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A complete isometry classification of 3-dimensional lattices

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Abstract A periodic lattice in Euclidean 3-space is the infinite set of all integer linear combinations of basis vectors. Any lattice can be generated by infinitely many different bases. This ambiguity was only partially resolved, but standard reductions remained discontinuous under perturbations modelling crystal vibrations. This paper completes a continuous classification of 3-dimensional lattices up to Euclidean isometry (or congruence) and similarity (with uniform scaling).

The new homogeneous invariants are uniquely ordered square roots of scalar products of four superbase vectors whose sum is zero and all pairwise angles are non-acute. These root invariants continuously change under perturbations of basis vectors. The geometric methods extend the work of Delone, Conway and Sloane.

Keywords Lattice · rigid motion · isometry · invariant · metric · continuity

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1 The hard problem to continuously classify lattices up to isometry

We extend the continuous isometry classification of 2-dimensional lattices [20] to dimension 3. A *lattice* $\Lambda \subset \mathbb{R}^n$ consists of integer linear combinations of basis vectors $v_1, \dots, v_n$. This basis spans a parallelepiped called a *unit cell* $U \subset \mathbb{R}^n$.

The problem to classify lattices up to isometry is motivated by periodic crystals whose structures are determined in a rigid form. Hence the most natural equivalence of crystals is rigid motion. We start from general isometries that also include mirror reflections because the sign of a lattice similar to [20, Definition 3.4] easily distinguishes mirror images. As in $\mathbb{R}^2$, the space of lattices up to rigid motion in $\mathbb{R}^3$ is a 2-fold cover of the smaller Lattice Isometry Space $\mathrm{LIS}(\mathbb{R}^3)$.

The previous work [20, section 1] provided important motivations for a continuous classification problem, which we state below for 3-dimensional lattices.

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Problem 1.1 (continuous classification of 3D lattices) *Find an invariant* $I :$ $\mathrm{LIS}(\mathbb{R}^3) \to \mathrm{Inv}$ *mapping the Lattice Isometry Space to a simpler space such that*

(1.1a) invariance *:* $I(\Lambda)$ *is independent of a lattice basis and is preserved under isometry of* $\mathbb{R}^3$*, so* I *has no false negatives : if* $\Lambda \cong \Lambda'$ *then* $I(\Lambda) = I(\Lambda')$*;*

(1.1b) completeness *: if* $I(\Lambda) = I(\Lambda')$*, then* Λ, Λ' *are isometric, so* I *has no false positives and defines a bijection (or a 1-1 map)* $I : \mathrm{LIS} \to \mathrm{Inv} = I(\mathrm{LIS})$*;*

(1.1c) continuity *:* $I(\Lambda)$ *is continuous under perturbations of a basis of* Λ*;*

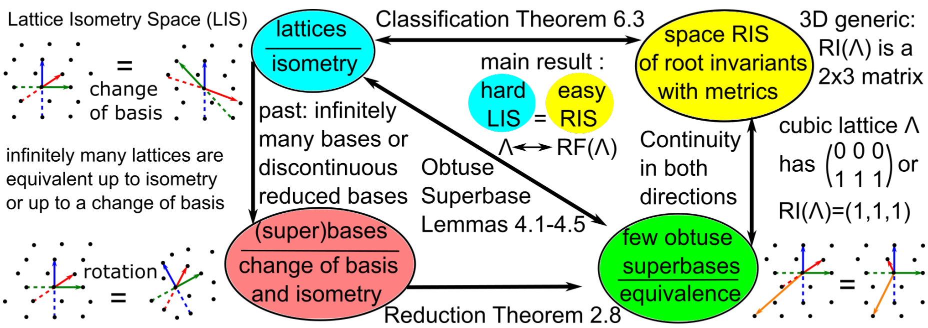
(1.1d) computability *:* $I(\Lambda)$ *can be explicitly computed from a suitable basis of* Λ*;*

(1.1e) inverse design *: a basis of* Λ *can be explicitly reconstructed from* $I(\Lambda)$*.* ■

About 30 years ago John Conway and Neil Sloane published a series of seven papers on low-dimensional lattices. The most relevant for Problem 1.1 is [13, item 1 on page 55] saying that certain lattice invariants (conorms) 'vary continuously with the lattice'. Unfortunately, there was no further discussion of continuity, which needs a metric on the space of lattices (LIS) and a metric on the space of invariants. The statement in [12, p. xxv] that "two [3-dimensional] lattices are isomorphic [isometric] if and only if the corresponding labelings differ only by an automorphism of the [projective] plane [of order 2]" holds only for generic 3D lattices of Voronoi type V_1, see Lemmas 4.1-4.5, Theorem 6.3 covering all cases.

In $\mathbb{R}^2$, [20, Problem 1.1] was stated and solved for stronger conditions (1.1c)-(1.1d) requiring a continuous and computable metric on lattices. This metric part of Problem 1.1 is postponed to the next paper, because the invariant part is already hard in $\mathbb{R}^3$. The orientation-aware equivalences (rigid motion and orientation-preserving similarity) are also postponed for future work. Fig. 1 summarises the past obstacles and a full solution to Problem 1.1. The space Inv will be the root invariant space (RIS), where any root invariant consists of up to six parameters.

Fig. 1 Vectors of an obtuse superbase of a lattice $\Lambda \subset \mathbb{R}^3$ have ordered scalar products that form the root invariants continuously parameterising the Lattise Isometry Space $\mathrm{LIS}(\mathbb{R}^3)$.



2 Main definitions and an overview of past work and new results

The previous work defined the main concepts for any dimension $n \geq 2$ in [20, section 2]. For simplicity, we remind these concepts only for $n = 3$. Any point p

in Euclidean space $\mathbb{R}^3$ can be represented by the vector from the origin $0 \in \mathbb{R}^n$ to p. This vector is also denoted by p, An equal vector p can be drawn at any initial point. The *Euclidean* distance between points $p, q \in \mathbb{R}^3$ is $|p - q|$.

Definition 2.1 (a lattice Λ, a primitive unit cell U) *Let vectors v_1, v_2, v_3 form a linear* basis *in $\mathbb{R}^3$ so that any vector $v \in \mathbb{R}^3$ can be written as $v = c_1v_1 + c_2v_2 + c_3v_3$ for some real $c_i \in \mathbb{R}$, and if $v = 0$ then $c_1 = c_2 = c_3 = 0$. A* lattice *Λ in $\mathbb{R}^3$ consists of $c_1v_1 + c_2v_2 + c_3$ for $c_i \in \mathbb{Z}$. The parallelepiped $U(v_1, v_2, v_3) = \{c_1v_1 + c_2v_2 + c_3v_3 : c_i \in [0, 1)\}$ is a* primitive unit cell *of Λ.* ▲

The conditions $0 \leq c_i < 1$ on the coefficients c_i above guarantee that the copies of unit cells $U(v_1, v_2, v_3)$ translated by all $v \in \Lambda$ are disjoint and cover $\mathbb{R}^3$.

Definition 2.2 (orientation, isometry, rigid motion, similarity) *For a basis v_1, v_2, v_3 of $\mathbb{R}^3$, the* signed volume *of $U(v_1, v_2, v_3)$ is the determinant of the 3×3 matrix with columns v_1, v_2, v_3. The sign of this $\det(v_1, v_2, v_3)$ can be called an* orientation *of the basis v_1, v_2, v_3. An* isometry *is any map $f : \mathbb{R}^3 \to \mathbb{R}^3$ such that $|f(p) - f(q)| = |p - q|$ for any $p, q \in \mathbb{R}^3$. The unit cells $U(v_1, v_2, v_3)$ and $U(f(v_1), f(v_2), f(v_3))$ have non-zero volumes with equal absolute values. If these volumes have equal signs, f is* orientation-preserving*, otherwise f is* orientation-reversing. *Any orientation-preserving isometry f is a composition of translations and rotations, and can be included into a continuous family of isometries f_t (a* rigid motion*), where $t \in [0, 1]$, f_0 is the identity map and $f_1 = f$. A* similarity *is a composition of isometry and uniform scaling $v \mapsto sv$ for a fixed scalar $s > 0$.* ▲

Any lattice Λ can be generated by infinitely many bases or unit cells. This ambiguity was traditionally resolved by a reduced basis, which can be defined in several ways [18]. All these reduced bases including Niggli's basis [24] are discontinuous under perturbations, which was highlighted in [16, section 1], see an example extendable to any dimension by adding long orthogonal basis vectors in [20, Fig. 3] and a formal proof in [28, Theorem 15]. Experimentally, discontinuity of Niggli's basis was demonstrated in the seminal work [1] and motivated the subsequent progress of Larry Andrews and Herbert Bernstein [2,3,21,4] in Problem 1.1.

The proposed solution is based on the *Voronoi domain* [26], also called the *Wigner-Seitz cell*, *Brillouin zone* or *Dirichlet cell*. We use the word *domain* to avoid a confusion with a unit cell in Definition 2.1. Though the Voronoi domain can be defined for any point of a lattice, it suffices to consider only the origin 0.

Definition 2.3 (Voronoi domain $V(\Lambda)$) *The* Voronoi domain *of a lattice $\Lambda \subset \mathbb{R}^3$ is the neighbourhood $V(\Lambda) = \{p \in \mathbb{R}^3 : |p| \leq |p - v| \text{ for any } v \in \Lambda\}$ of the origin $0 \in \Lambda$ consisting of all points p that are non-strictly closer to* 0 *than to other points $v \in \Lambda$. A vector $v \in \Lambda$ is a* Voronoi vector *if the bisector hyperspace $H(0, v) = \{p \in \mathbb{R}^n : p \cdot v = \frac{1}{2}v^2\}$ between 0 and v intersects $V(\Lambda)$. If $V(\Lambda) \cap H(0, v)$ is a 2-dimensional face of $V(\Lambda)$, then v is called a* strict *Voronoi vector.* ▲

Voronoi [26] proved any lattice $\Lambda \subset \mathbb{R}^3$ has one of the Voronoi types below:

Voronoi type V_1: a truncated octahedron;

Voronoi type V_2: a hexa-rhombic dodecahedron;

Voronoi type V_3: a rhombic dodecahedron;

Voronoi type V_4: a hexagonal prism;

Voronoi type V_5: a cuboid (an orthogonal parallelepiped or a rectangular box).

Any lattice is determined by its Voronoi domain by [20, Lemma A.1]. However, the combinatorial structure of $V(\Lambda)$ is discontinuous under perturbations. Almost any perturbation of an orthogonal basis in $\mathbb{R}^3$ (whose lattice has a cuboid Voronoi domain) gives a generic lattice whose Voronoi domain of type V_1. Hence any integer-valued descriptors of $V(\Lambda)$ such as the numbers of vertices or edges are always discontinuous and unsuitable for continuous quantification of similarities between arbitrary crystals or periodic point sets.

Optimal geometric matching of Voronoi domains with a shared centre led [22] to two continuous metrics (up to orientation-preserving isometry and similarity) on lattices. The minimisation over infinitely many rotations was implemented in [22] by sampling and gave approximate algorithms for these metrics. The complete invariant isoset [7] for periodic point sets in $\mathbb{R}^n$ has a continuous metric that can be approximated [6] with a factor $O(n)$. The metric on invariant density functions [16] required a minimisation over $\mathbb{R}$, so far without approximation guarantees.

Lemma 2.4 shows how to find all Voronoi vectors of any lattice $\Lambda \subset \mathbb{R}^n$. The doubled lattice is $2\Lambda = \{2v \,:\, v \in \Lambda\}$. Vectors $u, v \in \Lambda$ are called *2Λ-equivalent* if $u-v \in 2\Lambda$. Then any vector $v \in \Lambda$ generates its 2Λ-class $v+2\Lambda = \{v+2u \,:\, u \in \Lambda\}$, which is 2Λ translated by v and containing $-v$. All classes of 2Λ-equivalent vectors form the quotient space $\Lambda/2\Lambda$.

Lemma 2.4 (a criterion for Voronoi vectors [13, Theorem 2]) *For any lattice $\Lambda \subset \mathbb{R}^n$, a non-zero vector $v \in \Lambda$ is a Voronoi vector of Λ if and only if v is a shortest vector in its 2Λ-class $v + 2\Lambda$. Also, v is a strict Voronoi vector if and only if $\pm v$ are the only shortest vectors in the 2Λ-class $v + 2\Lambda$.* ∎

We use the notations from [13], though obtuse superbases and their conorms were studied earlier by Selling [25] for $n = 3$ and Delone for any $n \geq 2$ [15].

Definition 2.5 (obtuse superbase, conorms p_{ij}) *For any basis v_1, v_2, v_3 in $\mathbb{R}^n$, the* superbase *includes the vector $v_0 = -v_1-v_2-v_3$. The* conorms *$p_{ij} = -v_i \cdot v_j$ are the negative scalar products of the vectors above. The superbase is* obtuse *if all conorms $p_{ij} \geq 0$, so all angles between vectors v_i, v_j are non-acute for distinct indices $i, j \in \{0, 1, 2, 3\}$. The superbase is* strict *if all $p_{ij} > 0$.* ▲

[13, formula (1)] has a typo initially defining p_{ij} as exact Selling parameters, but later Theorems 3, 7, 8 use the non-negative conorms $p_{ij} = -v_i \cdot v_j \geq 0$.

The indices of a conorm p_{ij} are distinct and unordered. We set $p_{ij} = p_{ji}$ for all i, j. Any superbase of $\mathbb{R}^3$ has six conorms $p_{12}, p_{13}, p_{23}, p_{01}, p_{02}, p_{03}$.

