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On the enumeration of the combinatorial types of primitive parallelohedra in E^d, $2 \le d \le 6$

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The cone of positive-definite quadratic forms is subdivided into subcones of combinatorial types of primitive parallelohedra in E^d, $2 \le d \le 6$. A new algorithm is described and recent results on the enumeration are given.

1. Introduction

Following Fedorov (1885), a convex body which tiles space by translations is called a *parallelogon* in two- and a *parallelohedron* in three-dimensional space. Voronoï (1908*a*,*b*) used the term parallelohedron for any dimension d. Translation lattices and their associated quadratic forms play an important role in mathematics and in crystallography, where the periodically arranged atomic building blocks are a fundamental property of crystals. Fedorov (1885) determined the two combinatorial types of parallelogons in E^2 and the five combinatorial types of parallelohedra in E^3. He stated the following necessary conditions for a parallelohedron. With his Theorems 3, 4, 23 and 35 he proved:

(i) *Each parallelohedron is centrosymmetric*; and from his Theorem 42 follows the condition

(ii) *Each facet is centrosymmetric*; and his Theorem 41 proves

(iii) *Each belt consists of four or six facets*.

As a main achievement Venkov (1954), and independently McMullen (1980), proved that conditions (i) to (iii) are necessary and sufficient for a convex polytope in E^d to be a parallelohedron.

A famous result of Minkowski (1897*a*,*b*) states that the number of facets of a parallelohedron is $N_{\rm f} \le 2(2^d - 1)$ and Voronoï (1908*a*,*b*) proved that for primitive parallelohedra the equal sign holds. But for $d \ge 4$ there exist non-primitive parallelohedra which have the maximal number of facets.

Voronoï (1908*a*,*b*) determined the three combinatorial types of primitive parallelohedra in E^4. In Engel (2000, 2011), for the first time, a complete enumeration of the 222 combinatorial types of primitive parallelohedra in E^5, and their classification into contraction and similarity types, was performed.

2. Basic notations

Let $\Lambda^d := \{\mathbf{t} \mid \mathbf{t} = t_1\mathbf{a}_1 + \ldots + t_d\mathbf{a}_d,\ t_i \in \mathbb{Z}\}$ be a *translation lattice* in Euclidean space E^d with origin O, lattice basis

$$\mathbf{a}_1, \ldots, \mathbf{a}_d, \tag{1}$$

and Gram matrix $\mathsf{Q} := \{q_{ij} \mid q_{ij} = \mathbf{a}_i\mathbf{a}_j,\ i, j = 1, \ldots, d\}$. A *dual basis* is given by

$$\mathbf{a}_1^*, \ldots, \mathbf{a}_d^*, \tag{2}$$

where $\mathbf{a}_i^*$, $i = 1, \ldots, d$, is the outer product of $\{\mathbf{a}_1, \ldots, \mathbf{a}_d\} \setminus \{\mathbf{a}_i\}$. It holds that $\mathbf{a}_i\mathbf{a}_j^* = \delta_{ij}$ and $\mathsf{Q}^* = \mathsf{Q}^{-1}$.

The *Dirichlet parallelohedron* (Dirichlet, 1850*a*,*b*) of Λ^d at O is defined by

$$\mathsf{P}(\mathsf{Q}) := \{\mathbf{x} \in E^d \mid \mathbf{x}^t\mathsf{Q}\mathbf{x} \le (\mathbf{x} - \mathbf{t})^t\mathsf{Q}(\mathbf{x} - \mathbf{t}), \forall \mathbf{t} \in \Lambda^d\}.$$

It is a special kind of parallelohedron.

Geometrically, a parallelohedron P(Q) is obtained as the intersection of a set of closed half-spaces $\mathsf{H}_\mathbf{t}$ each being determined through the hyperplane perpendicular to the lattice vector $\mathbf{t}$ and bisecting it (Engel, 1986),

$$\mathsf{P}(\mathsf{Q}) = \bigcap_{\mathbf{t} \in \Lambda^d \setminus \{\mathsf{O}\}} \mathsf{H}_\mathbf{t}. \tag{3}$$

Only lattice vectors $\mathbf{t}$ within a ball of finite radius $2R$ contribute to P, where R is the radius of the largest interstitial ball of Λ^d having its centre at an extreme vertex of P. It follows that every parallelohedron has a finite number of facets only.

The k-faces of a polytope P, $k = 0, \ldots, d$, are partially ordered with respect to inclusion. The 0-faces are the vertices, the 1-faces the edges and the $(d-1)$-faces the facets of P. The d-face is the polytope P. The k-faces of P, together with the empty set $\{\emptyset\}$, determine the *face lattice* $\mathcal{L}(\mathsf{P})$. A lattice vector $\mathbf{t}$ is called a *facet vector* of P if $\mathsf{P} \cap \mathsf{P} + \mathbf{t} = \mathsf{F}$ is a facet of P. It is called a *corona vector* of P if $\mathsf{P} \cap \mathsf{P} + \mathbf{t} \ne \emptyset$. The set of facet vectors and the set of all corona vectors are denoted by F and C, respectively. For primitive parallelohedra it holds that $F = C$.

Translations of a Dirichlet parallelohedron P completely cover Euclidean space E^d *facet-to-facet*; that is, the intersection of any two tiles is either empty, or a k-face of each. Following Voronoï (1908*a*,*b*), a parallelohedron P in a facet-to-facet tiling of E^d is denoted as being *primitive* if in every k-face of P, $k = 0, \ldots, d-1$, exactly $d - k + 1$ adjacent parallelohedra meet, and he proved that a parallelohedron is primitive if, and only if, in every vertex of it $d + 1$ contiguous parallelohedra

Table 1
Numbers N_k of k-faces of primitive parallelohedra in E^d, $2 \le d \le 6$.

d	N_0	N_1	N_2	N_3	N_4	N_5	Belts
2	6	6					6_1
3	24	36	14				6_6
4	120	240	150	30			6_{25}
5	720	1800	1560	540	62		6_{90}
	708	1770	1536	534	62		6_{89}
6	5040	15120	16800	8400	1806	126	6_{301}
	5012	15036	16710	8360	1800	126	6_{300}
	4984	14952	16620	8320	1794	126	6_{299}
	4956	14868	16530	8280	1788	126	6_{298}
	4928	14784	16440	8240	1782	126	6_{297}
	4900	14700	16350	8200	1776	126	6_{296}
	4872	14616	16260	8160	1770	126	6_{295}
	4844	14532	16170	8120	1764	126	6_{294}
	4816	14448	16080	8080	1758	126	6_{293}
	4788	14364	15990	8040	1752	126	6_{292}
	4760	14280	15900	8000	1746	126	6_{291}
	4732	14196	15810	7960	1740	126	6_{290}
	4704	14112	15720	7920	1734	126	6_{289}
	4676	14028	15630	7880	1728	126	6_{288}
	4648	13944	15540	7840	1722	126	6_{287}
	4620	13860	15450	7800	1716	126	6_{286}
	4592	13776	15360	7760	1710	126	6_{285}

meet. If two primitive parallelohedra are contiguous then they meet in a common facet.

