

Fundamental D-V cells for \mathbb{E}^4 space groups on the 2D-screen

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Abstract

As an introduction we describe two algorithms for determining fundamental domains (D-V cells) of **XIX.27/01/01** and **XXII.31/05/02/002** [BBNWZ] space groups. With the first algorithm we obtain a 4-polytope as fundamental domain of **XIX.27/01/01** space group [AM01] belonging to the decagonal crystal family. The second algorithm determines a fundamental domain of a space group with broken translations [AM02].

Then we describe a method for orthogonal projection of \mathbb{E}^d -pictures on 2D-screen, and we can illustrate the edge structure of D-V cells for 25 space groups to the decagonal and icosahedral families of \mathbb{E}^4 .

Key Words: crystallographic group, four-dimensional space group, decagonal family, icosahedral family, fundamental domain, Dirichlet-Voronoi cell

MSC 2000: 20H15, 51F15

1. Description of Space Groups in \mathbb{E}^d

A *space group* Γ is defined in space \mathbb{E}^d as a group of isometries with a *compact* (bounded and closed) *fundamental domain* \mathcal{F} i.e.

$$\bigcup_{\gamma \in \Gamma} \gamma \mathcal{F} = \mathbb{E}^d \quad \text{and} \quad \text{Int}\mathcal{F} \cap \text{Int}\gamma\mathcal{F} = \emptyset \quad \text{for any } \gamma \in \Gamma \setminus \{\mathbf{1}\}$$

(“Int” abbreviates interior, $\gamma\mathcal{F}$ is the γ -image of \mathcal{F} , $\mathbf{1}$ denotes the identity map). Any element α of Γ associates each point X with its image $\alpha X =: Y$ by $(d+1)$ -row-column multiplication as usual:

$$\begin{pmatrix} \mathbf{y} \\ 1 \end{pmatrix} := \begin{pmatrix} \mathbf{A} & \mathbf{a} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ 1 \end{pmatrix} = \begin{pmatrix} \mathbf{Ax+a} \\ 1 \end{pmatrix}; X \begin{pmatrix} \mathbf{x} \\ 1 \end{pmatrix}, Y \begin{pmatrix} \mathbf{y} \\ 1 \end{pmatrix}$$

are introduced. We write $\alpha(\mathbf{a}; \mathbf{A})$ as well. The $d \times d$ matrix \mathbf{A} is called the *linear part* of α , the column vector \mathbf{a} is its *translational part*. All these are expressed in a coordinate system $(O, \mathbf{e}_1, \dots, \mathbf{e}_d)$ with an origin O , and a so called *lattice basis* $(\mathbf{e}_1, \dots, \mathbf{e}_d)$. \mathbf{L} is the *integral linear combinations* of the basis vectors $(\mathbf{e}_1, \dots, \mathbf{e}_d)$

$$\mathbf{L} = \{\mathbf{l} = \mathbf{e}_1 l^1 + \dots + \mathbf{e}_d l^d : (l^1, \dots, l^d) \in \mathbb{Z}^d\},$$

where \mathbb{Z} denotes the set of integers.

1.1. D-V Cell and Fundamental Domain

The D-V cell of the kernel point P to its Γ -orbit is

$$\mathcal{D}_\Gamma(P) = \{X \in \mathbb{E}^d : \rho(P, X) \leq \rho(\gamma P, X) \text{ for each } \gamma \in \Gamma\}$$

2. Fundamental domain for space group

XIX.27/01/01

The Gramian matrix in the decagonal family is:

$$G_d = \begin{pmatrix} a & b & -\frac{1}{2}(a+2b) & -\frac{1}{2}(a+2b) \\ b & a & b & -\frac{1}{2}(a+2b) \\ -\frac{1}{2}(a+2b) & b & a & b \\ -\frac{1}{2}(a+2b) & -\frac{1}{2}(a+2b) & b & a \end{pmatrix}.$$

To simplify our discussion, $b = -\frac{1}{4}a$ will be assumed, since we want to find a fundamental domain as simple as possible. The point group Γ_{05} of space group 27/01/01 = Γ_5 has one generator: γ_5 , mapping

$$\mathbf{e}_1 \rightarrow \mathbf{e}_4 \rightarrow \mathbf{e}_2 \rightarrow -\mathbf{e}_1 - \mathbf{e}_2 - \mathbf{e}_3 - \mathbf{e}_4 \rightarrow \mathbf{e}_3 \rightarrow \mathbf{e}_1$$

cyclically, thus γ_5 is a transform of order five, indeed.

