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THE 24-CELL CONJECTURE IN THE ALL-CONTACT CASE AND NEAR D_4

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Abstract. The 24-cell conjecture states that every Voronoi cell of a packing of unit balls in $\mathbb{R}^4$ has volume at least 8, the volume of the regular 24-cell. It implies that no packing of equal balls in $\mathbb{R}^4$ is denser than the lattice packing D_4. We prove the conjecture for two classes of cells; in each class, equality holds only for the D_4 root configuration. The first consists of the cells whose ball touches every ball centred at distance less than $2\sqrt{2}$ from its centre, and its proof uses a certificate at the second level of the Lasserre hierarchy. The second consists of the cells whose 24 nearest centres lie in an explicit neighbourhood of the D_4 configuration, whatever the other centres are. For them the volume is at least 8 plus a fixed multiple of the total outward displacement of the 24 centres, which we prove by a quantitative rigidity estimate and a second-order expansion of the volume about D_4. Our proofs for both classes are computer-assisted and partly formalised in Lean.

1. Introduction

Let $\mathcal{P} \subset \mathbb{R}^4$ be the set of centres of a packing of unit balls, so that distinct centres are at distance at least 2. The Voronoi cell of $c \in \mathcal{P}$ is

$$V_c = \{x \in \mathbb{R}^4 : \ |x - c| \le |x - y| \text{ for all } y \in \mathcal{P}\}.$$

For the lattice D_4, scaled to minimal distance 2, every Voronoi cell is a regular 24-cell with inradius 1 and volume 8. The *24-cell conjecture* states that $\mathrm{vol}(V_c) \ge 8$ for every packing and every centre.

The conjecture implies that the density of a packing of equal balls in $\mathbb{R}^4$ is at most $\pi^2/16$, the density of D_4, so that D_4 would be the densest packing in $\mathbb{R}^4$ [14]. Among lattice packings this was proved by Korkine and Zolotareff [10], while for general packings the best proved upper bound on the density is 0.63611, from the three-point bounds of Cohn, de Laat and Salmon [5]. In dimension three the analogous volume statement for the densest lattice packing is false: by the dodecahedral theorem of Hales and McLaughlin [9], the smallest Voronoi cell of a packing of unit balls is the regular dodecahedron of inradius 1, not the cell of the face-centred cubic lattice [14]. A proof of the full conjecture has been announced by Bhattacharjee, Bhattacharya, Mandal and Bhattacharya [2]. The subsection at the end of this section relates our results to it and to their later draft [3].

The centres that touch a given ball form a kissing configuration. In dimension 4 the kissing number is 24, the number of contacts in D_4, by Musin's theorem [13], and the configuration of 24 contact points is unique up to isometry [11]. Musin [14] proposed to approach the conjecture itself by semidefinite bounds for the centres around a given one, extending those for spherical codes, together with isoperimetric inequalities for polyhedra. Our proof of Theorem 1.1 below combines the two kissing theorems with the semidefinite part of this proposal.

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The conjecture is sharp at D_4, where the 24 nearest centres touch the central ball and every other centre is at distance at least $2\sqrt{2}$. Our first result treats the cells in which, as in D_4, every centre at distance less than $2\sqrt{2}$ touches the central ball.

Theorem 1.1. *Let $c \in \mathcal{P}$, and suppose that every centre $y \in \mathcal{P}$ with $0 < |y-c| < 2\sqrt{2}$ satisfies $|y-c| = 2$. Then $\mathrm{vol}(V_c) \geq 8$, with equality if and only if the centres at distance 2 from c form a translate of a D_4 root system scaled by $\sqrt{2}$.*

The proof bounds $\mathrm{vol}(V_c)$ from below by a quantity T_3, obtained from the caps that the neighbouring centres cut from the ball $B = B(c, \sqrt{2})$ by inclusion–exclusion truncated at the third order. For contact configurations, T_3 depends only on the kissing configuration $C \subset S^3$ of contact directions. An exact certificate for the second level of the Lasserre hierarchy, in the form developed by de Laat, Leijenhorst and de Muinck Keizer [11], together with interval bounds for the polynomial approximations it uses, shows $T_3(C) > 8$ whenever $|C| \leq 23$. The two kissing theorems recalled above dispose of $|C| \geq 24$. We also show that, for every packing, no point of B lies in five caps (Proposition 2.1), which identifies the loss in this bound exactly.

Our second result concerns configurations close to that of D_4. Let $u_1, \dots, u_{24}$ be the vectors of the D_4 root system scaled to unit length. For unit vectors $W = (w_1, \dots, w_{24})$ put

$$d(W) = \min_{R \in O(4)} \min_{\pi} \Big(\sum_{i=1}^{24} |w_{\pi(i)} - R u_i|^2 \Big)^{1/2},$$

the minimum over orthogonal maps R and permutations π of $\{1, \dots, 24\}$.

Theorem 1.2. *Let $c \in \mathcal{P}$, and let $y_1, \dots, y_{24} \in \mathcal{P} \setminus \{c\}$ be distinct. Put $\delta_i = |y_i - c| - 2$ and $w_i = (y_i - c)/|y_i - c|$, and suppose that*

$$d(W) \leq \tfrac{2}{5} \qquad \text{and} \qquad \sum_{i=1}^{24} \delta_i \leq \tfrac{3}{100}.$$

Then

$$\mathrm{vol}(V_c) \;\geq\; 8 + 0.2437 \cdot \frac{1}{2} \sum_{i=1}^{24} \delta_i.$$

In particular $\mathrm{vol}(V_c) \geq 8$, with equality if and only if $\{y_1 - c, \dots, y_{24} - c\} = 2R\{u_1, \dots, u_{24}\}$ for some $R \in O(4)$. In that case V_c is the regular 24-cell cut out by these 24 centres.

The packing condition gives $\delta_i \geq 0$, and nothing is assumed about the other centres of $\mathcal{P}$. The bound $d(W) \leq \frac{2}{5}$ only starts the rigidity argument, which then confines $d(W)$ below 0.022; in particular, $y_1, \dots, y_{24}$ are the 24 centres nearest to c (Remark 7.12). The proof shows that the first-order gain from the outward displacement outweighs all losses (Section 7 begins with an outline).

We develop the truncated bound in Section 2, give the certificate in Section 3, control its polynomial approximations in Section 4 and complete the proof of Theorem 1.1 in Section 5. Section 6 contains remarks on the relaxation, and we prove Theorem 1.2 in Section 7. Results marked *computer-assisted* rest on finite computations, which Section 8 describes together with the parts of both proofs that are formalised in Lean. Appendix A contains the longer proofs of Section 7.

Relation to [2] and [3]. The proof of the full conjecture announced in [2] treats cells according to their number of contacts, using a covering estimate, a semidefinite certificate and the uniqueness of the D_4 root system. The later public draft [3] states the bound for every cell

except those with 24 to 27 other centres within distance $\sqrt{6}$ of the centre, not all at distance 2. For part of this excluded class it has further results, among them a local result near D_4 and the bound for the 24 centres of the root configuration pushed outwards along their own directions.

The statement of [3] covers the cells of Theorem 1.1, for which we give an independent proof, based on an exact certificate for the second level of the Lasserre hierarchy. The configurations of Theorem 1.2 with $\sum_i \delta_i > 0$ lie in the excluded class (Remark 7.12). Theorem 1.2 contains the local result of [3], allows a total outward displacement 7.5 times larger and gives an explicit linear bound.

From [2] we take the truncated inclusion–exclusion bound and its value at D_4, which we reprove in Section 2; the distance $d(W)$; and the rigidity operator of the D_4 contact graph with its constant stress (Lemma 7.1) and its spectrum, which we recheck. From [3] we take the inversion hull (Lemma 7.2) and the rigidity argument with slack (Lemma 7.4).

2. The truncated cell

Fix a packing and translate so that $c = 0$. Let $B = \{x : |x| < \sqrt{2}\}$. For a centre $y \neq 0$ put

$$H_y = \{x : \ \langle x, y\rangle > |y|^2/2\} = \{x : \ |x - y| < |x|\}, \qquad K_y = H_y \cap B.$$

Since V_0 is closed and each H_y is open, $V_0 = \mathbb{R}^4 \setminus \bigcup_y H_y$, so $V_0 \cap B = B \setminus \bigcup_y K_y$. If $|y| \geq 2\sqrt{2}$, then every $x \in H_y$ has $|x| \geq \langle x, y\rangle/|y| > |y|/2 \geq \sqrt{2}$, so $K_y = \emptyset$. Write Y for the finite set of centres with $0 < |y| < 2\sqrt{2}$, and let S_k be the sum, over all k-element subsets of Y, of the volumes of the intersections of the corresponding caps.

Proposition 2.1. *No point of B lies in five of the sets K_y. Consequently*

$$\mathrm{vol}(V_0 \cap B) = 2\pi^2 - S_1 + S_2 - S_3 + S_4.$$

Proof. Let $x \in B$ lie in $K_{y_1}, \ldots, K_{y_m}$, and put $p_0 = 0$ and $p_i = y_i$. Each p_i satisfies $|p_i - x| \leq |x|$, and $|p_i - p_j| \geq 2$ for $i \neq j$. Hence

$$\langle p_i - x,\, p_j - x\rangle = \tfrac{1}{2}\big(|p_i - x|^2 + |p_j - x|^2 - |p_i - p_j|^2\big) \leq |x|^2 - 2 < 0.$$

The $m + 1$ vectors $p_i - x$ are nonzero and have pairwise negative inner products. In $\mathbb{R}^4$ there are at most five such vectors, so $m \leq 4$. Inclusion–exclusion over the caps covering a point therefore ends at order four, and $\mathrm{vol}(B) = 2\pi^2$. □

Put

$$T_3(Y) = 2\pi^2 - S_1 + S_2 - S_3.$$

Since at most four caps meet, S_4 is the volume of the set of points of B that lie in four caps.

Corollary 2.2. $\mathrm{vol}(V_0) \ \geq \ \mathrm{vol}(V_0 \cap B) \ = \ T_3(Y) + S_4 \ \geq \ T_3(Y)$.

The inequality $\mathrm{vol}(V_0 \cap B) \geq T_3(Y)$ is [2, Lemma 7.32], stated there for contact configurations together with its equality case. Corollary 2.2 shows that, in every packing, its loss is exactly S_4.

Proposition 2.3. *If a centre moves radially outward, or is removed, then $T_3(Y)$ does not decrease. Moving a centre of Y radially inward strictly decreases it.*

Proof. For $x \in B$ let $k(x)$ be the number of caps containing x. Then $T_3(Y) = \int_B b(k(x))\,dx$ with $b(k) = 1 - k + \binom{k}{2} - \binom{k}{3}$, and $b(k) - b(k-1) = -(k-2)(k-3)/2 \leq 0$ for $k \geq 1$. Moving y outward along its ray shrinks H_y, and removing y removes it, so $k(x)$ does not increase anywhere. For an inward move of $y \in Y$ the gained region contains points near $y/2$. This point lies in no other half-space $H_{y'}$, because the packing condition gives $|y/2 - y'|^2 - |y/2|^2 = \frac{1}{2}\big(|y'|^2 + |y - y'|^2 - |y|^2\big) \geq (8 - |y|^2)/2 > 0$. There k goes from 0 to 1 and b from 1 to 0. □

Contact configurations. Suppose now that every $y \in Y$ has $|y| = 2$. Then $y = 2w$ with $w \in S^3$, and $|y - y'| \geq 2$ means $\langle w, w' \rangle \leq \frac{1}{2}$. The directions form a *kissing configuration* $C \subset S^3$: a finite set of unit vectors with pairwise inner products in $[-1, \frac{1}{2}]$. All caps are cut off by hyperplanes at distance 1. Let ω_1 be the volume of one such cap of B, let $\omega_2(u)$ be the volume of the intersection of two caps whose normals have inner product u, and let $\omega_3(u, v, t)$ be the analogous volume for three caps. Then

$$T_3(C) = 2\pi^2 - \omega_1|C| + \sum_{\{w,w'\}\subset C} \omega_2(\langle w, w' \rangle) - \sum_{\{w,w',w''\}\subset C} \omega_3(\langle w, w' \rangle, \langle w, w'' \rangle, \langle w', w'' \rangle).$$

Lemma 2.4. *If k caps of a contact configuration share a point of B, then their normals have pairwise positive inner products. In particular $\omega_2(u) = 0$ for $u \leq 0$. For three of the normals, with Gram matrix G and pairwise inner products $u, v, t \leq \frac{1}{2}$, we have $\omega_3(u, v, t) > 0$ if and only if*

$$q(u, v, t) = 4uvt - (u + v + t - 1)^2 = 2 \det G - \mathbf{1}^\top \operatorname{adj}(G)\, \mathbf{1} > 0.$$

Proof. If $x \in B$ satisfies $\langle x, w_i \rangle > 1$, then the angle between x and w_i has cosine greater than $1/|x| > 1/\sqrt{2}$. Any two of the w_i are therefore at angle less than $\pi/2$. Now let three caps meet in B. By the first part their inner products u, v, t lie in $(0, \frac{1}{2}]$, so $\det G = 1 + 2uvt - u^2 - v^2 - t^2 \geq \frac{1}{4}$. The entries of $\operatorname{adj}(G)\mathbf{1}$ are $(1 - t)(1 + t - u - v)$ and its cyclic analogues, all positive. Let $x_0 \in \operatorname{span}\{w_1, w_2, w_3\}$ satisfy $\langle x_0, w_i \rangle = 1$ for each i. Then $x_0 = \sum_i \lambda_i w_i$ with $\lambda = G^{-1}\mathbf{1} > 0$, and $|x_0|^2 = \mathbf{1}^\top G^{-1}\mathbf{1}$. Every x in the intersection of the three closed half-spaces satisfies

$$|x|^2 \;\geq\; |x_0|^2 + 2\langle x - x_0, x_0 \rangle \;=\; |x_0|^2 + 2\sum_i \lambda_i \big(\langle x, w_i \rangle - 1\big) \;\geq\; |x_0|^2,$$

so $\mathbf{1}^\top G^{-1}\mathbf{1} < 2$. Since $\operatorname{adj} G = (\det G)\, G^{-1}$, we get $q = \det G\,(2 - \mathbf{1}^\top G^{-1}\mathbf{1}) > 0$. Conversely, let $q > 0$. If $\det G = 0$, then $\operatorname{adj} G$ is positive semidefinite and $q = -\mathbf{1}^\top \operatorname{adj}(G)\mathbf{1} \leq 0$. Hence $\det G > 0$ and $|x_0|^2 = \mathbf{1}^\top G^{-1}\mathbf{1} < 2$, and for small $\varepsilon > 0$ the point $(1 + \varepsilon)x_0$ lies in all three caps. The identity for q is a direct expansion. □

Lemma 2.5 ([2, Prop. 7.34])**.** *For the D_4 root system, normalised to unit vectors, $T_3 = 8$.*

Proof. The Voronoi cell of $\sqrt{2}D_4$ is the regular 24-cell with inradius 1, circumradius $\sqrt{2}$ and volume 8, so $\operatorname{vol}(V_0 \cap B) = 8$. The lattice $\sqrt{2}D_4$ has no vectors of length strictly between 2 and $2\sqrt{2}$, so Y consists of the 24 contacts. The inner products of distinct roots lie in $\{-1, -\frac{1}{2}, 0, \frac{1}{2}\}$. The eight roots at inner product $\frac{1}{2}$ with a fixed root form the vertices of a cube, two of them being at inner product $\frac{1}{2}$ exactly when they are adjacent. A cube has no triangles, so no four roots have all six inner products equal to $\frac{1}{2}$. By Lemma 2.4 no point of B lies in four caps, so $S_4 = 0$, and Corollary 2.2 gives $T_3 = 8$. □

Numerically,

$$\omega_1 \approx 0.7460119958, \qquad \omega_2(\tfrac{1}{2}) \approx 0.0760762771, \qquad \omega_3(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) \approx 0.0118567031,$$

and Lemma 2.5 reads $2\pi^2 - 24\omega_1 + 96\,\omega_2(\frac{1}{2}) - 96\,\omega_3(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) = 8$.