Voronoï (1908*a*,*b*) conjectured that each parallelohedron is affinely equivalent to a Dirichlet parallelohedron P of a certain translation lattice, and he proved the conjecture for primitive parallelohedra. Therefore, we may use Dirichlet's construction [equation (3)] in order to completely derive the combinatorial types of primitive parallelohedra in E^d.

For a primitive parallelohedron P, let $\mathbf{f}_1, \ldots, \mathbf{f}_d$ be the d facet vectors whose corresponding facets meet in a common vertex $\mathbf{v} \subset \mathsf{P}$. We calculate the determinant $\omega := \det(\mathbf{f}_1, \ldots, \mathbf{f}_d)$. The parallelohedron P is said to be *principal primitive* if for all vertices of P it holds that $\omega = 1$. For $d \le 4$, $d = 5$ and $d = 6$, the maximal value of ω is 1, 2 and 3, respectively (Ryshkov & Baranovskiî, 1998). Sets of vertices of P having the same ω occur in multiples of $2(d+1)$.

Following Voronoï (1908*a*,*b*), the number of k-faces N_k, $0 \le k < d$, of a parallelohedron in E^d is

$$N_k \le (d+1-k)\sum_{l=0}^{d-k}(-1)^{d-k-l}\binom{d-k}{l}(1+l)^d. \qquad (4)$$

The equal sign holds for principal primitive parallelohedra (see Table 1).

The components of a lattice vector depend on the choice of the lattice basis B. For any $\mathsf{A} \in GL_d(\mathbb{Z})$, $B' = \mathsf{A}B$ is an equivalent lattice basis and $\mathsf{Q}' = \mathsf{AQA}^t$ is *arithmetically equivalent* to Q. A lattice vector transforms according to $\mathbf{t}' = \mathsf{A}^\circ\mathbf{t}$, where $\mathsf{A}^\circ = (\mathsf{A}^t)^{-1}$. A dual vector transforms according to $\mathbf{z}^{*\prime} = \mathsf{A}\mathbf{z}^*$. A lattice basis is called *optimal* if it minimizes the magnitudes of the components of all lattice vectors within a given ball of fixed finite radius. In Engel (1988) the concept of an optimal basis was introduced. It simultaneously reduces the Gram matrices Q and Q^{-1} such that $\Delta_{\rm opt} := {\rm tr}(\mathsf{Q}_{\rm opt} - \rho^2\mathsf{Q}_{\rm opt}^{-1})^2$ is minimal, where $\rho := [\det(\mathsf{Q})]^{1/d}$. We obtain

$$\Delta_{\rm opt} = \min_{\mathsf{A}\in GL_d(\mathbb{Z})} {\rm tr}(\mathsf{AQA}^t - \rho^2\mathsf{A}^\circ\mathsf{Q}^{-1}\mathsf{A}^{-1})^2. \qquad (5)$$

Table 2
The maximal number of belts of primitive parallelohedra in E^d, $2 \le d \le 8$.

d	2	3	4	5	6	7	8
$N_{\rm b}$	1	6	25	90	301	966	3025

A quadratic form is defined by $\varphi(\mathbf{x}) := \mathbf{x}^t\mathsf{Q}\mathbf{x}$. We denote by

$$\mathcal{C}^+ := \{\mathsf{Q} \mid \varphi(\mathbf{x}) > 0, \forall \mathbf{x} \in E^d \setminus \{\mathbf{0}\}\}$$

the *cone of positive-definite quadratic forms*. Its closure is denoted by $\mathcal{C} := {\rm clos}(\mathcal{C}^+)$ and its boundary by $\mathcal{C}^o := \mathcal{C} \setminus \mathcal{C}^+$. Given a basis $\mathbf{e}_1, \ldots, \mathbf{e}_d$ of $\mathbb{R}^d$, a basis of $\mathbb{R}^{d\times d}$ is obtained by the tensor products

$$\mathbf{e}_{ij} := \mathbf{e}_i \otimes \mathbf{e}_j, \quad 1 \le i, j \le d, \qquad (6)$$

with $\mathbf{e}_{ij}\mathbf{e}_{kl} = \delta_{ik}\delta_{jl}$. We denote by $\mathbf{q}$ the vector representing the Gram matrix Q in $\mathbb{R}^{d\times d}$,

$$\mathbf{q} = q_{11}\mathbf{e}_{11} + q_{12}\mathbf{e}_{12} + \ldots + q_{dd}\mathbf{e}_{dd}. \qquad (7)$$

Similarly, let $\mathbf{i}$ be the vector representing the identity matrix I. In $\mathbb{R}^{d\times d}$, $\mathcal{C}$ is a cone of rotation with axis given by $\mathbf{i}$. The aperture angle with respect to $\mathbf{i}$ becomes (Engel, 2000)

$$\cos\varphi = 1/d^{1/2}. \qquad (8)$$

From the commutativity of the scalar product it follows that Q is symmetric, $\mathsf{Q} = \mathsf{Q}^t$, and therefore the cone $\mathcal{C}^+$ can be restricted to a subspace of dimension $\binom{d+1}{2}$, defined by $\mathbf{e}_{ij} = \mathbf{e}_{ji}$, $i \le j = 1, \ldots, d$. In order to keep the same metric as in $\mathbb{R}^{d\times d}$, we take for $i \ne j$, $\mathbf{e}'_{ij} := 2^{1/2}\mathbf{e}_{ij}$.