2.1. Algorithm for the fundamental domain \mathcal{F}_5 of space group Γ_5

First: We choose the kernel point $P_1(1; 1; 1; 1)$, and determine the 3-plane bisectors of P_1 and γP_1 , $\gamma \in \Gamma_{05}$ (P_1 lies in negative halfspaces of the former 3-planes).

The transforms and the equations of 3-planes will be

$$\gamma_5 : \begin{pmatrix} 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, -z = 0; \quad \gamma_5^2 : \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, -x = 0;$$

$$\gamma_5^3 : \begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, -w = 0; \quad \gamma_5^4 : \begin{pmatrix} 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, -y = 0.$$

Thus we get a pyramidal domain \mathcal{F}_{05} with apex O that will contain \mathcal{F}_5 .

Second: We determine the equations of *bisector 3-planes of the origin O and its Γ_5 -images, now the lattice points with 0, 1, -1 coordinates*. In case of Γ_5 it will be enough to take points with 0, 1 coordinates. The origin O always lies in negative halfspaces of the above 3-planes. Thus we can intersect the pyramid by new 3-planes

The lattice points and the equations of 3-planes:

$$(1; 1; 1; 1; 1)^T, x + y + z + w - 2 = 0$$

$$(1; 0; 0; 0; 1)^T, 4x - y - z - w - 2 = 0,$$

$$(0; 1; 0; 0; 1)^T, -x + 4y - z - w - 2 = 0,$$

$$(0; 0; 1; 0; 1)^T, -x - y + 4z - w - 2 = 0,$$

$$(0; 0; 0; 1; 1)^T, -x - y - z + 4w - 2 = 0,$$

$$(1; 1; 0; 0; 1)^T, 3x + 3y - 2z - 2w - 3 = 0,$$

$$(1; 0; 1; 0; 1)^T, 3x - 2y + 3z - 2w - 3 = 0,$$

$$(1; 0; 0; 1; 1)^T, 3x - 2y - 2z + 3w - 3 = 0,$$

$$(0; 1; 1; 0; 1)^T, -2x + 3y + 3z - 2w - 3 = 0,$$

$$(0; 1; 0; 1; 1)^T, -2x + 3y - 2z + 3w - 3 = 0,$$

$$(0; 0; 1; 1; 1)^T, -2x - 2y + 3z + 3w - 3 = 0,$$

$$(1; 1; 1; 0; 1)^T, 2x + 2y + 2z - 3w - 3 = 0,$$

$$(1; 1; 0; 1; 1)^T, 2x + 2y - 3z + 2w - 3 = 0,$$

$$(1; 0; 1; 1; 1)^T, 2x - 3y + 2z + 2w - 3 = 0,$$

$$(0; 1; 1; 1; 1)^T, -3x + 2y + 2z + 2w - 3 = 0.$$

Third: We start with five suitable equations of 3-planes and determine the 5 vertices of a starting simplex (5-cell). We take a new 3-plane, substitute the coordinates of all vertices of the convex 4-dimensional polyhedron into its equation. If at least one vertex exists in the positive halfspace of the 3-plane, then we cut the polyhedron, otherwise leave it.

Finally, the fundamental domain \mathcal{F}_5 has 19 geometric 3-faces and 65 proper vertices.

