

REMARKS ON THE DENSITY OF SPHERE PACKINGS
IN THREE DIMENSIONS

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This paper shows how the density of sphere packings of spheres of equal radius may be studied using the Delaunay decomposition. Using this decomposition, a local notion of density for sphere packings in \mathbb{R}^3 is defined. Conjecturally this approach should yield a bound of $0.740873\dots$ on sphere packings in \mathbb{R}^3 , and a small perturbation of this approach should yield the bound of $\pi/\sqrt{18}$. The face-centered-cubic and hexagonal-close-packings provide local maxima (in a strong sense defined below) to the function which associates to every saturated sphere packing in \mathbb{R}^3 its density. The local measure of density coincides with the actual density for the face-centered cubic and hexagonal-close-packings.

Introduction

An old conjecture states that in three dimensions no sphere packing has density exceeding that of the packing obtained by placing spheres of unit radius at the lattice points

$$m_1v_1 + m_2v_2 + m_3v_3, \quad v_1 = (2, 0, 0), \quad v_2 = (1, \sqrt{2}, 1), \quad v_3 = (0, 0, 2), \quad m_i \in \mathbb{Z}.$$

This lattice is called the face-centered-cubic lattice or the A_3 -lattice. Denote it by Λ_{fcc} . Other packings have the same density, notably the hexagonal-close-packing Λ_{hcp} .

The purpose of this note is to take a few steps towards the solution of this problem. We describe a continuous function f on a compact subset K of Euclidean space which gives a compact bound on the density of sphere packings in three dimensions in the following sense. If Λ is the set of centers of a saturated sphere packing we obtain a map $\varphi = \varphi_\Lambda$

$$\varphi: \Lambda \rightarrow K$$

such that the density of the packing Λ does not exceed $\sup_{\Lambda} f \circ \varphi$. The map φ is local in the sense that $\varphi(v)$ depends on Λ only through the points $B_4(v) \cap \Lambda$ where $B_4(v)$ is the ball of radius 4 about v .

Of course other compact bounds (f, K) have been proposed in the past. However, the construction given here has the following remarkable properties.

1. $f(\varphi(v))$ is independent of $v \in \Lambda_{\text{fcc}}$.
2. $f(\varphi(v))$, $v \in \Lambda_{\text{fcc}}$ is equal to the density of the packing Λ_{fcc} .
3. $\varphi(\Lambda_{\text{fcc}})$ is finite.
4. Each $p \in \varphi(\Lambda_{\text{fcc}})$ is a local maximum of f on K .

The same statements hold with Λ_{fcc} replaced by Λ_{hcp} . An early version of this paper incorrectly conjectured that the global maximum of f on K is $\pi/\sqrt{18}$. However, there is considerable numerical evidence described in [4] that the global maximum of f will give an extremely good bound on sphere packings: $0.740873\dots$. By perturbing f to closely related functions f_1 discussed in [4], numerical evidence strongly suggests that we may also obtain the bound of $\pi/\sqrt{18}$ from this method.

The set K may be thought of as the set of configurations of a finite number of spheres around a fixed central sphere. Although we have made no attempt to obtain the best possible bound on the number of spheres one must consider, we show that every such configuration consists of at most 53 spheres around a fixed central sphere.

The most extensively studied compact bound of lattice packings, that based on Voronoi cells, does not satisfy property 4. Our approach, which is based on the Delaunay decomposition, is dual to that approach.

By applying our construction to the packing of disks in the plane, we recover the simple proof of L. Fejes Tóth [2] that no packing in two dimensions has density exceeding $\pi/\sqrt{12}$. Recent work of W.-Y. Hsiang, carried out some time after this paper was written, studies sphere packings using Voronoi cells. The paper of J. H. Lindsey II [5] makes implicit use of Delaunay simplices.

Since K is compact and f is the restriction to K of a piecewise analytic function one may investigate the behavior of f on K numerically. This line of investigation is pursued in [4]. All of the calculations that follow are elementary. We hope that this might convince some readers that this part of Hilbert's 18th problem is not beyond reach.

Section 1

This section gives a bound on the density of sphere packings based on the Delaunay decomposition associated to a packing.

A sphere packing in \mathbb{R}^n is a set of points $\Lambda \subseteq \mathbb{R}^n$ such that $d(v, w) \geq 2$ for all $v, w \in \Lambda$, $v \neq w$, $d(v, w) = \text{Euclidean distance on } \mathbb{R}^n$. The density δ_Λ of a sphere packing Λ is defined as

$$\sup_{w \in \mathbb{R}^n} \limsup_{N \rightarrow \infty} \frac{\sum_{v \in \Lambda} \text{vol}(B_N(w) \cap B_1(v))}{\text{vol}(B_N(w))},$$

where $B_t(w)$, $t \in \mathbb{R}_+$, $w \in \mathbb{R}^n$ is the open ball of radius t centered at $w \in \mathbb{R}^n$. We always take $B_t(w)$ to be open, and the various polytopes in this paper to be closed.

If there exists $w' \in \mathbb{R}^n$ such that $d(v, w') \geq 2$ for all $v \in \Lambda$, then $\Lambda' = \Lambda \cup \{w'\}$ is a sphere packing and $\delta_{\Lambda'} \geq \delta_\Lambda$. When looking for packings of high density we shall assume without loss of generality that the packing has the property: For all $w' \in$

\mathbb{R}^n , $\exists v \in A$ such that $d(v, w') \leq 2$. A packing A with this property will be called *saturated*.

A saturated packing A determines a decomposition of \mathbb{R}^n into Voronoi cells. For each $v \in A$, the points of \mathbb{R}^n at least as close to v as to any other point $w \in A$ is a compact convex connected region surrounding v called the Voronoi cell attached to v . Each Voronoi cell is bounded by a finite number of hyperplanes. The Voronoi cell at v contains $B_1(v)$.

The Voronoi cells fill \mathbb{R}^n and their interiors are disjoint. Since in a saturated packing A no point in \mathbb{R}^n lies at a distance greater than 2 from a point in A , the Voronoi cell at v lies in $B_2(v)$.

The Delaunay decomposition of \mathbb{R}^n associated to a saturated packing A is dual to the Voronoi decomposition. Perturbing the packing A by replacing each $v \in A$ by v' , $d(v, v') \leq \varepsilon$, (ε small), we may assume that the set of points in \mathbb{R}^n equidistant from any $v_1, \dots, v_\ell \in A'$ has dimension $n+1-\ell$ (A' the set formed from the v'). Although A' may no longer be a saturated packing, this does not matter: there is still a Voronoi decomposition and the Voronoi cells remain compact for small perturbations.

If w is a vertex of a Voronoi cell of A' there are $n+1$ closest points in A' to w . To the vertex w we associate the closed simplex whose vertices are these $n+1$ points of A' . Deforming the simplex slightly so that its vertices lie in A , we have a Delaunay simplex. The Delaunay simplices fill \mathbb{R}^n , and their interiors are disjoint [6]. Notice that there is more than one choice of a Delaunay decomposition when there are points of \mathbb{R}^n equidistant from more than $n+1$ points of A . It follows from the saturation of A that the edges of a Delaunay simplex have length at least 2 and at most 4.