A *belt* of a parallelohedron P is a complete set of parallel $(d-2)$-faces of P. A belt contains either four or six $(d-2)$-faces. Primitive parallelohedra contain sixfold belts only. Thus the number $N_{\rm b}$ of belts of a primitive parallelohedron can be obtained by dividing the number of $(d-2)$-faces by 6,

$$N_{\rm b} = \frac{N_{(d-2)}}{6}.$$

Using equation (4) for $N_{(d-2)}$ we obtain

$$N_{\rm b} \le \frac{1 - 2^{(d+1)} + 3^d}{2}.$$

The equal sign holds for principal primitive parallelohedra. Numbers $N_{\rm b}$ are given in Table 2.

A *zone* of a parallelohedron P is the set of all 1-faces (edges) E that are parallel to a zone vector $\mathbf{z}^*$, $\mathsf{Z} := \{\mathsf{E} \subset \mathsf{P} \mid \mathsf{E} \parallel \mathbf{z}^*\}$. In each 1-face $\mathsf{E} \subset \mathsf{P}$ at least $d-1$ facets meet. The zone vector $\mathbf{z}^*$ is the outer product of the corresponding facet vectors. Referring to the dual basis [equation (2)], $\mathbf{z}^*$ has integer components $z_1^*, \ldots, z_d^*$. We assume that the greatest common divisor $gcd(z_1^*, \ldots, z_d^*) = 1$. With respect to any zone vector $\mathbf{z}^*$ we can classify the lattice vectors in *layers*

$$L_i(\mathbf{z}^*) := \{\mathbf{t} \in \Lambda^d \mid \mathbf{t}\mathbf{z}^* = i, \quad | i | = 0, 1, 2, \ldots\}. \tag{9}$$

A zone Z is called *closed*, if every 2-face of P contains either two edges of Z, or else none, otherwise it is called *open*. For the number N_z^c of closed zones the following holds:

$$N_z^c \le \binom{d+1}{2}.$$

The equal sign holds for the unique class of principal primitive zonohedral parallelohedra in E^d (see Engel, 2005). It is represented by the root lattice A_d^*.

The edges of a zone Z are collected into subsets S_j^Z, $j = 1, \ldots, s(\mathsf{Z})$, according to their length l_j, $l_1 < l_2 < \ldots < l_{s(\mathsf{Z})}$. Each subset contains a multiple of $2d$ edges. Zonohedral parallelohedra have edges of the same length within each zone. By *zone contraction* $\mathsf{P}^\downarrow$, we understand the process of contracting every edge of a closed zone Z by the amount of its shortest edges. All zone contractions of P define the *zone-contraction lattice* $\mathcal{Z}(\mathsf{P})$. If all zones of P are open, then P is said to be *totally contracted*. The *zone extension* $\mathsf{P}^\uparrow$ is the inverse operation of the zone contraction $\mathsf{P}^\downarrow$. An open zone of P(Q) having zone vector $\mathbf{z}^*$ is said to be extendable if it can be extended to a closed zone. For the corresponding Gram matrix this means that (Engel, 2000)

$$\mathsf{Q}' = \mathsf{Q} + \lambda(\mathbf{z}^* \otimes \mathbf{z}^*), \tag{10}$$

where $\lambda \in \mathbb{R} \ge 0$. The ray vector $\mathbf{z}^* \otimes \mathbf{z}^*$ has zero determinant and lies on the boundary $\mathcal{C}^o$. From equation (10) Theorem 1 immediately follows.

Theorem 1. A zone Z of a parallelohedron P is closed, or extendable if, and only if, the facet vectors of P lie in layers $L_i(\mathbf{z}^*)$, $|i| \le 1$, only.

Proof. By equation (3), P(Q) is contained in a ball of radius R. Choose $\lambda \gg R$ such that by equation (10) $| \mathbf{z}^*\mathbf{v}_i | < 1$ for all $\mathbf{v}_i \subset \mathsf{P}'(\mathsf{Q}')$. Thus, lattice vectors $\mathbf{t} \in L_2$ cannot be facet vectors. *Vice versa*, if there are only facet vectors in L_i, $| i | \le 1$, then $\lambda > 0$ can be freely chosen, and therefore Z is closed. □

Two parallelohedra P and P′ are said to be combinatorially equivalent, $\mathsf{P}' \overset{\text{comb}}{\simeq} \mathsf{P}$, and belong to the same *combinatorial type*, if there exists a combinatorial isomorphism $\tau : \mathcal{L}(\mathsf{P}) \to \mathcal{L}(\mathsf{P}')$.

A rough identification of the combinatorial type is obtained by the subordination scheme. For any k, $1 < k < d$, let $n_i^{(k)}$ be the number of k-faces of P which have subordinated $f_i^{(k)}$ $(k-1)$-faces, $i = 1, \ldots, r$. The *k-subordination symbol* is defined by

$$f_1^{(k)}{}_{n_1^{(k)}} f_2^{(k)}{}_{n_2^{(k)}} \ldots f_r^{(k)}{}_{n_r^{(k)}},$$

with $f_1^{(k)} < f_2^{(k)} < \ldots < f_r^{(k)}$. As *subordination scheme* we denote the concatenation of the k-subordination symbols. For primitive parallelohedra in E^d, $d \le 5$, the $(d-1)$-subordination symbol was found to be sufficient for a unique identification. In rare cases in E^6, parallelohedra of different combinatorial type were found, which have the same subordination scheme but are distinguished by the number of closed and open zones. A complete identification is obtained by the *unified polytope scheme* described in Engel (1991) which, however, becomes very large in E^6 and is time-consuming to determine.

3. Subdivision of the cone $\mathcal{C}$

We partition $\mathcal{C}^+ := \{\mathsf{Q} \mid \mathbf{x}^t\mathsf{Q}\mathbf{x} > 0\}$ into connected open *subcones of equivalent combinatorial types of primitive parallelohedra* (Engel, 2003)

$$\Phi^+(\mathsf{P}) = \{\mathsf{Q}' \in \mathcal{C}^+ \mid \mathsf{P}(\mathsf{Q}') \overset{\text{comb}}{\simeq} \mathsf{P}\}.$$

By Φ we denote the closure of Φ^+, and its boundary by $\Phi^o := \Phi \setminus \Phi^+$. Inside a domain Φ, the length of at least one edge $\mathsf{E} \subset \mathsf{P}$ diminishes for some $\mathsf{Q}' \in \Phi^+$ approaching the boundary Φ^o, and when Q' hits Φ^o both vertices subordinated to the edge E coincide. Since P is primitive, it follows that at the point of coincidence $d+1$ facets meet in a common vertex $\mathbf{v} \subset \mathsf{P}'$. Let $\mathbf{f}_1, \ldots, \mathbf{f}_{d+1}$ be the corresponding facet vectors.

