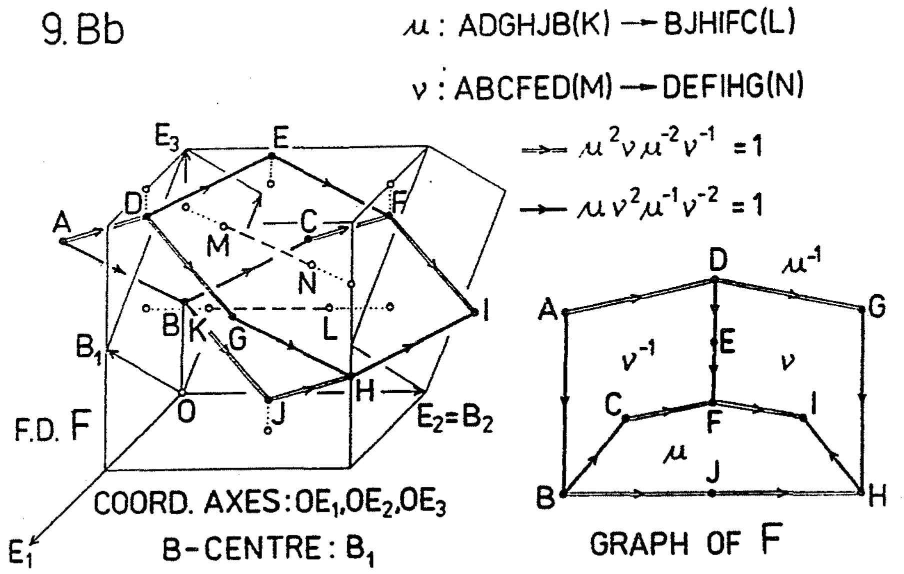


Fig. 5.3. **The minimally presenting concave fundamental 'tetrahedron' F realizing Bb by (5.18) with 4 faces, 6 + 6 edges and 10 vertices**

in a very nice symmetric form. From the paper of E. MOLNÁR (1987) the surprising concave fundamental 'tetrahedron' is pictured here in *Fig. 5.3*, which geometrically realizes the algebraic presentation (5.18) in the sense detailed in (1.18).

Again, we remark that **Bb** is a fixed point free space group, thus the orbit space $\mathcal{E}^3/\mathbf{Bb}$ represents a *non-orientable* Euclidean space form. This is geometrically realized by any fundamental domain $\mathcal{F}_{\mathbf{Bb}}$ (see *Fig. 5.2* or *5.3*), analogously as described at **Pb** above.

Asking for the densest ball packing by **Bb**, we obtain again $\delta = \pi/\sqrt{18} \approx 0.7405$, the same as at the densest lattice-like packing. The extremal orbit $X^{\mathbf{Bb}}$ will be given with the Gramians

$$((\mathbf{e}_i;\mathbf{e}_j)) = \begin{pmatrix} 8 & 0 & 0 \\ 0 & 8 & 0 \\ 0 & 0 & 8 \end{pmatrix} \quad \text{or} \quad ((\mathbf{b}_i;\mathbf{b}_j)) = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 8 & 0 \\ 0 & 0 & 4 \end{pmatrix} \tag{5.19}$$

and with a centre $X(x\mathbf{e}_1 + y\mathbf{e}_2 + \frac{1}{4}\mathbf{e}_3 = (x+\frac{1}{4})\mathbf{b}_1 + y\mathbf{b}_2 + (\frac{1}{4} - x)\mathbf{b}_3)$. Then the ball radius is 1, the packing itself has the self-symmetry group $\mathbf{Fm\bar{3}m}$.