The Delaunay star (as opposed to a Delaunay simplex) associated to $v \in A$ is defined as the union of all Delaunay simplices with v as a vertex. If w is an interior point of a Delaunay simplex then it lies in exactly $n+1$ stars corresponding to the various vertices of the simplex. We write $D^*(v)$ for a Delaunay star associated to $v \in A$.

Now we associate a value $\Gamma_\delta(D^*)$ to each Delaunay star $D^* = D^*(v)$ of A depending on a parameter $\delta \in \mathbb{R}_+$. Set

$$\Gamma_\delta(D^*) = -\delta \operatorname{vol}(D^*) + \sum_{w \in A} \operatorname{vol}(D^* \cap B_1(w)).$$

Let

$$\Gamma_\delta(A) = \sup_{\{D^*\}} \Gamma_\delta(D^*)$$

as D^* runs over all Delaunay stars of A .

The following theorem will show that the bound $\Gamma_\delta(A)$ on the Delaunay stars D^* of A leads to a bound on the density of a saturated packing A . The rough idea is simple enough. The Delaunay stars of a saturated packing A cover space evenly $n+1$ times. Thus to obtain a bound on the density of A it is enough to obtain a good inequality relating the volume of a Delaunay star $\operatorname{vol}(D^*)$ to the volume of the spheres inside the Delaunay star. Since $\Gamma_\delta(D^*)$ is a linear combination of the volume of D^* and the volume of the spheres inside D^* , an upper bound on $\Gamma_\delta(D^*)$ (namely $\Gamma_\delta(A)$) leads us directly to a bound on density.

Theorem 1. Let Λ be a saturated packing. Suppose $1 > \delta > 0$ is chosen so that $\sigma < 1$ where

$$\sigma \stackrel{\text{def}}{=} \frac{\Gamma_\delta(\Lambda)}{(n+1)\text{vol}(B_1(0))}.$$

Then

$$\delta_\Lambda \leq \frac{\delta}{1-\sigma}.$$

Proof. Fix $w \in \mathbb{R}^n$, $v \in \Lambda$, let $D^*(v)$ denote the Delaunay star associated to v . Let $\Lambda_N = \{v \in \Lambda \mid D^*(v) \subseteq B_N(w)\}$, $N \gg 0$ and let $\Lambda_N^{\text{ERR}} = \{v \in \Lambda \mid v \notin \Lambda_N\}$.

$$\begin{aligned} & \sum_{v \in \Lambda} \text{vol}(B_N(w) \cap B_1(v)) \\ &= \sum_{w' \in \Lambda_N} \sum_{v \in \Lambda} \frac{\text{vol}(D^*(w') \cap B_1(v))}{n+1} + E_1(N), \\ & \left(\text{with } E_1(N) = \sum_{w' \in \Lambda_N^{\text{ERR}}} \sum_{v \in \Lambda} \frac{\text{vol}(B_N(w) \cap D^*(w') \cap B_1(v))}{n+1} \right) \\ &= \sum_{w' \in \Lambda_N} \frac{[\Gamma_\delta(D^*(w')) + \delta \text{vol}(D^*(w'))]}{n+1} + E_1(N) \\ &\leq \sum_{w' \in \Lambda_N} \frac{\Gamma_\delta(\Lambda)}{n+1} + \delta \text{vol}(B_N(w)) - E_2(N) + E_1(N), \\ & \left(\text{with } E_2(N) = \frac{\delta}{n+1} \sum_{w' \in \Lambda_N^{\text{ERR}}} \text{vol}(B_N(w) \cap D^*(w')) \right) \\ & \sum_{v \in \Lambda} \frac{\text{vol}(B_N(w) \cap B_1(v))}{\text{vol}(B_N(w))} \leq \frac{|\Lambda_N| \Gamma_\delta(\Lambda)}{(n+1)\text{vol}(B_N(w))} + \delta + \frac{E_1(N) - E_2(N)}{\text{vol}(B_N(w))}. \end{aligned}$$

Take $\limsup_{N \rightarrow \infty}$, using $E_1(N)$, $E_2(N) = O(N^{n-1})$, $\text{vol}(B_N(w)) = cN^n$, $c \neq 0$.

$$\limsup_{N \rightarrow \infty} \sum_{v \in \Lambda} \frac{\text{vol}(B_N(w) \cap B_1(v))}{\text{vol}(B_N(w))} \leq \delta + \frac{\Gamma_\delta(\Lambda)}{(n+1)\text{vol}(B_1(0))} \cdot \limsup_{N \rightarrow \infty} \left[\frac{|\Lambda_N| \text{vol}(B_1(0))}{\text{vol}(B_N(w))} \right].$$

Now

$$\limsup_{N \rightarrow \infty} \frac{|\Lambda_N| \text{vol}(B_1(0))}{\text{vol}(B_N(w))} \leq \delta_\Lambda$$

by the definition of δ_Λ . So we obtain

$$\delta_\Lambda \leq \delta + \sigma \cdot \delta_\Lambda, \quad \sigma = \frac{\Gamma_\delta(\Lambda)}{(n+1)\text{vol}(B_1(0))}.$$

By assumption $\sigma < 1$ so the conclusion follows. ■

Section 2

This section gives an expression for $\Gamma_\delta(D^*)$.

Lemma 2.1. *If $D^* = D^*(v)$, $v \in \Lambda$, is a Delaunay star of a saturated packing Λ then $B_1(v) \subseteq D^*(v)$.*

Proof. Let S be a Delaunay simplex with vertex v . It is enough to show that $B_1(v)$ does not intersect the face of S opposite v , for then $B_1(v)$ cannot meet the boundary of $D^*(v)$.

The sphere Σ circumscribing S has radius $1 \leq r \leq 2$ and center θ . Let H denote the hyperplane between v and θ distance 1 from v normal to the line through v and θ . If w lies on the sphere Σ on the same side of H as v then $d(v, w) \leq d(v, w_0)$ where w_0 lies on $H \cap \Sigma$. Now $d(v, w_0)$, considered as a function of the radius r , is increasing in r and takes the value 2 when $r = 2$. hence $d(v, w) \leq d(v, w_0)|_{r=2} = 2$. But if w' is a vertex of S ($w' \neq v$) then $d(w', v) \geq 2$. Consequently every vertex of S other than v lies across H from v . Thus the open ball $B_1(v)$ does not meet the face of S opposite v . ■

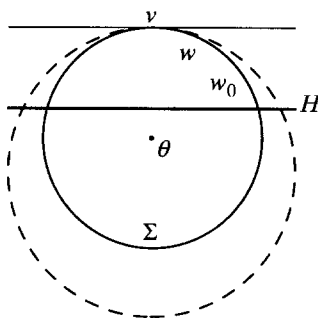


Fig. 1

If S is any Delaunay n -simplex $\subseteq \mathbb{R}^n$ define

$$(*) \quad \Gamma_\delta(S) = -\delta \operatorname{vol}(S) + \sum_v \operatorname{vol}(S \cap B_1(v)).$$

Here v runs over the vertices of S . If S is a Delaunay simplex with vertices at v_0, \dots, v_n write $\varrho_i(S) = \operatorname{vol}(S \cap B_1(v_i))$, $i = 0, \dots, n$, and $\varrho(S) = \sum_0^n \varrho_i(S)$, so that $\Gamma_\delta(S) = -\delta \operatorname{vol}(S) + \varrho(S)$. Also by Lemma 2.1, if D^* is a Delaunay star

$$(2.2) \quad \Gamma_\delta(D^*) = \sum_{S \subseteq D^*} \Gamma_\delta(S)$$

(the sum running over Delaunay simplices lying in D^*).