A boundary surface of Φ is determined in the following way. If a facet F_i, $i = 1, \ldots, d+1$, contains the vertex $\mathbf{v}$ then the corresponding facet vector $\mathbf{f}_i$ fulfils the equation

$$\mathbf{v}^t\mathsf{Q}\mathbf{f}_i = \tfrac{1}{2}\mathbf{f}_i^t\mathsf{Q}\mathbf{f}_i, \quad i = 1, \ldots, d+1.$$

As a sufficient condition that $d+1$ facets meet in vertex $\mathbf{v}$ we have that the determinant

$$\begin{vmatrix} \sum q_{1j}f_{1j} & \ldots & \sum q_{dj}f_{1j} & \mathbf{f}_1^t\mathsf{Q}\mathbf{f}_1 \\ \vdots & & \vdots & \vdots \\ \sum q_{1j}f_{dj} & \ldots & \sum q_{dj}f_{dj} & \mathbf{f}_d^t\mathsf{Q}\mathbf{f}_d \\ \sum q_{1j}f_{d+1,j} & \ldots & \sum q_{dj}f_{d+1,j} & \mathbf{f}_{d+1}^t\mathsf{Q}\mathbf{f}_{d+1} \end{vmatrix} = 0.$$

Since $\mathbf{f}_1, \ldots, \mathbf{f}_d$ form a basis of a sublattice of Λ^d of index ω, it follows that

$$\mathbf{f}_{d+1} = \alpha_1\mathbf{f}_1 + \ldots + \alpha_d\mathbf{f}_d, \quad \alpha_i \in \mathbb{Z}/\omega. \tag{11}$$

Hence, the determinant can be transformed to

$$\begin{vmatrix} \sum q_{1j}f_{1j} & \ldots & \sum q_{dj}f_{1j} & \mathbf{f}_1^t\mathsf{Q}\mathbf{f}_1 \\ \vdots & & \vdots & \vdots \\ \sum q_{1j}f_{dj} & \ldots & \sum q_{dj}f_{dj} & \mathbf{f}_d^t\mathsf{Q}\mathbf{f}_d \\ 0 & \ldots & 0 & A \end{vmatrix} = 0,$$

where

$$A := \sum_{i=1}^{d} \alpha_i(\alpha_i - 1)\mathbf{f}_i^t\mathsf{Q}\mathbf{f}_i + 2\sum_{i=1}^{d-1}\sum_{j=i+1}^{d} \alpha_i\alpha_j\mathbf{f}_i^t\mathsf{Q}\mathbf{f}_j. \tag{12}$$

We set

$$\Delta_d = \begin{vmatrix} \sum q_{1j}f_{1j} & \ldots & \sum q_{dj}f_{1j} \\ \vdots & & \vdots \\ \sum q_{1j}f_{dj} & \ldots & \sum q_{dj}f_{dj} \end{vmatrix}.$$

The determinant thus becomes

$$A\,\Delta_d = A\det(\mathsf{Q})\det(\mathbf{f}_1, \ldots, \mathbf{f}_d) = 0.$$

This product gives, in terms of the Gram matrix Q, the condition that the $d+1$ facets meet in the vertex $\mathbf{v}$. Either factor can be zero.

(i) First consider the case $A = 0$. The term A is linear in q_{ij} and hence it determines a flat wall $\mathsf{W} \subset \Phi$. Since ω is finite, the term A can be represented by integral numbers n_{ij}. Thus the *wall equation* becomes

$$n_{11}q_{11} + n_{12}q_{12} + \ldots + n_{dd}q_{dd} = 0.$$

In order to determine the coefficients n_{ij} we have to solve equation (11) for α_i. Referring to the lattice basis [equation (1)] we have that $\mathbf{f}_i = f_{i1}\mathbf{a}_1 + \ldots + f_{id}\mathbf{a}_d$, $1 \le i \le d+1$, and thus we obtain

$$\begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_d \end{pmatrix} = \begin{pmatrix} f_{11} & \cdots & f_{d1} \\ \vdots & & \vdots \\ f_{1d} & \cdots & f_{dd} \end{pmatrix}^{-1} \begin{pmatrix} f_{d+1,1} \\ \vdots \\ f_{d+1,d} \end{pmatrix}.$$

Substituting α_i, $i = 1, \ldots, d$, in equation (12), we get the components n_{ij} relative to the basis [equation (6)]. The vector

$$\mathbf{n} = n_{11}\mathbf{e}_{11} + n_{12}\mathbf{e}_{12} + \ldots + n_{dd}\mathbf{e}_{dd} \qquad (13)$$

is the *wall normal* perpendicular to the wall W.

(ii) The case that $\det(\mathsf{Q}) = 0$, or $\det(\mathbf{f}_1, \ldots, \mathbf{f}_d) = 0$, means that Λ^d degenerates to Λ^k, $k < d$. It follows that Φ *is a rational polyhedral subcone of* $\mathcal{C}$, *having a finite number of walls defining its boundary*.

The k-faces of Φ, $0 \le k \le \binom{d+1}{2}$, determine the *face lattice* $\mathcal{L}(\Phi)$. The 0-face is the apex of the subcone at the origin O, the 1-faces are the edge forms and the $[\binom{d+1}{2} - 1]$-faces are the walls of Φ. The wall normal $\mathbf{n}$ is normalized such that for $\mathsf{Q} \in \Phi^+$ it holds that $\mathbf{nq} < 0$. By $\widehat{\mathbf{n}}$ we denote the unit wall normal having length 1.

Let $\widehat{\mathbf{w}}_i^*$, $i = 1, \ldots, r$, be the unit edge forms of a subcone Φ, then any set of $\lambda_i > 0$, $i = 1, \ldots, r$ gives a Gram matrix $\mathsf{Q} \in \Phi^+$ by

$$\mathsf{Q} = \sum_{i=1}^{r} \lambda_i \widehat{\mathbf{w}}_i^*.$$

Similarly, let $\widehat{\mathbf{w}}_j^*$, $j = 1, \ldots, p$, be the unit edge forms contained in a k-face of Φ^o, $0 < k < \binom{d+1}{2}$, then any set of $\lambda_j > 0$, $j = 1, \ldots, p$ gives a Gram matrix Q^o at the relative interior of the k-face by

$$\mathsf{Q}^o = \sum_{j=1}^{p} \lambda_j \widehat{\mathbf{w}}_j^*.$$

In particular, for a wall W and $\lambda_j = 1$, $j = 1, \ldots, p$,

$$\mathbf{q}' = \mathbf{q}^o + \mu\widehat{\mathbf{n}} \qquad (14)$$

lies in the neighbouring subcone Φ' relative to the wall W for some sufficiently small value $\mu > 0 \in \mathbb{R}$.