Definition 2.6 (partial sums v_S, vonorms v_S^2) *Let a lattice $\Lambda \subset \mathbb{R}^n$ have a superbase $B = \{v_0, v_1, v_2, v_3\}$. For any proper subset $S \subset \{0, 1, 2, 3\}$ of indices, consider its complement $\bar{S} = \{0, 1, 2, 3\} - S$ and the* partial sum *$v_S = \sum\limits_{i \in S} v_i$ whose squared lengths v_S^2 are called the* vonorms *of B and can be expressed as*

$$v_S^2 = \Big(\sum_{i \in S} v_i\Big)\Big(-\sum_{j \in \bar{S}} v_j\Big) = -\sum_{i \in S, j \in \bar{S}} v_j \cdot v_j = \sum_{i \in S, j \in \bar{S}} p_{ij}. \tag{2.6a}$$

For example, $v_i^2 = p_{ij}+p_{ik}+p_{il}$ for any unordered triple $\{j, k, l\} = \{0, 1, 2, 3\}-\{i\}$,

$v_{ij}^2 = (v_i + v_j)^2 = (-v_k - v_l)^2 = p_{ik} + p_{il} + p_{jk} + p_{jl}$ *for* $\{k, l\} = \{0, 1, 2, 3\} - \{i, j\}$. *For instance,* $v_0^2 = p_{01} + p_{02} + p_{03}$. *The six conorms are conversely expressed as*

$$p_{ij} = \frac{1}{2}(v_i^2 + v_j^2 - v_{ij}^2) \text{ for any distinct indices } i, j \in \{0, 1, 2, 3\}. \tag{2.6b}$$

The seven vonorms above have the relation $v_0^2 + v_1^2 + v_2^2 + v_3^2 = v_{01}^2 + v_{02}^2 + v_{03}^2$. ▲

Lemma 2.7 will help classify obtuse superbases for all five Voronoi domains.

Lemma 2.7 (Voronoi vectors v_S [13, Theorem 3]) *For any obtuse superbase* v_0, v_1, v_2, v_3 *of a lattice, all partial sums* v_S *from Definition 2.6 split into seven symmetric pairs* $v_S = -v_{\bar{S}}$*, which are Voronoi vectors representing distinct* 2Λ*-classes in* $\Lambda/2\Lambda$*. All Voronoi vectors* v_S *are strict if and only if all* $p_{ij} > 0$. ■

By Conway and Sloane [13, section 2], any lattice $\Lambda \subset \mathbb{R}^n$ that has an obtuse superbase is called a *lattice of Voronoi's first kind*. It turns out that any lattice in dimensions 2 and 3 is of Voronoi's first kind by Theorem 2.8, likely for any $n \geq 4$ because higher dimensions have 'more space' for obtuse superbases.

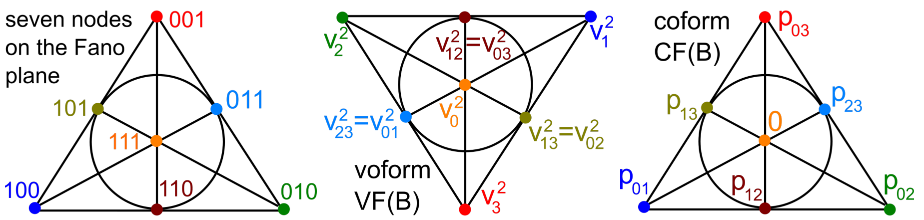
Theorem 2.8 (reduction to an obtuse superbase) *Any lattice* $\Lambda \subset \mathbb{R}^3$ *has an obtuse superbase* $\{v_0, v_1, v_2, v_3\}$ *so that all conorms* $p_{ij} = -v_i \cdot v_j \geq 0$. ▲

Conway and Sloane in [13, section 7] attempted to prove Theorem 2.8 for $n = 3$ by example whose details are corrected after the updated proof in appendix A.

3 Voforms and coforms of an obtuse superbase of a 3D lattice

For a lattice $\Lambda \subset \mathbb{R}^3$ with an obtuse superbase B, Definition 3.1 introduces the voform $\mathrm{VF}(B)$ and the coform $\mathrm{CF}(B)$, which will be converted into root invariants later. These forms are Fano planes marked by vonorms and conorms, respectively. The *Fano* projective plane of order 2 consists of seven non-zero classes (called *nodes*) of the space $\Lambda/2\Lambda$, arranged in seven triples (called *lines*). If we mark these nodes by binary numbers 001, 010, 011, 100, 101, 110, 111, the digit-wise sum of any two numbers in each line equals the third number modulo 2, see Fig. 2.

Fig. 2 **Left**: the Fano plane is a set of seven nodes arranged in triples shown by six lines and one circle. **Middle**: nodes of the voform $\mathrm{VF}(\Lambda)$ are marked by vonorms v_i^2 and v_{ij}^2. **Right**: nodes of the coform $\mathrm{CF}(\Lambda)$ are marked by conorms p_{ij} and 0.



Definition 3.1 (voform $\mathrm{VF}(B)$ and coform $\mathrm{CF}(B)$ of an obtuse superbase) *The* voform $\mathrm{VF}(B)$ *of any obtuse superbase $B = (v_0, v_1, v_2, v_3)$ in $\mathbb{R}^3$ is the Fano plane in Fig. 2 with four nodes marked by $v_0^2, v_1^2, v_2^2, v_3^2$ and three nodes marked by $v_{12}^2, v_{23}^2, v_{13}^2$ so that v_0^2 is in the centre, v_1^2 is opposite to v_{23}^2, etc. The* coform $\mathrm{CF}(B)$ *is the dual Fano plane in Fig. 2 with three nodes marked by p_{12}, p_{23}, p_{13} and three nodes marked by p_{01}, p_{02}, p_{03}, the centre is marked by 0.* ▲

Much earlier than [13], Delone represented an obtuse superbase B of $\vec{a}, \vec{b}, \vec{c}$, $\vec{d} = -\vec{a} - \vec{b} - \vec{c}$ by the skeleton of a tetrahedron with six (negative) scalar products on edges. This *Delone tetrahedron* is equivalent to the coform $\mathrm{CF}(B)$, which will be written in a matrix form in Definition 3.3. In 1975 [14, chapter 10.4, p. 154] claimed (without proof) a unique description of any lattice up to isometry by a 6-parameter Delone symbol satisfying sophisticated systems of equations and inequalities in 16 cases. Theorem 6.3 will give a simpler and proved solution by root invariants in Definition 5.1 based on only five Voronoi types.

The *zero* conorm $p_0 = 0$ at the centre of the coform $\mathrm{CF}(B)$ seems mysterious, because Conway and Sloane [13] gave no formula for p_0, which also wrongly became non-zero in their Fig. 5. This past mystery is explained by Lemma 3.2.

Lemma 3.2 (6 conorms $\leftrightarrow$ 7 vonorms) *For distinct indices $i, j \in \{0, 1, 2, 3\}$, the conorm p_{ij} in $\mathrm{CF}(B)$ of any superbase B defines the dual line in the voform $\mathrm{VF}(B)$ through the nodes marked by v_{ij}^2, v_k^2, v_l^2 for $\{k, l\} = \{0, 1, 2, 3\} - \{i, j\}$. Then*

$$4p_{ij} = v_i^2 + v_j^2 + v_{ik}^2 + v_{jk}^2 - v_{ij}^2 - v_k^2 - v_l^2, \tag{3.2a}$$

where the vonorms with negative signs are in the line of the voform $\mathrm{VF}(B)$ dual to p_{ij}. The zero conorm $p_0 = 0$ in $\mathrm{CF}(B)$ can be computed by the similar formula

$$4p_0 = v_0^2 + v_1^2 + v_2^2 + v_3^2 - v_{01}^2 - v_{02}^2 - v_{03}^2 = 0, \tag{3.2b}$$

where the line dual to the zero conorm p_0 is the 'circle' through $v_{01}^2, v_{02}^2, v_{03}^2$. ■

Proof Since all indices $i, j, k, l \in \{0, 1, 2, 3\}$ are distinct, formula (3.2a) is symmetric in k, l due to $v_{ik}^2 + v_{jk}^2 = v_{il}^2 + v_{jl}^2$ following from $v_{ik} = v_i + v_k = -(v_j + v_l) = -v_{jl}$, $v_{jk} = v_j + v_k = -(v_i + v_l) = -v_{il}$. To prove (3.2a), simplify its right hand side:

$$v_i^2 + v_j^2 + v_{ik}^2 + v_{jk}^2 - v_{ij}^2 - v_k^2 - v_l^2 = v_i^2 + v_j^2 + (v_i + v_k)^2 + (v_j + v_k)^2 - (v_i + v_j)^2 - v_k^2 -$$

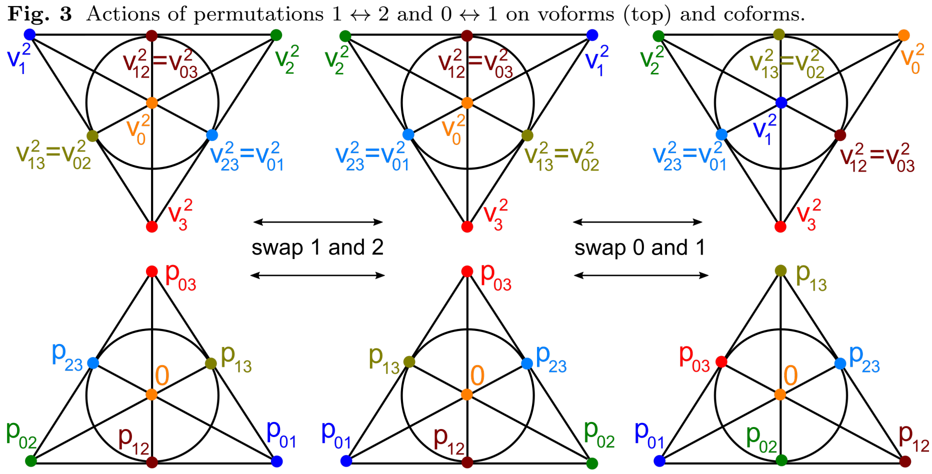
$$-(-v_i - v_j - v_k)^2 = v_i^2 + v_j^2 + (v_i^2 + 2v_i v_k + v_k^2) + (v_j^2 + 2v_j v_k + v_k^2) -$$

$$-(v_i^2 + 2v_i v_j + v_j^2) - v_k^2 - (v_i^2 + v_j^2 + v_k^2 + 2v_i v_j + 2v_i v_k + 2v_j v_k) = -4v_i v_j = 4p_{ij}.$$

(3.2b) follows from $v_0^2 + v_1^2 + v_2^2 + v_3^2 = v_{01}^2 + v_{02}^2 + v_{03}^2$ in Definition 3.1. □

Definition 3.3 (index-permutations on vonorms and conorms) *For any ordered obtuse superbase $B = \{v_0, v_1, v_2, v_3\}$, an* index-permutation *is a permutation $\sigma \in S_4$ of indices $0, 1, 2, 3$, which maps vonorms as follows: $v_i^2 \mapsto v_{\sigma(i)}^2$, $v_{ij}^2 \mapsto v_{\sigma(i)\sigma(j)}^2$, where $v_{ij}^2 = v_{ji}^2$. If we swap v_1^2, v_2^2, then we also swap only $v_{13}^2 = v_{02}^2$ and $v_{23}^2 = v_{01}^2$. If we swap v_0^2, v_1^2, then we also swap only $v_{12}^2 = v_{03}^2$ and $v_{02}^2 = v_{13}^2$, see Fig. 3. Any index-permutation $\sigma \in S_4$ maps conorms by $p_{ij} \mapsto p_{\sigma(i)\sigma(j)}$, where $p_{ij} = p_{ji}$. The group S_4 of all 24 index-permutations is generated by the three* index-transpositions $0 \leftrightarrow 1$, $1 \leftrightarrow 2$, $2 \leftrightarrow 3$. ▲

Fig. 3 Actions of permutations $1 \leftrightarrow 2$ and $0 \leftrightarrow 1$ on voforms (top) and coforms.



For any ordered superbase $\{v_0, v_1, v_2, v_3\}$, the voform can be written as the 2×3 matrix $\mathrm{VF}(B) = \begin{pmatrix} v_{23}^2 & v_{13}^2 & v_{12}^2 \\ v_1^2 & v_2^2 & v_3^2 \end{pmatrix}$, where $v_{23}^2 = v_{01}^2$ is above v_1^2 and so on. The 7th vonorm can be found as $v_0^2 = v_{23}^2 + v_{13}^2 + v_{12}^2 - v_1^2 - v_2^2 - v_3^2$ and is unnecessary to include into the matrix. A coform can be written as $\mathrm{CF}(B) = \begin{pmatrix} p_{23} & p_{13} & p_{12} \\ p_{01} & p_{02} & p_{03} \end{pmatrix}$.