6. The Bravais $\mathbb{Z}$-classes 2/mP and 2/mB

The monoclinic primitive lattice mP with the Gramian (1.11) obviously has a 2-fold rotation symmetry

$$\mathbf{2}: \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{pmatrix} \mapsto \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{pmatrix}. \tag{6.1}$$

Thus, we have a maximal (arithmetic) $\mathbb{Z}$-class, denoted by

$$\mathbf{2/mP}: \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{6.2}$$

The lattice mP with Gramian (1.11) does not allow a larger $\mathbb{Z}$-class, in general. Thus **2/mP** characterizes the monoclinic primitive lattice mP, therefore **2/mP** is called also a *Bravais $\mathbb{Z}$-class.*

The geometric crystal class, itself, is a point group

$$G_0 := \{\mathbf{1},\ \mathbf{2},\ \bar{\mathbf{1}},\ \mathbf{M}\} =: \mathbf{2/m}, \tag{6.3}$$

called also a *holohedry, as a maximal* $\mathbb{Q}$*-class leaving a Bravais lattice invariant.*

The same geometric class (6.3) describes also the symmetries of a monoclinic single face centred lattice $mS := mB$. The arithmetic class **2/mB** is expressed in the B-centred basis $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$ by formula (3.6)

$$\mathbf{2/mB}: \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}. \tag{6.4}$$

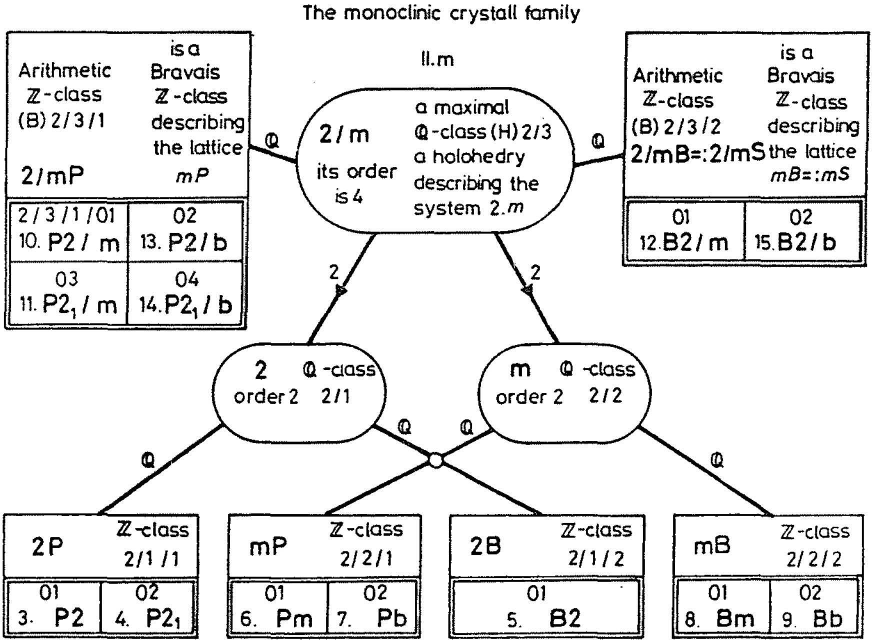
This is also said to be a Bravais $\mathbb{Z}$-class.

The (geometric) $\mathbb{Q}$-class $\mathbf{2/m}$ is also a holohedry for the Bravais lattice $mB =: mS$. Thus $2/m$ characterizes the monoclinic crystal system $2.m$, where the 6 $\mathbb{Z}$-classes fall into 3 $\mathbb{Q}$-classes and 2 Bravais flocks (by the Bravais lattices mP and mB).

As our examples have illustrated, we can determine all the space groups to any prescribed (arithmetic) $\mathbb{Z}$-class, and we can select them by

Table 6.1

The structure of the monoclinic crystal family *II. m* is described, based on the arithmetic $\mathbb{Z}$-classes. It contains 1 crystal system: *2.m*; 3 $\mathbb{Q}$-classes; 2 Bravais lattices (flocks); 6 $\mathbb{Z}$-classes; and 13 space group classes



the affine equivalence under formula (2.7). This is a problem for computer not detailed here.

Table 6.1 indicates by our cases, how to organize the structure of space group classes for a future data base. We are working on this problem, in order to investigate systematically actual questions, indicated in the paper and many others, by computer.

Nowadays, the procedure how to determine all the crystallographic groups for any space $\mathcal{E}^n$ is 'clear'.