For any pair $\mathsf{Q}, \mathsf{Q}' \in \Phi^+$, the corresponding parallelohedra P and P′, respectively, have sets of facet vectors $F' = F$. In particular, if $\mathsf{Q}' \in \Phi^o$, it holds that $F' \subseteq F$.

Theorem 2. Let P be a parallelohedron with $s \ge d$ closed zones with zone vectors $\mathbf{z}_i^*$, $i = 1, \ldots, s$. If $\mathbf{z}_1^*, \ldots, \mathbf{z}_s^*$ span a subspace of dimension d, then there exists a lattice basis referred to which the facet vectors of P have components in $\{\bar{1}, 0, 1\}$ only.

Proof. By assumption $\dim \operatorname{aff}(\mathbf{z}_1^*, \ldots, \mathbf{z}_s^*) = d$. There exists a basis such that $\mathbf{z}_1^{*\prime} = (1, 0, \ldots, 0), \ldots, \mathbf{z}_d^{*\prime} = (0, \ldots, 0, 1)$ (generally, the optimal basis has this property). $\lambda_1(\mathbf{z}_1^{*\prime} \otimes \mathbf{z}_1^{*\prime}), \ldots, \lambda_d(\mathbf{z}_d^{*\prime} \otimes \mathbf{z}_d^{*\prime})$, $\lambda_i > 0$, generates a d-face of the subcone of the zonohedral parallelohedra. Therefore, there exist $\mathsf{Q}' \in \Phi^+(\mathsf{P})$ within any ε-neighbourhood of the identity I. The corona vectors of the tiling with hypercubes have components in $\{\bar{1}, 0, 1\}$ only. By a small deformation $\mathsf{I} \to \mathsf{Q}'$ some of the corona vectors become facet vectors and others lose this property. Therefore, the facet vectors of P′ and thus of P have components in $\{\bar{1}, 0, 1\}$ only. □

For the first time in E^5, there exists one class of equivalent subcones for which $\dim \operatorname{aff}(\mathbf{z}_1^*, \ldots, \mathbf{z}_{10}^*) = 4$. Referring to the optimal basis the facet vectors have maximal components 2. In E^6 such cases are frequently met, but with reference to an optimal basis, we have found no components >2.

Corollary. Let P be a parallelohedron with $s \ge 1$ closed zones with zone vectors $\mathbf{z}_i^*$, $i = 1, \ldots, s$. If $\mathbf{z}_1^*, \ldots, \mathbf{z}_s^*$ span a subspace of dimension $k \le d$, then there exists a lattice basis in reference to which the facet vectors of P, in the first k positions, have components in $\{\bar{1}, 0, 1\}$ only.

Proof. By assumption $\dim \operatorname{aff}(\mathbf{z}_1^*, \ldots, \mathbf{z}_s^*) = k$. There exists a basis such that $\mathbf{z}_i^{*\prime}$ has component 1 in position i and all other components are 0, $1 \le i \le k$. By Theorem 1, $|\, \mathbf{z}_i^{*\prime}\mathbf{f}_j' \,| \le 1$, for all $\mathbf{f}_j' \in F$. Therefore, the ith components of $\mathbf{f}_j'$ have to lie in $\{\bar{1}, 0, 1\}$ only. □

In Engel (2011), an algorithm was described in order to determine the walls of a subcone $\Phi(\mathsf{P})$. We developed an alternative algorithm which is based on the contraction of the edges of P and which proved to be approximately five times faster than the original algorithm.

(i) Eliminate all edges of P which are equivalent by the centre of symmetry at the origin O. This is easily performed because the facets of P are determined in centrosymmetric pairs.

(ii) For each remaining edge, determine the wall normal [equation (13)] by contracting that edge.

(iii) Select $\binom{d+1}{2}$ wall normals which are linearly independent and calculate the initial simplicial subcone $\mathsf{K}_0 \supseteq \Phi$.

(iv) Recursively intersect K_i, $i = 0, 1, \ldots, s$, by a new wall, in order to obtain K_{i+1}. Note that most of the walls do not intersect K_i. Finally, after all wall normals are treated, we obtain $\mathsf{K}_s = \Phi$.

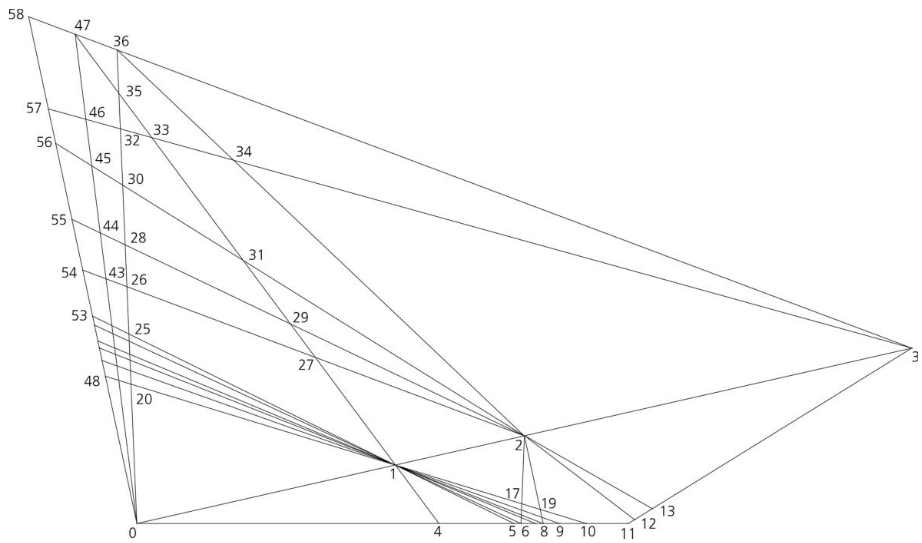

Figure 1
A two-dimensional section through the $\mathbf{E}_6 - \mathbf{F}_4$ cell complex of maximal totally zone-contracted parallelohedra.