Lemma 3.4 *For any ordered obtuse superbase $B = \{v_0, v_1, v_2, v_3\}$, all 24 index-permutations act on the coform $\mathrm{CF}(B)$ as compositions of the transpositions:*
(a) *$i \leftrightarrow j$ for non-zero $i \neq j$ swaps the columns i, j in $\mathrm{CF}(B)$, for example*

$$\begin{pmatrix} p_{13} & p_{23} & p_{12} \\ p_{02} & p_{01} & p_{03} \end{pmatrix} \overset{1\leftrightarrow 2}{\longleftrightarrow} \begin{pmatrix} p_{23} & p_{13} & p_{12} \\ p_{01} & p_{02} & p_{03} \end{pmatrix} \overset{0\leftrightarrow 1}{\longleftrightarrow} \begin{pmatrix} p_{23} & p_{03} & p_{02} \\ p_{01} & p_{12} & p_{13} \end{pmatrix}; \tag{3.4a}$$

(b) *$0 \leftrightarrow i$ for $i \neq 0$ diagonally swaps pairs in the columns of indices $j \neq i, 0$.*
Any even permutation from A_4 acts as composition of the following permutations:

$$\begin{pmatrix} p_{23} & p_{02} & p_{03} \\ p_{01} & p_{13} & p_{12} \end{pmatrix} \overset{0\leftrightarrow 1, 2\leftrightarrow 3}{\longleftrightarrow} \begin{pmatrix} p_{23} & p_{13} & p_{12} \\ p_{01} & p_{02} & p_{03} \end{pmatrix} \overset{0\mapsto 1\mapsto 2\mapsto 0}{\longleftrightarrow} \begin{pmatrix} p_{03} & p_{23} & p_{02} \\ p_{12} & p_{01} & p_{13} \end{pmatrix}. \tag{3.4b}$$

Proof By Definition 3.3 the action of any index-permutation $\sigma \in S_4$ on $\mathrm{CF}(B)$ follows by permuting the indices of conorms: $p_{ij} \mapsto p_{\sigma(i)\sigma(j)}$. In all cases, any two conorms from one column of $\mathrm{CF}(B)$ remain in one column. The composition of two transpositions such as $0 \leftrightarrow 1, 2 \leftrightarrow 3$ vertically swaps conorms in columns $2, 3$. The even permutation $1 \mapsto 2 \mapsto 3 \mapsto 1$ cyclically permutes columns $1, 2, 3$. Another even permutation $0 \mapsto 1 \mapsto 2 \mapsto 0$ involving index 0 cyclically permutes the triples

(p_{23}, p_{13}, p_{03}) of the coforms all including index 3 and the triple (p_{01}, p_{02}, p_{12}) of the coforms all excluding index 3. □

Lemma 3.4 shows that coforms of six conorms are easier than voforms, which essentially require seven vonorms since v_0^2 appears after the transposition $0 \leftrightarrow 1$.

$$\begin{pmatrix} v_{13}^2 & v_{23}^2 & v_{12}^2 \\ v_2^2 & v_1^2 & v_3^2 \end{pmatrix} \overset{1\leftrightarrow 2}{\longleftrightarrow} \mathrm{VF}(B) = \begin{pmatrix} v_{23}^2 & v_{13}^2 & v_{12}^2 \\ v_1^2 & v_2^2 & v_3^2 \end{pmatrix} \overset{0\leftrightarrow 1}{\longleftrightarrow} \begin{pmatrix} v_{23}^2 & v_{12}^2 & v_{13}^2 \\ v_0^2 & v_2^2 & v_3^2 \end{pmatrix}$$

Definition 3.5 (odd-sum and even-sum vectors, digital sums) *For any basis v_1, v_2, v_3 in $\mathbb{R}^3$, write the partial sums v_S from Lemma 2.7 in coordinates:*

(3.5o) $v_1 = (1, 0, 0)$, $v_2 = (0, 1, 0)$, $v_3 = (0, 0, 1)$, $v_0 = (-1, -1, -1)$;

(3.5e) $v_{12} = v_1 + v_2 = (1, 1, 0)$, $v_{23} = v_2 + v_3 = (0, 1, 1)$, $v_{13} = v_1 + v_3 = (1, 0, 1)$.

The four vectors (and their opposites) from (3.5o) are called odd-sum *vectors, because the sum of their coordinates is odd. The three vectors (and their opposites) from (3.5e) are called* even-sum *vectors. For any vector $v = (x_1, x_2, x_3)$ with coordinates $x_1, x_2, x_3 \in \mathbb{Z}$, its* digital *image is $[v] = 100x_1 + 10x_2 + x_3$.* ▲

Lemma 3.6 (digital sums sufficiency) *For any basis v_1, v_2, v_3, let u, v be sums of at most four vectors v_S in Lemma 2.7. Then $u = v$ if and only if $[u] = [v]$.* ■

Proof Any partial sum or its opposite from (3.5o,e) has all coordinates in the range $[-1, 1]$. Both u, v have coordinates in the range $[-4, 4]$. The equality between $[v] = 100x_1 + 10x_2 + x_3$ and $[u] = 100y_1 + 10y_2 + y_3$ is equivalent to $100(x_1 - x_2) + 10(y_1 - y_2) + (z_1 - z_2) = 0$. Since each integer difference in the brackets is within $[-8, 8]$, the last equality can hold only if all differences vanish, so $u = v$. □

4 An explicit description all obtuse superbases of 3D lattices

In this section Lemmas 4.1-4.5 describe all possible obtuse superbases of any lattice $\Lambda \subset \mathbb{R}^3$. Any obtuse superbase $\{v_0, v_1, v_2, v_3\}$ has its dual $\{-v_0, -v_1, -v_2, -v_3\}$ related by the central symmetry with respect to 0. Lemmas 4.1-4.5 describe all obtuse superbases and their coforms separately for each Voronoi type.

Even in the generic case, [14, chapter 7.5, p. 130] missed the following step and went straight to Delone paramaters of a single obtuse superbase. Lemma 4.1 proves that any lattice Λ of a Voronoi type V_1 has only one pair centrally symmetric obtuse superbases. There will be more non-isometric obtuse superbases for higher symmetry types in Lemmas 4.2-4.5.

Lemma 4.1 (obtuse superbases for Voronoi type V_1) *Let a lattice $\Lambda \subset \mathbb{R}^3$ have Voronoi type V_1, so the Voronoi domain $V(\Lambda)$ is a truncated octahedron.*

(a) *Λ has two obtuse superbases related by the central symmetry $v \leftrightarrow -v$;*

(b) *coforms of all obtuse superbases of Λ are related by 24 index-permutations.* ■

Proof **(a)** Let $\{v_0, v_1, v_2, v_3\}$ be any obtuse superbase of Λ, which exists by Theorem 2.8. Since the Voronoi domain $V(\Lambda)$ is a truncated octahedron with seven pairs of parallel opposite faces. The lattice Λ has seven pairs of strict Voronoi vectors orthogonal to these faces. By Lemma 2.7 all these seven pairs of Voronoi vectors should coincide with the partial sums and their opposites $\pm v_S$ from (3.5o,e).

The Voronoi domain $V(\Lambda)$ has four pairs of opposite hexagonal faces obtained by cutting corners in four pairs of opposite triangular faces of an octahedron. The normal vectors of these hexagons are Voronoi odd-sum vectors $\pm v_i$, $i = 0, 1, 2, 3$. The Voronoi even-sum vectors $v_{ij} = v_i + v_j$ are normal to the three pairs of opposite parallelogram faces obtained by cutting three pairs of opposite vertices.

The seven pairs of Voronoi vectors have these digital sums from Definition 3.5:
(4.1o) Voronoi odd-sums $[\pm v_1] = \pm 100$, $[\pm v_2] = \pm 10$, $[\pm v_3] = \pm 1$, $[\pm v_0] = \mp 111$.

(4.1e) Voronoi even-sum vectors $[\pm v_{12}] = \pm 110$, $[\pm v_{23}] = \pm 11$, $[\pm v_{13}] = \pm 101$.

If an obtuse superbase $\{u_0, u_1, u_2, u_3\}$ consists of four odd-sum vectors, by Lemma 3.6 the condition $u_0 + u_1 + u_2 + u_3 = 0$ is equivalent to $[u_0] + [u_1] + [u_2] + [u_3] = 0$ for some digital sums from (4.1o). The only possibility $100 + 10 + 1 + (-111) = 0$ up to a sign gives the known obtuse superbases $\pm\{v_0, v_1, v_2, v_3\}$. If an obtuse superbase has one even-sum vector u_0, then it should have one more, say u_1, otherwise an odd sum $[u_1] + [u_2] + [u_3]$ cannot become 0 after adding an even integer $[u_0]$. For any choice of $u_0 \neq \pm u_1$ from (4.1e), by Lemma 2.7 the sum $u_0 + u_1$ should be another even-sum vector from (4.1e). But there is no choice of signs such that $\pm 110 \pm 11 \pm 101 = 0$.

(b) By part (a) all obtuse superbases B of Λ differ either by re-ordering vectors of B or by the central symmetry with respect to the origin of $\mathbb{R}^3$, which keeps the coform $\mathrm{CF}(B)$ invariant. Lemma 3.4(c) implies that coforms $\mathrm{CF}(B)$ of all obtuse superbases B of Λ are related by 24 index-permutations from Definition 3.3. $\square$

Lemma 4.2 (obtuse superbases for Voronoi type V_2) *Let a lattice $\Lambda \subset \mathbb{R}^3$ have Voronoi type V_2, so the Voronoi domain is a hexa-rhombic dodecahedron.*

(a) *Λ has an obtuse superbase $\{v_0, v_1, v_2, v_3\}$ with one pair of orthogonal vectors, say $v_2 \cdot v_3 = 0$. Then any obtuse superbase B of Λ is isometric to one of*

(4.2) *obtuse superbases* $B_1 = \{v_0, v_1, v_2, v_3\}$ *and* $B_2 = \{v_0 + v_3, v_1 + v_3, v_2, -v_3\}$.

(b) *Let an obtuse superbase $B = \{v_0, v_1, v_2, v_3\}$ with $v_1 \cdot v_2 = 0$ have a coform* $\mathrm{CF}(B_1) = \begin{pmatrix} 0 & p_{13} & p_{12} \\ p_{01} & p_{02} & p_{03} \end{pmatrix}$ *with $p_{23} = 0$. Then another obtuse superbase* $B_2 = \{v_0 + v_3, v_1 + v_3, v_2, -v_3\}$ *has the coform* $\mathrm{CF}(B_2) = \begin{pmatrix} 0 & p_{03} & p_{12} \\ p_{01} & p_{02} & p_{13} \end{pmatrix}$.

(c) *Any obtuse superbase B of Λ has exactly one zero conorm. The 24 index-permutations from Definition 3.3 allow us to write* $\mathrm{CF}(B) = \begin{pmatrix} 0 & p_{13} & p_{12} \\ p_{01} & p_{02} & p_{03} \end{pmatrix}$.

The above forms with $p_{23} = 0$ *over all obtuse superbases of* Λ *are related by the symmetry group* D_4 *(of a square) acting on the* 2×2 *submatrix* $\begin{pmatrix} p_{13} & p_{12} \\ p_{02} & p_{03} \end{pmatrix}$. ■

Proof **(a)** In comparison with the most generic Voronoi domain in Lemma 4.1, a hexa-rhombic dodecahedron $V(\Lambda)$ has six pairs of faces: two pairs of hexagons and four pairs parallelograms with one pair degenerated from one pair of hexagons and one pair of parallelograms disappeared. This degeneracy appears when exactly two of four superbase vectors become orthogonal, say $v_2 \cdot v_3 = 0$.

In addition to the seven pairs of Voronoi vectors $\pm v_S$ from Lemma 4.1, we have exactly one extra pair of the non-strict Voronoi vectors $\pm(v_3 - v_2)$ whose length equals $|v_3 + v_2|$ due to $v_2 \cdot v_3 = 0$. Now we have the extra choice of the Voronoi even-sum vector $v_3 - v_2 = (0, -1, 1)$ and its opposite. Here are the digital images of all $4 \times 2 + 4 \times 2$ Voronoi vectors.

(4.2o) Voronoi odd-sums $[\pm v_1] = \pm 100$, $[\pm v_2] = \pm 10$, $[\pm v_3] = \pm 1$, $[\pm v_0] = \mp 111$.

(4.2e) even : $[\pm v_{12}] = \pm 110$, $[\pm v_{23}] = \pm 11$, $[\pm v_{13}] = \pm 101$, $[\pm(v_3 - v_2)] = \mp 9$.

If an obtuse superbase has only four odd-sum vectors from (4.2e), we can get only $\pm B_1 = \pm\{v_0, v_1, v_2, v_3\}$ as in Lemma 4.1. Choosing an even-sum vector u_0 from (4.2e), we should include at least one more even-sum vector, say u_1. The negative partial sum $-u_0 - u_1$ by Lemma 2.7 should be among other Voronoi even-sum vectors in (4.2e) so that $[u_0] + [u_1] + [-u_0 - u_1] = 0$. Without a vector from the new pair $\pm(v_3 - v_2)$, no choice of signs gives $0 = \pm 110 \pm 11 \pm 101$.

The only possible identity $[u_0] + [u_1] + [-u_0 - u_1] = 0$ with a new digital sum 9 from (4.2e) is $110 - 101 - 9 = 0$ up to a permutation and an overall sign. Hence we can get another obtuse superbase (potentially not isometric to B_1) only by choosing $u_0 = -v_{12} = -v_1 - v_2 = v_0 + v_3$ with $[u_0] = -110$ and $u_1 = v_{13} = v_1 + v_3$ with $[u_1] = 101$ so that $u_0 + u_1 = v_3 - v_2$ with $[u_0] = -9$ (up to a sign and re-ordering).

Other superbase vectors u_2, u_3 should have the digital sum $[u_2]+[u_3] = -[u_0]-[u_1] = 110 - 101 = 9$. The remaining digital sums from (4.2o) and (4.2e) give only one splitting $9 = 10-1$, so $u_2 = v_2$, $u_3 = -v_3$. We got the second obtuse superbase from (4.2): $B_2 = \{u_0, u_1, u_2, u_3\} = \{v_0 + v_3, v_1 + v_3, v_2, -v_3\}$.