3. A level-two certificate

We use the second level of the Lasserre hierarchy for spherical codes in the form of [11], which built on [7]. The dual objects are a kernel K on $\mathcal{I}_2$, the subsets of S^3 of size at most

two, invariant under the orthogonal group and positive semidefinite in the sense of [11]. For a finite set S of at most four points put

$$A_2K(S) = \sum_{\substack{J,J'\in\mathcal{I}_2\\ J\cup J'=S}} K(J,J').$$

Positive semidefiniteness of K, applied to the indicator vector of the subsets of a finite code C, gives

$$0 \;\le\; \sum_{J,J'\subseteq C,\ |J|,|J'|\le 2} K(J,J') \;=\; K(\emptyset,\emptyset) + \sum_{\emptyset\neq S\subseteq C,\ |S|\le 4} A_2K(S). \tag{1}$$

In the symmetry-reduced form of [11], $A_2K(S)$ is an $S_{|S|}$-invariant polynomial in the pairwise inner products of S. We use the degree parameters $(d_1,\delta) = (14,16)$ of [11], and with these every such polynomial has degree at most 16.

The objective is encoded by right-hand sides on pieces of the configuration spaces. Write $D = [-1,\frac{1}{2}]$, and call a finite set of points *admissible* if its pairwise inner products lie in D and its Gram matrix is positive semidefinite. Let p_2 be a polynomial of degree at most 16 in one variable, and let p_3 be an S_3-invariant polynomial of degree at most 16 in three variables. The pieces are:

- singletons, with right-hand side $-\omega_1^+$, where ω_1^+ is a rational number with $\omega_1 \le \omega_1^+$;
- pairs with $u \in [-1,0]$, right-hand side 0, and pairs with $u \in [0,\frac{1}{2}]$, right-hand side $p_2(u)$;
- admissible triples with $q \le 0$, right-hand side 0, and admissible triples with $q \ge 0$, right-hand side $-p_3$;
- admissible quadruples, right-hand side 0.

On each piece we require an identity $A_2K(S) + \Sigma(S) = c(S)$, where Σ is a sum of terms $g\cdot h$ with h a sum of squares and g a polynomial that is nonnegative on the piece. Put $s(x) = (x+1)(\frac{1}{2}-x)$. For pairs on $[a,b]$ the polynomials g are 1 and $(u-a)(b-u)$. For triples they are 1, the elementary symmetric functions of $s(u), s(v), s(t)$, the Gram determinant, and $-q$ or q on the two triple pieces. For quadruples they are 1, the elementary symmetric functions of the values of s at the six inner products, the Gram determinant, and the elementary symmetric functions of the four 3×3 principal minors of the Gram matrix. In the singleton identity we add a variable $\mu \ge 0$, giving $A_2K(\{x\}) + r - \mu = -\omega_1^+$ with a constant $r \ge 0$.

Proposition 3.1. *Suppose the identities hold, with $\mu \ge 0$ and $K(\emptyset,\emptyset) + 23\mu = \kappa$. Then every kissing configuration C with $|C| \le 23$ satisfies*

$$F(C) := 2\pi^2 - \omega_1^+|C| + \sum_{\substack{\{w,w'\}\subset C\\ u\ge 0}} p_2(u) - \sum_{\substack{\text{triples}\\ q\ge 0}} p_3 \;\;\ge\;\; 2\pi^2 - \kappa.$$

Proof. Assign each pair with $u \ge 0$ to the second pair piece and every other pair to the first. Assign each triple with $q \ge 0$ to the second triple piece and every other triple to the first. Quadruples form a single piece. On the assigned piece $\Sigma \ge 0$, so $A_2K(S) \le c(S)$. For singletons, $A_2K(\{x\}) \le \mu - \omega_1^+$. Substituting into (1) gives $0 \le K(\emptyset,\emptyset) + |C|(\mu-\omega_1^+) + \sum p_2 - \sum p_3$. Since $|C|\mu \le 23\mu$, this becomes $F(C) \ge 2\pi^2 - K(\emptyset,\emptyset) - 23\mu = 2\pi^2 - \kappa$. □

Theorem 3.2 (computer-assisted)**.** *There is a solution of the identities above in exact rational arithmetic with $\mu > 0$ and $\kappa = 1828197/156250$. Hence $F(C) \ge 2\pi^2 - 1828197/156250 = 8.0387480021787\ldots$ for every kissing configuration with at most 23 points.*

The certificate, computed with the clustered low-rank solver of [12] and rounded to exact rationals, is in the supplement [16]. Each zonal matrix entry, indexed as in [11] by a signature $\lambda = (\lambda_1, \lambda_2)$, was checked to have degree $|\lambda| = \lambda_1 + \lambda_2$, and the sum-of-squares terms have degree at most 16 by construction. So both sides of each identity are polynomials of degree at most 16, and exact equality at the pair samples and on the principal lattices of Table 3, which are unisolvent for all such polynomials [15, 4], proves the identities.

4. The polynomial approximations

The function F uses ω_1^+, p_2 and p_3 in place of ω_1, ω_2 and ω_3. Lemma 4.1 below bounds the errors (Table 3). The volume ω_2 has a closed form. For ω_3 the partial derivative $\partial\omega_3/\partial u$ has a closed form in terms of a one-dimensional integral, and ω_3 is enclosed by certified one-dimensional integration [1]. The same formula bounds the derivatives of $\omega_3 - p_3$ over each box of a cover of the triple piece.

Lemma 4.1 (computer-assisted)**.** *Let $\varepsilon_2 = 2.8111 \cdot 10^{-12}$ and $\varepsilon_3 = 10^{-6}$. Then*

(1) $\omega_1 \le \omega_1^+$;
(2) $p_2(u) \le \omega_2(u) + \varepsilon_2$ *for* $u \in [0, \frac{1}{2}]$;
(3) $p_3(u, v, t) \ge \omega_3(u, v, t) - \varepsilon_3$ *for every admissible triple with* $q(u, v, t) \ge 0$.

By Lemma 2.4, $\omega_2 = 0$ on $[-1, 0]$ and $\omega_3 = 0$ on admissible triples with $q \le 0$. The right-hand side 0 on those pieces is therefore exact.

5. Proof of Theorem 1.1

By Corollary 2.2 it suffices to show $T_3(C) \ge 8$ for every kissing configuration $C \subset S^3$, with equality only for D_4. By [13] we have $|C| \le 24$, and by [11] a configuration with $|C| = 24$ is a D_4 root system, for which $T_3 = 8$ by Lemma 2.5.

Let $|C| \le 23$. Then C has at most 253 pairs and 1771 triples. Lemmas 2.4 and 4.1 give

$$T_3(C) \;\ge\; F(C) - 253\,\varepsilon_2 - 1771\,\varepsilon_3,$$

since the singleton term only improves, the pair and triple terms on the pieces with right-hand side 0 are exact, and each remaining term loses at most ε_2 or ε_3. Theorem 3.2 then gives

$$T_3(C) \;\ge\; 2\pi^2 - \frac{1828197}{156250} - 253\,\varepsilon_2 - 1771\,\varepsilon_3 = 8.0369770014675\ldots > 8.$$

If $\mathrm{vol}(V_0) = 8$, then $T_3(C) \le 8$ by Corollary 2.2, so C is a D_4 root system and V_0 is the regular 24-cell. Conversely, if the contacts form $\sqrt{2}$ times a D_4 root system, their half-spaces cut out a regular 24-cell of circumradius $\sqrt{2}$. Every other centre y has $|y| \ge 2\sqrt{2}$, so H_y lies in $\{|x| > \sqrt{2}\}$ and misses the cell. Hence V_0 is this 24-cell and $\mathrm{vol}(V_0) = 8$. □

6. Remarks on the relaxation

Remark 6.1 (The bound on the number of points). The values in this remark are floating-point solutions of the semidefinite programs. Without the constraint $|C| \le 23$, the relaxation gives only $T_3 \ge 7.9617$ at degrees $(14, 16)$ and 7.9932 at degrees $(16, 18)$; at $(14, 16)$ the numbers of pairs, triples and quadruples of its optimal moment vector are close to those of a mixture of a 23-point and a 24-point configuration, which the bound on $|C|$ excludes. The bound $|C| \le 23.5$, which is equivalent for integer sizes, gives 7.9807. For the exact truncated volume $T_3 + S_4$ of Corollary 2.2 the values are 7.9953 without a bound and 8.0239 with $|C| \le 23.5$. Whether the relaxation for $T_3 + S_4$ reaches 8 without a bound on $|C|$ at some degree is open.

Remark 6.2 (The packing constraint is needed). The bound concerns cells whose facets come from a kissing configuration. Without the angular constraint it fails. The polytope $\{x : \langle x, q_i\rangle \le 1,\ i = 1, \dots, 24\}$ for the rational vectors q_i listed in the supplement contains the unit ball and has 24 facets, yet its volume is $7.9655697\ldots < 8$. This was computed exactly, by two independent methods [16]. Its normals have minimal angle about $54.6°$. A volume below 8 in this setting was observed numerically in the code accompanying [2]. So no argument about facet directions alone, in the manner of Fejes Tóth's bound for polyhedra with twelve faces containing a ball [8], can give the conjecture. Any proof must use the $60°$ separation.

Remark 6.3 (Beyond contacts). For a general cell, the centres at distance between 2 and $2\sqrt{2}$ cut smaller caps from B, and Proposition 2.1 still applies. The natural extension of Theorem 3.2 is a level-two relaxation in which each point carries its distance as a label. By Proposition 2.3, rounding labels down is valid, but near D_4 the bound grows only linearly in the displacement, so such a relaxation must keep the labels continuous there. Theorem 1.2 treats the configurations near D_4 by a local argument instead.

7. A neighbourhood of D_4

This section proves Theorem 1.2. We translate so that $c = 0$ and write ρ and σ for the two bounds in the hypothesis, so that $d(W) \le \rho$ and $\sum_i \delta_i \le \sigma$. Put

$$h_i = \tfrac{1}{2}|y_i|, \qquad \eta_i = h_i - 1 = \tfrac{1}{2}\delta_i, \qquad s = \sum_{i=1}^{24} \eta_i, \qquad w_i = \frac{y_i}{|y_i|}.$$

The packing condition gives $\eta_i \ge 0$, and the hypothesis gives $\eta_i \le \bar\eta := \sigma/2$ and $s \le \sigma/2$, so that $|\eta|^2 \le \bar\eta s$. Since $H_{y_i} = \{x : \langle x, w_i\rangle > h_i\}$, the cell lies in the polytope

$$P = \{x :\ \langle x, w_i\rangle \le h_i,\ i = 1, \dots, 24\},$$

and we put $\mathcal{F} = \mathrm{vol}(P \cap B)$, with $B = \{|x| < \sqrt{2}\}$ as in Section 2. The argument works for any (ρ, σ) satisfying the conditions collected in Section 7.7, and it gives $\mathrm{vol}(V_0) \ge 8 + \Gamma s$ with an explicit constant $\Gamma = \Gamma(\rho, \sigma) > 0$. The values in Theorem 1.2 are one certified instance, the row $(\rho, \sigma) = (\frac{2}{5}, \frac{3}{100})$ of Table 1, which we call the *main row*.

The proof compares the first-order gain with the losses. By Lemma 7.2, the cell contains $P \cap J$, where J is the inversion hull of Section 7.2, so $\mathrm{vol}(V_0)$ is at least $\mathcal{F}$ minus the *hull deficit* $\mathrm{vol}((P \cap B) \setminus J)$. In Section 7.4 we write $\mathcal{F}$ as an inclusion–exclusion sum Φ, the analogue of T_3, up to a small term from squares of caps, and in Section 7.5 we expand Φ about D_4: to first order it grows by $\frac{4}{3}s$, the quadratic part is controlled by exact matrices, and the third-order remainder is explicit. In Section 7.6 we bound the hull deficit by quadratic terms. All these losses are quadratic in the tilt τ and the pushes η. The rigidity estimate of Section 7.3 bounds $|\tau|$ by a multiple of s, and $|\eta|^2 \le \bar\eta s$, so in the region of Theorem 1.2 the losses add up to less than $\frac{4}{3}s$, and the first-order gain dominates them. The budget and the assembly of the bound are in Section 7.7.

7.1. **The root system.** The roots of D_4 are the 24 vectors $\pm e_p \pm e_q$ with $p < q$, and u_i is the ith root divided by $\sqrt{2}$. Two distinct u_i, u_j have inner product $\frac{1}{2}$ on a set T of 96 pairs, 0 on a set O of 72 pairs, $-\frac{1}{2}$ on 96 pairs and -1 on 12. The pairs in T are the *contact pairs*. Each u_i lies in eight of them, and its eight contact neighbours sum to $4u_i$. A *contact triangle* is a set of three roots any two of which form a contact pair. There are 96 contact triangles, each contact pair lies in exactly three of them and each root in twelve, and no four roots are pairwise in contact (proof of Lemma 2.5).

The 24 *vertex directions* $v_1, \dots, v_{24}$ are the unit vectors $\pm e_p$ and $\frac{1}{2}(\pm 1, \pm 1, \pm 1, \pm 1)$. Each inner product $\langle u_i, v_k \rangle$ is 0 or $\pm 1/\sqrt{2}$. For each k the set $N(k) = \{i : \langle u_i, v_k \rangle = 1/\sqrt{2}\}$ has six elements. It consists of three orthogonal pairs $\{a_{kj}, a'_{kj}\}$, $j = 1, 2, 3$, and its other twelve pairs are contact pairs. With $f_{kj} = (u_{a_{kj}} - u_{a'_{kj}})/\sqrt{2}$, the vectors $v_k, f_{k1}, f_{k2}, f_{k3}$ are orthonormal, and the six roots in $N(k)$ are $(v_k \pm f_{kj})/\sqrt{2}$. In particular $u_{a_{kj}} + u_{a'_{kj}} = \sqrt{2}\, v_k$. Each orthogonal pair lies in exactly one set $N(k)$, each contact pair in exactly three and each root in exactly six. A *square* is the union of two orthogonal pairs of the same $N(k)$; there are 72 squares. The polytope

$$J_0 = \operatorname{conv}\{2u_1, \dots, 2u_{24}\} = \{x : \ \langle x, v_k \rangle \le \sqrt{2} \text{ for all } k\}$$

is a 24-cell with inradius $\sqrt{2}$. Its facet with normal v_k is the octahedron $\operatorname{conv}\{2u_b : b \in N(k)\}$, which touches the sphere $|x| = \sqrt{2}$ at $\sqrt{2}\, v_k$.

For each i fix a 4×3 matrix B_i whose columns form an orthonormal basis of $u_i^\perp$. A *tilt* is a vector $\tau = (\tau_1, \dots, \tau_{24}) \in (\mathbb{R}^3)^{24} = \mathbb{R}^{72}$, and we write $t_i = B_i \tau_i \in u_i^\perp$, so that $|\tau|^2 = \sum_i |t_i|^2$. The *rigidity operator* $\Lambda : \mathbb{R}^{72} \to \mathbb{R}^T$ and its analogue $\Lambda_O : \mathbb{R}^{72} \to \mathbb{R}^O$ on orthogonal pairs are

$$(\Lambda\tau)_{ij} = \langle t_i, u_j \rangle + \langle u_i, t_j \rangle \quad (\{i,j\} \in T), \qquad (\Lambda_O\tau)_{ij} = \langle t_i, u_j \rangle + \langle u_i, t_j \rangle \quad (\{i,j\} \in O).$$

The vector $\Lambda\tau$ is the first-order change of the contact inner products when each u_i moves to $u_i + t_i$.