The Delaunay star $D^*(v)$ about $v \in \Lambda$ determines a triangulation of the unit sphere at v – each spherical triangle is the intersection of the unit sphere with a Delaunay simplex. The spherical triangles cover the sphere and do not intercept except along geodesic edges. Let Λ be a saturated packing, D^* a Delaunay star of Λ about $v \in \Lambda$.

Lemma 2.3. *Every edge of the spherical triangulation of $B_1(v)$ has geodesic length at least $\pi/6$, and at most $2\pi/3$.*

Proof. Let v_X, v_P, v_Q be three vertices of a Delaunay simplex. Let θ be the center of the circle circumscribing v_X, v_P, v_Q . Since $d(v_P, v_Q) \geq 2 \geq d(\theta, v_P) = d(\theta, v_Q)$, we have $\angle v_P \theta v_Q \geq \pi/3$. Then $\angle v_P v_X v_Q = \frac{1}{2} \angle v_P \theta v_Q \geq \pi/6$. If two angles are at least $\pi/6$ the third is at most $2\pi/3$. ■

Now turn to packings in three dimensions. The volume $\text{vol}(S)$ of a simplex S with vertices $0, v_1, v_2, v_3$ is $|\det(v_1, v_2, v_3)|/6$ and hence depends analytically on the coordinates of v_1, v_2, v_3 on any open set for which $\det(v_1, v_2, v_3)$ has fixed sign. Now $3\rho_i(S)$ is the solid angle of S at v_i which is given by the classical formula for the area of a spherical triangle: $\alpha_1 + \alpha_2 + \alpha_3 - \pi$ where $\alpha_1, \alpha_2, \alpha_3$ (depending on i) are the angles of the spherical triangle cut out by S on the sphere of radius 1 at v_i .

We note that the spherical law of cosines states that if $\beta_1, \beta_2, \beta_3$ are the spherical lengths of the sides of a triangle with opposite angles $\alpha_1, \alpha_2, \alpha_3$ then

$$\cos \alpha_1 = \frac{\cos \beta_1 - \cos \beta_2 \cos \beta_3}{\sin \beta_2 \sin \beta_3}$$

and similarly for α_2 and α_3 . In particular, α_j and $\rho_i(S)$ depend analytically on the lengths β_j when β_j satisfy $0 < \beta_j < \pi$ and $\beta_j \neq |\beta_k \pm \beta_\ell|$, (j, k, ℓ a permutation of 1, 2, 3). Thus using Lemma 2.3, one sees that $\rho_j(S)$ is analytic when the triangle has positive area. Also, for instance, if S has vertices $0, v_1, v_2, v_3$, and $\beta_1, \beta_2, \beta_3$ are the spherical lengths (Euclidean angles) for the vertex of S at the origin, then $\cos \beta_j = v_k \cdot v_\ell / |v_k| |v_\ell|$ where again j, k, ℓ are a permutation of 1, 2, 3; and this gives $\rho(S)$ analytically in terms of the coordinates of the vertices of S provided S has positive volume.

Section 3

In this section, and in the remainder of the paper, we restrict to packings Λ in 3 dimensions. We state our results using the lattice packing Λ_{fcc} , but the same results also hold without modification for the hexagonal-close-packing Λ_{hcp} . The Delaunay decomposition of the lattice Λ_{fcc} is not unique. There is a unique choice $\delta = \delta_{\text{oct}}$ which insures that $\Gamma_\delta(D^*)$ is the same for all Delaunay stars D^* arising in any choice of a Delaunay decomposition of the packing Λ_{fcc} . Any other choice of δ would lead to unsatisfactory bounds. This section shows for the lattice Λ_{fcc} in 3 dimensions using this choice $\delta = \delta_{\text{oct}}$ that the bound

$$\delta_{\text{oct}} / (1 - \sigma_{\text{fcc}}), \quad \sigma_{\text{fcc}} \stackrel{\text{def}}{=} 3\Gamma_{\delta_{\text{oct}}}(\Lambda_{\text{oct}}) / 16\pi$$

on the density of Λ_{fcc} given in Theorem 1 coincides with the packing's true density $\delta_{\Lambda_{\text{fcc}}} = \frac{\pi}{\sqrt{18}}$. Write Γ_{oct} for $\Gamma_{\delta_{\text{oct}}}$. We set $\chi_0 = \arccos(1/\sqrt{3})$.

Let V_{oct} be a solid regular octahedron whose edges have length 2. Let v_1, \dots, v_6 denote the vertices of V_{oct} . We let δ_{oct} be the density of V_{oct} :

$$\delta_{\text{oct}} = \sum_{i=1}^6 \frac{\text{vol}(V_{\text{oct}} \cap B_1(v_i))}{\text{vol}(V_{\text{oct}})} = \frac{-3\pi + 12\chi_0}{2\sqrt{2}} = 0.7209029495 \dots$$

There are three types of Delaunay simplices in A_{fcc} .

Type I (regular tetrahedron with edge length 2)

Type II (tetrahedron with edges of length $2, 2, 2, 2, 2\sqrt{2}$)

Type III (tetrahedron of zero volume, edges of length $2, 2, 2, 2\sqrt{2}, 2\sqrt{2}$)

Four simplices of type II fit together to form a regular octahedron whose edges have length 2. There are several possible ways to break an octahedron such as this into 4 Delaunay simplices. In each case one obtains 4 simplices of type II and possibly one of type III. Three of these ways correspond to the three pairs of opposite vertices of the octahedron (depending on the perturbation of Λ chosen in the construction of the Delaunay decomposition).

Here we stress that with this choice $\delta = \delta_{\text{oct}}$, we have $\Gamma_{\delta_{\text{oct}}}(S) = \Gamma_{\text{oct}}(S) = 0$ for any type II or type III tetrahedron. Hence if D^* is any star of the fcc packing, then the value $\Gamma_{\text{oct}}(D^*)$ is independent of D^* , and is equal in fact to $8\Gamma_{\text{oct}}(S)$ where S is a tetrahedron of type I.