Using the transposition $2 \leftrightarrow 3$ of indices and respecting $v_2 \cdot v_3 = 0$, we get the obtuse superbase $\{v_0 + v_2, v_1 + v_2, v_3, -v_2\} = \{-v_1 - v_3, -v_0 - v_3, v_3, -v_2\}$. After re-ordering, the last superbase becomes opposite (isometric via $v \mapsto -v$) to B_2. Under the transposition $0 \leftrightarrow 1$, vectors are only permuted in both B_1, B_2.

(b) The conorms q_{ij} of the superbase $B_2 = \{v_0+v_3, v_1+v_3, v_2, -v_3\}$ are expressed via the conorms p_{ij} of $B_1 = \{v_0, v_1, v_2, v_3\}$ with $p_{23} = -v_2 \cdot v_3 = 0$ as follows:

$q_{23} = -v_2 \cdot (-v_3) = v_2 \cdot v_3 = 0$,

$q_{13} = -(v_1 + v_3) \cdot (-v_3) = (v_0 + v_2) \cdot (-v_3) = -v_0 \cdot v_3 = p_{03}$,

$q_{12} = -(v_1 + v_3) \cdot v_2 = -v_1 \cdot v_2 = p_{12}$,

$q_{01} = -(v_0+v_3)\cdot(v_1+v_3) = (v_1+v_2)\cdot(v_1+v_3) = v_1(v_1+v_2+v_3) = -v_1\cdot v_0 = p_{01}$,

$q_{02} = -(v_0 + v_3) \cdot v_2 = -v_0 \cdot v_2 = p_{02}$,

$$q_{03} = -(v_0+v_3)\cdot(-v_3) = (v_1+v_2)\cdot(-v_3) = p_{13}, \text{ so } \mathrm{CF}(B_2) = \begin{pmatrix} 0 & p_{03} & p_{12} \\ p_{01} & p_{02} & p_{13} \end{pmatrix}.$$

(c) By parts **(a,b)** and Lemma 3.4, the coform of any superbase of Λ up to 24 index-permutations is either $\mathrm{CF}(B_1) = \begin{pmatrix} 0 & p_{13} & p_{12} \\ p_{01} & p_{02} & p_{03} \end{pmatrix}$ or $\mathrm{CF}(B_2) = \begin{pmatrix} 0 & p_{03} & p_{12} \\ p_{01} & p_{02} & p_{13} \end{pmatrix}$ related by the transposition $p_{13} \leftrightarrow p_{03}$. Keeping the first column fixed, the index-permutations induced by $2 \leftrightarrow 3$ and $0 \leftrightarrow 1$ act on $\begin{pmatrix} p_{13} & p_{12} \\ p_{02} & p_{03} \end{pmatrix}$ by swapping the columns and by swapping diagonally opposite elements, see Definition 3.3.

Use $\mathbf{CF}(\boldsymbol{B_1})$: $\begin{pmatrix} p_{12} & p_{13} \\ p_{03} & p_{02} \end{pmatrix} \overset{2\leftrightarrow 3}{\leftarrow\!\mapsto} \begin{pmatrix} \boldsymbol{p_{13}} & \boldsymbol{p_{12}} \\ \boldsymbol{p_{02}} & \boldsymbol{p_{03}} \end{pmatrix} \overset{0\leftrightarrow 1}{\mapsto} \begin{pmatrix} p_{03} & p_{02} \\ p_{12} & p_{13} \end{pmatrix} \overset{2\leftrightarrow 3}{\mapsto} \begin{pmatrix} p_{02} & p_{03} \\ p_{13} & p_{12} \end{pmatrix}$.

Use $\mathbf{CF}(\boldsymbol{B_2})$: $\begin{pmatrix} p_{12} & p_{03} \\ p_{13} & p_{02} \end{pmatrix} \overset{2\leftrightarrow 3}{\leftarrow\!\mapsto} \begin{pmatrix} \boldsymbol{p_{03}} & \boldsymbol{p_{12}} \\ \boldsymbol{p_{02}} & \boldsymbol{p_{13}} \end{pmatrix} \overset{0\leftrightarrow 1}{\mapsto} \begin{pmatrix} p_{13} & p_{02} \\ p_{12} & p_{03} \end{pmatrix} \overset{2\leftrightarrow 3}{\mapsto} \begin{pmatrix} p_{02} & p_{13} \\ p_{03} & p_{12} \end{pmatrix}$. The eight arrangements above are realised by the symmetry group D_4 of a square.

Lemma 4.3 (obtuse superbases for Voronoi type V_3**)** *Let a lattice $\Lambda \subset \mathbb{R}^3$ have Voronoi type V_3, so the Voronoi domain $V(\Lambda)$ is a rhombic dodecahedron.*

(a) *In this case the lattice Λ has an obtuse superbase $B_1 = \{v_0, v_1, v_2, v_3\}$ with two different pairs of orthogonal vectors, say $v_0 \cdot v_1 = 0 = v_2 \cdot v_3$. Then any obtuse superbase of Λ is isometric to one of the following obtuse superbases:*

$$(4.3) \quad B_1, \quad B_2 = \{v_0+v_3, v_1+v_3, v_2, -v_3\}, \quad B_3 = \{v_0, -v_1, v_2+v_1, v_3+v_1\}.$$

(b) *Any obtuse superbase B of Λ has exactly two zero conorms in one column. The 24 index-permutations from Definition 3.3 allow us to write* $\mathrm{CF}(B) = \begin{pmatrix} 0 & p_{13} & p_{12} \\ 0 & p_{02} & p_{03} \end{pmatrix}$.
In the above form with $p_{23} = 0 = p_{01}$ for all obtuse superbases of Λ, the four non-zero conorms can be freely permuted by the symmetry group S_4. ■

Proof **(a)** In comparison with Lemma 4.2, a rhombic dodecahedron has five pairs of parallelograms degenerated from a 12-face hexa-rhombic dodecahedron due to another pair of orthogonal vectors, say $v_0 \cdot v_1 = 0$ in addition to $v_2 \cdot v_3 = 0$.

This degeneracy adds the 9th pair of non-strict Voronoi vectors $\pm(v_0 - v_1)$ whose lengths equals $|v_0 + v_1|$ since $v_0 \cdot v_1 = 0$. The first two superbases B_1, B_2 in (4.3) came from Lemma 4.2. The double transposition of indices $0 \leftrightarrow 2$, $1 \leftrightarrow 3$ respects $v_0 \cdot v_1 = 0 = v_2 \cdot v_3$ and maps $B_2 = \{v_0+v_3, v_1+v_3, v_2, -v_3\}$ as follows:

$$B_2 \overset{0\leftrightarrow 2,1\leftrightarrow 3}{\mapsto} \{v_2+v_1, v_1+v_3, v_0, -v_1\} = \{v_0, -v_1, v_2+v_1, v_3+v_1\} = B_3.$$

We will show that any other obtuse superbase is isometric to one of B_1, B_2, B_3. We have four pairs of odd-sum vectors and five pairs of even-sum vectors below:

(4.3o) Voronoi odd-sums $[\pm v_1] = \pm 100$, $[\pm v_2] = \pm 10$, $[\pm v_3] = \pm 1$, $[\pm v_0] = \mp 111$;

(4.3e) Voronoi even-sum vectors $[\pm v_{12}] = \pm 110$, $[\pm v_{23}] = \pm 11$, $[\pm v_{13}] = \pm 101$, and $[\pm(v_3 - v_2)] = \mp 9$, $[\pm(v_0 - v_1)] = \mp 211$.

Since the condition $v_0 \cdot v_1 = 0$ wasn't used in Lemma 4.2, it suffices to consider only superbases whose partial sums have a vector from the new pair $\pm(v_0 - v_1)$.

Looking for even-sum vectors u_0, u_1 and $-u_0-u_1$ from (4.2e), the only possible identity $[u_0] + [u_1] + [-u_0 - u_1] = 0$ with a new digital sum 211 from (4.2e) is $211 - 110 - 101 = 0$ up to a permutation and sign. We can get another obtuse superbase not isometric to B_1, B_2 from Lemma 4.2 only by choosing $u_0 = -v_{12} = -v_1 - v_2 = v_0 + v_3$, $[u_0] = -110$ and $u_1 = -v_{13} = -v_1 - v_3 = v_0 + v_2$, $[u_1] = -101$ so that $u_0 + u_1 = -v_1 - v_2 + v_0 + v_2 = v_0 - v_1$, $[u_0 + u_1] = -211$ (up to a sign and re-ordering). Other superbase vectors u_2, u_3 should have the digital sum $[u_2] + [u_3] = -[u_0] - [u_1] = 211$. The remaining digital sums from (4.2o) and (4.2e) give only $211 = 111 + 100$, so $u_2 = -v_0$, $u_1 = v_1$. This superbase $\{-v_1 - v_2, -v_3 - v_3, -v_0, v_1\}$ is opposite to $B_3 = \{v_0, -v_1, v_2 + v_1, v_3 + v_1\}$ up to re-ordering.

(b) If $B_1 = \{v_0, v_1, v_2, v_3\}$ with $v_0 \cdot v_1 = 0 = v_2 \cdot v_3$ has a coform $\mathrm{CF}(B_1) = \begin{pmatrix} 0 & p_{13} & p_{12} \\ 0 & p_{02} & p_{03} \end{pmatrix}$ with $p_{12} = 0 = p_{03}$, the superbase $B_2 = \{v_0 + v_3, v_1 + v_3, v_2, -v_3\}$ has $\mathrm{CF}(B_2) = \begin{pmatrix} 0 & p_{03} & p_{12} \\ 0 & p_{02} & p_{13} \end{pmatrix}$ by Lemma 4.2(b) with the extra restriction $p_{01} = 0$.

The obtuse superbase $B_3 = \{v_0, -v_1, v_2+v_1, v_3+v_1\}$ potentially non-isometric to B_1, B_2 has the conorms q_{ij} expressed via the conorms p_{ij} of B_1 as follows:
$q_{23} = -(v_2 + v_1) \cdot (v_3 + v_1) = -v_1 \cdot (v_1 + v_2 + v_3) = v_1 \cdot v_0 = 0$,
$q_{13} = v_1 \cdot (v_3 + v_1) = -v_1 \cdot (v_0 + v_2) = -v_1 \cdot v_2 = p_{12}$,
$q_{12} = v_1 \cdot (v_2 + v_1) = -v_1 \cdot (v_0 + v_3) = -v_1 \cdot v_3 = p_{13}$,
$q_{01} = -v_0 \cdot (-v_1) = 0$,
$q_{02} = -v_0 \cdot (v_2 + v_1) = -v_0 \cdot v_2 = p_{02}$,
$q_{03} = -v_0 \cdot (v_3 + v_1) = -v_0 \cdot v_3 = p_{03}$. Hence $\mathrm{CF}(B_3) = \begin{pmatrix} 0 & p_{12} & p_{13} \\ 0 & p_{02} & p_{03} \end{pmatrix}$.

By part **(a)** and Lemma 3.4, the coform of any superbase of Λ up to 24 index-permutations is one of the above coforms $\mathrm{CF}(B_1), \mathrm{CF}(B_2), \mathrm{CF}(B_3)$, which are related by the transpositions $p_{13} \leftrightarrow p_{03}$ and $p_{12} \leftrightarrow p_{13}$. Keeping the first column fixed in a coform, the index-permutations induced by $2 \leftrightarrow 3$ and $0 \leftrightarrow 1$ act on $\begin{pmatrix} p_{13} & p_{12} \\ p_{02} & p_{03} \end{pmatrix}$ by swapping the columns and by swapping diagonally opposite elements. All permutations above generate the full group S_4 permuting all non-zero conorms in the submatrix $\begin{pmatrix} p_{23} & p_{01} \\ p_{13} & p_{02} \end{pmatrix}$ of $\mathrm{CF}(B)$. □

Lemma 4.4 (obtuse superbases for Voronoi type V_4) *Let a lattice $\Lambda \subset \mathbb{R}^3$ have Voronoi type V_4, so the Voronoi domain $V(\Lambda)$ is a hexagonal prism.*

(a) *Then Λ has an obtuse superbase $B_1 = \{v_0, v_1, v_2, v_3\}$ with one vector (say) v_3 orthogonal to two others v_1, v_2. Any obtuse superbase of Λ is isometric to one of*

(4.4) B_1, $\quad B_2 = \{v_0 + v_3, v_1 + v_3, v_2, -v_3\}$, $\quad B_4 = \{v_0 + v_3, v_2 + v_3, v_1, -v_3\}$.

(b) *Any obtuse superbase B of Λ has exactly two zero conorms in one column. The 24 index-permutations from Definition 3.3 allow us to write* $\mathrm{CF}(B) = \begin{pmatrix} 0 & 0 & p_{12} \\ p_{01} & p_{02} & p_{03} \end{pmatrix}$.
In the above form with $p_{23} = 0 = p_{13}$ for all obtuse superbases of Λ, the conorms p_{12}, p_{01}, p_{02} can be freely permuted by the symmetry group S_3. ■

Proof A hexagonal prism $V(\Lambda)$ has four pairs of opposite parallel faces: one pair of hexagons and three pairs of rectangles. So $V(\Lambda)$ can be considered as a degenerate case of a hexa-rhombic dodecahedron from Lemma 4.2, not a rhombic dodecahedron. This degeneracy happens due to one vector (say) v_3 orthogonal to other two superbase vectors v_1, v_2. The first two superbases in (4.4) are inherited from Lemma 4.2. The last obtuse superbase in (4.4) is obtained from the second one by the transposition $1 \leftrightarrow 2$ of indices, which respects the new orthogonality conditions $v_1 \cdot v_3 = 0 = v_2 \cdot v_3$.