The exact computations in [16] use other coordinates: $t_i = B_i^{\mathrm{s}} \tau_i^{\mathrm{s}}$, where $\sqrt{2}\, B_i^{\mathrm{s}}$ is an integer 4×3 matrix whose columns are orthogonal, lie in $u_i^\perp$ and have lengths $\sqrt{2}, 1, 1$. So the columns of B_i^{s} have Gram matrix $\operatorname{diag}(1, \frac{1}{2}, \frac{1}{2})$. In the coordinates τ^{s}, the matrices of Λ and Λ_O are rational, and so are the matrices of the quadratic forms given by N_0 in Lemma 7.4 and by $\mathcal{H}$ in Lemma 7.9. Positive semidefiniteness, eigenvalues, Schur complements and norms refer to the Euclidean inner product and do not depend on the coordinates. In [16] they are computed exactly in the coordinates τ^{s}, with this Gram matrix.

Lemma 7.1. (1) *The eigenvalues of* $\Lambda^\top\Lambda$ *are* $0, 1, \frac{5}{2}, 3, 4$, *with multiplicities* $6, 29, 8, 21, 8$, *and* $\ker\Lambda = \{(B_i^\top A u_i)_i : \ A \in \mathfrak{so}(4)\}$. *Hence* $|\Lambda\tau| \ge |\tau|$ *for* $\tau \perp \ker\Lambda$, *and* $\|\Lambda\| = 2$.
(2) $\sum_{\{i,j\} \in T} (\Lambda\tau)_{ij} = 0$ *for every* τ.
(3) $\|\Lambda_O\| \le 2$.

Proof. Part (1) is [2, Lemma 7.50], where it is stated for the singular values of Λ. The vectors $(B_i^\top A u_i)_i$ lie in the kernel because $\langle Au_i, u_j \rangle + \langle u_i, Au_j \rangle = 0$, and they form a 6-dimensional space because the u_i span $\mathbb{R}^4$; since $\ker\Lambda$ has dimension 6, they form all of it. For (2), $\sum_T (\Lambda\tau)_{ij} = \sum_i \langle t_i, \sum_j u_j \rangle$, where j runs over the contact neighbours of i. This equals $\sum_i \langle t_i, 4u_i \rangle = 0$, which is the constant stress of [2, Cor. 7.49]. For (3), the six roots orthogonal to u_i are $\pm$ an orthonormal basis of $u_i^\perp$, so $\sum_{j \perp i} \langle t_i, u_j \rangle^2 = 2|t_i|^2$, and $\sum_O (\Lambda_O\tau)_{ij}^2 \le 2 \sum_i \sum_{j \perp i} \langle t_i, u_j \rangle^2 = 4|\tau|^2$. □

By (1) and (2), a tilt with $\Lambda\tau \le 0$ satisfies $\Lambda\tau = 0$ and is an infinitesimal rotation: the normalised root system is infinitesimally jammed, as shown in [6, Prop. 3.3]. Lemma 7.4 below is a quantitative form of this statement.

7.2. **The other centres.** Put $q_i = 4y_i/|y_i|^2 = 2w_i/h_i$, the image of y_i under inversion in the sphere of radius 2, and let

$$J = \operatorname{conv}\{0, q_1, \dots, q_{24}\}$$

be the *inversion hull*.

Lemma 7.2 (Inversion hull [3]). *For centres $y \neq z$, both different from 0, and $q_y = 4y/|y|^2$,*

$$\frac{|z|^2}{2} - \langle q_y, z\rangle = \frac{(|z|^2-4)(|y|^2-4) + 4(|y-z|^2-4)}{2|y|^2} \;\geq\; 0.$$

Consequently $V_0 \supseteq P \cap J$ and

$$\operatorname{vol}(V_0) \;\geq\; \mathcal{F} - \operatorname{vol}\big((P\cap B)\setminus J\big).$$

Proof. Since $2\langle y,z\rangle = |y|^2 + |z|^2 - |y-z|^2$,

$$2|y|^2\Big(\frac{|z|^2}{2} - \langle q_y, z\rangle\Big) = |y|^2|z|^2 - 4\big(|y|^2+|z|^2-|y-z|^2\big) = (|z|^2-4)(|y|^2-4) + 4(|y-z|^2-4),$$

and the three brackets are nonnegative by the packing condition. Hence, for every centre $z \notin \{0, y_1, \dots, y_{24}\}$, the closed half-space $\{x : \langle x, z\rangle \leq |z|^2/2\}$ contains 0 and every q_i, and therefore contains J. The cell V_0 is the intersection of P with these half-spaces, so $V_0 \supseteq P\cap J$ and $\operatorname{vol}(V_0) \geq \operatorname{vol}(P\cap J\cap B) = \mathcal{F} - \operatorname{vol}((P\cap B)\setminus J)$. □

7.3. **Gauge and rigidity.** Choose, as in [2, Theorem 7.51], a labelling and an $R \in O(4)$ that attain $d(W)$. Applying R^{-1} to the packing changes neither the hypotheses nor the volume, so we may assume $R = I$. Then the identity minimises $R' \mapsto \sum_i |w_i - R'u_i|^2$ over $O(4)$. Put

$$d_i = w_i - u_i, \qquad \|d\| = \Big(\sum_i |d_i|^2\Big)^{1/2} = d(W) \leq \rho, \qquad n_i = \langle d_i, u_i\rangle, \qquad t_i = d_i - n_i u_i,$$

let $\tau \in \mathbb{R}^{72}$ be the tilt with $B_i\tau_i = t_i$, and write $\xi = (\tau, \eta) \in \mathbb{R}^{72}\times\mathbb{R}^{24}$. For $\{i,j\} \in T\cup O$ put $u_{ij} = \langle w_i, w_j\rangle$, and for $\{i,j\}\in T$ put $\Delta u_{ij} = u_{ij} - \frac12$. Let $\bar d$ be a number with $\max_i |d_i| \leq \|d\| \leq \bar d < 1$. At first $\bar d = \rho$, and Corollary 7.5 below replaces it by a much smaller value. Put

$$\chi = \frac{2}{1 + (1-\bar d^2)^{1/2}}, \qquad \varphi = 2\arcsin\frac{\bar d}{2}, \qquad \bar u = \tfrac12 - \cos\big(\tfrac{\pi}{3} + 2\varphi\big), \qquad \bar u_\perp = \sin 2\varphi.$$

Lemma 7.3. (1) $\tau \perp \ker\Lambda$.

(2) $n_i = -\frac12|d_i|^2$ *and* $|t_i|^2 \leq |d_i|^2 \leq \chi|t_i|^2$. *Hence* $|\tau| \leq \|d\| \leq \chi^{1/2}|\tau|$.

(3) *For $\{i,j\}\in T$ we have $\Delta u_{ij} = (\Lambda\tau)_{ij} + c_{ij}$ with $c_{ij} = \langle d_i, d_j\rangle - \frac14(|d_i|^2 + |d_j|^2)$. For $\{i,j\}\in O$ we have $u_{ij} = (\Lambda_O\tau)_{ij} + \langle d_i, d_j\rangle$. Moreover*

$$\sum_{\{i,j\}\in T} \Delta u_{ij} = Q_d := \sum_{\{i,j\}\in T} \langle d_i, d_j\rangle - 2\|d\|^2.$$

(4) $|c_{ij}| \leq \frac34(|d_i|^2 + |d_j|^2)$ *and* $(\sum_T c_{ij}^2)^{1/2} \leq 3\bar d\|d\|$. *With* $Q_t(\tau) = \sum_T\langle t_i, t_j\rangle - 2|\tau|^2$,

$$|Q_d - Q_t(\tau)| \leq \big(2\sqrt3\,\chi\bar d + \chi^2\bar d^2\big)|\tau|^2.$$

(5) *For $\{i,j\}\in T$,*

$$u_{ij} \;\leq\; a(h_i,h_j) \;\leq\; \tfrac12 + \tfrac12(\eta_i+\eta_j), \qquad a(h,h') = \frac{h^2+h'^2-1}{2hh'}.$$

(6) *If $2\varphi < \pi/6$, then $u_{ij} \geq \frac12 - \bar u$ for $\{i,j\}\in T$, $|u_{ij}| \leq \bar u_\perp$ for $\{i,j\}\in O$, and $u_{ij} < 0$ for all other pairs.*

Proof. (1) For $A \in \mathfrak{so}(4)$ the derivative of $s \mapsto \sum_i |w_i - e^{sA}u_i|^2$ at $s=0$ is $-2\sum_i\langle u_i + d_i, Au_i\rangle = -2\sum_i\langle t_i, Au_i\rangle$, because $\langle u_i, Au_i\rangle = 0$ and $d_i - t_i$ is a multiple of u_i. Minimality makes it vanish, so τ is orthogonal to every $(B_i^\top Au_i)_i$, and these span $\ker\Lambda$ by Lemma 7.1.

(2) Expanding $|u_i + d_i|^2 = 1$ gives $|d_i|^2 = -2n_i$. Hence $n_i^2 + 2n_i + |t_i|^2 = 0$, and since $\langle w_i, u_i\rangle = 1 + n_i = 1 - \frac{1}{2}|d_i|^2 > 0$ (as $|d_i| \le \bar{d} < 1$) we get $n_i = (1 - |t_i|^2)^{1/2} - 1$. So $|d_i|^2 = 2|t_i|^2/(1 + (1 - |t_i|^2)^{1/2}) \le \chi|t_i|^2$, while $|d_i|^2 = |t_i|^2 + n_i^2 \ge |t_i|^2$.

(3) For $\{i, j\} \in T$ we have $\langle u_i, d_j\rangle = \langle u_i, t_j\rangle + \frac{1}{2}n_j = \langle u_i, t_j\rangle - \frac{1}{4}|d_j|^2$, and expanding $\langle u_i + d_i, u_j + d_j\rangle$ gives the first identity. The second is the same expansion with $\langle u_i, u_j\rangle = 0$. For the sum, the contact neighbours of u_i sum to $4u_i$, so $\sum_T(\langle u_i, d_j\rangle + \langle d_i, u_j\rangle) = \sum_i \langle d_i, 4u_i\rangle = 4\sum_i n_i = -2\|d\|^2$.

(4) The bound on c_{ij} follows from $|\langle d_i, d_j\rangle| \le \frac{1}{2}(|d_i|^2 + |d_j|^2)$. Since each root lies in eight contact pairs, $\sum_T c_{ij}^2 \le \frac{9}{16}\sum_T(|d_i|^2 + |d_j|^2)^2 \le \frac{9}{8}\sum_T(|d_i|^4 + |d_j|^4) = 9\sum_i |d_i|^4 \le 9\bar{d}^2\|d\|^2$. For the last bound write $d_i = t_i + n_i u_i$. For $\{i, j\} \in T$ this gives $\langle d_i, d_j\rangle = \langle t_i, t_j\rangle + n_j\langle t_i, u_j\rangle + n_i\langle u_i, t_j\rangle + \frac{1}{2}n_i n_j$, and $\|d\|^2 = |\tau|^2 + \sum_i n_i^2$, so

$$Q_d - Q_t(\tau) = \sum_T \big(n_j\langle t_i, u_j\rangle + n_i\langle u_i, t_j\rangle + \tfrac{1}{2}n_i n_j\big) - 2\sum_i n_i^2.$$

Here $|\langle t_i, u_j\rangle| = |\langle t_i, u_j - \frac{1}{2}u_i\rangle| \le \frac{\sqrt{3}}{2}|t_i|$, $|n_i| \le \frac{\chi}{2}|t_i|^2$ and $|t_i| \le \bar{d}$. The cubic terms are therefore at most $\frac{\sqrt{3}\chi}{4}\bar{d}\sum_T(|t_i|^2 + |t_j|^2) = 2\sqrt{3}\chi\bar{d}|\tau|^2$. The quartic terms are at most $\frac{\chi^2}{16}\bar{d}^2\sum_T(|t_i|^2 + |t_j|^2) + \frac{\chi^2}{2}\bar{d}^2|\tau|^2 = \chi^2\bar{d}^2|\tau|^2$.

(5) The packing condition $|y_i - y_j|^2 = 4h_i^2 + 4h_j^2 - 8h_i h_j u_{ij} \ge 4$ is $u_{ij} \le a(h_i, h_j)$. With $h = 1 + \eta$ a direct expansion gives

$$\tfrac{1}{2}(\eta_i + \eta_j) - \big(a(h_i, h_j) - \tfrac{1}{2}\big) = \frac{\eta_i\eta_j(3 + \eta_i + \eta_j)}{2(1 + \eta_i)(1 + \eta_j)} \;\ge\; 0.$$

(6) The angle between w_i and u_i is $2\arcsin(|d_i|/2) \le \varphi$. Angles between points of S^3 satisfy the triangle inequality, so the angle between w_i and w_j differs by at most 2φ from the angle between u_i and u_j. This angle is $\pi/3$ on T, $\pi/2$ on O and at least $2\pi/3$ otherwise. Since $2\varphi < \pi/6$, this gives the three bounds. □

The next lemma is the rigidity argument of [2, Theorem 7.51], carried out with slack as in [3]: the contact inner products may exceed $\frac{1}{2}$ by the pushes.

Lemma 7.4 (computer-assisted)**.** *Let C_r be the supremum of $|\tau'|$ over all $\tau' \perp \ker\Lambda$ and $\eta' \in \mathbb{R}^{24}$ such that $\eta' \ge 0$, $\sum_i \eta'_i = 1$, and $(\Lambda\tau')_{ij} \le \frac{1}{2}(\eta'_i + \eta'_j)$ for all $\{i, j\} \in T$. Then C_r is finite, and $C_r^2 \le \frac{191}{100}$. In the setting of Lemma 7.3,*

$$|\tau| \;\le\; C_r\big(s + \tfrac{3}{2}\|d\|^2\big).$$

If moreover $|\tau| \le \bar{t}$ and $\beta := \frac{3}{2}C_r\chi\bar{t} < 1$, then $|\tau| \le C_r s/(1 - \beta)$.

Proof. First, $C_r \le 8$. Let (τ', η') be admissible. Since each root lies in eight contact pairs, $\sum_T(\Lambda\tau')_{ij}^+ \le \frac{1}{2}\sum_T(\eta'_i + \eta'_j) = 4$. By Lemma 7.1(2) the entries of $\Lambda\tau'$ sum to 0, so $\|\Lambda\tau'\|_1 = 2\sum_T(\Lambda\tau')_{ij}^+ \le 8$. By Lemma 7.1(1), $|\tau'| \le |\Lambda\tau'| \le \|\Lambda\tau'\|_1 \le 8$.

The bound $C_r^2 \le \frac{191}{100}$ comes from an identity

$$\tfrac{191}{100}\Big(\sum_i \eta'_i\Big)^2 - |\tau'_\perp|^2 = \xi'^{\top} N_0 \xi' + \sum_{k,l}(M_0)_{kl}\,\ell_k(\xi')\,\ell_l(\xi') \qquad \text{for all } \xi' = (\tau', \eta'),$$

where $\tau'_\perp$ is the component of τ' orthogonal to $\ker\Lambda$ and $\ell_1, \dots, \ell_{120}$ are the linear forms η'_i and $\frac{1}{2}(\eta'_i + \eta'_j) - (\Lambda\tau')_{ij}$ for $\{i, j\} \in T$. The matrix M_0 is symmetric with nonnegative rational entries, and N_0 is positive semidefinite (Table 3). On admissible (τ', η') every ℓ_k is nonnegative, so $|\tau'|^2 \le \frac{191}{100}$.