(v) According to equation (14), for every wall $\mathsf{W}_h \subset \Phi^o$ determine a Q' in the neighbouring subcone which shares the wall W_h.

4. Results

Starting from an arbitrary primitive parallelohedron $\mathsf{P}(\mathsf{Q})$ in E^d, $2 \le d \le 6$, we calculated its subcone $\Phi(\mathsf{P})$. In order to obtain an optimal basis, only transpositions $\mathbf{a}_i = \mathbf{a}_i \pm \mathbf{a}_j$, $1 \le i \ne j \le d$, for the matrix A in equation (5) were used which quickly leads to reasonable results for $d \le 6$. Referring to such an optimal basis, we found in E^6 that the maximal components for the facet vectors have magnitude 2. By determining for each wall $\mathsf{W}_j \subset \Phi$ a Q_j in its neighbouring subcone Φ_j, $j = 1, \ldots, N_{\rm w}$, and classifying their parallelohedra according to their combinatorial type, we possibly get new types. Repeating this process, we finally will obtain all combinatorial types of primitive parallelohedra in E^d. With respect to the number $N_z^{\rm c}$ of closed zones of P, the subcones Φ_i are arranged in shells $\mathcal{S}_{N_z^{\rm c}}$. For a primitive parallelohedron P with $N_z^{\rm c}$ closed zones, we found that its subcone Φ has only neighbouring subcones which share a common wall with it in shells $\mathcal{S}_{N_z^{\rm c}-1}, \mathcal{S}_{N_z^{\rm c}}$ and $\mathcal{S}_{N_z^{\rm c}+1}$, where $N_z^{\rm c} - 1 \ge 0$, $N_z^{\rm c} + 1 \le \binom{d+1}{2}$. Thus it is sufficient to calculate subcones in shell $\mathcal{S}_{N_z^{\rm c}}$ only, in order to obtain all combinatorial types of parallelohedra having $N_z^{\rm c}$ closed zones. A similar behaviour was also found for the vertices of a primitive parallelohedron in E^6. If P defining $\Phi(P)$ has N_0 vertices then P' which defines any neighbouring subcone that shares a common wall with Φ has $N_0 - 28$, N_0 or $N_0 + 28$ vertices, where $N_0 - 28 \ge 4592$ and $N_0 + 28 \le 5040$.

Fig. 1 shows a two-dimensional section through the complex of subcones $\mathcal{S}_0$ of totally zone-contracted primitive parallelohedra, which is referred to as the $\mathbf{E}_6 - \mathbf{F}_4$ cell complex. Vertices Nos. 0, 2 and 3 correspond to the Gram matrices of the root lattices

$$\mathbf{E}_6 := \begin{pmatrix} 2 & 1 & -1 & -2 & 0 & 1 \\ & 2 & 0 & -2 & -1 & 1 \\ & & 2 & 1 & -1 & -2 \\ & & & 4 & 1 & -2 \\ & & & & 2 & 1 \\ & & & & & 4 \end{pmatrix},$$

$$\mathbf{E}_6^* := \frac{1}{2} \begin{pmatrix} 4 & 1 & -2 & -2 & 1 & 1 \\ & 4 & 1 & -2 & -2 & 1 \\ & & 4 & 1 & -2 & -2 \\ & & & 4 & -2 & -2 \\ & & & & 4 & 1 \\ & & & & & 4 \end{pmatrix}$$

and

$$\mathbf{F}_4 := \begin{pmatrix} 2 & 0 & -1 & 0 & 1 & 0 \\ & 2 & 1 & 0 & -1 & 0 \\ & & 2 & 0 & -1 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 2 & 0 \\ & & & & & 0 \end{pmatrix},$$

respectively. The parallelohedron belonging to $\mathbf{F}_4$ is the unique totally zone-contracted type of parallelohedron in E^4. The Gram matrix of $\mathbf{F}_4$ lies in a ten-dimensional subspace which intersects the cone $\mathcal{C}^+$. The section exhibits 59 subcones which are described in Table 6. Each subcone is characterized by the numbers of walls and edge forms as $N_{\rm w}.N_{\rm e}$. The polygons defined by the vertices 2–31–33–34 and 2–12–11–10–19 correspond to the subcones C1 and C2, respectively, described by Dutour & Vallentin (2005). The shells $\mathcal{S}_h$, $h = 1, \ldots, \binom{d+1}{2}$, are arranged arround the central complex with main poles at $\mathbf{E}_6$ and $\mathbf{F}_4$.

In order to define the section of Fig. 1, the following Gram matrix was used in addition:

Table 3
The numbers of combinatorial types of primitive parallelohedra in E^d, $1 \le d \le 6$, with respect to closed zones (numbers in italics are lower bounds only).

N_z^c	$d = 1$	2	3	4	5	6
0						*2054178 (1613816)*
1	1					*2795540 (1935928)*
2						*4703482 (1786091)*
3		1				*28162447 (15217832)*
4						*205502480 (95095788)*
5						*56450677 (34509507)*
6			1			*9073375 (3427592)*
7						*19131264 (12155238)*
8						*21584349 (11182713)*
9				2		*37577836 (22034218)*
10				1	135 (16)	*56029825 (37537474)*
11					58 (4)	*47477880 (29908926)*
12					24 (1)	*37889356 (15659248)*
13					3	*35697164 (10669985)*
14					1	3355657 (766718)
15					1	123661 (16024)
16						4189 (274)
17						245 (11)
18						22
19						3
20						1
21						1
Total	1	1	1	3	222 (21)	567613632 (293517383)

$$\begin{pmatrix} 4.0 & 0.9 & -2.2 & -2.1 & 1.0 & 0.8 \\ & 4.0 & 0.9 & -1.8 & -1.8 & 0.8 \\ & & 4.4 & 1.3 & -1.9 & -1.6 \\ & & & 4.2 & 0.8 & -1.6 \\ & & & & 4.0 & 0.8 \\ & & & & & 3.8 \end{pmatrix}.$$

In Table 1, the general properties of primitive parallelohedra in E^d, $2 \le d \le 6$ are stated. For dimension $d \le 4$ it was found that all subcones Φ_i are simplicial cones each having $\binom{d+1}{2}$ walls. This is no longer true for dimensions $d \ge 5$. In Table 3 are given the numbers of combinatorial types of primitive parallelohedra in E^d, $2 \le d \le 6$ with respect to the number of closed zones. The numbers of non-principal primitive types are given in parentheses. For dimension $d = 6$, the numbers in italics are lower bounds only.