Fundamental domain of space group 27/01/01 (\mathcal{F}_5)

<i>Element generator</i>
$\gamma_5 = \begin{pmatrix} 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix};$
<i>3-faces</i>
$-x = 0, \quad -y = 0, \quad -z = 0, \quad -w = 0,$ $x+y+z+w-2=0, \quad 4x-y-z-w-2=0, \quad -x+4y-z-w-2=0,$ $-x-y+4z-w-2=0, \quad -x-y-z+4w-2=0, \quad 3x+3y-2z-2w-3=0,$ $3x-2y+3z-2w-3=0, \quad 3x-2y-2z+3w-3=0, \quad -2x+3y+3z-2w-3=0,$ $-2x+3y-2z+3w-3=0, \quad -2x-2y+3z+3w-3=0, \quad 2x+2y+2z-3w-3=0,$ $2x+2y-3z+2w-3=0, \quad 2x-3y+2z+2w-3=0, \quad -3x+2y+2z+2w-3=0;$

The diagram consists of two parts. The left part shows a perspective view of a polyhedron composed of several rectangular faces, some of which are shaded. A dashed line indicates an edge that is not visible from this angle. The right part shows a more complex, wireframe-like polyhedron with many edges drawn, also with some faces shaded. A vertical line extends downwards from the bottom of this structure.

3. Fundamental domain (\mathcal{F}_{05t}) for space group XXII.31/05/02/002

The icosahedral crystal family has two Bravais lattices with Gramians

$$\begin{pmatrix} a & -\frac{a}{4} & -\frac{a}{4} & -\frac{a}{4} \\ -\frac{a}{4} & a & -\frac{a}{4} & -\frac{a}{4} \\ -\frac{a}{4} & -\frac{a}{4} & a & -\frac{a}{4} \\ -\frac{a}{4} & -\frac{a}{4} & -\frac{a}{4} & a \end{pmatrix}, \begin{pmatrix} a & \frac{a}{2} & \frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & a & \frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & \frac{a}{2} & a & \frac{a}{2} \\ \frac{a}{2} & \frac{a}{2} & \frac{a}{2} & a \end{pmatrix},$$

for the primitive and its SN centred (seitenflächen-nebendiagonal-zentriert) lattices.

XXII.31/05/02/002 = Γ_{5t} is the richest space group for the SN centred lattice with broken translations [BBNWZ]. The 120 transform of its point group Γ_{05t} and all transforms of Γ_{5t} itself can be generated by homogeneous 5x5 matrices, as usual

$$\gamma_{4t} = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 1 & 1 & 1 & 1 & \frac{2}{3} \\ 0 & -1 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & -1 & \frac{2}{3} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \gamma_{5t} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & -1 & -1 & -1 & \frac{2}{3} \\ 1 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\gamma_{6t} = \begin{pmatrix} 0 & 0 & -1 & 0 & \frac{1}{3} \\ -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

3.1. Algorithm for the fundamental domain \mathcal{F}_{5t} of space group Γ_{5t}

First: We determine all broken translations of Γ_{5t} in increasing distances, say, to the origin O , at the same time we obtain the transforms without translations $\gamma_{05} \in \Gamma_{stab(O)} < \Gamma_{05t}$.

Second: We determine the equations of bisector 3-planes of the origin O and its broken translates.

Third: We choose the second kernel point $P_1(1; 1; 1; 1)$, and determine the pyramidal domain $\mathcal{F}_{Stab(O)}$ with γ_{05} 's fixing O .

Fourth: We apply the algorithm in the third point of previous chapter, and we obtain the equations of 3-planes and the vertices of the fundamental domain.

Our fundamental domain \mathcal{F}_{5t} will have 20 bisector 3-faces and 45 proper vertices.

Fundamental domain of space group 31/05/02/002 (\mathcal{F}_{5t})

<i>Generator elements</i>
$\gamma_{4t} = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 1 & 1 & 1 & 1 & \frac{2}{3} \\ 0 & -1 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & -1 & \frac{2}{3} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad \gamma_{5t} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & -1 & -1 & -1 & \frac{2}{3} \\ 1 & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$ $\gamma_{6t} = \begin{pmatrix} 0 & 0 & -1 & 0 & \frac{1}{3} \\ -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix};$

4. \mathbb{E}^d -pictures on 2-screen

Let $(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_d, \mathbf{a}_0)$ be a fixed homogeneous coordinate system of $\mathbb{E}^d \subset \mathcal{P}^d$ with given (possibly skew) Gramian

$$(<\mathbf{a}_i, \mathbf{a}_j>); \quad \mathbf{a}_{ij} = \mathbf{a}_{ji}, \quad \text{for } i, j = 1, \dots, d.$$