First step: Determine all the maximal irreducible unimodular groups leaving invariant an n-dimensional lattice. Arrange these into $\mathbb{Q}$-classes, and determine the Bravais $\mathbb{Z}$-lasses, up to unimodular $\mathbb{Z}$-equivalence.

Second step: Determine all the maximal reducible unimodular groups with the corresponding invariant sublattices of an n-dimensional lattice. Form again the possible centerings, $\mathbb{Q}$-classes, Bravais $\mathbb{Z}$-classes, again up to $\mathbb{Z}$-equivalence.

Third step: Form the possible subgroups of these unimodular groups in each Bravais $\mathbb{Z}$-class, up to $\mathbb{Z}$-equivalence again. Thus, we obtain all the arithmetic $\mathbb{Z}$-classes as finite unimodular $n \times n$ matrix groups.

Fourth step: To each arithmetic $\mathbb{Z}$-class determine all the vector systems (group cohomology classes). These bring screw motions, glide reflections into considerations, where the translational parts are broken lattice vectors, as our examples **Pb** and **Bb** illustrate. Here the affine conjugacy is important again. The so-called Zassenhaus algorithm (H. ZASSENHAUS, (1948)) leads to all the non-isomorphic space groups belonging to the given arithmetic $\mathbb{Z}$-class. In the sense of formula (2.7) we need the *$\mathbb{Z}$-normalizer of the given arithmetic class*. This means, if G_0 a $\mathbb{Z}$-class, then

$$N_{\mathbb{Z}}(G_0) := (\mathbf{F} \in GL_n(\mathbb{Z}) : \mathbf{F}^{-1}G_0\mathbf{F} = G_0)$$

defines this normalizer. The vector systems (cohomology classes), equivalent under $N_{\mathbb{Z}}(G_0)$, determine affine conjugate space groups.

This procedure has been carried out for $n = 2, 3, 4$ as a grandious result of a cooperation by H. BROWN et al. (1978). The computer promises many further results also in this field of research.

References

1. BIEBERBACH, L. (1912): Über die Bewegungsgruppe der Euklidischen Räume, (Zweite Abhandlung) Die Gruppen mit einem endlichen Fundamentalbereich. *Math. Ann.* Vol. 72, pp. 400–412.
2. BROWN, H. – BÜLOW, R. – NEUBÜSER, J. – WONDRATSCHEK, H. – ZASSENHAUS, H. (1978): Crystallographic Groups of Four-dimensional Space. Wiley-Interscience, New York–Chichester–Brisbane–Toronto.
3. BURCKHARDT, J. J. (1966): *Die Bewegungsgruppe der Kristallographie.* 2nd ed., Birkhäuser, Basel und Stuttgart.
4. COXETER, H. S. M. – MOSER, W. O. J. (1980): Generators and Relations for Discrete Groups. 4th ed., Springer, Berlin–Heidelberg–New York.
5. DADE, E. C. (1965): The Maximal Finite Groups of 4×4 matrices. *Ill. J. Math.* Vol. 9, pp. 99–122.
6. DELANEY, M. S. (1980): Quasi Symmetries of Space Group Orbits. Proc. of the ZiF-Conference on Crystallographic Groups, *Match* Vol. 9, pp. 73–80.
7. DELAUNAY, B. (1929): Sur la partition regulière de l'espace à 4 dimensions. I. II. *Izv. AN SSSR* 1929 No. 1, pp. 70–110, No. 2, pp. 147–167.
8. DRESS, A. W. M. (1987): Presentation of Discrete Groups, Acting on Simply Connected Manifolds in Terms of Parametrized Systems of Coxeter Matrices. – A systematic approach. *Advances in Math.* Vol. 63, pp. 196–212.
9. DRESS, A. W. M. – HUSON, D. – MOLNÁR, E. (1991): The classcfication of face-transitive periodic 3D-tilings. Preprint *Univ. Bielefeld, Combinatorics and its Applications* 1990/91, Zif-Nr 91/38, *Acta Crystallogr.*
10. FEDOROV, E. S.: (1891) Symmetry of regular systems of figures. *Proc.* S. Peterb. Mineral. Soc. **28**, 1–146 (Russian) Reguläre Plan- und Raumtheilung. *Abh. K. Bayer Akad. d. Wiss.* **11** (1899), *Cl. XX, Abth* 11, 465–588.
11. FEJES TÓTH, L.(1964): *Regular figures.* Pergamon, New York, *Reguläre Figuren*, Akadémiai Kiadó, Budapest 1965.