Recall that

$$\Gamma_{\text{oct}}(D^*(v)) = \sum_{S \subseteq D^*} \Gamma_{\text{oct}}(S) = \sum_{S \subseteq D^*} (-\delta_{\text{oct}} \text{vol}(S) + \varrho(S)).$$

By construction $\Gamma_{\text{oct}}(S) = 0$ for S of type II, and

$$\Gamma_{\text{oct}}(S) = \frac{11\pi}{3} - 12\chi_0 = 0.05537364567 \dots$$

for S of type I. Any Delaunay star of A_{fcc} has precisely 8 Delaunay simplices of type I. Therefore $\Gamma_{\text{oct}}(D^*) = 8\Gamma_{\text{oct}}(S)$ and $\text{vol}(B_1(0)) = \frac{4\pi}{3}$. So

$$1 - \frac{\delta_{\text{oct}}}{\frac{\Gamma_{\text{oct}}(D^*)}{4\text{vol}(B_1(0))}} = \frac{\pi}{\sqrt{18}}.$$

But $\frac{\pi}{\sqrt{18}}$ is the density of the sphere packing A_{fcc} .

Section 4

We continue to write $\Gamma_{\text{oct}}(\cdot)$ for $\Gamma_{\delta_{\text{oct}}}(\cdot)$. In this section we show that if D^* is sufficiently close to a Delaunay star D_{fcc}^* of the packing A_{fcc} then

$$\Gamma_{\text{oct}}(D^*) \leq \Gamma_{\text{oct}}(D_{\text{fcc}}^*)$$

with equality only if $D^* = D_{\text{fcc}}^*$. We state our arguments for the fcc packing but the same argument gives the same results for the hexagonal-close-packing as well.

The Delaunay star D_{fcc}^* is the union of four types of regions

- (A_{fcc}) a regular tetrahedron = a single Delaunay simplex of type I.
- (B_{fcc}) a regular octahedron = the union of four Delaunay simplices of type II.
- (C_{fcc}) half a regular octahedron = the union of two Delaunay simplices of type II (the other two Delaunay simplices of the given octahedron belong to a different Delaunay star).

(D_{fcc}) three quarters of a regular octahedron = the union of three Delaunay simplices of type II, and one of type III. In this case the long edges of the simplices lie along two different axes.

Note that there are always 2, 3, or 4 simplices of type II meeting at a vertex of an octahedron – no matter how the Delaunay decomposition is chosen. (There is always more than one simplex of type II at a vertex because the triangulation of a square always requires at least two triangles). Types B_{fcc} , C_{fcc} and D_{fcc} correspond respectively to 4, 2 and 3 simplices of type II meeting at a vertex.

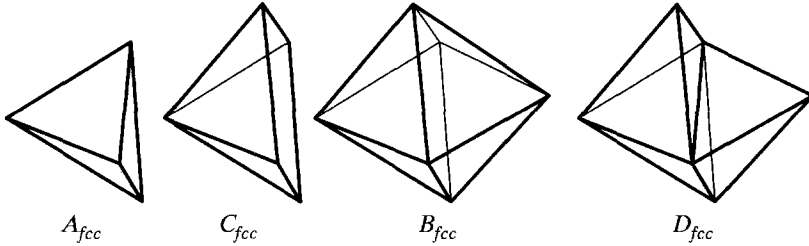


Fig. 2

Thus it is enough to show that

$$\Gamma_{\text{oct}}(X) \leq \Gamma_{\text{oct}}(X_{\text{fcc}}) \quad (X, X_{\text{fcc}}) \in \{(A, A_{\text{fcc}}), (B, B_{\text{fcc}}), (C, C_{\text{fcc}}), (D, D_{\text{fcc}})\}$$

where A, B, C, D are perturbations of $A_{\text{fcc}}, B_{\text{fcc}}, C_{\text{fcc}}, D_{\text{fcc}}$.

We begin with the case (A, A_{fcc}) . We use coordinates (t_1, \dots, t_6) to describe the tetrahedron A where $t_i + 2$ is the length of the i th edge of A (edges labelled in any order). The tetrahedron A_{fcc} then has coordinates $(t_1, \dots, t_6) = (0, 0, \dots, 0)$. Both the volume of A and the solid angles of A are analytic functions of (t_1, \dots, t_6) in a neighborhood of $(0, \dots, 0)$, thus (by Section 2) $\Gamma_{\text{oct}}(A)$ may be considered an analytic function of (t_1, \dots, t_6) . We consider a first order approximation

$$\Gamma_{\text{oct}}(A) = \Gamma_{\text{oct}}(A_{\text{fcc}}) + \sum_1^6 t_i \frac{\partial \Gamma_{\text{oct}}(A_{\text{fcc}})}{\partial t_i} + \text{higher order terms.}$$

By symmetry $\frac{\partial \Gamma}{\partial t_i}(A_{\text{fcc}}, \delta_{\text{oct}}) = \alpha_0$ independent of i . So

$$\Gamma_{\text{oct}}(A) = \Gamma_{\text{oct}}(A_{\text{fcc}}) + \alpha_0 t_0 + \text{higher order terms}$$

where $t_0 + 12$ is the perimeter of A . Along the curve A_t : $(t_1, \dots, t_6) = (t, \dots, t)$ we have

$$\Gamma_{\text{oct}}(A_t) = -\delta_{\text{oct}} \text{vol}(A_t) + \sum_v \text{vol}(A_{\text{fcc}} \cap B_1(v)) \quad (\text{sum over vertices of } A_{\text{fcc}})$$

$$\left. \frac{d\Gamma_{\text{oct}}(A_t)}{dt} \right|_{t=0} = 6\alpha_0 = -\delta_{\text{oct}} \left. \frac{d}{dt} \text{vol}(A_t) \right|_{t=0} = -\delta_{\text{oct}} \sqrt{2} < 0.$$

The requirement for A to be a Delaunay simplex now forces $t_i \geq 0$, $i = 1, \dots, 6$ or $t_0 \geq 0$ so that

$$\begin{aligned}\Gamma_{\text{oct}}(A) &= \Gamma_{\text{oct}}(A_{\text{fcc}}) + \alpha_0 t_0 + \text{higher order terms} \\ &< \Gamma_{\text{oct}}(A_{\text{fcc}}) \text{ for } 0 < t_0 < \varepsilon.\end{aligned}$$

Now turn to the octahedral case (B, B_{fcc}) . $\Gamma_{\text{oct}}(B)$ depends analytically on the lengths of the edges of the simplices comprising B . These consist of the edges of B and a diagonal of B . Moreover the length of the diagonal of B is an analytic function of the lengths of its edges. Thus we may let (t_1, \dots, t_{12}) be the coordinates of B near B_{fcc} with $t_i + 2$ the length of the i th edge of B .