The 2D lattice Λ_2 has two pairs of obtuse superbases $\pm\{v_1, v_2, -v_1 - v_2\}$. We can choose any two of the three vectors $v_1, v_2, -v_1 - v_2$ and complement this pair u_2, u_3 by $u_1 = -v_3$ and $u_0 = -u_1 - u_2 - u_3$. The resulting three superbases are isometric to B_1, B_2, B_4 in (4.4). For example, the superbase with $u_1 = v_1$, $u_2 = v_2$, $u_3 = -v_3$, $u_0 = -v_1 - v_2 + v_3$ is isometric to B_1 by $v_1 \mapsto v_1$, $v_2 \mapsto v_2$, $v_3 \mapsto -v_3$.

We check that any obtuse superbases of Λ is isometric to one of B_1, B_2, B_4. In addition to the eight pairs of Voronoi vectors $\pm v_0, \pm v_1, \pm v_2, \pm v_3, \pm v_{12}, \pm v_{23}, \pm v_{13}$ and $\pm(v_3 - v_2)$ in Lemma 4.2, we have two more pairs of non-strict Voronoi vectors $\pm(v_3 - v_1)$ and $\pm(v_1 + v_2 - v_3)$ whose lengths are equal to $|v_3 + v_1|$ and $|v_0| = |v_1 + v_2 + v_3|$, respectively, due to $v_1 \cdot v_3 = 0 = v_2 \cdot v_3$. We have 5+5 pairs:

(4.3o) Voronoi odd-sum vectors: $[\pm v_1] = \pm 100$, $[\pm v_2] = \pm 10$, $[\pm v_3] = \pm 1$, and $[\pm v_0] = \mp 111$, $[\pm(v_1 + v_2 - v_3)] = \pm 109$;

(4.3e) Voronoi even-sum vectors: $[\pm v_{12}] = \pm 110$, $[\pm v_{23}] = \pm 11$, $[\pm v_{13}] = \pm 101$, and $[\pm(v_3 - v_2)] = \mp 9$, $[\pm(v_3 - v_1)] = \mp 99$.

Since Lemma 4.2 didn't use the condition $v_1 \cdot v_3 = 0$, it suffices to check only superbases whose partial sums have a vector from $\pm(v_3 - v_1)$, $\pm(v_1 + v_2 - v_3)$.

Case of four odd-sum vectors. Trying to find four digital sums from (4.4e) to fit $[u_0] + [u_1] + [u_2] + [u_3] = 0$, we conclude that one of ± 100 and one of ± 10 should be used, because three other pairs have odd digital sums. Choosing one positive sign of (say) 100, we have two sums 100 ± 10. The sum 90 cannot be split as a sum of two numbers from $\{\pm 1, \pm 111, \pm 109\}$. The only splitting $110 = 111 - 1$ of another sum misses ± 109 and leads to the first superbase $B_1 = \{v_0, v_1, v_2, v_3\}$.

Case of at least two even-sum vectors. Looking for even-sum vectors u_0, u_1 and $-u_0 - u_1$ from (4.4e), the only possible identity $[u_0] + [u_1] + [-u_0 - u_1] = 0$ with a new digital sum 99 is $110 - 11 - 99 = 0$ up to a sign and re-ordering.

We can get another obtuse superbase not isometric to B_1, B_2 from Lemma 4.2 only by choosing $u_0 = -v_1 - v_2 = v_0 + v_3$, $[u_0] = -110$ and $u_1 = v_{23} = v_2 + v_3$, $[u_1] = 11$ so that $u_0 + u_1 = v_3 - v_1$, $[u_0 + u_1] = -99$ up to a sign and re-ordering.

Other vectors u_2, u_3 should have the digital sum $[u_2]+[u_3] = -[u_0]-[u_1] = 99$. The remaining digital sums from (4.4o) and (4.4e) can give only one new splitting $99 = 100-1$, because we have already used $99 = 110-11$ above. Choosing $u_2 = v_1$ and $u_3 = -v_3$ (up to a swap), we get $B_4 = \{v_0 + v_3, v_2 + v_3, v_1, -v_3\}$ from (4.4).

(b) If $B_1 = \{v_0, v_1, v_2, v_3\}$ with $v_1 \cdot v_3 = 0 = v_2 \cdot v_3$ has a coform $\mathrm{CF}(B_1) = \begin{pmatrix} 0 & 0 & p_{12} \\ p_{01} & p_{02} & p_{03} \end{pmatrix}$ with $p_{23} = 0 = p_{13}$, the superbase $B_2 = \{v_0 + v_3, v_1 + v_3, v_2, -v_3\}$ has $\mathrm{CF}(B_2) = \begin{pmatrix} 0 & p_{03} & p_{12} \\ p_{01} & p_{02} & 0 \end{pmatrix}$ by Lemma 4.2(b) with the extra restriction $p_{13} = 0$. The index-permutation induced by $0 \leftrightarrow 1$ from Definition 3.3 transforms the above coform into $\mathrm{CF}(B_2) = \begin{pmatrix} 0 & 0 & p_{02} \\ p_{01} & p_{12} & p_{03} \end{pmatrix}$ with $p_{23} = 0 = p_{13}$ as in $\mathrm{CF}(B_1)$.

The obtuse superbase $B_4 = \{v_0+v_3, v_2+v_3, v_1, -v_3\}$ potentially non-isometric to B_1, B_2 has the conorms q_{ij} expressed via the conorms p_{ij} of B_1 as follows:
$q_{23} = -v_1 \cdot (-v_3) = 0$,
$q_{13} = -(v_2 + v_3) \cdot (-v_3) = (v_0 + v_1) \cdot (-v_3) = -v_0 \cdot v_3 = p_{03}$,
$q_{12} = -(v_2 + v_3) \cdot v_1 = -v_2 \cdot v_1 = p_{12}$,
$q_{01} = -(v_0+v_3)\cdot(v_2+v_3) = (v_0+v_3)\cdot(v_0+v_1) = v_0(v_0+v_1+v_3) = -v_0\cdot v_2 = p_{02}$,
$q_{02} = -(v_0 + v_3) \cdot v_1 = -v_0 \cdot v_1 = p_{01}$,
$q_{03} = -(v_0 + v_3) \cdot (-v_3) = (v_1 + v_2) \cdot (-v_3) = 0$.

The index-permutation induced by $0 \leftrightarrow 1$ from Definition 3.3 transforms the resulting coform $\begin{pmatrix} 0 & p_{03} & p_{12} \\ p_{02} & p_{01} & 0 \end{pmatrix}$ into $\mathrm{CF}(B_4) = \begin{pmatrix} 0 & 0 & p_{01} \\ p_{02} & p_{12} & p_{03} \end{pmatrix}$. Comparing $\mathrm{CF}(B_1)$, $\mathrm{CF}(B_2)$, $\mathrm{CF}(B_4)$, which all have $p_{23} = 0 = p_{13}$, we notice that p_{03} remains at the same place. Actually, $p_{03} = -v_0 \cdot v_3 = (v_1 + v_2 + v_3) \cdot v_3 = v_3^2$ is invariant as the squared length of the vector v_3 orthogonal to v_2, v_3. The other three conorms p_{01}, p_{02}, p_{12} have three arrangements in $\mathrm{CF}(B_1)$, $\mathrm{CF}(B_2)$, $\mathrm{CF}(B_4)$. If we swap the first two columns by the index-permutation $1 \leftrightarrow 2$, we get all six arrangements. Hence p_{12}, p_{01}, p_{02} can be freely permuted by the group S_3. $\square$

As an alternative to Lemma 4.4 for any lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type V_4, the index-permutation induced by $1 \leftrightarrow 2, 0 \leftrightarrow 3$ from Definition 3.3 re-writes $\mathrm{CF}(\Lambda)$ as $\begin{pmatrix} p_{12} & p_{01} & p_{02} \\ 0 & 0 & p_{03} \end{pmatrix}$ with fixed p_{03} and freely permutable conorms in the top row.

Lemma 4.5 (obtuse superbases for Voronoi type V_5) *Let a lattice $\Lambda \subset \mathbb{R}^3$ have Voronoi type V_4, so the Voronoi domain $V(\Lambda)$ is a cuboid. Then any obtuse superbase of Λ belongs to one of the four isometry classes of obtuse superbases.*

(4.5o) One class of 8 odd superbases *: $\{v_0, \pm v_1, \pm v_2, \pm v_3\}$ for any choice of signs. Any coform can be written as* $\begin{pmatrix} 0 & 0 & 0 \\ |v_1|^2 & |v_2|^2 & |v_3|^2 \end{pmatrix}$ *up to 24 index-permutations.*

(4.5e) Three classes each consisting of 8 even superbases $\{v_i, v_j, v_k - v_i, -v_k - v_j\}$ *for pairwisely orthogonal basis vectors $v_i, v_j, v_k \in \{\pm v_1, \pm v_2, \pm v_3\}$ with distinct $i, j, k \in \{1, 2, 3\}$. Any coforms can be written as* $\begin{pmatrix} 0 & 0 & |v_i|^2 \\ 0 & |v_k|^2 & |v_j|^2 \end{pmatrix}$ *up to 24 index-permutations, where $k = 1, 2, 3$ determines a class, but i, j can be swapped.* ▲

Proof A cuboid V_5 has 13 pairs of Voronoi vectors pointing at 26 lattice points $xv_1 + yv_2 + zv_3$ with coefficients $x, y, z \in \{0, \pm 1\}$ excluding the origin $x = y = z = 0$. In any obtuse superbase $\{u_0, u_1, u_2, u_3\}$ of Λ, all four vectors cannot have even sums of coordinates in the basis v_1, v_2, v_3, otherwise they cannot express the vector $v_1 = (1, 0, 0)$. Then at least one vector (say) u_0 has an odd sum ± 1 or ± 3.

The first case is an odd sum $[u_0] = \pm 3$. Applying reflections in the x, y, z-axes, we can assume that $u_0 = (-1, -1, -1) = -v_1 - v_2 - v_3$. Then each u_i, $i = 1, 2, 3$ has no coordinate -1, the sum $u_0 + u_i$ has coordinate -2, which contradicts Lemma 2.7 saying that all partials sum of an obtuse superbase are Voronoi vectors with coordinates $x, y, z \in \{0, \pm 1\}$. If all u_1, u_2, u_3 are even-sum vectors, the only remaining choice (up to permutation) is $u_1 = (1, 1, 0)$, $u_2 = (1, 0, 1)$, $u_3 = (0, 0, 1)$, but all these vectors pairwisely have acute angles. Hence one vector (say) u_1 has $[u_1] = 1$ and we can assume that $u_0 = v_1 = (1, 0, 0)$ up to permutation. The sum $[u_0] + [u_1] = -3 + 1 = -2$ can be neutralised only by Voronoi vectors u_2, u_3 with non-negative coordinates and $[u_2] = 1 = [u_3]$, so the only choice (up to a swap) is $u_2 = v_2 = (0, 1, 0)$ and $u_3 = (0, 0, 1)$. By reflections, this superbase $\{v_0, v_1, v_2, v_3\}$ generates all eight odd superbases in (4.5o), which are isometric to each other and have the coform with zeros in the top row and $p_{0i} = -v_0 \cdot v_i = |v_i|^2$.

The second case is an odd sum $[u_0] = \pm 1$. Permutions and reflections in the x, y, z-axes allow us to assume that $u_0 = (1, 0, 0)$. Since u_0 has non-acute angles with each u_i, $i = 1, 2, 3$, the first coordinates of u_i is 0 or (-1). Since the x-coordinates of u_i cannot have opposite signs, the projections of u_1, u_2, u_3 to the (y, z)-plane cannot have larger pairwise scalar products than the original vectors. Hence these projections u_1', u_2', u_3' form an obtuse superbase for the rectangular lattice Λ_2 that they generate. In this 2-dimensional case, all four obtuse superbases of Λ_2 have the form $u_2' = \pm v_2$, $u_3' = \pm v_3$, $u_1' = -u_2' - u_3'$.

Without loss of generality, assume that $u'_2 = (1,0)$, $u'_3 = (0,1)$. To lift these projections to $\mathbb{R}^3$, if we complement both u'_2, u'_3 by the first coordinate 0, we get one of the odd superbases above. If we complement u'_2 by (-1), then $u_2 = (-1,1,0)$. Since u_3 cannot have the first coordinate (-1), the only choice is $u_3 = (0,0,1)$, then $u_1 = -u_0 - u_2 - u_3 = (0,-1,-1)$. The resulting obtuse superbase $\{v_1, -v_2 - v_3, v_2 - v_1, v_3\}$ is $\{v_i, v_j, v_k - v_i, -v_k - v_j\}$ for $v_i = v_1$, $v_j = v_3$, $v_k = v_2$. For any fixed $k = 1,2,3$, we can choose three signs of pairwisely orthogonal basis vectors $\pm v_i, \pm v_j, \pm v_k$ in 8 ways. Then (4.5e) has 3×8 even obtuse superbases.

Up to index-permutations, these 24 even obtuse superbases have coforms in (4.5o) computed from $u_0 = v_i$, $u_1 = v_j$, $u_2 = v_k - v_i$, $u_3 = -v_k - v_j$ as follows: $p_{23} = (v_k - v_i)\cdot(v_k + v_j) = |v_k|^2$, $p_{13} = v_j \cdot (v_k + v_j) = |v_j|^2$, $p_{12} = v_j \cdot (v_k - v_i) = 0$, $p_{01} = -v_i \cdot v_j = 0$, $p_{02} = -v_i \cdot (v_k - v_i) = |v_i|^2$, $p_{03} = v_i \cdot (v_k + v_j) = 0$.