By Lemma 7.3(3)–(5), $(\Lambda\tau)_{ij} = \Delta u_{ij} - c_{ij} \le \frac{1}{2}(\eta_i + \eta_j) + \frac{3}{4}(|d_i|^2 + |d_j|^2)$ on T. So $\eta_i' := \eta_i + \frac{3}{2}|d_i|^2 \ge 0$ satisfies $(\Lambda\tau)_{ij} \le \frac{1}{2}(\eta_i' + \eta_j')$, and $\tau \perp \ker\Lambda$ by Lemma 7.3(1). If $\sum_i \eta_i' > 0$, scaling gives $|\tau| \le C_r \sum_i \eta_i' = C_r(s + \frac{3}{2}\|d\|^2)$. If $\sum_i \eta_i' = 0$, then $\Lambda\tau \le 0$ with entries summing to 0, so $\Lambda\tau = 0$ and $\tau = 0$. Finally $\|d\|^2 \le \chi|\tau|^2 \le \chi\bar{t}|\tau|$, so $|\tau| \le C_r s + \beta|\tau|$. □

Iterating Lemma 7.4 improves the bound $\bar{d}$.

Corollary 7.5. *Let $D_0 = \rho$, and for $n \ge 0$ let $\chi_n = 2/(1 + (1 - D_n^2)^{1/2})$, $\beta_n = \frac{3}{2} C_r \chi_n D_n$ and*

$$D_{n+1} = \min\Big(D_n,\ \chi_n^{1/2}\,\frac{C_r\,\sigma/2}{1-\beta_n}\Big).$$

If $\beta_0 < 1$, then for every n we have $\|d\| \le D_n$, hence $\max_i |d_i| \le D_n$, and

$$|\tau| \ \le\ C_r''\, s \ \le\ \tau_{\max} := C_r''\,\sigma/2, \qquad C_r'' = \frac{C_r}{1-\beta_n}.$$

Proof. By induction on n. If $\|d\| \le D_n$, then $|\tau| \le \|d\| \le D_n$, so Lemma 7.4 applies with $\bar{d} = \bar{t} = D_n$ and $\beta = \beta_n \le \beta_0 < 1$. It gives $|\tau| \le C_r s/(1-\beta_n) \le C_r(\sigma/2)/(1-\beta_n)$, and then $\|d\| \le \chi_n^{1/2}|\tau| \le D_{n+1}$ by Lemma 7.3(2). □

We write D_{eff} for the value of D_n used below (the computation of Section 7.7 takes $D_{\text{eff}} = D_{12}$). From now on $\bar{d} = D_{\text{eff}}$, the quantities $\chi, \varphi, \bar{u}, \bar{u}_\perp$ are computed from it, and we assume $2\varphi < \pi/6$, so that Lemma 7.3(6) applies. At $\rho = \frac{2}{5}$ the first step has $\beta_0 = 0.8653\ldots$, and at the main row the iteration gives the value D_{eff} of Table 1.

7.4. **The truncated volume of P.** For heights $h_1, \ldots, h_m \ge 1$ and unit vectors $w_1, \ldots, w_m$ with Gram entries u_{ab}, the volume of

$$\{x :\ |x| < \sqrt{2},\ \langle x, w_a\rangle > h_a \text{ for } a = 1, \ldots, m\}$$

depends only on the h_a and the u_{ab}. For $m = 1, 2, 3$ we denote it by $S(h_1)$, $\Pi(h_1, h_2; u_{12})$ and $\Theta(h_1, h_2, h_3; u_{12}, u_{13}, u_{23})$. Thus $S(h_i) = \mathrm{vol}(K_{y_i})$, and at $h = 1$ these are the functions $\omega_1, \omega_2, \omega_3$ of Section 2. Define

$$\Phi(h, u_T) = 2\pi^2 - \sum_i S(h_i) + \sum_{\{i,j\}\in T} \Pi(h_i, h_j; u_{ij}) - \sum_{\{a,b,c\}} \Theta(h_a, h_b, h_c; u_{ab}, u_{ac}, u_{bc}),$$

the last sum over the 96 contact triangles. This is a function of the 24 heights and the 96 contact inner products. At $\zeta_0 = (h = 1,\ u_T = \frac{1}{2})$ it equals $T_3(D_4) = 8$, by Lemma 2.5.

The next lemma describes two half-spaces in a frame adapted to them.

Lemma 7.6. *Let w, w' be unit vectors with $u = \langle w, w'\rangle \in (-1, 1)$, and let $h, h' \ge 1$. Put $\alpha = ((1+u)/2)^{1/2}$, $\alpha' = ((1-u)/2)^{1/2}$, $p = (w + w')/(2\alpha)$, $n = (w - w')/(2\alpha')$, $\hat{h} = \frac{1}{2}(h + h')$, $\check{h} = (h - h')/(2\alpha')$, $\hat{c} = \hat{h}/\alpha$ and $\hat{g} = \sqrt{2} - \hat{c}$. Then p, n are orthonormal, and $\langle x, w\rangle > h$ and $\langle x, w'\rangle > h'$ hold if and only if $\alpha\langle x, p\rangle > \hat{h} + \alpha'|\langle x, n\rangle - \check{h}|$. If some x with $|x| < \sqrt{2}$ satisfies both, then $\hat{g} > 0$, $u > 0$ and $\hat{g} \le u/\sqrt{2}$, and every such x satisfies*

$$\hat{c} < \langle x, p\rangle < \sqrt{2}, \qquad |\langle x, n\rangle - \check{h}| < \frac{\alpha}{\alpha'}\big(\langle x, p\rangle - \hat{c}\big), \qquad |x - \sqrt{2}p|^2 < (2 - \hat{c}^2) + \hat{g}^2.$$

Proof. We have $w = \alpha p + \alpha' n$ and $w' = \alpha p - \alpha' n$. The two inequalities read $\alpha\langle x, p\rangle > h - \alpha'\langle x, n\rangle$ and $\alpha\langle x, p\rangle > h' + \alpha'\langle x, n\rangle$, and the larger right-hand side is $\hat{h} + \alpha'|\langle x, n\rangle - \check{h}|$. This gives $\langle x, p\rangle > \hat{c}$ and the bound on $\langle x, n\rangle - \check{h}$, and $\langle x, p\rangle \le |x| < \sqrt{2}$. Next, $|x - \sqrt{2}p|^2 = (|x|^2 - \langle x, p\rangle^2) + (\sqrt{2} - \langle x, p\rangle)^2 < (2 - \hat{c}^2) + \hat{g}^2$. Since $h, h' \ge 1$ we have $\hat{c} \ge 1/\alpha = (2/(1+u))^{1/2}$, so $\hat{c} < \sqrt{2}$ forces $u > 0$, and $\hat{g} \le \sqrt{2}(1 - (1+u)^{-1/2}) \le u/\sqrt{2}$. □

For $x \in B$ let $A(x) = \{i : \ x \in K_{y_i}\}$, and put

$$c_0 = \Big(\frac{2}{1+\bar u_\perp}\Big)^{1/2}, \qquad \zeta_O = \big((2-c_0^2) + (\sqrt2 - c_0)^2\big)^{1/2} + 4\bar d.$$

Lemma 7.7. *Suppose $\zeta_O \le 1 - \sqrt2\,\bar d$, and let $x \in B$. Either any two elements of $A(x)$ form a contact pair, and then $A(x)$ has at most three elements, or $A(x) \subseteq N(k)$ for some k.*

Proof. Let $x \in K_{y_i} \cap K_{y_j}$ with $\{i,j\} \notin T$. By Lemma 7.6, $u_{ij} > 0$, so $\{i,j\} \in O$ by Lemma 7.3(6). Let k be the vertex with $\{i,j\} \subseteq N(k)$, so that $u_i + u_j = \sqrt2\, v_k$. Lemma 7.6 gives $|x - \sqrt2 p| < ((2-\hat c^2) + \hat g^2)^{1/2}$, and $\hat c \ge (2/(1+u_{ij}))^{1/2} \ge c_0$. The right-hand side decreases in $\hat c$, so it is at most $((2-c_0^2) + (\sqrt2 - c_0)^2)^{1/2}$. Since $|(w_i + w_j) - (u_i + u_j)| \le 2\bar d$ and $|u_i + u_j| = \sqrt2$, and $|a/|a| - b/|b|| \le 2|a-b|/|b|$ for nonzero vectors, we get $|p - v_k| \le 2\sqrt2\,\bar d$. Hence $|x - \sqrt2 v_k| < \zeta_O$. If also $x \in K_{y_l}$, then

$$1 \le h_l < \langle x, w_l\rangle \le \sqrt2 \langle v_k, w_l\rangle + \zeta_O \le \sqrt2 \langle v_k, u_l\rangle + \sqrt2\,\bar d + \zeta_O,$$

so $\langle v_k, u_l\rangle > 0$. Hence $\langle v_k, u_l\rangle = 1/\sqrt2$, that is, $l \in N(k)$. So $A(x) \subseteq N(k)$ as soon as $A(x)$ contains a pair outside T. Otherwise its elements are pairwise in contact, and there are at most three of them. □

Lemma 7.8. *Suppose $\zeta_O \le 1 - \sqrt2\,\bar d$ and $64\bar d^2 < 1$. Then $\mathcal F = \Phi(h, u_T) + \mathcal N$, where*

$$\mathcal N = \int_B \nu(A(x))\,dx, \qquad \nu(A) = [A = \emptyset] - 1 + |A| - e_T(A) + t_T(A),$$

and $e_T(A)$, $t_T(A)$ are the numbers of contact pairs and contact triangles contained in A. The function $\nu(A(x))$ takes values in $\{-1, 0, 1\}$, and it equals -1 exactly when $A(x)$ is a square. Moreover

$$\mathcal N \ \ge \ -\sum_Q \operatorname{vol}\Big(\bigcap_{a\in Q} K_{y_a}\Big) \ \ge \ -A_{\mathrm{sq}}|\tau|^2,$$

the sum over the 72 squares Q, where $A_{\mathrm{sq}} = \frac12 k_{\mathrm{sq}}\,\bar g^{3/2}(2 + \sqrt3\,\bar d\chi^{1/2})^2$ with

$$k_{\mathrm{sq}} = \frac{32}{15}\,2^{3/4}\,\frac{1+\bar u_\perp}{1-\bar u_\perp}\,(1 - 64\bar d^2)^{-1/2}, \qquad \bar g = \bar u_\perp/\sqrt2.$$

Proof. Up to a null set, $P \cap B = \{x \in B : A(x) = \emptyset\}$. The numbers $S(h_i)$, $\Pi(h_i, h_j; u_{ij})$ and $\Theta(\dots)$ are the volumes of the caps K_{y_i} and of their intersections, so $\sum_i S(h_i) = \int_B |A(x)|\,dx$, $\sum_T \Pi = \int_B e_T(A(x))\,dx$ and $\sum \Theta = \int_B t_T(A(x))\,dx$. With $\operatorname{vol}(B) = 2\pi^2$ this gives $\mathcal F - \Phi = \mathcal N$. By Lemma 7.7, $A(x)$ is a set of at most three pairwise contacts, where $\nu = 0$, or lies in some $N(k)$. In $N(k)$ the contact pairs are the twelve edges of an octahedron, the orthogonal pairs its three diagonals and the contact triangles its eight faces. A subset without a diagonal lies in a face, where $\nu = 0$. For subsets containing a diagonal we have $\nu = 1$ for $|A| = 2$ and $\nu = 0$ for $|A| = 3$. For $|A| = 4$, $\nu = -1$ for two diagonals, which is a square, and $\nu = 0$ for one diagonal together with one vertex of each other diagonal. Finally $\nu = 0$ for $|A| = 5$ and $\nu = 1$ for $|A| = 6$. This proves the statement about ν, and with it the first inequality. The second is proved in Appendix A.1. □

7.5. **The smooth part.** By the symmetry of D_4, the first partial derivatives of Φ at ζ_0 are $g_h = \partial\Phi/\partial h_i$ and $g_u = \partial\Phi/\partial u_{ij}$, the same for all i and all $\{i,j\} \in T$. Write $\Phi_{hh}, \Phi_{hu}, \Phi_{uu}$ for the blocks of the Hessian $D^2\Phi(\zeta_0)$, and define the quadratic form

$$\widetilde{\mathcal H}(\xi,\xi) = 2g_u\,Q_t(\tau) + D^2\Phi(\zeta_0)\big[(\eta, \Lambda\tau)\big]^2, \qquad \xi = (\tau,\eta) \in \mathbb R^{72} \times \mathbb R^{24},$$

with Q_t as in Lemma 7.3(4). By Lemma 7.3(3), $\frac{1}{2}\widetilde{\mathcal{H}}(\xi,\xi)$ is the second-order part of $\xi \mapsto \Phi(h, u_T)$. Let M_σ be the 24×72 matrix with $(M_\sigma\tau)_k = \sigma_k(\tau) := \sum_{j=1}^{3} (\Lambda_O \tau)_{a_{kj}a'_{kj}}$, the sum of the first-order changes of the three orthogonal inner products at the vertex v_k. Let E be the 24×24 matrix with $E_{kb} = 1$ if $b \in N(k)$ and $E_{kb} = 0$ otherwise.

Lemma 7.9 (computer-assisted)**.** (1) *$|g_h - \frac{4}{3}| \le 10^{-22}$ and $|g_u - \frac{1}{4}| \le 10^{-22}$. The entries of Φ_{hh}, Φ_{hu} and Φ_{uu} differ by at most 10^{-22} from those of the rational matrices Φ^0_{hh}, Φ^0_{hu} and Φ^0_{uu} given by $(\Phi^0_{hh})_{kk} = -4$, $(\Phi^0_{hh})_{kl} = 1$ if $\{k,l\} \in T$ and 0 for the other $k \neq l$, $(\Phi^0_{hu})_{k,ij} = -1$ if $k \in \{i,j\}$, $\frac{1}{3}$ if $\{i,j,k\}$ is a contact triangle and 0 otherwise, and $(\Phi^0_{uu})_{ee} = 1$, $(\Phi^0_{uu})_{ef} = -\frac{1}{6}$ if the distinct contact pairs e, f lie in a common contact triangle and 0 otherwise. Moreover $\|\Phi^0_{hu}\| = 4$ and $0 \preceq \Phi^0_{uu} \preceq \frac{3}{2} I$.*

(2) *Let $D^2\Phi^0$ be the symmetric matrix with blocks $\Phi^0_{hh}, \Phi^0_{hu}, \Phi^0_{uu}$, and define the quadratic form $\mathcal{H}(\xi,\xi) = \frac{1}{2}Q_t(\tau) + D^2\Phi^0\big[(\eta, \Lambda\tau)\big]^2$. Then $\|\widetilde{\mathcal{H}} - \mathcal{H}\| \le 1.3 \cdot 10^{-20}$, and the blocks of $\mathcal{H}$ satisfy:*

- (a) *$0 \preceq \mathcal{H}_{\tau\tau}$, with largest eigenvalue $\frac{5}{3}$;*
- (b) *$\mathcal{H}_{\eta\tau}$ vanishes on $\ker \mathcal{H}_{\tau\tau}$; hence $L := \mathcal{H}^+_{\tau\tau}\mathcal{H}_{\tau\eta}$ satisfies $\mathcal{H}_{\tau\tau}L = \mathcal{H}_{\tau\eta}$, and $\|L\|^2 = 12$;*
- (c) *the Schur complement $Z = \mathcal{H}_{\eta\eta} - \mathcal{H}^\top_{\tau\eta}L$ satisfies $Z \succeq -8I$;*
- (d) *$9\,\mathcal{H}_{\tau\tau} - M_\sigma^\top M_\sigma \succeq 0$ and $\|E + M_\sigma L\| = 6$.*

The blocks of $\mathcal{H}$, the pseudo-inverse in (2)(b) and the matrices M_σ, L are taken in the orthonormal coordinates $\tau \in \mathbb{R}^{72}$, $\eta \in \mathbb{R}^{24}$ (cf. Section 7.1). The form $\mathcal{H}$ is the Hessian at $\xi = 0$ of the volume of P (Table 3). The draft [3] also computes this Hessian at the 24-cell. Part (2)(b) gives, for $\tau' = \tau + L\eta$,

$$\mathcal{H}(\xi,\xi) = \tau'^\top \mathcal{H}_{\tau\tau}\tau' + \eta^\top Z \eta \;\ge\; \tau'^\top \mathcal{H}_{\tau\tau}\tau' - 8|\eta|^2. \tag{2}$$

So the quadratic part of the expansion is bounded below by $-4|\eta|^2 \ge -4\bar{\eta}s$. The tilts do not enter at first order: the first-order term in u_T is $g_u \sum_T \Delta u_{ij} = g_u Q_d$, which is of second order by Lemma 7.3(3); this is where the constant stress enters.