Proceeding as in the previous case, we find

$$\Gamma_{\text{oct}}(B) = \Gamma_{\text{oct}}(B_{\text{fcc}}) + \beta_0 t_0 + \text{higher order terms}$$

where

$$\beta_0 = \frac{-\sqrt{2}}{3} \delta_{\text{oct}} < 0,$$

and

$$t_0 + 24 = \text{the perimeter of } B.$$

The edges of a Delaunay simplex must have length at least 2, and

$$\Gamma_{\text{oct}}(B) = \Gamma_{\text{oct}}(B_{\text{fcc}}) + \beta_0 t_0 + \dots < \Gamma_{\text{oct}}(B_{\text{fcc}}) \text{ for } 0 < t_0 < \varepsilon.$$

Next, turn to half an octahedron (C, C_{fcc}) . We take C_{fcc} to be the convex hull of $0, v_1, v_2, v_3, v_4$ where $d(0, v_i) = 2$, $d(v_i, v_{i+1}) = 2$, $d(v_i, v_{i+2}) = 2\sqrt{2}$, $\forall i$.

Take w_1, w_2, w_3, w_4 to be vectors near v_1, v_2, v_3, v_4 . Take $t_i + 2$, $i = 1, \dots, 4$ to be the lengths of the edges running from 0 to w_i . Take $t_i + 2$, $i = 5, \dots, 8$, to be the lengths of the edges from the vertex w_i to the vertex w_{i+1} (subscripts modulo 4). Let θ be the center of the sphere circumscribing the simplex with vertices $0, w_1, w_3, w_4$. Define $t_9 = d(\theta, w_4)^2 - d(\theta, w_1)^2 = w_4 \cdot w_4 - 2\theta \cdot w_4$. Then we take (t_1, \dots, t_9) to be the coordinates for C in a neighborhood of C_{fcc} .

Note that every small neighborhood of C_{fcc} is a union of two regions. On one, the Delaunay decomposition gives two simplices with vertices $\{0, w_1, w_2, w_3\}$ and $\{0, w_1, w_3, w_4\}$. On the other, the Delaunay decomposition gives two simplices with vertices $\{0, w_2, w_3, w_4\}$ and $\{0, w_4, w_1, w_2\}$. If $\Gamma_{\text{oct}}(C) \leq \Gamma_{\text{oct}}(C_{\text{fcc}})$ on one of these regions then the inequality holds on both regions. We define an analytic function $\hat{\Gamma}_{\text{oct}}(C)$ of local parameters (t_1, \dots, t_9) which is equal to $\Gamma_{\text{oct}}(C)$ on the first of these regions. Let S_1 be the simplex with vertices $\{0, w_1, w_2, w_3\}$ and let S_2 be the simplex with vertices $\{0, w_1, w_3, w_4\}$. Set $C = S_1 \cup S_2$, and define $\hat{\Gamma}_{\text{oct}}(C) = \Gamma_{\text{oct}}(S_1) + \Gamma_{\text{oct}}(S_2)$. It can be checked using the explicit formulas of Section 2 that the function $\hat{\Gamma}_{\text{oct}}(C)$ depends analytically on (t_1, \dots, t_9) near C_{fcc} .

A calculation using Mathematica (the code is available upon request) shows that

$$\begin{aligned}\hat{\Gamma}_{\text{oct}}(C) &= \Gamma_{\text{oct}}(C_{\text{fcc}}) + \gamma_0^a(t_1 + t_3) + \gamma_0^b(t_2 + t_4) + \gamma_0^c(t_5 + t_6 + t_7 + t_8) + \gamma_0^d t_9 \\ &\quad + \text{higher orders}\end{aligned}$$

where

$$\begin{aligned}\gamma_0^a &= -\frac{2}{3} + \frac{4}{3\sqrt{2}}(1 - \delta_{oct}) = -0.403531444 \dots < 0 \\ \gamma_0^b &= \frac{2(1 - \sqrt{2})}{3} = -0.2761423749 \dots < 0 \\ \gamma_0^c &= \frac{-\delta_{oct}}{3\sqrt{2}} = -0.1699184547 \dots < 0 \\ \gamma_0^d &= -\frac{1}{6} + \frac{1}{3\sqrt{2}} - \frac{\delta_{oct}}{6\sqrt{2}} = -0.01592363363 \dots < 0.\end{aligned}$$

For a Delaunay simplex the edges have length at least 2, so that $t_1, t_2, \dots, t_8 \geq 0$.

By the obvious symmetry of the configuration we may assume that S_1 and S_2 are two Delaunay simplices in C . Thus by the construction of Delaunay simplices $d(\theta, w_4) \geq d(\theta, w_i)$, $i = 1, 2, 3$, so that $t_9 \geq 0$. This shows that $\Gamma_{oct}(C) \leq \Gamma_{oct}(C_{fcc})$.

The final case (D, D_{fcc}) is similar to the others. We let $2+t_1, \dots, 2+t_{12}$ be the lengths of the edges of the octahedron spanned by the vertices of D . D consists of four Delaunay simplices. Three of the simplices are perturbations of simplices of type II. The fourth is a nearly flat simplex which collapses into a simplex of no volume for $D = D_{fcc}$. We consider D as an octahedron with one Delaunay simplex removed. Call this excised simplex S_0 , and let the longest edge of S_0 be denoted ℓ . Then we divide the coordinates into four sets:

$2+t_1, 2+t_2, 2+t_3, 2+t_4$ the lengths of the edges ($\neq \ell$) of S_0 which meet ℓ at a vertex,

$2+t_5$ the length of the edge of S_0 opposite ℓ ,

$2+t_6, 2+t_7, 2+t_8, 2+t_9$ the lengths of the edges of the simplices in D sharing a vertex with ℓ ,

$2+t_{10}, 2+t_{11}, 2+t_{12}$ the remaining edges.

Note that all of these edges are taken to be external edges of the octahedron. Then a Mathematica calculation shows

$$\begin{aligned}\Gamma_{oct}(D) &= \Gamma_{oct}(D_{fcc}) + \delta_0^a(t_1 + t_2 + t_3 + t_4) + \delta_0^b t_5 + \delta_0^c(t_6 + t_7 + t_8 + t_9) \\ &\quad + \delta_0^d(t_{10} + t_{11} + t_{12}) + \text{higher orders}\end{aligned}$$

where

$$\begin{aligned}\delta_0^a &= \frac{1}{6} - \frac{1}{3\sqrt{2}} - \frac{\delta}{6\sqrt{2}} = -0.1539948211 \dots < 0 \\ \delta_0^b &= -\frac{1}{2} + \frac{1}{\sqrt{2}} - \frac{\delta}{2\sqrt{2}} = -0.0477709009 \dots < 0 \\ \delta_0^c &= -\frac{1}{6} + \frac{1}{3\sqrt{2}} - \frac{5\delta}{6\sqrt{2}} = -0.3557605431 \dots < 0 \\ \delta_0^d &= \frac{1}{6} - \frac{1}{3\sqrt{2}} - \frac{\delta}{2\sqrt{2}} = -0.3239132758 \dots < 0.\end{aligned}$$

Thus $\Gamma_{oct}(D) < \Gamma_{oct}(D_{fcc})$ for $t_1, \dots, t_{12} > 0$.