Let $(\mathbf{e}_1(t), \mathbf{e}_2(t), \mathbf{e}_0(t))$ be Cartesian homogeneous coordinate system of the screen, moving by the time t , expressed in \mathbf{a}_i :

$$\mathbf{e}_\alpha(t) = \mathbf{a}_i \mathbf{e}_\alpha^i(t), \quad \alpha = 0, 1, 2; \quad i = 0, 1, \dots, d;$$

with the projective freedom of non-zero **R**-factor, and the orthogonality

$$e_{\alpha\beta} := <\mathbf{e}_\alpha, \mathbf{e}_\beta> = <\mathbf{a}_r \mathbf{e}_\alpha^r, \mathbf{a}_s \mathbf{e}_\beta^s> = e_\alpha^r a_{rs} e_\beta^s = \delta_{\alpha\beta} \quad \alpha, \beta \in \{1, 2\}; \quad r, s \in \{1, 2, \dots, d\}.$$

Any point $X(\mathbf{x} = \mathbf{a}_i x^i)$ will be orthogonally projected onto the screen

$$(\mathbf{e}_1(t), \mathbf{e}_2(t), \mathbf{e}_0(t)),$$

and the image $Y(t)(\mathbf{y}(t) = \mathbf{e}_\alpha(t) y^\alpha(t))$ of X is to express by (x^i) , (a_{rs}) , $e_\alpha^k(t)$.

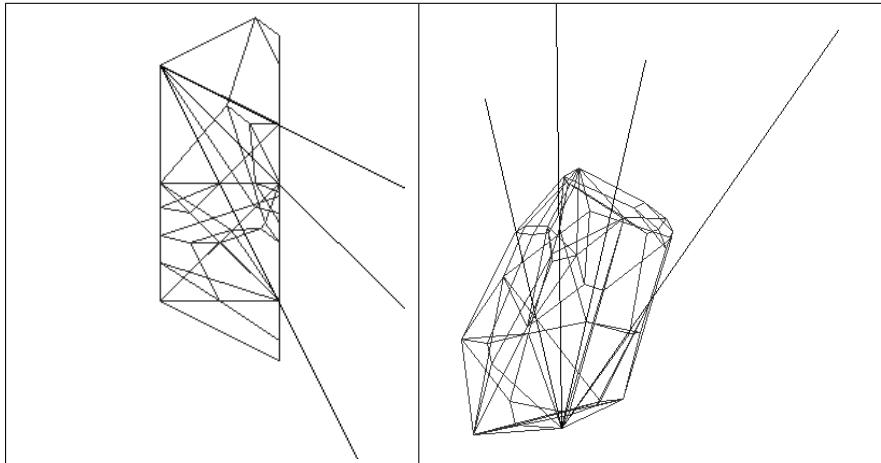
The crucial assumption is

$$\overrightarrow{XY} \perp (\mathbf{e}_1(t), \mathbf{e}_2(t), \mathbf{e}_0(t)) \quad \text{i.e.} \\ <\mathbf{a}_i e_\alpha^i(t) y^\alpha(t) - \mathbf{a}_i x^i c(t), \mathbf{a}_k e_\beta^k(t) - \mathbf{a}_k e_0^k(t) d_\beta(t)> = 0$$

Here the “functions” $c(t)$ and $d_\beta(t)$ are determined by

$$e_\alpha^0(t) y^\alpha(t) = x^0 c(t), \\ \text{and} \\ e_\beta^0(t) = e_0^0(t) d_\beta(t),$$

in general, but $x^0 = 1$, $e_0^0(t) = 1, e_1^0 = e_2^0 = 0$, thus $y^0 = 1$, $c(t) = 1$, $d_0(t) = 1, d_1(t) = d_2(t) = 0$ can be assumed from the beginning for any time t later. The cases $x^0 = 0$ lead $y^0 = 0$, i.e. ideal points have ideal images (at the infinity).



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