Let $\varepsilon_0 = 10^{-20}$. For $b_e, b_u > 0$ let $\mathbf{B}(b_e, b_u)$ be the box of heights $h_a \in [1, 1 + b_e]$ and inner products $u_{ab} \in [\frac{1}{2} - b_u, \frac{1}{2} + b_e]$.

Lemma 7.10 (computer-assisted)**.** *Suppose that $\bar{\eta} \le b_e$ and $\bar{u} \le b_u$ for one of the boxes $\mathbf{B}_m = \mathbf{B}(m/100, m/50)$, $m = 1, \dots, 5$. Then*

$$\Phi(h, u_T) - 8 - \big(\tfrac{4}{3} - \varepsilon_0\big)s - \tfrac{1}{2}\mathcal{H}(\xi,\xi) \;\ge\; -A^{(3)}_e|\eta|^2 - A^{(3)}_t|\tau|^2,$$

with the constants $A^{(3)}_e, A^{(3)}_t$ of Appendix A.3, which depend on $\bar{\eta}$, $\bar{d}$, a weight $\kappa_1 > 0$ and bounds for the third partial derivatives of Π and Θ on the box.

The proof is in Appendix A.3, which also describes how the bounds on the third derivatives are obtained. The certification of Theorem 1.2 leaves some room in these inputs: it still succeeds if all bounds on third derivatives are multiplied by 4.09, or if only $C_r \le 1.444$ is used in place of $C_r^2 \le \frac{191}{100}$.

7.6. **The hull deficit.** The cell can lose volume only near the 24 points $\sqrt{2}\,v_k$, where J_0 touches the sphere $|x| = \sqrt{2}$. There the hull J is close to the facet $\operatorname{conv}\{2u_b : b \in N(k)\}$ of J_0. Put $e_{kj} = \eta_{a_{kj}} + \eta_{a'_{kj}}$. To first order, the part of $(P \cap B) \setminus J$ near $\sqrt{2}\,v_k$ is empty unless $e_{kj} > u_{a_{kj}a'_{kj}}$ for $j = 1, 2, 3$, and its depth and its widths in the directions f_{kj} are bounded by these excesses. So its volume is of fourth order [3].

Lemma 7.11. *Let $\kappa_2, \kappa_3 > 0$, and suppose that the region condition* (4) *of Appendix A.2 holds at every step of the iteration described there. Then, with $\tau' = \tau + L\eta$,*

$$\operatorname{vol}\big((P \cap B) \setminus J\big) \;\le\; A_\sigma \sum_{k=1}^{24} \sigma_k(\tau')^2 + A_e^{\mathrm{h}} |\eta|^2 + A_t^{\mathrm{h}} |\tau|^2,$$

where $A_\sigma, A_e^{\mathrm{h}}, A_t^{\mathrm{h}}$ are given by (5) *in terms of $\bar\eta$, $\bar d$, κ_2 and κ_3.*

The proof is in Appendix A.2. By Lemma 7.9(2)(d), $\sum_k \sigma_k(\tau')^2 = |M_\sigma \tau'|^2 \le 9\, \tau'^{\top} \mathcal{H}_{\tau\tau} \tau'$. So the first term is absorbed by the nonnegative term in (2) when $9A_\sigma \le \frac{1}{2}$.

7.7. **Proof of Theorem 1.2.** Let $\kappa_1, \kappa_2, \kappa_3, \kappa_4 > 0$ be weights. We use the following conditions on (ρ, σ), with $\bar d = D_{\mathrm{eff}}$:

(C1) $\beta_0 < 1$ in Corollary 7.5;
(C2) $2\varphi < \pi/6$;
(C3) $\zeta_O \le 1 - \sqrt{2}\,\bar d$, $64\bar d^2 < 1$, and $\varepsilon_q < \sqrt{2}$, where $\varepsilon_q = 2\bar\eta/(1+\bar\eta) + 2\bar d$;
(C4) $\bar\eta \le b_e$ and $\bar u \le b_u$ for one of the boxes $\mathbf{B}_m$;
(C5) the region condition (4) at every step of the iteration of Appendix A.2;
(C6) $\Gamma > 0$, where Γ is defined in (3) below.

By Lemma 7.2, $\operatorname{vol}(V_0) \ge \mathcal{F} - \operatorname{vol}((P\cap B)\setminus J)$. By Lemma 7.8, $\mathcal{F} \ge \Phi - A_{\mathrm{sq}}|\tau|^2$. Lemma 7.10, inequality (2) and Lemma 7.11 then give

$$\operatorname{vol}(V_0) - 8 \;\ge\; \big(\tfrac{4}{3} - \varepsilon_0\big) s + \big(\tfrac{1}{2} - 9A_\sigma\big) \tau'^{\top} \mathcal{H}_{\tau\tau} \tau' - (4 + A_e)|\eta|^2 - A_t |\tau|^2,$$

with $A_e = A_e^{(3)} + A_e^{\mathrm{h}}$ and $A_t = A_t^{(3)} + A_{\mathrm{sq}} + A_t^{\mathrm{h}}$. If $9A_\sigma \le \frac{1}{2}$, the middle term is nonnegative and we drop it. Otherwise we use $\mathcal{H}_{\tau\tau} \preceq \frac{5}{3} I$ and $|\tau'|^2 \le (1+\kappa_4)|\tau|^2 + (1+\kappa_4^{-1})\|L\|^2 |\eta|^2$ with $\|L\|^2 = 12$, and add $(9A_\sigma - \frac{1}{2})\frac{5}{3}(1+\kappa_4)$ to A_t and $(9A_\sigma - \frac{1}{2})\frac{5}{3}(1+\kappa_4^{-1}) \cdot 12$ to A_e. Finally $|\eta|^2 \le \bar\eta s$, and $|\tau|^2 \le \tau_{\max} C_r'' s$ by Corollary 7.5. Hence

$$\operatorname{vol}(V_0) - 8 \;\ge\; \Gamma s, \qquad \Gamma = \tfrac{4}{3} - \varepsilon_0 - (4 + A_e)\,\bar\eta - A_t\, \tau_{\max} C_r''. \tag{3}$$

All quantities in (C1)–(C6) are explicit. They were evaluated, together with the choice between the two cases for $9A_\sigma$, using $C_r = (191/100)^{1/2}$, the third-derivative bounds of Lemma 7.10 and 300 steps of the iteration of Appendix A.2 (Table 3). At the main row the computation gives $\Gamma \ge 0.2437$ (Table 2), which proves the inequality of Theorem 1.2. Every row of Table 1 gives a theorem of the same form; for instance, $d(W) \le \frac{9}{20}$ and $\sum_i \delta_i \le \frac{1}{125}$ imply $\operatorname{vol}(V_0) \ge 8 + 1.3111\, s$. At the main row the depth bound $\hat\Delta$ of Appendix A.2 keeps its starting value ε_q; the iteration there improves only $\bar Y$ and $\tilde Y$.

Equality. If $s > 0$, then $\operatorname{vol}(V_0) - 8 \ge \Gamma s > 0$. If $s = 0$, Corollary 7.5 gives $|\tau| \le C_r'' s = 0$, so $t_i = 0$, $d_i = 0$ and $y_i = 2u_i$ for all i, in the labelling and frame fixed in Section 7.3. Then $q_i = 2u_i$ and $J = J_0$, and $P = \{x : \langle x, u_i\rangle \le 1\}$ is the regular 24-cell with vertices $\sqrt{2}\, v_k$. These satisfy $\langle \sqrt{2} v_k, v_{k'}\rangle \le \sqrt{2}$, so $P \subseteq J_0$. By Lemma 7.2, $V_0 \supseteq P \cap J = P$, and $V_0 \subseteq P$, so $V_0 = P$ and $\operatorname{vol}(V_0) = 8$. The same argument shows that $\operatorname{vol}(V_0) = 8$ whenever $\{y_1, \dots, y_{24}\} = 2R\{u_1, \dots, u_{24}\}$ for some $R \in O(4)$. This completes the proof of Theorem 1.2. □

Remark 7.12 (Effective size and nearest centres). We prove the claims made after Theorem 1.2. Corollary 7.5 gives $d(W) = \|d\| \le D_{\mathrm{eff}} < 0.021709$, so no 24 centres of a packing containing 0 with $d(W)$ between this value and $\frac{2}{5}$ have $\sum_i \delta_i \le \frac{3}{100}$. The hypothesis $d(W) \le \frac{2}{5}$ gives the starting value $D_0 = \frac{2}{5}$ of the iteration of Corollary 7.5, for which condition (C1) is checked.

TABLE 1. Certified pairs (ρ, σ): with the weights and box listed, conditions (C1)–(C6) hold, and $\mathrm{vol}(V_0) \geq 8 + \Gamma s$ whenever $d(W) \leq \rho$ and $\sum_i \delta_i \leq \sigma$. The column Γ gives the certified lower bound rounded down to four decimals, and the column D_{eff} the certified upper bound rounded up to six decimals.

ρ	σ	$\Gamma \geq$	D_{eff}	$(\kappa_1, \kappa_2, \kappa_3, \kappa_4)$	box
2/5	1/125	1.3111	0.005593	$(1, 8, 1, \frac{1}{2})$	$\mathbf{B}_1$
9/20	1/125	1.3111	0.005593	$(1, 8, 1, \frac{1}{2})$	$\mathbf{B}_1$
2/5	1/50	1.1951	0.014242	$(\frac{1}{2}, 4, 4, \frac{1}{2})$	$\mathbf{B}_2$
2/5	1/40	0.9535	0.017944	$(\frac{1}{2}, 2, 4, \frac{1}{2})$	$\mathbf{B}_2$
2/5	3/100	0.2437	0.021709	$(\frac{1}{2}, 2, 4, 2)$	$\mathbf{B}_2$
2/5	31/1000	0.0026	0.022470	$(\frac{1}{2}, 2, 4, 2)$	$\mathbf{B}_2$

TABLE 2. The budget of (3) at the main row of Table 1, with the weights $(\frac{1}{2}, 2, 4, 2)$ and the box $\mathbf{B}_2$, per unit of s. The losses are rounded as shown, and Γ is rounded down. They follow, as in Section 7.7, from the constants recorded for the main row in the supplement [16].

term	per unit of s
first-order gain (Lemma 7.10)	$\frac{4}{3} - \varepsilon_0$
hull deficit (Lemma 7.11), including the term added because $9A_\sigma > \frac{1}{2}$	-0.94
other losses: third-order remainder (Lemma 7.10), quadratic part (2), square overlaps (Lemma 7.8)	-0.15
total loss, using $\lvert\tau\rvert^2 \leq \tau_{\max} C_r'' s$ (Corollary 7.5)	-1.0896
Γ	0.243742

Next, every centre $z \notin \{0, y_1, \ldots, y_{24}\}$ satisfies $|z| > 2.72$. Indeed, the 24-cell $\{x : \langle x, u_i\rangle \leq 1\}$ has circumradius $\sqrt{2}$, so $\langle z, u_i\rangle \geq |z|/\sqrt{2}$ for some i, and then $|z - 2u_i|^2 \leq |z|^2 - 2\sqrt{2}|z| + 4 = (|z| - \sqrt{2})^2 + 2$. In the frame of Section 7.3, $|y_i - 2u_i| \leq 2\eta_i + 2|d_i| < 0.0735$, so $|z - 2u_i| > 2 - 0.0735$ by the packing condition. Since $|z| \geq 2$, this gives $(|z| - \sqrt{2})^2 > 1.9265^2 - 2 > 1.7114$ and $|z| > 2.72$. So $y_1, \ldots, y_{24}$ are the 24 centres nearest to 0, and the only centres within distance $\sqrt{6}$.

Remark 7.13 (Sharpness). The coefficient $\frac{4}{3}$ is g_h, and it cannot be improved. Let the packing consist of 0 and the centres $2u_i$, except that $y_1 = 2(1 + \eta)u_1$ with $0 < \eta < 1$; this is a packing, and $d(W) = 0$. The cell is the 24-cell with one facet moved from $\langle x, u_1\rangle = 1$ to $\langle x, u_1\rangle = 1 + \eta$. The hyperplanes of the eight neighbouring facets pass through $2u_1$, and the pyramid over the facet with apex $2u_1$ has height 1, like the pyramid with apex 0, so its volume is $8/24 = \frac{1}{3}$. The cell gains the part of this pyramid at height at most η, so $\mathrm{vol}(V_0) = 8 + \frac{1}{3}(1 - (1 - \eta)^4)$, and $(\mathrm{vol}(V_0) - 8)/s = (1 - (1 - \eta)^4)/(3\eta) < \frac{4}{3}$ (this example is also in [3]). For the largest push allowed by Theorem 1.2, $\eta = \frac{3}{200}$, the ratio equals $1.3036\ldots$, slightly less than $\frac{4}{3}$. Numerically, configurations with exact rational coordinates sampled at the corner of the region of Theorem 1.2, including extreme tilts and further centres, never give a smaller exact ratio than this single push [16]. The certified constant is far below these values.

Remark 7.14 (Limits of the method). In σ, the method is limited by the second-order terms of the hull deficit: at $\rho = \frac{2}{5}$ the certified constant falls to 0.0026 at $\sigma = \frac{31}{1000}$, and with the weights

$(\frac{1}{2}, 2, 8, 2)$ the computation gives a negative lower bound for Γ at $\sigma = \frac{1}{25}$. In ρ, the method is limited by the first step of the rigidity iteration: (C1) fails at $(\frac{23}{50}, \frac{1}{125})$, and at $(\frac{9}{20}, \frac{1}{50})$ the iteration of Corollary 7.5 does not reduce D_n below $\frac{9}{20}$, so (C2) fails.

8. Verification

Table 3 lists, for the results behind Theorems 1.1 and 1.2, how each is checked and what is formalised in Lean. The computations are done by the programs of the supplement [16]. Unless ball or interval arithmetic [1] is stated, they are exact, in rational or in modular arithmetic. A comparison made in ball or interval arithmetic holds for every point of the balls or intervals involved.