Finally, if $\Gamma_{oct}(D^*) = \Gamma_{oct}(D_{fcc}^*)$ then we must have $t_i = 0 \ \forall i$ in all of the preceding cases. Then $A = A_{fcc}$, $B = B_{fcc}$, $C = C_{fcc}$, $D = D_{fcc}$ and $D^* = D_{fcc}^*$.

Section 5

We continue to work with packings in three dimensions. The main result of this section is Theorem 5.4 which eliminates the hypothesis ($\sigma < 1$) in Theorem 1, so that any saturated packing Λ has density at most $\delta_{\text{oct}}/(1 - 3\Gamma_0/(16\pi))$, $\Gamma_0 = \sup_{D^*} \Gamma_{\text{oct}}(D^*)$. We lead up to Theorem 5.4 with 3 technical lemmas. Let t_0 be the positive root of the quadratic equation $3t_0^2 - 1 = 2/\delta_{\text{oct}}$. Set $t'_0 = (t_0 - 1)^2(2t_0 + 1)/3$. So $t_0 = 1.12165\dots$, $t'_0 = 0.015999\dots$

Lemma 5.1. *Let S be any Delaunay simplex. Its volume is at least*

$$\varrho(S)/\delta_{\text{oct}} - 4\pi t'_0.$$

Lemma 5.2. *Let S be any Delaunay simplex. There are at most two vertices v of S such that the distance from v to the face of S opposite v is less than t_0 .*

Lemma 5.3. *Let S be any Delaunay simplex. Then*

$$\Gamma_{\text{oct}}(S) \leq 4\pi\delta_{\text{oct}}t'_0 < 0.15.$$

Theorem 5.4. *Every Delaunay star D^* satisfies*

$$\Gamma_{\text{oct}}(D^*) < 16\pi/3.$$

We begin this sequence of proofs by introducing some temporary notation and terminology. We call a vertex v of a simplex which comes within t_0 of the face opposite v an *osculating* vertex. If the point closest to v on the triangular face opposite v lies on an edge of the triangle we say that v is an *outer* vertex. If the point lies in the interior of the triangular face we say v is an *inner* vertex. We denote triangles by expressions such as $\Delta v_A v_B v_C$, edges by expressions such as $v_A v_B$, and angles by expressions such as $\angle v_A v_B v_C$.

Proof of 5.2. Suppose for a contradiction that there is a simplex S with at least 3 osculating vertices. We denote them by v_X, v_A, v_B , and denote the remaining vertex by v_C .

Case 1: *Suppose that v_X is an inner vertex.* Let \bar{v}_X denote the orthogonal projection of v_X onto the interior of the triangle $\Delta v_A v_B v_C$. Since $d(v_B, v_X) \geq 2$, $d(v_X, \bar{v}_X) \leq t_0$, the Pythagorean theorem gives $d(v_B, \bar{v}_X) \geq \sqrt{4 - t_0^2} \geq 1.6$ and similarly $d(v_A, \bar{v}_X) \geq 1.6$. Either $\angle v_C \bar{v}_X v_A$ or $\angle v_C \bar{v}_X v_B$ is obtuse, say $\angle v_C \bar{v}_X v_B$. If $\angle v_A \bar{v}_X v_B$ were also obtuse,

$$1.2 \geq t_0 \geq d(v_B, \Delta v_X v_A v_C) \geq d(v_B, \Delta \bar{v}_X v_A v_C) = d(v_B, \bar{v}_X) \geq 1.6,$$

a contradiction. So $\angle v_A \bar{v}_X v_B$ is acute, and this forces both $\angle v_A \bar{v}_X v_C$ and $\angle v_B \bar{v}_X v_C$ to be obtuse.

Either $\angle v_A v_B \bar{v}_X$ or $\angle v_B v_A \bar{v}_X$ is acute, say $\angle v_A v_B \bar{v}_X$. Let \bar{v}_A be the projection of v_A onto the segment $\bar{v}_X v_B$. Then

$$t_0 \geq d(v_B, \Delta v_X v_A v_C) \geq d(v_B, \Delta \bar{v}_X v_A v_C) \geq d(v_B, \bar{v}_X v_A) \geq d(v_B, \bar{v}_A)$$

$$t_0 \geq d(v_A, \Delta v_X v_B v_C) \geq d(v_A, \Delta \bar{v}_X v_B v_C) = d(v_A, \bar{v}_A).$$

The Pythagorean theorem gives the contradiction in case 1:

$$4 \leq d(v_A, v_B)^2 = d(v_A, \bar{v}_A)^2 + d(\bar{v}_A, v_B)^2 \leq t_0^2 + t_0^2 < 3.$$

In the remaining case we keep the assumption of three osculating vertices, but we assume that the situation of Case 1 holds for none of the vertices, that is:

Case 2: Suppose the simplex has at least 3 osculating outer vertices. Let $v_1 v_2 v_3$ be vertices of a triangle with sides of length between 2 and 4. Assume that $d(v_1, \bar{v}_1) \leq t_0$ where \bar{v}_1 is the orthogonal projection of v_1 onto the segment $v_2 v_3$. Then

$$d(v_2, \bar{v}_1)^2 = d(v_2, v_1)^2 - d(v_1, \bar{v}_1)^2 \geq 4 - t_0^2 > 1.6^2.$$

Similarly, $d(\bar{v}_1, v_3) > 1.6$, so also

$$d(v_2, v_3) = d(v_2, \bar{v}_1) + d(\bar{v}_1, v_3) > 3.2.$$

$$d(v_3, \bar{v}_1) = d(v_3, v_2) - d(v_2, \bar{v}_1) \leq 4 - 1.6 = 2.4$$

$$d(v_1, v_3)^2 = d(v_1, \bar{v}_1)^2 + d(\bar{v}_1, v_3)^2 \leq t_0^2 + 2.4^2 < 2.7^2.$$

Similarly $d(v_1, v_2) < 2.7$. In summary, the adjacent edges $v_1 v_2, v_1 v_3$ of a outer osculating vertex v_1 are *short* (meaning of length < 2.7) and the opposite edge $v_2 v_3$ of an outer osculating vertex v_1 is *long* (meaning of length > 3.2).

Suppose there were a simplex with three or more osculating outer vertices. For this, the simplex would need at least three short edges (leaving at most 3 long edges) and at least two long edges. We illustrate the five possible combinatorial patterns with two or three long edges and mark with an asterisk the vertices possibly satisfying the 1-opposite&long-2-adjacent&short edge condition given above. The long edges are indicated by bold edges. Only one of these configurations has 3 or more vertices marked with an asterisk. It has 2 non-adjacent long edges.