In E^6, we found up till now 567 613 632 combinatorial types of primitive parallelohedra, of which 293 517 383 are non-principal primitive. The final numbers will be much larger still. Altogether, we determined 29 167 228 subcones. We note that non-principal primitive types become predominant with increasing dimension d. With decreasing numbers of closed zones, the subcones exhibit an increasing number of walls. Table 5 shows preliminary results on the maximal number N_w^m of walls of the subcones with respect to the number N_z^c of closed zones. It means that subcones of parallelohedra with few open zones are hard to calculate. Of interest is the distribution of combinatorial types of non-principal primitive parallelohedra. Among them a few subcones were found that have all subcones adjacent to a common wall lying in the same shell $\mathcal{S}_h$. Also relatively few types were found, each having 14 vertices with $\omega = 3$. Table 4 gives the distribution of combinatorial types of primitive parallelohedra with the minimal number, 4592, of vertices.

Table 4
Numbers N_0^{4592} of primitive parallelohedra with 4592 vertices with respect to closed zones N_z^c (numbers in italics are lower bounds only).

N_z^c	12	11	10	9	8	7
N_0^{4592}	234	15576	*387465*	*1148851*	*1105211*	*1069396*

N_z^c	6	5	4	3	2	1	0
N_0^{4592}	*553283*	*134343*	*20180*	1898	175	12	5

Table 5
Maximal numbers N_w^m of walls of Φ with respect to closed zones N_z^c (numbers in italics are lower bounds only).

N_z^c	21	20	19	18	17	16	15	14	13	12	11	10
N_w^m	21	21	25	21	30	38	45	47	*55*	*68*	*69*	*65*

N_z^c	9	8	7	6	5	4	3	2	1	0
N_w^m	*60*	*61*	*68*	*67*	*75*	*87*	*89*	*89*	*104*	*130*

Of particular interest are the edge forms of the subcones because their Dirichlet parallelohedra are unique up to a scale factor and are totally zone-contracted. We characterize their combinatorial types by the symbol $N_5.N_0$, where N_5, N_0 give the numbers of facets and vertices, respectively. Again their number is very large. We have determined 11 763 877 non-equivalent edge forms, but the final number will be much larger still. Among them are 182 605 edge forms having parallelohedra with the maximal number of facets, $N_5 = 126$, and $720 \le N_0 \le 4184$ vertices. The type 126.720 corresponds to the root lattice E_6^*. In Table 7 are given edge forms having parallelohedra with small numbers $60 \le N_5 \le 76$ of facets. There exist parallelohedra having less than 60 facets, but those are not totally zone-contracted. They result from parallelohedra in E^5 enhanced to E^6. The column 'Order' states for each type of parallelohedron the order of its automorphism group aut(P). In E^d, $d \ge 5$, it is still an open problem if aut(P) can be realized by an isomorphic symmetry group sym(P′) (group of isometries) for some $\mathsf{P}' \overset{comb}{\simeq} \mathsf{P}$. The types 60.76, 72.54 and 76.160 correspond to the root lattices D_6, E_6 and D_6^*, respectively, and are well known in the literature (*e.g.* Moody & Patera, 1995). Remarkably, the following parallelohedra given in Table 7 have all verices lying on a 5-sphere of radius R *viz*. 66.240, $R = 2^{1/2}$, 70.106, $R = 6^{1/2}/2$, 72.54, $R = 12^{1/2}/3$, 76.160, $R = 6^{1/2}/2$. We have calculated the order of the automorphism group for 1 141 584 edge forms, using the unified polytope scheme (Engel, 1991). Among them 89% have order 2, 10% have order 4 and only 1% have order greater than 4, and up to $2^8 3^4 5 = 103\,680$ for the root lattice E_6 and its dual E_6^*. Generally, the edge forms exhibit automorphism groups of higher order than the generic forms. Therefore, the minimal symmetry C_i is predominant among all combinatorial types of parallelohedra in E^6.

Table 6
Subcones of maximal non-contractible primitive parallelohedra shown in Fig. 1.

No.	Polygon	Subcone	No.	Polygon	Subcone
1	0-1-4	76.637527	31	8-15-16-18	80.235615
2	0-1-20	76.111796	32	9-10-19-18	92.881305
3	0-20-37	65.43437	33	16-17-19-18	86.466226
4	0-37-48	65.43437	34	20-21-38-37	65.60671
5	1-2-17	90.1570695	35	21-22-39-38	66.129686
6	1-2-27	96.1195174	36	22-23-40-39	58.25883
7	1-4-5	80.605460	37	23-24-41-40	64.65722
8	1-5-6	80.87293	38	24-25-42-41	59.33535
9	1-6-14	82.228648	39	25-26-43-42	92.1496875
10	1-14-15	84.270744	40	26-27-29-28	83.633810
11	1-15-16	88.442178	41	26-28-44-43	75.308235
12	1-16-17	92.716200	42	28-29-31-30	95.563079
13	1-20-21	76.203112	43	28-30-45-44	85.587340
14	1-21-22	77.515382	44	30-31-33-32	116.2108874
15	1-22-23	69.156668	45	30-32-46-45	105.†
16	1-23-24	75.434010	46	32-33-35	73.58314
17	1-24-25	70.257378	47	32-35-47-46	71.114426
18	1-25-26-27	99.595852	48	33-34-36-35	90.283494
19	2-3-13	81.45329	49	35-36-47	65.52293
20	2-3-34	99.1629746	50	37-38-49-48	65.60671
21	2-12-11-10-19	100.2257616	51	38-39-50-49	66.129686
22	2-12-13	75.176608	52	39-40-51-50	58.25883
23	2-17-19	92.1059050	53	40-41-52-51	64.65722
24	2-27-29	77.193693	54	41-42-53-52	59.33535
25	2-29-31	99.595852	55	42-43-54-53	92.1496875
26	2-31-33-34	130.7145429	56	43-44-55-54	75.308235
27	3-34-36	72.112930	57	44-45-56-55	86.587340
28	6-7-14	72.95308	58	45-46-57-56	104.†
29	7-8-15-14	76.112771	59	46-47-58-57	71.114426
30	8-9-18	84.476144			

† The subcone is not completely determined.