Parts of Sections 2–5 and of Section 7 are formalised in Lean 4 with Mathlib. A theorem is *kernel-checked* if its only axioms are the three standard ones of Lean, so that every step has been checked by Lean's kernel. It is *native* if some finite computations are evaluated by compiled code, which adds the Lean compiler, its runtime and the compiled libraries to the trusted base. In the formal statements, space is $\mathbb{R}^4$ with Lebesgue measure, half-spaces and the ball B are open as in Section 2, and a packing is any set of points, possibly infinite, at mutual distance at least 2. For the arithmetic of the certificate, the kernel works on a copy of the certificate in Lean, whose agreement with the deposited certificate is verified by independent programs outside Lean. For Theorem 3.2, native evaluation shows that each row of the certificate is the value at its sample point of a row function built by a Lean reimplementation of the zonal assembly of [11], and that the triple row functions are invariant under relabelling, as the invariant sample sets require. The versions of Theorems 3.2 and 1.1 specialised to the certificate make two assumptions on the certificate:

- (H1) inequality (1) holds, for every kissing configuration, for the kernel that the 60 kernel blocks of the certificate define through the zonal functions of the reimplementation;
- (H2) the row function of the quadruple piece, an explicit polynomial in the six inner products, is invariant under the relabellings of the four points.

Hypothesis (H1) contains the positivity theorem of [11], the faithfulness of the reimplementation to the construction there, and the correctness of the zonal entries, which agree with those computed by the code of [11]. The formal proof of Theorem 1.2 assumes, for every packing and centres $y_1, \dots, y_{24}$ as in the theorem with $c = 0$, and in (h1)–(h4) for every labelling and R as in (h0), with certified upper bounds for the constants of the main row:

- (h0) a labelling and an $R \in O(4)$ attaining $d(W)$ exist, which follows from the compactness of $O(4)$;
- (h1) the bound of Lemma 7.8 holds;
- (h2) the inequality of Lemma 7.11 holds;
- (h3) the bounds on $|\tau|$ of Corollary 7.5 hold;
- (h4) the inequality of Lemma 7.10 holds.

The supplement [16] gives these constants exactly, states the hypotheses in full and documents the formal proofs.

Appendix A. Proofs for Section 7

Throughout, the notation of Section 7 is in force, with $\bar{d} = D_{\text{eff}}$ and conditions (C2)–(C4) of Section 7.7. In particular $\bar{d}$ bounds $\|d\|$ and every $|d_i|$, and $0 \le \eta_i \le \bar{\eta}$.

TABLE 3. Verification. "Kernel" means kernel-checked, and "native" that some finite computations are evaluated by compiled code.

result	how it is checked	in Lean
the results of Section 2 and Proposition 3.1	proofs in the text	kernel; Lemma 2.5 via the covolume of $\sqrt{2}D_4$, without identifying V_0 as the 24-cell
the certificate of Theorem 3.2	identities at the sample points and the identity fixing κ, right-hand sides $-\omega_1^+$, p_2, $-p_3$, 0: exact blocks positive definite: Cholesky, ball arithmetic unisolvence of the sample sets (17 points for pairs; 204 and 3679, the dimensions of the S_3- and S_4-invariant polynomials of degree ≤ 16): full rank modulo a prime triple and quadruple identities on the principal lattices $\{a/16 :\ a \in \mathbb{Z}^m_{\ge 0},\ \lvert a\rvert \le 16\}$, $m = 3, 6$, without invariance assumptions: exact	polynomials g of Section 3 nonnegative on their pieces: kernel these facts, except those on the principal lattices, and $K(\emptyset,\emptyset) + 23\mu = 1828197/156250$ with $\mu > 0$: kernel Theorem 3.2 for the certificate: native, under (H1) and (H2)
Lemma 4.1	interval arithmetic (Section 4)	(1): kernel, with ω_1^+ read natively from the certificate (2): closed form of ω_2 kernel, inequality native (3): not formalised
Theorem 1.1	proof in Section 5	kernel, from the bound of Theorem 3.2, Lemma 4.1, [13] and [11] for the certificate: native, under (H1), (H2), Lemma 4.1(3), [13] and [11]
facts on D_4 and J_0 (Section 7.1)	exact, with J_0 by vertex enumeration	counts of roots, contact pairs and contact triangles: kernel
Lemma 7.1	spectrum of $\Lambda^\top\Lambda$: exact, in two coordinate systems	$\ker\Lambda$, $\lvert\Lambda\tau\rvert \ge \lvert\tau\rvert$ for $\tau \perp \ker\Lambda$, $\lVert\Lambda\rVert = 2$ and the constant stress: kernel the rest of the spectrum: not formalised
$C_r^2 \le 191/100$ (Lemma 7.4)	exact identity; $M_0 \ge 0$ entrywise, $N_0 \succeq 0$ of rank 90 by $LDL^\top$	the certificate: kernel; it enters only through (h3)
$\mathcal{H}$ (Lemma 7.9(2))	exact $LDL^\top$ and spectra eigenvalues of $\mathcal{H}_{\tau\tau}$: $0, 1/6, 2/3, 1, 4/3, 5/3$, multiplicities $15, 16, 12, 12, 9, 8$ characteristic polynomial of Z: $(x+8)^{14}(x+20/3)^9(x-4)$ in the coordinates τ^{s}, equal to the Hessian of the volume of P computed in [16]	parts (a)–(d), with the eigenvalue $5/3$ and $\lVert L\rVert^2 = 12$ as upper bounds, (c) as $\mathcal{H}(\xi,\xi) \ge -8\lvert\eta\rvert^2$, without $\lVert E + M_\sigma L\rVert = 6$; the characteristic polynomial of Z; the identity with the matrix of [16]: kernel
Lemma 7.9(1)	derivatives of S, Π, Θ at ζ_0: ball arithmetic, within 10^{-22} of the rationals $\lVert\Phi^0_{hu}\rVert = 4$ and $0 \preceq \Phi^0_{uu} \preceq (3/2)I$: exact	the derivative values: not formalised
Lemma 7.10	third derivatives of Π, Θ on $\mathbf{B}_1, \dots, \mathbf{B}_5$: Taylor models in ball arithmetic (Appendix A.3)	not formalised; enters as (h4)
(C1)–(C6) and Γ (Tables 1 and 2)	ball arithmetic	$\Gamma \ge 0.2437$ from the certified constants: kernel
Theorem 1.2	proof in Section 7	kernel, from (h0)–(h4), for $c = 0$, without identifying V_0 with the regular 24-cell Lemma 7.2 and inequality (2): kernel

A.1. **The square overlaps.** We prove the second inequality of Lemma 7.8. Let Q be a square at the vertex v_k, formed by the orthogonal pairs $\{a_1, a_1'\}$ and $\{a_2, a_2'\}$. Apply Lemma 7.6 to each pair, with $w = w_{a_r}$, $w' = w_{a_r'}$, $h = h_{a_r}$ and $h' = h_{a_r'}$, and denote the resulting quantities by $\alpha_r, \alpha_r', p_r, n_r, \check{h}_r, \hat{c}_r, \hat{g}_r$ for $r = 1, 2$. Suppose the four caps of Q meet, so that $\hat{g}_1, \hat{g}_2 > 0$. By Lemma 7.6, a common point x satisfies

$$\hat{c}_1 < \langle x, p_1\rangle < \sqrt{2}, \qquad |\langle x, n_1\rangle - \check{h}_1| < \frac{\alpha_1}{\alpha_1'}\big(\langle x, p_1\rangle - \hat{c}_1\big), \qquad |\langle x, n_2\rangle - \check{h}_2| < \frac{\alpha_2}{\alpha_2'}\,\hat{g}_2,$$

the last because $\langle x, p_2\rangle < \sqrt{2}$. Let $\Pr$ be the orthogonal projection onto the plane orthogonal to p_1 and n_1. For fixed $\langle x, p_1\rangle$ and $\langle x, n_1\rangle$, the projection $\Pr x$ lies in a disc of radius $(2-\langle x, p_1\rangle^2)^{1/2}$ and in a strip of width $2(\alpha_2/\alpha_2')\hat{g}_2/|\Pr n_2|$. Put $\lambda = \sqrt{2} - \langle x, p_1\rangle \in (0, \hat{g}_1)$. Then $\langle x, p_1\rangle - \hat{c}_1 = \hat{g}_1 - \lambda$ and $2 - \langle x, p_1\rangle^2 \le 2\sqrt{2}\,\lambda$, so

$$\operatorname{vol}\Big(\bigcap_{a\in Q} K_{y_a}\Big) \le \int_0^{\hat{g}_1} 2\frac{\alpha_1}{\alpha_1'}(\hat{g}_1 - \lambda)\cdot 4\frac{\alpha_2}{\alpha_2'}\frac{\hat{g}_2}{|\Pr n_2|}(2\sqrt{2}\,\lambda)^{1/2}\,d\lambda = \frac{32}{15}2^{3/4}\frac{\alpha_1\alpha_2}{\alpha_1'\alpha_2'}\frac{\hat{g}_1^{5/2}\hat{g}_2}{|\Pr n_2|},$$

and the same holds with 1 and 2 exchanged. By Lemma 7.3(6), $\alpha_r/\alpha_r' = ((1+u)/(1-u))^{1/2} \le ((1+\bar{u}_\perp)/(1-\bar{u}_\perp))^{1/2}$. As in the proof of Lemma 7.7, $|p_r - v_k| \le 2\sqrt{2}\,\bar{d}$, and likewise $|n_r - f_{kj_r}| \le 2\sqrt{2}\,\bar{d}$, where j_r is the index of the pair. Since f_{kj_2} is orthogonal to v_k and f_{kj_1}, we get $|\langle n_2, p_1\rangle|, |\langle n_2, n_1\rangle| \le 4\sqrt{2}\,\bar{d}$ and $|\Pr n_2|^2 \ge 1 - 64\bar{d}^2$. With $\hat{g}_r \le u_{a_r a_r'}/\sqrt{2} \le \bar{g}$ (Lemma 7.6) this gives

$$\operatorname{vol}\Big(\bigcap_{a\in Q} K_{y_a}\Big) \le k_{\mathrm{sq}}\,\hat{g}_1\hat{g}_2\min(\hat{g}_1, \hat{g}_2)^{3/2} \le \tfrac{1}{2}k_{\mathrm{sq}}\,\bar{g}^{3/2}\big(\hat{g}_1^2 + \hat{g}_2^2\big).$$

Each orthogonal pair lies in exactly two squares, and $\hat{g}^+ \le u^+/\sqrt{2}$ for each pair, so the sum over all squares is at most $\frac{1}{2}k_{\mathrm{sq}}\bar{g}^{3/2}\sum_O (u_{ij}^+)^2$. By Lemma 7.3(3) and Lemma 7.1(3),

$$\Big(\sum_O u_{ij}^2\Big)^{1/2} \le \|\Lambda_O\|\,|\tau| + \Big(\sum_O |d_i|^2|d_j|^2\Big)^{1/2} \le \big(2 + \sqrt{3}\,\bar{d}\chi^{1/2}\big)|\tau|,$$

because each root lies in six orthogonal pairs, so that $\sum_O |d_i|^2|d_j|^2 \le \frac{\bar{d}^2}{2}\sum_O(|d_i|^2 + |d_j|^2) = 3\bar{d}^2\|d\|^2 \le 3\bar{d}^2\chi|\tau|^2$. This proves $\mathcal{N} \ge -A_{\mathrm{sq}}|\tau|^2$.

A.2. **The hull deficit.** We prove Lemma 7.11. Put $\varepsilon_q = 2\bar{\eta}/(1+\bar{\eta}) + 2\bar{d}$. Then $|q_i - 2u_i| \le 2(1-1/h_i) + 2|d_i| \le \varepsilon_q$ for all i. By (C3), $\varepsilon_q < \sqrt{2}$; on the certified pairs of Table 1, $\varepsilon_q \le 0.0755$. This condition is used three times: for the positive factor $1 - \varepsilon_q/\sqrt{2}$ in (a), for $\langle x, v_k\rangle > 0$ on C_k, which makes t_* well defined in Lemma A.1(2), and for $\sqrt{2} - \hat{\Delta} > 0$ in $t_{\max}$.

(a) Localisation. For a unit vector e, the support functions satisfy $h_J(e) \ge \max_i\langle q_i, e\rangle \ge h_{J_0}(e) - \varepsilon_q \ge (1-\varepsilon_q/\sqrt{2})\,h_{J_0}(e)$, because $h_{J_0} \ge \sqrt{2}$. Since $1-\varepsilon_q/\sqrt{2} > 0$, the right-hand side is the support function of $(1-\varepsilon_q/\sqrt{2})J_0$, so $J \supseteq (1-\varepsilon_q/\sqrt{2})J_0 = \{x : \langle x, v_k\rangle \le \sqrt{2} - \varepsilon_q \text{ for all } k\}$. So $(P\cap B)\setminus J$ is contained in the union of the sets $X_k = (P\cap C_k)\setminus J$, where $C_k = \{x \in B : \langle x, v_k\rangle > \sqrt{2} - \varepsilon_q\}$. For $x \in C_k$ we have $\langle x, v_k\rangle > \sqrt{2} - \varepsilon_q > 0$, and the vector $z = x - \sqrt{2}v_k$ satisfies $|z|^2 = |x|^2 - 2\sqrt{2}\langle x, v_k\rangle + 2 < 2\sqrt{2}(\sqrt{2} - \langle x, v_k\rangle) < 2\sqrt{2}\,\varepsilon_q$.

Fix k for the rest of the proof, and write $v = v_k$ and $f_j = f_{kj}$. For $j = 1, 2, 3$ write $j+ = a_{kj}$ and $j- = a_{kj}'$, so that $u_{j\pm} = (v \pm f_j)/\sqrt{2}$. For $b \in N(k)$ let $j(b)$ be its pair and $s_b = \pm 1$ its sign. For $x \in \mathbb{R}^4$ write $z = x - \sqrt{2}v = z_0 v + z_\perp$ with $z_\perp = \sum_l z_l f_l$. Since $q_b = (2/h_b)(u_b + d_b)$,

$$q_b - \sqrt{2}v = \theta_b v + P_b, \qquad P_b = s_b\sqrt{2}\,f_{j(b)} + r_b,$$

with $\theta_b = \sqrt{2}(h_b^{-1}-1)+2h_b^{-1}\langle v,d_b\rangle$ and $r_b = s_b\sqrt{2}(h_b^{-1}-1)f_{j(b)}+2h_b^{-1}(d_b-\langle v,d_b\rangle v)$. If b' is the partner of b, then $v=(u_b+u_{b'})/\sqrt{2}$, so $\langle v,d_b\rangle = (\langle u_{b'},t_b\rangle + n_b)/\sqrt{2}$ and $|\langle v,d_b\rangle| \le \bar\nu|d_b|$ with $\bar\nu = (1+\bar d/2)/\sqrt{2}$. Hence $|\theta_b| \le \sqrt{2}\eta_b + 2\bar\nu|d_b|$ and $|r_b| \le \sqrt{2}\eta_b + 2|d_b|$. Put $\bar\theta_j = \frac12(\theta_{j+}+\theta_{j-})$, $\mathrm{spr}_j = \max_{l\ne j,\pm}|\theta_{l\pm}-\bar\theta_j|$ and $\bar r = \max_b |r_b|$.

(b) Height of the hull. Let $\Omega = \mathrm{conv}\{q_b : b\in N(k)\} \subseteq J$, and let $\Omega^\perp$ be its orthogonal projection to $v^\perp$, which is the convex hull of the P_b. For $y\in\Omega^\perp$ let $\mathrm{hup}(y)$ and $\mathrm{low}(y)$ be the largest and the smallest t with $\sqrt{2}v+y+tv\in\Omega$. For $y\in v^\perp$ write $y_l = \langle y, f_l\rangle$ and $|y|_1 = \sum_l |y_l|$.