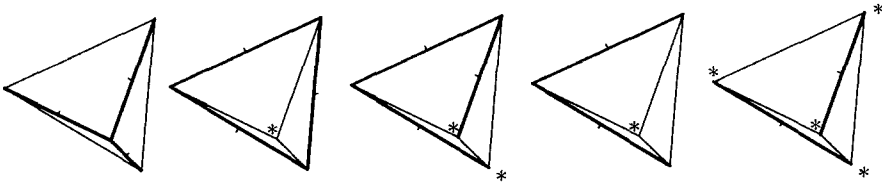


Fig. 3

To complete case 2, we show that such a simplex with three outer vertices and 2 non-adjacent long edges does not exist. Let a simplex with vertices v_X, v_A, v_B, v_C be given with $v_X v_B, v_A v_C$ long (i.e. $d(v_X, v_B), d(v_A, v_C) \geq 3.2$). Exchanging v_A, v_C with v_X, v_B if necessary, we may assume both v_X and v_B are osculating outer vertices. We deform the simplex by lengthening the segment $v_X v_B$ keeping the lengths of the other edges fixed until v_X, v_A, v_B, v_C are coplanar. It is enough to

show that in this elongated planar configuration $d(v_X, v_B) \leq 3$ contradicting the hypothesis that $v_X v_B$ is a long edge.

Let \bar{v}_X (resp. \bar{v}_B) be the orthogonal projection of v_X (resp. v_B) onto the segment $v_A v_C$. Interchanging v_X and v_B if necessary, assume without loss of generality that \bar{v}_X is between \bar{v}_B and v_C . We have

$$d(v_C, \bar{v}_X)^2 = d(v_C, v_X)^2 - d(v_X, \bar{v}_X)^2 \geq 4 - t_0^2 > 1.65^2.$$

Similarly $d(v_A, \bar{v}_B) \geq 1.65$. Then

$$d(\bar{v}_B, \bar{v}_X) = -d(\bar{v}_B, v_A) + d(v_A, v_C) - d(v_C, \bar{v}_X) \leq 4 - 2(1.65) = .7.$$

This gives the contradiction

$$d(v_B, v_X) \leq d(v_B, \bar{v}_B) + d(\bar{v}_B, \bar{v}_X) + d(\bar{v}_X, v_X) \leq t_0 + .7 + t_0 < 3. \quad \blacksquare$$

Proof of 5.1. Let S be a Delaunay simplex. Set $S_i = S \cap B_{t_0}(v_i)$, $i = 1, 2, 3, 4$; it is the region inside S and inside a ball of radius t_0 centered at the i th vertex v_i of S .

If i, j, k are distinct then $S_i \cap S_j \cap S_k = \emptyset$. For such a point in the intersection would be within distance t_0 of all vertices of a triangle with sides of length ≥ 2 (vertices v_i, v_j, v_k). But for a contradiction we observe that no triangle of sides ≥ 2 is contained in a circle of radius $t_0 < 2/\sqrt{3}$. Hence by the inclusion-exclusion principle, the volume of S is at least

$$\sum_{i=1}^4 \text{vol}(S_i) - \sum_{1 \leq i < j \leq 4} \text{vol}(S_i \cap S_j).$$

To complete the proof, we give a lower bound on $\text{vol}(S_i)$ and an upper bound on $\text{vol}(S_i \cap S_j)$.

The volume of the smaller region bounded by a sphere of radius t_0 and a plane at distance $x_0 \geq 1$ from the center of the sphere is

$$\pi f(x_0) = \pi \int_{x_0}^{t_0} t_0^2 - t^2 dt \leq \pi \int_1^{t_0} t_0^2 - t^2 dt = \pi t'_0.$$

If v_i has distance t_0 or more from the face of S opposite v_i then $\text{vol}(S_i) = t_0^3 \varrho_i(S)$. If v_i comes within distance x_0 , $x_0 \leq t_0$ (note that $x_0 \geq 1$ by Lemma 2.1) then intersecting $B_{t_0}(v_i)$ with the simplex will cut a slice of width $t_0 - x_0$ of volume at most $\pi f(x_0) \leq \pi t'_0$ from the sphere $B_{t_0}(v_i)$. By Lemma 5.2 at most two vertices come within t_0 of their opposite face so

$$\sum \text{vol}(S_i) \geq t_0^3 \sum \varrho_i(S) - 2\pi t'_0 = t_0^3 \varrho(S) - 2\pi t'_0.$$

Consider $S_i \cap S_j$. If $d(v_i, v_j) \geq 2t_0$, then $S_i \cap S_j = \emptyset$. More generally if $d(v_i, v_j) = 2x_0$, $1 \leq x_0 \leq t_0$ the perpendicular bisecting plane between v_i and v_j breaks $B_{t_0}(v_i) \cap B_{t_0}(v_j)$ into two regions of equal volume, each of volume $\pi f(x_0) \leq \pi t'_0$. If we intersect $B_{t_0}(v_i) \cap B_{t_0}(v_j)$ with S , we retain only a sector of some angle $\alpha_{ij} \leq \pi$, $i \neq j$. So the two volumes intersected with S each have upper bound

$\pi f(x_0)\alpha_{ij}/(2\pi) \leq \alpha_{ij}t'_0/2$. We count both pieces by summing over $i \neq j$ instead of $i < j$. Summing then gives the upper bound $\sum_{i \neq j} \alpha_{ij}t'_0/2$. The area of the spherical triangle cut out by S on the unit sphere at v_i is $-\pi + \sum_{j \neq i} \alpha_{ij}$ (i fixed). Hence $\varrho_i(S) = (1/3)(-\pi + \sum_{j \neq i} \alpha_{ij})$ (i fixed), or summing over i :

$$\varrho(S) = (1/3)(-4\pi + \sum_{i \neq j} \alpha_{ij}), \quad \text{and} \quad \sum_{i \neq j} \alpha_{ij} = 3\varrho(S) + 4\pi.$$

Hence

$$\sum_{i < j} \text{vol}(S_i \cap S_j) \leq (3\varrho(S) + 4\pi)t'_0/2.$$

Combine with the earlier estimate of $\text{vol}(S_i)$ to obtain

$$\text{vol}(S) \geq t_0^3 \varrho(S) - (3/2)t'_0 \varrho(S) - 2\pi t'_0 - 2\pi t'_0 = \varrho(S)/\delta_{\text{oct}} - 4\pi t'_0. \quad \blacksquare$$

Proof of 5.3. This follows immediately from $\Gamma_{\text{oct}}(D^*) = -\delta_{\text{oct}} \text{vol}(S) + \varrho(S)$ and Lemma 5.1. \blacksquare

Proof of 5.4. A Delaunay star D^* gives a triangulation of the unit sphere with the property that every edge has length at least $\pi/6$ (Lemma 2.3). In fact every pair of vertices are at least $\pi/6$ apart. A classical result [3] states that the number of triangles in a triangulation never exceeds $4\pi/A$ where A is the area of a spherical equilateral triangle whose edges have geodesic length equal to the geodesic distance separating the closest pair of vertices of a triangle. Thus the triangulation determined by D^* has at most $4\pi/A = 4\pi/(-\pi + 3\arccos(-3 + 2\sqrt{3})) = 102.218813\dots$ triangles. Hence D^* is made up of at most 102 simplices. By Lemma 5.3, and Equation 2.2 we have

$$\Gamma_{\text{oct}}(D^*) \leq 102 \max_S \Gamma_{\text{oct}}(S) \leq 102(0.15) < 16\pi/3. \quad \blacksquare$$

Remark. By Euler's formula, the bound of 102 simplices also gives the bound of $53 = 2 + 102/2$ spheres mentioned in the introduction.