The resulting coform $\begin{pmatrix} |v_k|^2 & |v_j|^2 & 0 \\ 0 & |v_i|^2 & 0 \end{pmatrix}$ can be re-written as $\begin{pmatrix} 0 & 0 & |v_i|^2 \\ 0 & |v_k|^2 & |v_j|^2 \end{pmatrix}$ using the index-permutation induced by the composition of $0 \leftrightarrow 1$ and $0 \leftrightarrow 3$. The index-permutation induced by the composition $0 \leftrightarrow 2$, $1 \leftrightarrow 3$ swaps $|v_i|^2, |v_j|^2$.

The 24 even superbases split into three isometry classes, each having its own squared lengths $|v_i|^2, |v_j|^2, |v_i|^2 + |v_k|^2, |v_j|^2 + |v_k|^2$. These unordered quadruples differ for $k = 1,2,3$ if $|v_1|^2, |v_2|^2, |v_3|^2$ and their pairwise sums are all different. $\square$

In 1874, Selling tried to describe all possible obtuse superbases without proof but the V_5 case [25, p. 173, item 9] described only 24 coforms, not 32 as in Lemma 4.5. In 1934, the book [8, Fig. 64 on page 170] said that the numbers of isometry classes of obtuse superbases for Voronoi types V_2, V_3, V_4, V_5 are $2, 3, 3, 1+2$, respectively, also without proof, then added on the same page that, for Voronoi type V_5, "one class has eight superbases, each of the other two classes has three pairs of opposite superbases (six in each class)". In 1975, the survey [14, Fig. 13 on page 101] repeated the same picture with 1+2 classes for the 5th Voronoi (Dirichlet) type but added that "there are twelve pairs of such quadrilaterals [obtuse superbases], of which the first four can differ from the second four and the third four". In 2009, the book [17, p. 77] mentioned 32 pairs of centrally symmetric obtuse superbases for a cuboid, which has exactly 16 such pairs, see Table 4.

Lemma 4.5 corrects the above numbers to $1+3$ classes, where each of the three even classes in (4.5e) consists of eight isometric superbases, see Table 4.

Lemma 4.5 can be considered as a limit case of both Lemmas 4.3–4.4. Indeed,
$\{-v_1 - v_2, v_1 + v_3, v_2, -v_3\} = \{v_i, v_j, v_k - v_i, -v_k - v_j\}$, $v_i = v_2$, $v_j = -v_3$, $v_k = v_1$.
$\{v_0, -v_1, v_2 + v_1, v_3 + v_1\} = \{v_i, v_j, v_k - v_i, -v_k - v_j\}$, $v_i = v_0$, $v_j = -v_1$, $v_k = v_2$.
$\{v_0 + v_3, v_2 + v_3, v_1, -v_3\} = \{v_i, v_j, v_k - v_i, -v_k - v_j\}$, $v_i = v_1$, $v_j = -v_3$, $v_k = -v_0$.

5 A root form and a unique root invariant of a 3-dimensional lattice

Lemmas 4.1-4.5 showed that coforms of any lattice $\Lambda \subset \mathbb{R}^3$ should be considered up to different permutations for five Voronoi types. To reduce the ambiguity of

Table 1 For a primitive orthorhombic lattice, $(1+3)\times 8$ obtuse superbases split into $1+3$ isometry classes from Lemma 4.5 and can be distinguished by lengths of vectors.

8 odd superbases	1st even class in (4.5e)	2nd even class in (4.5e)	3rd even class in (4.5e)
$v_1 = (\pm 1, 0, 0)$	$v_1 = (\pm 1, 0, 0)$	$v_1 = (\pm 1, 0, 0)$	$v_2 = (0, \pm 2, 0)$
$v_2 = (0, \pm 2, 0)$	$v_2 = (0, \pm 2, 0)$	$v_3 = (0, 0, \pm 3)$	$v_3 = (0, 0, \pm 3)$
$v_3 = (0, 0, \pm 3)$	$v_3 - v_1 = (\mp 1, 0, \pm 3)$	$v_2 - v_1 = (\mp 1, \pm 2, 0)$	$v_1 - v_2 = (\pm 1, \mp 2, 0)$
$v_0 = (\mp 1, \mp 2, \mp 3)$	$-v_3 - v_2 = (0, \mp 2, \mp 3)$	$-v_2 - v_3 = (0, \mp 2, \mp 3)$	$-v_1 - v_3 = (\mp 1, 0, \mp 3)$
lengths $1, 2, 3, \sqrt{14}$	lengths $1, 2, \sqrt{10}, \sqrt{13}$	lengths $1, 3, \sqrt{5}, \sqrt{13}$	lengths $2, 3, \sqrt{5}, \sqrt{10}$
$\mathrm{CF} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 4 & 9 \end{pmatrix}$	$\mathrm{CF} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 9 & 4 \end{pmatrix}$	$\mathrm{CF} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 4 & 9 \end{pmatrix}$	$\mathrm{CF} = \begin{pmatrix} 0 & 0 & 4 \\ 0 & 1 & 9 \end{pmatrix}$

coforms, Definition 5.1 introduces below a root form $\mathrm{RF}(B)$ and root invariant $\mathrm{RI}(B)$, which will be proved to be a complete invariant of $\Lambda \subset \mathbb{R}^3$ up to isometry.

Since any obtuse superbase B has only non-negative conorms, the *root products* $r_{ij} = \sqrt{p_{ij}}$ are well-defined for all distinct indices $i, j \in \{0, 1, 2, 3\}$ and have the same units as coordinates of basis vectors, for example Angstroms: $1\mathring{A} = 10^{-10}$m. The six root products can combined into a 2×3 matrix called a root form $\mathrm{RF} = \begin{pmatrix} r_{23} & r_{13} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$, which will be considered up to permutations from Lemmas 4.1-4.5. The root invariant $\mathrm{RI}(B)$ will finally reduce the ambiguity $\mathrm{RF}(B)$ to 6, 5, 4, 4, 3 root products for Voronoi types V_1, V_2, V_3, V_4, V_5, respectively. Theorem 5.3 will show that the invariant $\mathrm{RI}(\Lambda)$ depends only on the isometry class of Λ.

Definition 5.1 (root form $\mathrm{RF}(B)$, root invariant $\mathrm{RI}(B)$) (V_5) *By Lemma 4.5 any obtuse superbase B of a lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type V_5 has exactly three non-zero root products. Up to 24 index-permutations, the* root form *is* $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & 0 \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$ *for any odd superbase B and* $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & r_{01} \\ 0 & r_{02} & r_{03} \end{pmatrix}$ *for any even superbase B, where all non-zero root products are freely permutable. The* root invariant $\mathrm{RI}(B)$ *is an ordered triple of the non-zero root products r_{01}, r_{02}, r_{03}.*

(V_4) *For any lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type V_4, any obtuse superbase B has two zero root products in different columns. A* root form *is* $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$*, where $r_{23} = 0 = r_{13}$, and the root products r_{12}, r_{01}, r_{02} are freely permutable. The* root invariant $\mathrm{RI}(B) = \{(r_{12}, r_{01}, r_{02}), r_{03}\}$ *consists of $3+1$ root products, where the triple (r_{12}, r_{01}, r_{02}) should be written in increasing order.*

(V_3) *For any lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type V_3, any obtuse superbase B of Λ has exactly two zero root products in the same column. A* root form *is* $\mathrm{RF}(B) =$

$\begin{pmatrix} 0 & r_{13} & r_{12} \\ 0 & r_{02} & r_{03} \end{pmatrix}$ *with* $r_{23} = 0 = r_{03}$*, and* $r_{13}, r_{12}, r_{02}, r_{03}$ *are freely permutable. The* root invariant $\mathrm{RI}(B)$ *consists of the four non-zero root products in increasing order.*

(V_2) *For any lattice* $\Lambda \subset \mathbb{R}^3$ *of Voronoi type* V_2*, any obtuse superbase* B *of* Λ *has exactly one zero root product. A root form is* $\mathrm{RF}(B) = \begin{pmatrix} 0 & r_{13} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$*, where* $r_{23} = 0$ *and the* 2×2 *submatrix* $\begin{pmatrix} r_{13} & r_{12} \\ r_{02} & r_{03} \end{pmatrix}$ *can be changed by the symmetry group* D_4*, which can guarantee (without changing indices for simplicity) that* $r_{13} = \min\{r_{13}, r_{12}, r_{02}, r_{03}\}$ *and also* $r_{12} \leq r_{02}$*. The* root invariant *consists of* $1+3+1$ *root products:* $\mathrm{RI}(B) = \{r_{01}, (r_{13}, r_{12}, r_{02}), r_{03}\}$*, where* $r_{03} \geq r_{13} \leq r_{12} \leq r_{02}$*.*

(V_1) *For any obtuse superbase* B *of a lattice* $\Lambda \subset \mathbb{R}^3$ *of Voronoi type* V_1*, a* root form $\mathrm{RF}(B)$ *is the matrix* $\begin{pmatrix} r_{23} & r_{13} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$*, where root products can be rearranged by the 24 index-permutations from Definition 3.3. A permutation of indices 1, 2, 3 as in (3.3a) allows us to arrange the three columns in any order. The composition of transpositions* $0 \leftrightarrow i$ *and* $j \leftrightarrow k$ *for distinct* $i, j, k \neq 0$ *vertically swaps the root products in columns* j *and* k*, for example apply the transposition* $2 \leftrightarrow 3$ *to the result of* $0 \leftrightarrow 1$ *in (3.3b). So we can put* $r_{min} = \min\{r_{ij}\}$ *into the top left position (*r_{23}*). Then we consider the four root products in columns 2 and 3. Keeping column 1 fixed, we can put the minimum of these four into the top middle position (*r_{13}*). Then the resulting root products in the top row should be in increasing order.*

If the top left and top middle root products are equal ($r_{23} = r_{13}$*), we can put their counterparts (*r_{01} *and* r_{02}*) in the bottom row of columns 1,2 in increasing order. If the top middle and top right root products are equal (*$r_{13} = r_{12}$*), we can put their counterparts (*r_{02} *and* r_{03}*) in the bottom row of columns 2 and 3 in increasing order. The resulting uniquely ordered matrix is the* root invariant $\mathrm{RI}(B)$ *and can be visualised as in Fig. 2 (right) with root products instead of conorms.* ▲

Lemma 5.2 (equivalence of $\mathrm{VF}, \mathrm{CF}, \mathrm{RF}$**)** *For any obtuse superbase* B*, its voform* $\mathrm{VF}(B)$*, coform* $\mathrm{CF}(B)$*, and* $\mathrm{RI}(B)$ *are reconstructable from each other.* ■

Proof The six conorms p_{ij} are uniquely expressed via the seven vonorms v_i^2, v_{ij}^2 by formulae (3.1ab) and vice versa. The root invariant $\mathrm{RI}(B)$ is uniquely defined by a tailored ordering of root products $r_{ij} = \sqrt{p_{ij}}$ in Definition 5.1.

Important Lemmas 4.1–4.5 imply in Theorem 5.3 below that $\mathrm{RI}(B)$, which was initially defined for an obtuse superbase B, is an isometry invariant of Λ.

The 2-dimensional analogue was the much simpler result in [20, Theorem 3.7] saying that all obtuse superbases of any lattice $\Lambda \subset \mathbb{R}^2$ are isometric to each other.

Theorem 5.3 (isometry invariance of $\mathrm{RI}(\Lambda)$**)** *If obtuse superbases* B, B' *generate isometric lattices* $\Lambda, \Lambda' \subset \mathbb{R}^3$*, respectively, then* $\mathrm{RI}(B) = \mathrm{RI}(B')$*. Hence* RI *is an isometry invariant of a lattice* Λ *and can be denoted by* $\mathrm{RI}(\Lambda)$. ■

Proof Any isometry f between given lattices Λ, Λ' maps B to a new obtuse superbase $f(B)$ of Λ' and preserves all lengths and scalar products of vectors, so $\mathrm{RF}(B) = \mathrm{RF}(f(B))$, hence $\mathrm{RI}(B) = \mathrm{RI}(f(B))$. Now the lattice Λ' has two obtuse superbases B' and $f(B)$. Lemmas 4.1–4.5 explicitly described all potentially non-isometric superbases of the same lattice for five types of Voronoi domains.

In all cases, Definition 5.1 introduced the root invariant $\mathrm{RI}(B)$ whose root products are uniquely ordered, resolving the ambiguity of obtuse superbases. Hence $\mathrm{RI}(B) = \mathrm{RI}(f(B)) = \mathrm{RI}(B')$, so $\mathrm{RI}(\Lambda)$ is an isometry invariant of the lattice Λ. □

Example 5.4 (root invariants of primitive orthorhombic lattices) *The primitive orthorhombic lattice* Λ *with edge-lengths* $0 \le a \le b \le c$ *has the obtuse superbase* $v_1 = (a,0,0)$, $v_2 = (0,b,0)$, $v_3 = (0,0,c)$, $v_0 = (-a,-b,-c)$*, whose root form is* $\mathrm{RF}(\Lambda) = \begin{pmatrix} 0 & 0 & 0 \\ a & b & c \end{pmatrix}$*, so the root invariant is* $\mathrm{RI}(\Lambda) = (a,b,c)$*. If we re-order vectors, columns of* $\mathrm{RF}(\Lambda)$ *are re-ordered accordingly, but* $\mathrm{RI}(\Lambda)$ *remains the same. Another obtuse superbase* $v_1 = (a,0,0)$, $v_2 = (0,b,0)$, $v_3' = (-a,0,c)$, $v_0' = (0,-b,-c)$ *has* $\mathrm{RF}(\Lambda) = \begin{pmatrix} 0 & 0 & a \\ 0 & b & c \end{pmatrix}$*, but* $\mathrm{RI}(\Lambda) = (a,b,c)$ *is the same.* ▲

Lemma 5.5 (invariants of mirror-symmetric lattices) ***(a)*** *If the root invariant* $\mathrm{RI}(\Lambda)$ *of a lattice* $\Lambda \subset \mathbb{R}^3$ *has two equal columns with identical root products, for example* $r_{12} = r_{13}$ *and* $r_{02} = r_{03}$*, then* Λ *is a mirror reflection of itself.*

(b) *If the rows of* $\mathrm{RF}(\Lambda)$ *coincide,* Λ *is a Face-centred Orthorhombic lattice.* ■

Proof **(a)** If $r_{12} = r_{13}$ and $r_{02} = r_{03}$, then the vectors v_2, v_3 have the same length by formulae of Definition 3.1: $v_2^2 = p_{02} + p_{12} + p_{23} = p_{03} + p_{13} + p_{23} = v_3^2$. Then v_2, v_3 are mirror images with respect to their bisector plane P. The identity $p_{02} = p_{03}$ implies that v_0 has the same angles with the vectors v_2, v_3 of equal lengths, also v_1 due to $p_{12} = p_{13}$. Then both v_0, v_1 belong to the bisector plane P between v_2, v_3. Hence the superbase is invariant under the mirror reflection in P.