Table 7
Edge forms having totally contracted parallelohedra with a small number of facets $60 \le N_5 \le 76$ in E^6.

Type	Order	Zones	Belts	Gram matrix $q_{i,j}$, $1 \le i \le j \le 6$					
60.76	$2^6 6!$	38	6_{80}	211111	21111	2011	211	21	2
66.164	$2^8 3$	33	$4_{13}6_{88}$	$2\bar{1}0\bar{1}11$	$200\bar{1}\bar{1}$	$2\bar{1}\bar{1}0$	$30\bar{1}$	30	2
66.194	$2^6 3^2$	33	$4_{12}6_{88}$	321222	31212	2011	421	31	3
66.240	$2^8 3^2$	33	$4_{18}6_{88}$	$40\bar{1}\bar{1}\bar{1}2$	21110	2010	$41\bar{2}$	20	4
66.286	$2^8 3$	31	$4_{15}6_{88}$	422222	42223	4023	421	42	4
66.374	2^7	34	$4_{22}6_{88}$	$4\bar{1}\bar{1}\bar{2}22$	$200\bar{1}\bar{1}$	$20\bar{1}\bar{1}$	$4\bar{1}\bar{2}$	40	4
66.386	$2^5 3$	32	$4_{19}6_{93}$	$411\bar{2}\bar{1}1$	$20\bar{1}\bar{1}\bar{1}$	$2\bar{1}00$	$4\bar{1}\bar{1}$	42	4
68.194	$2^5 3^2$	39	$4_9 6_{101}$	211111	32111	3011	320	30	2
70.106	$2^6 3^2 5$	48	6_{110}	211111	21111	2011	320	30	2
72.54	$2^8 3^4 5$	63	6_{120}	211111	21111	2011	210	21	2
72.330	$2^4 3^3$	57	$4_9 6_{119}$	432223	42223	4022	421	42	4
74.336	$2^5 3$	37	$4_{13}6_{113}$	321222	42222	3011	431	41	3
74.350	2^6	37	$4_{13}6_{112}$	$3\bar{1}\bar{1}\bar{1}21$	$200\bar{1}\bar{1}$	$4\bar{1}\bar{2}\bar{1}$	$30\bar{1}$	40	3
74.460	$2^3 3$	44	$4_{10}6_{116}$	422232	42222	4022	421	42	3
74.490	2^6	37	$4_{17}6_{112}$	$21002\bar{1}$	$3102\bar{1}$	$4\bar{2}2\bar{1}$	$4\bar{2}0$	$6\bar{2}$	3
74.694	2^8	37	$4_{20}6_{112}$	$43121\bar{2}$	$6022\bar{1}$	$624\bar{3}$	$42\bar{2}$	$6\bar{3}$	4
76.160	$2^6 6!$	30	$4_{15}6_{96}$	$3\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}$	20000	2000	200	20	2
76.308	$2^{10} 3$	30	$4_{14}6_{96}$	$4\bar{1}\bar{1}\bar{1}\bar{2}\bar{1}$	20000	2000	200	40	2
76.340	$2^6 5!$	30	$4_{10}6_{96}$	$4\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}$	20000	2000	200	20	2
76.400	$2^8 3$	30	$4_{13}6_{96}$	$5\bar{2}\bar{1}\bar{1}\bar{2}\bar{1}$	40000	2000	200	40	2
76.414	2^5	36	$4_{13}6_{120}$	211111	43122	4022	420	41	3
76.526	$2^3 3$	38	$4_{13}6_{119}$	422233	42222	4022	531	52	4
76.566	2^5	36	$4_{17}6_{120}$	$51\bar{3}\bar{2}12$	$52\bar{3}\bar{3}1$	$60\bar{3}\bar{2}$	$52\bar{2}$	52	4
76.680	$2^3 3$	36	$4_{15}6_{119}$	$511\bar{2}\bar{2}1$	$20\bar{1}\bar{1}\bar{1}$	$3\bar{1}\bar{1}\bar{1}$	$5\bar{1}\bar{1}$	63	6

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References

Dirichlet, P. G. L. (1850*a*). *J. Reine Angew. Math.* **40**, 209–227.

Dirichlet, P. G. L. (1850*b*). *Oeuvre*, **2**, 41–59.

Dutour, M. & Vallentin, F. (2005). *Proc. Inst. Math. Acad. Sci. Ukraine*, **55**, 102–108.

Engel, P. (1986). *Geometric Crystallography.* Dordrecht: D. Reidel Publishing Company.

Engel, P. (1988). *Comput. Math. Appl.* **16**, 425–436.

Engel, P. (1991). *Discrete Math.* **91**, 9–31.

Engel, P. (2000). *Acta Cryst.* A**56**, 491–496.

Engel, P. (2003). *Trans. Ukr. Math. Congress Sect. Geom. Topol.*, edited by C. I. Maksimenko, pp. 22–47. Kiev: Institute of Mathematics, National Academy of Sciences of Ukraine.

Engel, P. (2005). *Proc. Inst. Math. Acad. Sci. Ukraine*, **55**, 109–125.

Engel, P. (2011). *Acta Cryst.* A**67**, 402–408.

Fedorov, E. S. (1885). *Verh. Russ. Kais. Mineral. Ges. St Petersburg*, **21**, 1–279. [Reprint: Akad. Nauk SSSR, 1953.]

McMullen, P. (1980). *Mathematica*, **27**, 113–121.

Minkowski, H. (1897*a*). *Nachr. Akad. Wiss. Göttingen. Math.-Phys. Kl.* (1897), pp. 215–219.

Minkowski, H. (1897*b*). *Gesammelte Abh.* **2**, 117–121.

Moody, R. V. & Patera, J. (1995). *Can. J. Math.* **47**, 573–605.

Ryshkov, S. S. & Baranovskiî, E. P. (1998). *Proc. Inst. Math. Acad. Sci. Ukraine*, **21**, 115–124.

Venkov, B. A. (1954). *Vestn. Leningr. Univ. Ser. Mat. Fiz. Khim.* **9**, 11–31.

Voronoï, G. M. (1908*a*). *J. Reine Math.* **134**, 198–287.

Voronoï, G. M. (1908*b*). *J. Reine Math.* **135**, 67–181.