The pair (f, K) of the introduction is described in the remainder of this section. Fix a Delaunay star D^* with vertices at $0, v_1, v_2, \dots, v_n$. We fix an ordering on the vertices of each Delaunay star, considering two Delaunay stars distinct if they differ by a permutation of the indices of the vertices. Let $I = I(D^*)$ be the set of triples $I = \{(i, j, k)\}$ of integers such that $i < j < k$ and $(0, v_i, v_j, v_k)$ are the vertices of a Delaunay simplex S in D^* . The set of all Delaunay stars (endowed with fixed indexing on vertices) forms a topological space which we now describe. We require that the map $D^* \rightarrow I(D^*)$ be continuous (with respect to the discrete topology on the set of triples). In other words, stars with different indexing sets I are to belong to different connected components of the space. Given I we define $n = n(I)$ to be the largest integer coordinate of an element of I . On a given component (indexed by I) the Delaunay stars are in 1-1 correspondence with $v_1, \dots, v_n \in \mathbb{R}^3$ such that the following conditions hold. Let θ_{ijk} denote the circumcenter of the simplex with vertices $0, v_i, v_j, v_k$.

- (I) $2 \leq d(v_i, v_j), \quad \forall i < j \leq n.$
- (II) $2 \leq d(0, v_i) \leq 4, \quad \forall i \leq n.$
- (III) $d(0, \theta_{ijk}) \leq 2, \quad \forall (i, j, k) \in I.$ (In particular, the circumspheres never degenerate into planes.)
- (IV) $d(v_\ell, \theta_{ijk}) \geq d(0, \theta_{ijk}), \quad \forall \ell \leq n, \forall (i, j, k) \in I.$

The topology on the component indexed by I is determined by the condition that this bijection with a subset of \mathbb{R}^{3n} be a homeomorphism. When we wish to stress that we are considering a Delaunay star as a point in this space rather than as a union of Delaunay simplices, we refer to a star as an *abstract Delaunay star*. The space of all Delaunay stars is the space K of the introduction. The function f of the introduction is $\delta_{\text{oct}}/(1 - \sigma(D^*))$ where $\sigma(D^*) = 3\Gamma_{\text{oct}}(D^*)/(16\pi)$.

Appendix

Let Λ be a saturated packing. For $v \in \Lambda$ let $\text{Vor}(v)$ denote the Voronoi cell containing v . Then we obtain a compact bound (f, K) by setting $K =$ the space of all Voronoi cells contained in a ball of radius 2 (associated to saturated packings)

$$\varphi = \varphi_\Lambda, \quad \varphi: \Lambda \rightarrow K, \quad v \mapsto \text{Vor}(v), \quad f: K \rightarrow \mathbb{R}, \quad f(\text{Vor}(v)) = \frac{\text{vol}(B_1(0))}{\text{vol}(\text{Vor}(v))}.$$

Then no saturated packing has density exceeding $\sup_{\Lambda} f \circ \varphi$. This appendix justifies the claim made in the introduction that $\varphi(v) = \text{Vor}(v)$, $v \in \Lambda_{\text{fcc}}$ is not even a local maximum for f on K .

To show this we consider a curve in K connecting the cuboctahedron to the icosahedron. Their vertices are to lie on a sphere Σ of radius 2. Such a curve is described in [1]. We pair the vertices of the cuboctahedron into pairs (v_i, w_i) with $d(v_i, w_i) = 2\sqrt{2}$ as in the following diagram.

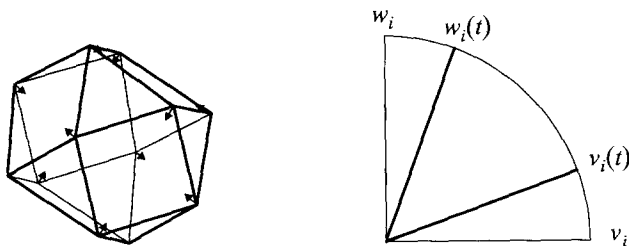


Fig. 4

Then $v_i, w_i \in \Sigma$ is such a pair we set

$$\begin{aligned} v_i(t) &= v_i \cos t + w_i \sin t \\ w_i(t) &= w_i \cos t + v_i \sin t \end{aligned} \quad i = 1, \dots, 6.$$

Then $t \mapsto \{v_i(t), w_i(t)\}_{i \leq 6}$ for $0 \leq t \leq t_{\max}$, describes a curve in K from the cuboctohedron to the icosahedron where t_{\max} is given by

$$(\cos(t_{\max}), \sin(t_{\max})) = \left(\sqrt{\frac{1}{2} + \frac{\sqrt{5}}{5}}, \sqrt{\frac{1}{2} - \frac{\sqrt{5}}{5}} \right).$$

Let Vor_t denote the Voronoi cell about 0 determined by placing spheres at the points $\{v_i(t), w_i(t)\}$.

A Mathematica calculation shows that

$$f(t) \stackrel{\text{def}}{=} \frac{\text{vol}(B_1(0))}{\text{vol}(\text{Vor}_t)} = \frac{-\sqrt{2}\pi \cos(t) (1 + 4\cos(t)^2 - 4\cos(t)^4 + 4\cos(t) \sin(t))}{6 (-3 + 2\cos(t)^2 - 4\cos(t) \sin(t))}.$$

The derivatives at $t=0, t_{\max}$ are $f'(0)=0$, $f'(t_{\max})=0$, and $f''(t_{\max}) < 0$.

We compare this to the bound based on the Delaunay decomposition. Let D_t^* denote the Delaunay star dual to Vor_t . Then D_t^* is in fact the convex hull of $\{v_i(t), w_i(t)\}$. Set

$$g(t) \stackrel{\text{def}}{=} \frac{\delta_{\text{oct}}}{1 - \Gamma_{\text{oct}}(D_t^*) / (4 \text{vol } B_1(0))}.$$

The graphs of $f(t)$ and $g(t)$ are illustrated.

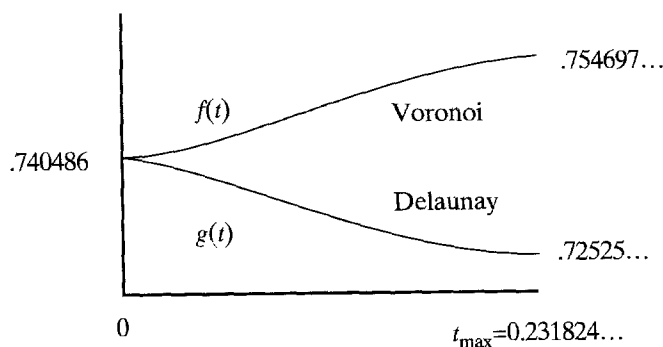


Fig. 5

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