(b) If $p_{01} = p_{23}$, $p_{02} = p_{13}$, $p_{03} = p_{12}$, the formulae of Definition 3.1 imply that the vectors v_0, v_1, v_2, v_3 have the same squared length equal to $p_{01}+p_{02}+p_{03}$. The three other partial sums $v_0 + v_i$, $i = 1,2,3$, are orthogonal to each other. Indeed,

$$(v_0+v_i)\cdot(v_0+v_j) = v_0^2+v_0\cdot v_i+v_0\cdot v_j+v_i\cdot v_j = (p_{01}+p_{02}+p_{03})-p_{0i}-p_{0j}-p_{ij} = 0,$$

because $p_{ij} = p_{0k}$ when all indices $i,j,k \in \{1,2,3\}$ are distinct. Hence the vectors $v_0 + v_i$ form a non-primitive orthogonal basis of Λ. Parameters a,b,c of a Face-centred Orthorhombic lattice (oF) can be found similarly to Example 5.4. □

6 Root invariants classify all 3-dimensional lattices up to isometry

Proposition 6.1 substantially reduces the ambiguity of lattice representations by their bases. Any fixed lattice $\Lambda \subset \mathbb{R}^3$ has infinitely many (super)bases but only a few obtuse superbases, maximum 32 (or two non-isometric classes) in Lemma 4.5.

Proposition 6.1 (obtuse superbases of isometric lattices in $\mathbb{R}^3$) *Lattices in $\mathbb{R}^3$ are isometric if and only if any of their obtuse superbases B, B' are isometric to each other or to a couple of obtuse superbases in one of Lemmas 4.1–4.5.* ▲

Proof Part *only if* ($\Rightarrow$): any isometry f between lattices Λ, Λ' maps any obtuse superbase B of Λ to the obtuse superbase $f(B)$ of Λ'. Then B' and $f(B)$ are isometric to each other or to obtuse superbases listed in one of Lemmas 4.1–4.5 for the Voronoi type of the given isometric lattices $\Lambda \cong \Lambda'$.

Part *if* ($\Leftarrow$): the given conditions on B, B' mean that there is an isometry $B \to B'$ extending to an isometry of their lattices $\Lambda \to \Lambda'$, or B, B' are isometric to a couple of obtuse superbases in one of Lemmas 4.1–4.5, so $\Lambda \cong \Lambda'$. □

Proposition 6.1 above formalises the key difference between dimensions 2 and 3 for an isometry classification of lattices. The 2D analogue in [20, Theorem 3.7] says that any lattices $\Lambda \subset \mathbb{R}^2$ are isometric if and only if any their superbases are isometric. Proposition 6.1 needs much more sophisticated Lemmas 4.1–4.5, because lattices in $\mathbb{R}^3$ can have several non-isometric superbases.

Lemma 6.2 (superbase reconstruction) *An obtuse superbase of any lattice $\Lambda \subset \mathbb{R}^3$ can be reconstructed up to isometry from its root invariant* $\mathrm{RI}(\Lambda)$. ■

Proof The root invariant $\mathrm{RI}(\Lambda)$ can be lifted to a 2×3 matrix of a root form $\mathrm{RF}(\Lambda)$ for each of five Voronoi types of lattices in Definition 5.1. The positions of root products $r_{ij} = \sqrt{-v_i \cdot v_j}$ in $\mathrm{RF}(\Lambda)$ allow us to compute the lengths $|v_i|$ from the formulae of Definition 3.1, for example $|v_0| = \sqrt{r_{01}^2 + r_{02}^2 + r_{03}^2}$. Up to rigid motion in $\mathbb{R}^3$, one can fix v_0 along the positive x-axis in $\mathbb{R}^3$.

The angle $\angle(v_i, v_j) = \arccos \dfrac{v_i \cdot v_j}{|v_i| \cdot |v_j|} \in [0, \pi)$ between the vectors v_i, v_j can be found from the vonorms v_i^2, v_j^2 and root product $r_{ij} = \sqrt{-v_i \cdot v_j}$. The found length $|v_1|$ and angle $\angle(v_0, v_1)$ allow us to fix v_1 in the xy-plane of $\mathbb{R}^3$. The vector v_2 with the known length $|v_2|$ and two angles $\angle(v_0, v_2)$ and $\angle(v_1, v_2)$ has two positions that are isometric by the mirror reflection in the xy-plane. □

Theorem 6.3 (3D lattices/isometry $\leftrightarrow$ root invariants) *Any lattices $\Lambda, \Lambda' \subset \mathbb{R}^3$ are isometric if and only if their root invariants coincide:* $\mathrm{RI}(\Lambda) = \mathrm{RI}(\Lambda')$. ▲

Proof The part *only if* ($\Rightarrow$) is Theorem 5.3 implying that any isometric lattices Λ, Λ' have equal root invariants: $\mathrm{RI}(\Lambda) = \mathrm{RI}(\Lambda')$. The part *if* ($\Leftarrow$) follows from Lemma 6.2 by reconstructing a superbase of Λ from its root invariant $\mathrm{RI}(\Lambda)$. □

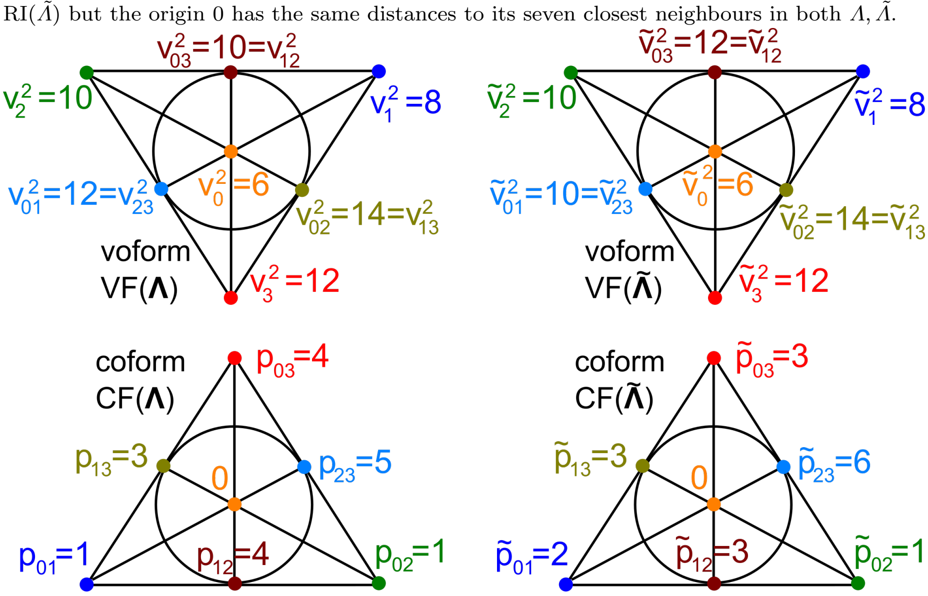
Corollary 6.4 (3D lattices/similarity $\leftrightarrow$ proportional RI) *Any lattices in $\mathbb{R}^3$ are related by similarity (a composition of isometry and uniform scaling) if and only if their root invariants are proportional by a factor $s > 0$.* ▲

Proof Scaling a lattice $\Lambda \subset \mathbb{R}^3$ by a factor $s > 0$ multiplies all root products r_{ij}, hence all components of $\mathrm{RI}(\Lambda)$, by s. The corollary follows from Theorem 6.3. $\square$

Example 6.5 (non-isometric lattices with $DC^7 = 0$) *Fig. 6.5 shows that we cannot freely permute vonorms or conorms (equivalently, root products) without changing the isometry class of a lattice. The voforms in Fig. 6.5 differ by a single transposition* $10 \leftrightarrow 12$ *for the vonorms* $v_{12}^2 = v_{03}^2$ *and* $v_{23}^2 = v_{01}^2$. *This transposition is not among the 24 index-permutations from Definition 3.1. The coforms in Fig. 6.5 are computed from the voforms by formulae (3.1b). These coforms include different conorms, for example value 5 appear in* $\mathrm{CF}(\Lambda)$ *but not in* $\mathrm{CF}(\tilde{\Lambda})$. *Then* $\mathrm{RI}(\Lambda) \neq \mathrm{RI}(\Lambda')$ *define non-isometric lattices* $\Lambda \not\cong \tilde{\Lambda}$ *by Theorem 6.3.*

In these lattices $\Lambda, \tilde{\Lambda} \subset \mathbb{R}^3$ *the origin* 0 *has the same distances* $|v_0|$, $|v_1|$, $|v_2|$, $|v_3|$, $|v_{12}|$, $|v_{23}|$, $|v_{13}|$ *to its seven closest Voronoi neighbours. Hence the function* DC^7 *taking the Euclidean distance between these 7-dimensional distance vectors [5] vanishes for* $\Lambda, \tilde{\Lambda}$. *Our colleagues Larry Andrews and Herbert Bernstein quickly checked that* $\Lambda, \tilde{\Lambda}$ *can be distinguished by the 8th distance from the origin to its 8th closest neighbour. However, the example in Fig. 6.5 can be extended to an infinite 6-parameter family of non-isometric lattices* $\Lambda, \tilde{\Lambda}$ *with* $DC^7(\Lambda, \tilde{\Lambda}) = 0$ *as follows.*

Fig. 4 The lattices $\Lambda, \tilde{\Lambda}$ defined by the coforms $\mathrm{CF}(\Lambda), \mathrm{CF}(\tilde{\Lambda})$ are not isometric due to $\mathrm{RI}(\Lambda) \neq \mathrm{RI}(\tilde{\Lambda})$ but the origin 0 has the same distances to its seven closest neighbours in both $\Lambda, \tilde{\Lambda}$.



Add any conorms $q_{ij} \geq 0$ to $\mathrm{CF}(\Lambda), \mathrm{CF}(\tilde{\Lambda})$ in the 'conorm-wise' way. Formulae (3.1a) imply that the voforms $\mathrm{VF}(\Lambda), \mathrm{VF}(\tilde{\Lambda})$ consist of the same 7 numbers:

$$\Lambda : \begin{cases} v_0^2 &= (p_{01}+q_{01})+(p_{02}+q_{02})+(p_{03}+q_{03}) = 1+4+1+q_{01}+q_{02}+q_{03}, \\ v_1^2 &= (p_{01}+q_{01})+(p_{12}+q_{12})+(p_{13}+q_{13}) = 1+4+3+q_{01}+q_{12}+q_{13}, \\ v_2^2 &= (p_{02}+q_{02})+(p_{12}+q_{12})+(p_{23}+q_{23}) = 1+4+5+q_{02}+q_{12}+q_{23}, \\ v_3^2 &= (p_{03}+q_{03})+(p_{13}+q_{13})+(p_{23}+q_{23}) = 4+3+5+q_{03}+q_{13}+q_{23}, \\ v_{01}^2 &= (p_{02}+q_{02})+(p_{03}+q_{03})+(p_{12}+q_{12})+(p_{13}+q_{13}) = \\ &= 1+4+4+3+q_{02}+q_{03}+q_{12}+q_{13} = 12+(q_{02}+q_{03}+q_{12}+q_{13}), \\ v_{02}^2 &= (p_{01}+q_{01})+(p_{03}+q_{03})+(p_{12}+q_{12})+(p_{23}+q_{23}) = \\ &= 1+4+4+5+q_{01}+q_{03}+q_{12}+q_{23} = 14+(q_{01}+q_{03}+q_{12}+q_{23}), \\ v_{03}^2 &= (p_{01}+q_{01})+(p_{02}+q_{02})+(p_{13}+q_{13})+(p_{23}+q_{23}) = \\ &= 1+1+3+5+q_{01}+q_{02}+q_{13}+q_{23} = 10+(q_{01}+q_{02}+q_{13}+q_{23}); \end{cases}$$

$$\tilde{\Lambda} : \begin{cases} \tilde{v}_0^2 &= (\tilde{p}_{01}+q_{01})+(\tilde{p}_{02}+q_{02})+(\tilde{p}_{03}+q_{03}) = 2+1+3+q_{01}+q_{02}+q_{03}, \\ \tilde{v}_1^2 &= (\tilde{p}_{01}+q_{01})+(\tilde{p}_{12}+q_{12})+(\tilde{p}_{13}+q_{13}) = 2+3+3+q_{01}+q_{12}+q_{13}, \\ \tilde{v}_2^2 &= (\tilde{p}_{02}+q_{02})+(\tilde{p}_{12}+q_{12})+(\tilde{p}_{23}+q_{23}) = 1+3+6+q_{02}+q_{12}+q_{23}, \\ \tilde{v}_3^2 &= (\tilde{p}_{03}+q_{03})+(\tilde{p}_{13}+q_{13})+(\tilde{p}_{23}+q_{23}) = 3+3+6+q_{03}+q_{13}+q_{23}, \\ \tilde{v}_{01}^2 &= (\tilde{p}_{02}+q_{02})+(\tilde{p}_{03}+q_{03})+(\tilde{p}_{12}+q_{12})+(\tilde{p}_{13}+q_{13}) = \\ &= 1+3+3+3+q_{02}+q_{03}+q_{12}+q_{13} = 10+(q_{02}+q_{03}+q_{12}+q_{13}), \\ \tilde{v}_{02}^2 &= (\tilde{p}_{01}+q_{01})+(\tilde{p}_{03}+q_{03})+(\tilde{p}_{12}+q_{12})+(\tilde{p}_{23}+q_{23}) = \\ &= 2+3+3+6+q_{01}+q_{03}+q_{12}+q_{23} = 14+(q_{01}+q_{03}+q_{12}+q_{23}), \\ \tilde{v}_{03}^2 &= (\tilde{p}_{01}+q_{01})+(\tilde{p}_{02}+q_{02})+(\tilde{p}_{13}+q_{13})+(\tilde{p}_{23}+q_{23}) = \\ &= 2+1+3+6+q_{01}+q_{02}+q_{13}+q_{23} = 12+(q_{01}+q_{02}+q_{13}+q_{23}). \end{cases}$$