Lemma A.1. (1) *If $|y|_1 + \sqrt{3}\,\bar r \le \sqrt{2}$, then $y\in\Omega^\perp$ and, for each j, with l_1,l_2 the other two indices,*

$$\mathrm{hup}(y) \;\ge\; \bar\theta_j - \frac{|y_j|+\bar r}{2\sqrt{2}}\,|\theta_{j+}-\theta_{j-}| - \frac{|y_{l_1}|+|y_{l_2}|+2\bar r}{\sqrt{2}}\,\mathrm{spr}_j.$$

(2) *Let $x\in C_k$, $z = x-\sqrt{2}v$ and $\hat\theta \ge \max_b|\theta_b|$, and suppose that $t|z_\perp|_1+\sqrt{3}\,\bar r<\sqrt{2}$ for all $t\in[1,t_*]$, where $t_* = (\sqrt{2}+\hat\theta)/(\sqrt{2}+z_0)$; note that $t_*>1$, because $z_0<0$ for $x\in B$. If $x\notin J$, then $z_0 > \mathrm{hup}(z_\perp)$.*

Proof. (1) For $y'\in v^\perp$ define $\lambda^0(y')\in\mathbb{R}^{N(k)}$ by $\lambda^0_{l\pm}(y') = \max(\pm y'_l,0)/\sqrt{2}$ for $l\ne j$ and $\lambda^0_{j\pm}(y') = \frac12(1-a(y'))\pm y'_j/(2\sqrt{2})$, where $a(y') = (|y'_{l_1}|+|y'_{l_2}|)/\sqrt{2}$. Then λ^0 is continuous, $\sum_b\lambda^0_b = 1$, $\sum_b \lambda^0_b(y')\,s_b\sqrt{2}f_{j(b)} = y'$, and $\lambda^0(y')\ge 0$ if and only if $|y'|_1\le\sqrt{2}$. On the closed ball of radius $\bar r$ about y we have $|y'|_1\le|y|_1+\sqrt{3}|y'-y|\le\sqrt{2}$, so $\lambda^0\ge 0$ there, and the continuous map $y'\mapsto y-\sum_b\lambda^0_b(y')r_b$ maps this ball into itself. By Brouwer's theorem it has a fixed point y^*. With $\lambda=\lambda^0(y^*)$ we get $\lambda\ge0$, $\sum_b\lambda_b=1$ and $\sum_b\lambda_bP_b = y^*+\sum_b\lambda_b r_b = y$. So $y\in\Omega^\perp$, and $\sum_b\lambda_b q_b = \sqrt{2}v+y+(\sum_b\lambda_b\theta_b)v\in\Omega$, whence $\mathrm{hup}(y)\ge\sum_b\lambda_b\theta_b$. For $l\ne j$ only one of $\lambda_{l+},\lambda_{l-}$ is nonzero, so

$$\sum_b\lambda_b\theta_b = \bar\theta_j + \frac{y^*_j}{2\sqrt{2}}(\theta_{j+}-\theta_{j-}) + \sum_{l\ne j}\frac{|y^*_l|}{\sqrt{2}}\big(\theta_{l,\pm}-\bar\theta_j\big),$$

with the sign of y^*_l in $\theta_{l,\pm}$. Since $|y^*_l|\le|y_l|+\bar r$, the bound follows.

(2) We show that $z_0\le\mathrm{hup}(z_\perp)$ implies $x\in J$; here $z_\perp\in\Omega^\perp$ by (1). For $t\ge1$ we have $tx = \sqrt{2}v+tz_\perp+\varrho(t)v$ with $\varrho(t) = t(\sqrt{2}+z_0)-\sqrt{2}$. Since $\sqrt{2}+z_0 = \langle x,v\rangle>0$, ϱ is increasing, and $\varrho(t_*)=\hat\theta$. By (1), every $tz_\perp$ with $t\in[1,t_*]$ lies in the interior of $\Omega^\perp$, where hup is concave and low is convex, hence both are continuous. Every point of Ω has height in $[\min_b\theta_b,\max_b\theta_b]$, so $\mathrm{low}\le\mathrm{hup}\le\hat\theta$. If $z_0\ge\mathrm{low}(z_\perp)$, then $x\in\Omega$. Otherwise $\varrho(t)-\mathrm{low}(tz_\perp)$ is negative at $t=1$ and nonnegative at $t=t_*$, so it vanishes at some $t_1\in(1,t_*]$. Then $\mathrm{low}(t_1z_\perp)=\varrho(t_1)\le\mathrm{hup}(t_1z_\perp)$, so $t_1x\in\Omega$ and $x=t_1^{-1}(t_1x)\in\mathrm{conv}(\{0\}\cup\Omega)\subseteq J$. □

Let $\hat\Delta\ge-z_0$, $\tilde Y\ge\max_l|z_l|$ and $\hat r\ge\bar r$ be bounds valid on X_k, and $\hat\theta\ge\max_b|\theta_b|$. Then $t_*\le t_{\max} := 1+(\hat\theta+\hat\Delta)/(\sqrt{2}-\hat\Delta)$ on X_k. If

$$3\,t_{\max}\tilde Y + \sqrt{3}\,\hat r < \sqrt{2}, \tag{4}$$

then Lemma A.1(2) applies on X_k, and every $x\in X_k$ satisfies $z_0>\bar\theta_j-\mathrm{err}_j(z)$ for each j, where

$$\mathrm{err}_j(z) = \frac{|z_j|+\bar r}{2\sqrt{2}}\,|\theta_{j+}-\theta_{j-}| + \frac{|z_{l_1}|+|z_{l_2}|+2\bar r}{\sqrt{2}}\,\mathrm{spr}_j.$$

(c) Volume. For $b\in N(k)$ put $\psi_b = h_b-\sqrt{2}\langle v,w_b\rangle = \eta_b-\sqrt{2}\langle v,d_b\rangle$, and for each pair l put $m_l = (\psi_{l+}+\psi_{l-})/\sqrt{2}$ and $o_l = (\psi_{l+}-\psi_{l-})/\sqrt{2}$. Let $x\in X_k$. Then $z_0<0$ because

$\langle x, v\rangle \le |x| < \sqrt{2}$, and the facet inequalities $\langle x, w_{l\pm}\rangle \le h_{l\pm}$ read $(z_0 \pm z_l)/\sqrt{2} \le \psi_{l\pm} - \langle z, d_{l\pm}\rangle$. Hence z_l lies in the interval

$$I_l = \big[\, o_l - (m_l - z_0) - \sqrt{2}|z||d_{l-}|,\ \ o_l + (m_l - z_0) + \sqrt{2}|z||d_{l+}|\,\big].$$

Let $\bar{Y} \ge \sup_{X_k} |z|$, put $\Delta_j = -\bar{\theta}_j + \sup_{X_k} \mathrm{err}_j$ and $\Delta_* = \min_j \Delta_j$, and for $l = 1, 2, 3$ put

$$H_l = m_l + \Delta_* + \frac{\bar{Y}}{\sqrt{2}}\big(|d_{l+}| + |d_{l-}|\big), \qquad H_l^+ = \max(H_l, 0).$$

By (b), $0 < -z_0 < \Delta_*$ on X_k, so $X_k = \emptyset$ if $\Delta_* \le 0$. For $x \in X_k$ the interval I_l has length $2(m_l - z_0) + \sqrt{2}|z|(|d_{l+}| + |d_{l-}|) \le 2H_l$, so $X_k = \emptyset$ if some $H_l < 0$. In every case X_k lies in the set of z with $0 < -z_0 < \Delta_*^+$ and each z_l in an interval of length $2H_l^+$, and integrating over z_1, z_2, z_3 and then over z_0 gives

$$\mathrm{vol}(X_k) \le \Delta_*^+ \prod_{l=1}^{3} 2H_l^+.$$

Put $\alpha_j = \sqrt{2}\,\Delta_j^+$, $\gamma_l = \sqrt{2}\,\big(m_l + \frac{\bar{Y}}{\sqrt{2}}(|d_{l+}| + |d_{l-}|)\big)^+$, $W_k = \sum_j \max(\alpha_j, \gamma_j)$ and $\alpha_{\min} = \min_j \alpha_j = \sqrt{2}\,\Delta_*^+ \le W_k/3$. If $\Delta_* \le 0$, then $X_k = \emptyset$ and the next display holds trivially. If $\Delta_* > 0$, then $\sqrt{2}\,H_l^+ \le \gamma_l + \alpha_{\min}$ for each l: if $H_l \ge 0$ this follows from the definitions, and otherwise the left-hand side is 0. By the arithmetic–geometric mean inequality,

$$\mathrm{vol}(X_k) \le 2\alpha_{\min} \prod_l (\gamma_l + \alpha_{\min}) \le 2\alpha_{\min}\Big(\frac{W_k}{3} + \alpha_{\min}\Big)^3 \le \frac{16}{81} W_k^4.$$

(d) Second-order bookkeeping. Write $e_j = \eta_{j+} + \eta_{j-}$ and $u_j = u_{j+,j-}$. From $\langle v, d_{j+} + d_{j-}\rangle = \big(u_j - \langle d_{j+}, d_{j-}\rangle - \frac{1}{2}(|d_{j+}|^2 + |d_{j-}|^2)\big)/\sqrt{2}$, $0 \le 1 - h_b^{-1} \le \eta_b$ and $|\langle v, d_b\rangle| \le \bar{\nu}|d_b|$ we get

$$-\bar{\theta}_j \le \frac{e_j - u_j}{\sqrt{2}} + \varpi_j, \qquad m_j \le \frac{e_j - u_j}{\sqrt{2}} + \varpi_j',$$

with $\varpi_j = (\bar{d}/\sqrt{2} + \bar{\nu}\bar{\eta})(|d_{j+}| + |d_{j-}|)$ and $\varpi_j' = (\bar{d}/\sqrt{2})(|d_{j+}| + |d_{j-}|)$. By Lemma 7.3(3), $u_j = (\Lambda_O \tau)_{j+,j-} + \langle d_{j+}, d_{j-}\rangle$. Put

$$R_{kj} = 2|\langle d_{j+}, d_{j-}\rangle| + \sqrt{2}\big(\varpi_j + \varpi_j' + \sup_{X_k} \mathrm{err}_j\big) + \bar{Y}\big(|d_{j+}| + |d_{j-}|\big), \qquad R_k = \sum_j R_{kj}.$$

If $X_k \ne \emptyset$, every Δ_j is positive, and α_j and γ_j are at most $e_j - (\Lambda_O\tau)_{j+,j-} + R_{kj}$, which is therefore positive. Summing over j gives $W_k \le \sum_j e_{kj} - \sigma_k(\tau) + R_k$, so

$$\mathrm{vol}(X_k) \le \tfrac{16}{81}\bar{M}^2\Big(\sum_j e_{kj} - \sigma_k(\tau) + R_k\Big)^2$$

for any bound $\bar{M} \ge W_k$.

A priori bounds. Put $d_2 = \sqrt{2}\,\bar{d} \ge |d_{l+}| + |d_{l-}|$ and

$$\bar{u}_O = \min\big(\bar{u}_\perp,\ d_2 + \tfrac{1}{2}\bar{d}^2\big), \quad \hat{\theta} = \sqrt{2}\bar{\eta} + 2\bar{\nu}\bar{d}, \quad \hat{r} = \sqrt{2}\bar{\eta} + 2\bar{d}, \quad \widehat{\Delta\theta} = \sqrt{2}\bar{\eta} + 2\bar{\nu}d_2,$$
$$\widehat{\mathrm{spr}} = \hat{\theta} + \sqrt{2}\bar{\eta} + \bar{\nu}d_2, \quad \hat{o} = \bar{\eta}/\sqrt{2} + \bar{\nu}d_2, \quad \hat{\varpi} = (\bar{d}/\sqrt{2} + \bar{\nu}\bar{\eta})d_2, \quad \hat{\varpi}' = (\bar{d}/\sqrt{2})d_2,$$
$$\hat{m} = (2\bar{\eta} + \bar{u}_O)/\sqrt{2} + \hat{\varpi}', \qquad \hat{K} = (2\bar{\eta} + \bar{u}_O)/\sqrt{2} + \hat{\varpi}.$$

These bound $|u_l|$ on O, $|\theta_b|$, $|r_b|$, $|\theta_{j+} - \theta_{j-}|$, spr_j, $|o_l|$, ϖ_j, ϖ_j', m_l and $-\bar{\theta}_j$, respectively. Start with $\hat{\Delta} = \varepsilon_q$ and $\bar{Y} = (2\sqrt{2}\,\varepsilon_q)^{1/2}$, which are valid by (a), and repeat the following step.

Put $\tilde{Y} = \hat{o} + \hat{m} + \hat{\Delta} + \sqrt{2}\bar{Y}\bar{d}$, which bounds $|z_l|$ by (c); replace $\bar{Y}$ by $\min(\bar{Y}, \hat{\Delta} + \sqrt{3}\tilde{Y})$ and recompute $\tilde{Y}$; check (4); put

$$\mathrm{err} = \frac{\tilde{Y} + \hat{r}}{2\sqrt{2}}\,\widehat{\Delta\theta} + \frac{2\tilde{Y} + 2\hat{r}}{\sqrt{2}}\,\widehat{\mathrm{spr}} \;\geq\; \sup_{X_k} \mathrm{err}_j,$$

and replace $\hat{\Delta}$ by $\min(\hat{\Delta}, \hat{K} + \mathrm{err})$. Each step derives valid bounds from valid ones, so the bounds after any number of steps may be used. Then $R_k \leq R_{\max} := 3\big(\frac{1}{2}d_2^2 + \sqrt{2}\hat{\varpi} + \sqrt{2}\hat{\varpi}' + \sqrt{2}\,\mathrm{err} + \bar{Y}d_2\big)$. By (d), α_j and γ_j are at most $2\bar{\eta} + \bar{u}_O + R_{\max}/3$, so $\bar{M} = 3(2\bar{\eta} + \bar{u}_O) + R_{\max}$ bounds W_k.