12. FROBENIUS, F. G. (1911): Über den von L. Bieberbach gefundenen Beweis eines Satzes von C. Jordan. *Sitzungsber. Preuss. Akad. Wiss. Berlin, Phys. Math. Kl.* (1911) pp. 241–248. *Gesammelte Abhandlungen* III, Springer, Berlin, 1968, pp. 493–500.
13. GRÜNBAUM, B. – SHEPHARD, G. C. (1987): Tilings and Patterns. W. H. Freeman and Company, New York.
14. HURLEY, A. C. – NEUBÜSER, J.–WONDRATSCHEK, H. (1967): Crystal Classes of Four-dimensional Space R^4. *Acta Crystallogr.* Vol. 22, p. 605.
15. *International Tables for X-ray Crystallography,* Vol. 1, HENRY, N. F. M. – LONSDALE, K. (1969): Symmetry groups. Kynoch, Birmingham. New edition by HAHN, T. (1983), Vol. A, Reidel Co, Dordrecht.
16. MINKOWSKI, H. (1905): Diskontinuitätsbereich für arithmetische Äquivalenz. *J. Reine Angew. Math.* Vol. 129, pp. 220–274. *GesammelteAbhandlungen*III.Teubner,Leipzig, 1911, pp. 53–100.
17. MOLNÁR, E.: (1983) Konvexe Fundamentalpolyeder und einfache D-V-Zellen für 29 Raumgruppen, die Coxetersche Spiegelungsuntergruppen enthalten. *Beiträge zur Algebra und Geometrie* Vol. 14, pp. 33–75.
18. MOLNÁR, E.: (1987) Minimal presentation of the 10 compact Euclidean space forms by fundamental domains. *Studia Sci. Math. Hung.* Vol. 22, pp. 19–51.
19. MOLNÁR, E.: (1988) Minimal presentation of crystallographic groups by fundamental polyhedra. *Comput. Math Aplic.* Vol. 16, pp. 507–520.
20. MOLNÁR, E. – PROK, I.: (1988) A polyhedron algorithm for finding space groups. *Proc. of 3rd Int. Conf. on Engineering Graphics and Descriptive Geometry,* Wienna Vol. 2, pp. 37–44.
21. MOLNÁR, E.: (1983) Polyhedron complexes with simply transitive group actions and their realizations. *Acta Math. Hung.* Vol. 59 (1-2), pp. 175-216
22. PLESKEN, W. – POHST, M. (1975): On Maximal Finite Irreducible Subgroups of $GL(n, \mathbb{Z})$ I. The Five and Seven Dimensional Case. II. The Six Dimensional Case. Preprint, Dept. of Math., California Inst. of Technology, Pasadena, 1975. *Math. Comput* Vol. 31 (1977), pp. 536–573; Vol. 34 (1980), pp. 245–301.
23. RYSHKOV, S. S. (1972): Maximal Finite Groups of Integral $n \times n$ Matrices and Full Groups of Integral Automorphisms of Positive Quadratic Forms (Bravais models). *Trudy. Mat. Inst. Steklov* Vol. 128, pp. 183–211. *Proc. Steklov Inst. Math.* Vol. 128 pp. 217–250.
24. SCHOENFLIES, A.: (1891) *Kristallsysteme und Kristallstruktur.* Teubner, Leipzig. (2. Aufl. *Theorie der Kristallstrukturen,* Berlin 1923
25. SCHWARZENBERGER, R. L. E. (1980): *N-dimensional Crystallography.* Pitman Adv. Publ. Program, San Francisco–London–Melburne.
26. ZASSENHAUS, H. (1948): Über einen Algorithmus zur Bestimmung der Raumgruppen. *Comment. Math. Helv.* Vol. 21, pp. 117–141.

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