Notice that almost all vonorms coincide: $v_i^2 = \tilde{v}_i^2$ and $v_{02}^2 = \tilde{v}_{02}^2$ except the couple of swapped values: $v_{01}^2 = \tilde{v}_{03}^2$ and $v_{03}^2 = \tilde{v}_{01}^2$. So both lattices $\Lambda, \tilde{\Lambda}$ have the same ordered distances from the origin to its seven closest neighbours: $DC^7(\Lambda, \tilde{\Lambda}) = 0$.

Now we show that the new coforms $\mathrm{CF}(\Lambda), \mathrm{CF}(\tilde{\Lambda})$ lead to different root invariants for almost all free parameters $q_{ij} \geq 0$ in the generic case of Lemma 4.1 when all conorms are positive. Under $4! = 24$ index-permutations from Definition 3.1, any two conorms from a common column remain together in a (possibly another) *column. The coforms* $\mathrm{CF}(\Lambda), \mathrm{CF}(\tilde\Lambda)$ *have the following column sums*

$$\Lambda : \begin{cases} p_{23} + p_{01} = (5 + q_{23}) + (1 + q_{01}) = 6 + q_{23} + q_{01}, \\ p_{13} + p_{02} = (3 + q_{13}) + (1 + q_{02}) = 4 + q_{13} + q_{02}, \\ p_{12} + p_{03} = (4 + q_{12}) + (4 + q_{03}) = 8 + q_{12} + q_{03}; \end{cases}$$

$$\tilde\Lambda : \begin{cases} \tilde p_{23} + \tilde p_{01} = (6 + q_{23}) + (2 + q_{01}) = 8 + q_{23} + q_{01}, \\ \tilde p_{13} + \tilde p_{02} = (3 + q_{13}) + (1 + q_{02}) = 4 + q_{13} + q_{02}, \\ \tilde p_{12} + \tilde p_{03} = (3 + q_{12}) + (3 + q_{03}) = 6 + q_{12} + q_{03}. \end{cases}$$

Two sums from the above triples coincide: $p_{13}+p_{02} = \tilde p_{13}+\tilde p_{02}$ *for any* $q_{ij} \geq 0$. *Since the first sums and third sums clearly differ, the above triples of sums can coincide only if the remaining pairs of sums are swapped, so* $p_{23} + p_{01} = \tilde p_{12} + \tilde p_{03}$ *and* $p_{12} + p_{03} = \tilde p_{12} + \tilde p_{03}$*, which both are equivalent to* $q_{23} + q_{01} = q_{12} + q_{03}$*. If* $q_{23} + q_{01} \neq q_{12} + q_{03}$*, the above triples of sums differ, so* $\mathrm{CF}(\Lambda), \mathrm{CF}(\tilde\Lambda)$ *are not related by index-permutations. The underlying lattices* $\Lambda, \tilde\Lambda$ *are not isometric by Theorem 6.3. To distinguish the lattices* $\Lambda \not\cong \tilde\Lambda$ *in this 6-parameter family by 8 or more distances from the origin to its neighbours, a theoretical proof is needed.* ▲

Lemma 6.6 below implies that the root products r_{ij} continuously change under perturbations of an obtuse superbase measured in the Minkowski metric M_∞.

Lemma 6.6 (bounds for root products [20, Lemma 7.3]) *Let vectors* $u_1, u_2, v_1, v_2 \in \mathbb{R}^n$ *have a maximum length* l*, have non-positive scalar products* $u_1 \cdot u_2, v_1 \cdot v_2 \leq 0$*, and* $|u_i - v_i| \leq \delta$ *for* $i = 1, 2$*. Then*

$$|u_1 \cdot u_2 - v_1 \cdot v_2| \leq 2l\delta \qquad \text{and} \qquad |\sqrt{-u_1 \cdot u_2} - \sqrt{-v_1 \cdot v_2}| \leq \sqrt{2l\delta}. \qquad \blacksquare$$

The next paper [19] will prove a stronger continuity result by defining metrics on root invariants. Justifying metric axioms will be much harder than in $\mathbb{R}^2$ [20, section 5], because we need to glue five Voronoi type subspaces of $\mathrm{LIS}(\mathbb{R}^3)$ in a non-trivial way not covered by the classical theory [9, Part I, Lemma 5.24]. These continuous metrics will define real-valued chiralities of 3D lattices by continuously measuring a deviation from a higher-symmetry neighbour as in [20, section 6].

The more recent Pointwise Distance Distributions [27] are continuous, complete for distance-generic crystals and helped establish the *Crystal Isometry Principle* saying that all real periodic crystals can be distinguished up to isometry by their geometric structures of atomic centres without chemical data. Hence all periodic crystals live in the common Crystal Isometry Space (CRISP), which can be projected to the Lattice Isometry Space $\mathrm{LIS}(\mathbb{R}^3)$ parameterised in Problem 1.1.

The companion papers in dimension 2 [10] and 3 [11] discuss many continuous maps of real crystal lattices from the Cambridge Structural Database.

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A Proof of reduction: any 3D lattice has an obtuse superbase

The previous paper [20, Appendix A] includes some basic definitions and proofs of past results outlined by Delone, Conway and Sloane [13]. This appendix corrects (in the next update) the example in [13, Fig. 8 in section 7] used in the proof of [13, Theorem 8]. Below we give a more detailed argument for this Reduction Theorem 2.8 by using Lemma A.1 as a typical reduction step.

Lemma A.1 (reduction) *Let* $B = (v_0, v_1, v_2, v_3)$ *be any superbase of a lattice* $\Lambda \subset \mathbb{R}^3$. *For any distinct* $i, j, k, l \in \{0, 1, 2, 3\}$, *let the new superbase vectors be* $u_i = -v_i$, $u_j = v_j$, $u_k = v_{ik} = v_i + v_k$, $u_l = v_{il} = v_i + v_l$. *Then all vonorms remain the same or swap their places, and the only change is* $u_{ij}^2 = v_{ij}^2 - 4\varepsilon$, *where* $\varepsilon = v_i \cdot v_j$. *The conorms* $q_\bullet$ *of the new vectors* $u_\bullet$ *are updated as in Fig. 5*

$$(A.1)\quad q_{ij} = \varepsilon,\ q_{jk} = p_{jk} - \varepsilon,\ q_{jl} = p_{jl} - \varepsilon,\ q_{ik} = p_{il} - \varepsilon,\ q_{il} = p_{ik} - \varepsilon,\ q_{kl} = p_{kl} + \varepsilon.$$

Proof If initial vectors $v_\bullet$ form a superbase, which means that $v_i + v_j + v_k + v_l = 0$, then so do the new vectors: $u_i + u_j + u_k + u_l = (-v_i) + v_j + (v_i + v_k) + (v_i + v_l) = 0$.

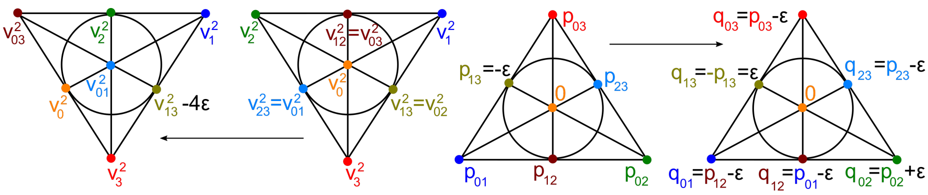

Fig. 5 Lemma A.1 for $i = 1$, $k = 2$, $j = 3$, $l = 0$ says that the new superbase $u_1 = -v_1$, $u_2 = v_{12}$, $u_3 = v_3$, $u_0 = v_{01}$ has the new voform VF and coform CF shown above.

For the new superbase $u_i = -v_i$, $u_j = v_j$, $u_k = v_{ik}$, $u_l = v_{il}$, two vonorms remain the same: $u_i^2 = v_i^2$ and $u_j^2 = v_j^2$. Two pairs of vonorms swap values: $u_k^2 = v_{ik}^2$, $u_{jl}^2 = u_{ik}^2 = (u_i + u_k)^2 = v_k^2$ and $u_l^2 = v_{il}^2$, $u_{jk}^2 = u_{il}^2 = (u_i + u_l)^2 = v_l^2$. The final vonorm is

$$u_{ij}^2 = u_{kl}^2 = (v_j - v_i)^2 = (v_i + v_j)^2 - 4 v_i \cdot v_j = v_{ij}^2 + 4p_{ij} = v_{ij}^2 - 4\varepsilon, \text{ see Fig. 5.}$$

We similarly check (A.1) illustrated in Fig. 5 for $i = 1$, $k = 2$, $j = 3$, $l = 0$.
$q_{ij} = -u_i \cdot u_j = v_i \cdot v_j = -p_{ij} = \varepsilon$
$q_{jk} = -u_j \cdot u_k = -v_j \cdot (v_i + v_k) = -v_i \cdot v_j - v_j \cdot v_k = p_{jk} - \varepsilon$
$q_{jl} = -u_j \cdot u_l = -v_j \cdot (v_i + v_l) = -v_i \cdot v_j - v_j \cdot v_l = p_{jl} - \varepsilon$
$q_{ik} = -u_i \cdot u_k = v_i \cdot (v_i + v_k) = v_i \cdot (-v_j - v_l) = -v_i \cdot v_l - v_i \cdot v_j = p_{il} - \varepsilon$
$q_{il} = -u_i \cdot u_l = v_i \cdot (v_i + v_l) = v_i \cdot (-v_j - v_k) = -v_i \cdot v_k - v_i \cdot v_j = p_{ik} - \varepsilon$
$q_{kl} = -u_k \cdot u_l = -(v_i + v_k)(v_i + v_l) = -v_i(v_i + v_k + v_l) - v_k \cdot v_l = v_i \cdot v_j + p_{kl} = p_{kl} + \varepsilon.$

Notice that all the formulae of Definition 2.6 hold for the new vonorms and conorms, while the conorm p_0 at the centre of CF remains zero by formula (3.2b):

$$4p_0 = u_i^2+u_j^2+u_k^2+u_l^2-u_{ij}^2-u_{ik}^2-u_{il}^2 = v_i^2+v_j^2+(v_i+v_k)^2+(v_i+v_l)^2-(v_j-v_i)^2-v_k^2-v_l^2$$

$$= v_i^2+v_j^2+(v_i^2+2v_iv_k+v_k^2)+(v_j+v_k)^2-(v_i^2-2v_iv_j+v_j^2)-v_k^2-(v_i+v_j+v_k)^2 =$$

$$= v_i^2+v_j^2+v_k^2+2v_iv_j+2v_jv_k+2v_iv_k-(v_i+v_j+v_k)^2 = 0.$$

Hence all central conorms p_0 in [13, Fig. 5] should be 0. □

Proof (of Theorem 2.8 for $n=3$) We will reduce any superbase $B=(v_0,v_1,v_2,v_3)$ of a lattice $\Lambda \subset \mathbb{R}^3$ to make all conorms p_{ij} non-negative. Starting from a negative conorm $p_{ij}=-\varepsilon<0$ (largest by absolute value), change the superbase by Lemma A.1. This reduction leads to the positive conorm $q_{ij}=\varepsilon$, not zero wrongly written in [13, Fig. 4(b)]. Four conorms decrease by $\varepsilon>0$ and can potentially become negative, which requires a new reduction by Lemma A.1 and so on.

To prove that the reduction process always finishes, notice that six vonorms keep or swap their values, but one vonorm decreases by $4\varepsilon>0$ at every step. Every reduction can make superbase vectors only shorter, but not shorter than a minimum distance between points of Λ. The angle between v_i, v_j can have only finitely many values when lengths of v_i, v_j are bounded. Hence the scalar product $\varepsilon = v_i \cdot v_j > 0$ cannot converge to 0. Since every reduction makes one partial sum v_S shorter by a positive constant, while other six vectors v_S keep or swap their lengths, the reductions by Lemma A.1 should finish in finitely many steps. □

A reduction of lattice bases for real crystals has many efficient implementations. Theoretical estimates for reduction steps are discussed in [23].