Summation. Put $f_1 = \frac{1}{2}(\tilde{Y} + \hat{r})$ and $f_2 = 2(\tilde{Y} + \hat{r})$. Then $\sqrt{2}\sup_{X_k}\mathrm{err}_j \leq f_1|\theta_{j+} - \theta_{j-}| + f_2\,\mathrm{spr}_j$, and

$$|\theta_{j+} - \theta_{j-}| \leq \sqrt{2}|\eta_{j+} - \eta_{j-}| + 2\bar{\nu}(|d_{j+}| + |d_{j-}|),$$
$$\mathrm{spr}_j \leq \sqrt{2}\sum_{b\notin j}\eta_b + 2\bar{\nu}\sum_{b\notin j}|d_b| + \frac{e_j}{\sqrt{2}} + \bar{\nu}(|d_{j+}| + |d_{j-}|),$$

where $b \notin j$ runs over the four elements of $N(k)$ outside the pair j. With $2|\langle d_{j+}, d_{j-}\rangle| \leq \frac{1}{2}d_2(|d_{j+}| + |d_{j-}|)$ this gives

$$R_{kj} \leq C_1(|d_{j+}| + |d_{j-}|) + C_2|\eta_{j+} - \eta_{j-}| + C_3\sum_{b\notin j}\eta_b + C_4\sum_{b\notin j}|d_b| + C_5 e_j,$$

with $C_1 = \frac{1}{2}d_2 + 2\bar{d} + \sqrt{2}\bar{\nu}\bar{\eta} + \bar{Y} + 2\bar{\nu}f_1 + \bar{\nu}f_2$, $C_2 = \sqrt{2}f_1$, $C_3 = \sqrt{2}f_2$, $C_4 = 2\bar{\nu}f_2$ and $C_5 = f_2/\sqrt{2}$. Sum over the 72 pairs (k, j). Each root lies in six orthogonal pairs and in six sets $N(k)$, so

$$\sum(|d_{j+}|^2 + |d_{j-}|^2) = 6\|d\|^2, \qquad \sum\sum_{b\notin j}|d_b|^2 = 12\|d\|^2,$$
$$\sum|\eta_{j+} - \eta_{j-}|^2 \leq 6|\eta|^2, \qquad \sum e_j^2 \leq 12|\eta|^2, \qquad \sum\sum_{b\notin j}\eta_b^2 = 12|\eta|^2,$$

and $\|d\|^2 \leq \chi|\tau|^2$. By $(\sum_j R_{kj})^2 \leq 3\sum_j R_{kj}^2$ and the Cauchy–Schwarz inequality $(\sum_i c_i y_i)^2 \leq (\sum_i c_i)(\sum_i c_i y_i^2)$ for $c_i \geq 0$, with $C_{\mathrm{tot}} = 2C_1 + C_2 + 4C_3 + 4C_4 + C_5$,

$$\sum_k R_k^2 \leq S_t|\tau|^2 + S_e|\eta|^2, \qquad S_t = 3C_{\mathrm{tot}}(6C_1 + 12C_4)\chi, \qquad S_e = 3C_{\mathrm{tot}}(6C_2 + 12C_3 + 12C_5).$$

Finally put $w(\eta) = (E + M_\sigma L)\eta$. Since $\sum_j e_{kj} = (E\eta)_k$ and $\sigma_k(\tau) = \sigma_k(\tau') - (M_\sigma L\eta)_k$, we have $\sum_j e_{kj} - \sigma_k(\tau) = w_k(\eta) - \sigma_k(\tau')$, and $|w(\eta)| \leq 6|\eta|$ by Lemma 7.9(2)(d). For $\kappa_2, \kappa_3 > 0$ it follows that

$$\sum_k \mathrm{vol}(X_k) \leq \tfrac{16}{81}\bar{M}^2\Big[(1+\kappa_2)\sum_k \sigma_k(\tau')^2 + (1+\kappa_2^{-1})\big((1+\kappa_3)\,36|\eta|^2 + (1+\kappa_3^{-1})(S_t|\tau|^2 + S_e|\eta|^2)\big)\Big],$$

which is Lemma 7.11 with

$$A_\sigma = \tfrac{16}{81}\bar{M}^2(1+\kappa_2), \qquad A_t^{\mathrm{h}} = \tfrac{16}{81}\bar{M}^2(1+\kappa_2^{-1})(1+\kappa_3^{-1})S_t,$$
$$A_e^{\mathrm{h}} = \tfrac{16}{81}\bar{M}^2(1+\kappa_2^{-1})\big(36(1+\kappa_3) + (1+\kappa_3^{-1})S_e\big). \tag{5}$$

A.3. **The third-order remainder.** We prove Lemma 7.10. By the symmetry of D_4, which acts transitively on roots, contact pairs and contact triangles, and the symmetry of Π in h_1, h_2 and of Θ under permutations of its three vectors, the derivatives of Φ at ζ_0 are $g_h = -S' + 8\Pi_{h_1} - 12\Theta_{h_1}$ and $g_u = \Pi_u - 3\Theta_{u_{12}}$, and

$$(\Phi_{hh})_{kl} = \begin{cases} -S'' + 8\Pi_{h_1h_1} - 12\Theta_{h_1h_1} & \text{if } k = l, \\ \Pi_{h_1h_2} - 3\Theta_{h_1h_2} & \text{if } \{k,l\} \in T, \\ 0 & \text{otherwise,} \end{cases}$$

$$(\Phi_{hu})_{k,ij} = \begin{cases} \Pi_{h_1u} - 3\Theta_{h_1u_{12}} & \text{if } k \in \{i,j\}, \\ -\Theta_{h_3u_{12}} & \text{if } \{i,j,k\} \text{ is a contact triangle}, \\ 0 & \text{otherwise,} \end{cases}$$

$$(\Phi_{uu})_{ef} = \begin{cases} \Pi_{uu} - 3\Theta_{u_{12}u_{12}} & \text{if } e = f, \\ -\Theta_{u_{12}u_{13}} & \text{if } e \neq f \text{ lie in a common contact triangle}, \\ 0 & \text{otherwise,} \end{cases}$$

with all partial derivatives of S, Π, Θ taken at $h = 1$, $u = \frac{1}{2}$. These partial derivatives, of order at most two, are enclosed in ball arithmetic with radius at most $6 \cdot 10^{-37}$, and the resulting values lie within 10^{-22} of $\frac{4}{3}, \frac{1}{4}, -4, 1, -1, \frac{1}{3}, 1, -\frac{1}{6}$, which is Lemma 7.9(1). Hence $D^2\Phi(\zeta_0) - D^2\Phi^0$ is a symmetric matrix with at most 29 nonzero entries in each row ($9 + 20$ in a row of a height, $5 + 7$ in a row of an inner product), all at most 10^{-22} in absolute value, and its norm is at most $2.9 \cdot 10^{-21}$. Since

$$\widetilde{\mathcal{H}}(\xi,\xi) - \mathcal{H}(\xi,\xi) = \big(2g_u - \tfrac{1}{2}\big)Q_t(\tau) + \big(D^2\Phi(\zeta_0) - D^2\Phi^0\big)\big[(\eta, \Lambda\tau)\big]^2,$$

$|Q_t(\tau)| \le 6|\tau|^2$ (each root lies in eight contact pairs) and $\|\Lambda\| = 2$, we obtain $|\widetilde{\mathcal{H}}(\xi,\xi) - \mathcal{H}(\xi,\xi)| \le 1.2 \cdot 10^{-21}|\tau|^2 + 2.9 \cdot 10^{-21}(|\eta|^2 + 4|\tau|^2) \le 1.3 \cdot 10^{-20}|\xi|^2$, which is the first claim of Lemma 7.9(2). Consequently $g_h \ge \frac{4}{3} - \varepsilon_0$ and $0 < g_u \le \frac{1}{4} + \varepsilon_0$. The matrix $\Phi_{hu} - \Phi^0_{hu}$ has at most 20 nonzero entries in each row and 5 in each column, all at most ε_0, so $\|\Phi_{hu}\| \le 4 + 10\varepsilon_0$. The matrix $\Phi_{uu} - \Phi^0_{uu}$ has at most 7 nonzero entries in each row, so $\|\Phi_{uu}\| \le \frac{3}{2} + 7\varepsilon_0$ and $\Phi_{uu} \succeq -7\varepsilon_0 I$. Finally $\|\widetilde{\mathcal{H}} - \mathcal{H}\| \le 1.3 \cdot 10^{-20} \le 96\,\varepsilon_0$.

Each local term $f \in \{S(h_i), \Pi(h_i, h_j; u_{ij}), \Theta(\dots)\}$ is real-analytic on the box: its closed form is valid there, the vertex of the corresponding cone lying inside the ball [16]. The box is convex and contains ζ_0 and, by Lemma 7.3(5),(6), the actual arguments. So $f(\zeta_0 + \Delta) = f(\zeta_0) + Df[\Delta] + \frac{1}{2}D^2f[\Delta]^2 + \frac{1}{6}D^3f(\zeta^*)[\Delta]^3$ for some ζ^* on the segment. Summing over the local terms and substituting $\Delta h = \eta$, $\Delta u = \Lambda\tau + c$ and $\sum_T \Delta u_{ij} = Q_d$ (Lemma 7.3(3)) gives

$$\Phi = 8 + g_h s + \tfrac{1}{2}\widetilde{\mathcal{H}}(\xi,\xi) + g_u\big(Q_d - Q_t(\tau)\big) + D^2\Phi(\zeta_0)\big[(\eta,\Lambda\tau),(0,c)\big] + \tfrac{1}{2}c^\top\Phi_{uu}c + R_\Phi,$$

where R_Φ is the sum of the cubic terms. We bound the terms in turn. First, $g_h s \ge (\frac{4}{3} - \varepsilon_0)s$ and $\frac{1}{2}\widetilde{\mathcal{H}}(\xi,\xi) \ge \frac{1}{2}\mathcal{H}(\xi,\xi) - 48\varepsilon_0(|\tau|^2 + |\eta|^2)$. By Lemma 7.3(4), $g_u(Q_d - Q_t) \ge -(\frac{1}{4} + \varepsilon_0)(2\sqrt{3}\chi\bar{d} + \chi^2\bar{d^2})|\tau|^2$. The next term is $\eta^\top\Phi_{hu}c + (\Lambda\tau)^\top\Phi_{uu}c$, and $|c| \le 3\bar{d}\|d\| \le c_*|\tau|$ with $c_* = 3\bar{d}\chi^{1/2}$. So for any $\kappa_1 > 0$ it is at least

$$-(4 + 10\varepsilon_0)c_*|\eta||\tau| - 2(\tfrac{3}{2} + 7\varepsilon_0)c_*|\tau|^2 \;\ge\; -c_*\Big((2 + 5\varepsilon_0)\big(\kappa_1^{-1}|\eta|^2 + \kappa_1|\tau|^2\big) + (3 + 14\varepsilon_0)|\tau|^2\Big).$$

Further, $\frac{1}{2}c^\top\Phi_{uu}c \ge -\frac{7}{2}\varepsilon_0 c_*^2|\tau|^2$.

For the cubic terms let M_{abc} be an upper bound for $|\partial_a\partial_b\partial_c f|$ on the box, for each local term f and each multi-index of order three. These bounds come from closed forms of lower

derivatives. For the pair term,

$$\frac{\partial\Pi}{\partial h_1} = -\frac{\pi}{3}\Big(2(2-h_1^2)^{3/2} - 3(2-h_1^2)\frac{h_2-uh_1}{(1-u^2)^{1/2}} + \frac{(h_2-uh_1)^3}{(1-u^2)^{3/2}}\Big),$$
$$\frac{\partial\Pi}{\partial u} = \frac{\pi}{4(1-u^2)^{1/2}}\Big(2 - \frac{h_1^2+h_2^2-2uh_1h_2}{1-u^2}\Big)^2,$$

and symmetrically in h_2. For the triple term,

$$\frac{\partial\Theta}{\partial u_{ab}} = \frac{1}{2(1-u_{ab}^2)^{1/2}}\int_{F_{ab}} (2-|x|^2)\,dA,$$
$$\frac{\partial^2\Theta}{\partial h_a\partial h_b} = \frac{|F_{ab}|}{(1-u_{ab}^2)^{1/2}}\quad (a\neq b), \qquad \frac{\partial^2\Theta}{\partial h_a^2} = \frac{h_a|\mathcal{S}_a|}{(2-h_a^2)^{1/2}} - \sum_{b\neq a}\frac{u_{ab}|F_{ab}|}{(1-u_{ab}^2)^{1/2}},$$

where F_{ab} is the two-dimensional face of the region $\{|x|<\sqrt{2},\ \langle x,w_c\rangle > h_c\ \forall c\}$ in the plane $\langle x,w_a\rangle = h_a$, $\langle x,w_b\rangle = h_b$ (a circular segment), and $\mathcal{S}_a$ is the part of the sphere $|x|=\sqrt{2}$ on the boundary of its face in the hyperplane $\langle x,w_a\rangle = h_a$ (the intersection of two spherical caps). These have closed forms in square roots and inverse cosines, valid on the boxes [16]. A third partial derivative with an index u is a second derivative of one of the forms for $\partial\Pi/\partial u$ or $\partial\Theta/\partial u_{ab}$, and the others are derivatives of the remaining forms. On each box these forms are expanded as Taylor models in ball arithmetic [1] on a cover of the box by cells. The required derivatives of the Taylor models are bounded on each cell, and the maxima over the cells, rounded up with a small safety factor, are the M_{abc} (Table 3). Then $\frac{1}{6}|D^3f(\zeta^*)[\Delta]^3| \le \frac{1}{6}\sum_{a,b,c} M_{abc}|\Delta_a||\Delta_b||\Delta_c|$, the sum over ordered triples of local variables. We use $|\Delta h_a|\le\bar\eta$ and $|\Delta u_b|\le\Delta_u := \max(\bar u,\bar\eta)$, and group the triples by the number of Gram variables. With the symmetric nonnegative matrices $\mathcal{M}_{xy}[a,b] = \sum_{c\in y} M_{abc}$ for a,b of type x ($x,y\in\{h,u\}$), and $\|\mathcal{M}\|_\infty$ the largest row sum of $\mathcal{M}$,

$$\tfrac{1}{6}|D^3f(\zeta^*)[\Delta]^3| \le \tfrac{1}{6}\Big[\big(\Delta_u\|\mathcal{M}_{uu}\|_\infty + 3\bar\eta\|\mathcal{M}_{uh}\|_\infty\big)|\Delta u_{\mathrm{loc}}|^2 + \big(3\Delta_u\|\mathcal{M}_{hu}\|_\infty + \bar\eta\|\mathcal{M}_{hh}\|_\infty\big)|\Delta h_{\mathrm{loc}}|^2\Big],$$

where Δu_{loc} and Δh_{loc} are the local variables of f. Each Δu_{ij}^2 occurs in one Π term and three Θ terms, and each η_i^2 in one S term, eight Π terms and twelve Θ terms. On $[1,1+\bar\eta]$ we have $|S'''(h)| = 8\pi(h^2-1)(2-h^2)^{-1/2} \le M_S := 8\pi\bar\eta(2+\bar\eta)(2-(1+\bar\eta)^2)^{-1/2}$. Hence $|R_\Phi| \le R_u|\Delta u|^2 + R_h|\eta|^2$, where

$$R_u = \tfrac{1}{6}\big[\Delta_u\lambda_{uu}(\Pi) + 3\bar\eta\lambda_{uh}(\Pi) + 3\big(\Delta_u\lambda_{uu}(\Theta) + 3\bar\eta\lambda_{uh}(\Theta)\big)\big],$$
$$R_h = \tfrac{1}{6}\big[M_S\bar\eta + 8\big(3\Delta_u\lambda_{hu}(\Pi) + \bar\eta\lambda_{hh}(\Pi)\big) + 12\big(3\Delta_u\lambda_{hu}(\Theta) + \bar\eta\lambda_{hh}(\Theta)\big)\big],$$

where $\lambda_{xy}(f) = \|\mathcal{M}_{xy}\|_\infty$ for the local term f, and $|\Delta u| \le |\Lambda\tau| + |c| \le (2+c_*)|\tau|$. For $\sigma = \frac{1}{125}$ (box $\mathbf{B}_1$) this gives $R_u \le 0.049195$ and $R_h \le 0.819561$, and for the row $(\rho,\sigma) = (\frac{2}{5},\frac{3}{100})$ of Table 1 (box $\mathbf{B}_2$) it gives $R_u \le 0.207857$ and $R_h \le 3.389261$. Collecting the terms proves Lemma 7.10 with

$$A_t^{(3)} = \big(\tfrac14+\varepsilon_0\big)\big(2\sqrt3\chi\bar d + \chi^2\bar d^2\big) + c_*\big((2+5\varepsilon_0)\kappa_1 + 3 + 14\varepsilon_0\big) + \tfrac72\varepsilon_0c_*^2 + R_u(2+c_*)^2 + 48\varepsilon_0,$$
$$A_e^{(3)} = c_*(2+5\varepsilon_0)/\kappa_1 + R_h + 48\varepsilon_0.$$

Data availability

The certificate and its checker, the interval-arithmetic proofs of Lemma 4.1, the construction scripts, the exact computation behind Remark 6.2, the programs and logs behind Section 7 and the Lean projects of Section 8 are in [16].

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