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The sphere packing problem

Thomas C. Hales

Department of Mathematics, University of Chicago, IL 60637, United States

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Abstract

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The sphere packing problem asks whether any packing of spheres of equal radius in three dimensions has density exceeding that of the face-centered-cubic lattice packing (of density $\pi/\sqrt{18}$). This paper sketches a solution to this problem.

Keywords: Sphere packing; Delaunay triangulation; packing and covering; spherical geometry; Hilbert's problems; Voronoi cells.

1. Outline of method

We begin with a general discussion of the strategy of the proof that no packing of equal spheres in three dimensions has density exceeding $\pi/\sqrt{18}$. The density of any packing may be improved by adding spheres as long as there is sufficient room to do so. When there is no longer room to add additional spheres, we say that the packing is *saturated*. We assume that our packings are saturated. We take our spheres to be of radius 1. Thus in a saturated packing no point of space lies more than distance 2 from a sphere center. The sphere centers are called the *packing points*.

Every saturated packing gives rise to a decomposition of space into simplices called the *Delaunay decomposition*. The simplices are called *Delaunay simplices*. Each vertex of a simplex lies at a packing point. Every sphere (abstract sphere, not packing sphere) circumscribing a simplex has the property that none of the packing points lie in the interior of the sphere. In fact, this property is enough to completely determine the Delaunay decomposition except for certain degeneracies.

When all of the simplices sharing a common vertex are grouped together, the resulting polytope is called a *Delaunay star*. Thus each Delaunay star is the union of Delaunay simplices.

Correspondence to: Prof. T.C. Hales, Department of Mathematics, University of Chicago, 5734 S. University, Chicago, IL 60637, United States.

Each Delaunay simplex has four vertices, and consequently forms part of four distinct Delaunay stars. In other words, the union of all Delaunay stars cover Euclidean space four times over.

Without much difficulty one can make a list of properties that characterize the polytopes that may arise as the Delaunay star coming from the Delaunay decomposition of some saturated sphere packing. Such polytopes form the points of a compact topological space known as the *space of abstract Delaunay stars* and the points are called *abstract Delaunay stars* or simply *Delaunay stars*. As a matter of notation we write D^* for a Delaunay star and if v is the center of a packing sphere, we write $D^*(v)$ for the abstract Delaunay star formed by taking the Delaunay simplices which have v as a vertex. The vertex v is called the *center* of the star. We say that an edge of a simplex is a *spoke* of a star if one of its endpoints is the center of the star.

We relate the space of Delaunay stars to the density of sphere packings as follows. Start with the following simple objective function, called the *compression* of a star, on the space of abstract Delaunay stars

$$-\delta \operatorname{vol}(D^*) + \sigma(D^*).$$

Here δ may be any constant, $\operatorname{vol}(D^*)$ is defined as the volume of the Delaunay star D^* and $\sigma(D^*)$ is the volume of the region obtained by intersecting D^* with the union of balls of radius 1 placed at every vertex and the center of D^* . Let M be the maximum of this function on the space of abstract Delaunay stars. Then if v is any packing point,

$$-\delta \operatorname{vol}(D^*(v)) + \sigma(D^*(v)) \leq M.$$

Now sum this inequality over the points of a packing contained in a large finite container. The first term will be approximately -4δ times the volume of the container since the Delaunay stars will fill the container four times over, except near the boundary of the container. Similarly, the second term will be approximately four times the number of spheres in the container times the volume of a sphere. The right-hand side will be the number of spheres in the container times M . This is then an inequality relating the number of spheres in the container to the volume of the container, and in this elementary manner we obtain a bound on the density of spheres in the container. The constant obtained by replacing M by $-\delta \operatorname{vol}(D^*) + \sigma(D^*)$ is called the *effective density* of a Delaunay star. The effective density estimates the density that would be attained in a sphere packing in which every Delaunay star were identical to D^* .

Numerical studies, using $\delta = 0.72090\dots$, show that this method gives an extremely good numerical bound on density: $0.740873\dots$. However this numerical constant exceeds $\pi/\sqrt{18}$. The main purpose of this paper is to argue that by adding suitable correction terms to our original function we are able to sharpen the bound to $\pi/\sqrt{18}$.

We add two types of corrections. The first comes from the Voronoi decomposition. There is a second approach to the theory of sphere packings based on the Voronoi decomposition. If we associate to each packing point the set of all points which lie at least as close to that packing point as to any other, we obtain a set of points forming a convex polyhedron called the *Voronoi cell* about that point. The Voronoi cells for all packing points fill space and overlap only on their boundaries. This decomposition of space into convex polyhedra is called the *Voronoi decomposition*. The density of the sphere packing cannot exceed the greatest density attained in

a Voronoi cell. Thus the ratio of the volume of a sphere to the smallest possible Voronoi cell is a bound on the density of sphere packings.

Associated to each abstract Delaunay star is a dual Voronoi cell obtained by forming a Voronoi cell using the vertices of the Delaunay simplices associated to the star instead of packing points. This notion agrees with the usual definition of Voronoi cell when the abstract Delaunay star arises from a saturated sphere packing (since the vertices of simplices are then packing points). By adding to the function above a term proportional to the volume of the Voronoi cell we obtain improved bounds on the density. The amount of improvement depends on the constant of proportionality. With respect to a choice given below the numerical bound on packing density becomes $0.740755\dots$. The bound obtained by this interpolation is a weighted harmonic average of the effective densities obtained by the approaches of Delaunay and Voronoi. The method cannot give the bound $\pi/\sqrt{18}$. Further refinements are needed.

Further examination of numerical evidence shows that the abstract Delaunay stars that give effective densities larger than $\pi/\sqrt{18}$ all lie in a small neighborhood of a single abstract Delaunay star. This Delaunay star has the shape of a pentagonal prism, terminated on both ends by a pentagonal pyramid. The pentagonal cross-sections are not regular but one edge is stretched slightly to allow the tips of the pyramids and the ten vertices of the prism all to lie at distance 2 from a central point in the prism. The height of the prism and the other four edges of the pentagon also have length 2.

The question of whether any sphere packing has density greater than $\pi/\sqrt{18}$ then depends on whether a packing can be created which has such pentagonal-prism-dipyramid (PPDP) configurations in sufficient abundance to yield a packing better than the face-centered-cubic packing. The second type of correction term is designed to rule out the possibility of such pentagonal-prism-dipyramid packings. The feature of the pentagonal-prism-dipyramid that we exploit is that two of its edges have length $\frac{8}{9}\sqrt{6}$, somewhat greater than 2. This means that if this configuration is used in a packing, some neighboring Delaunay star will also have a simplex with a spoke greater than 2. When a star has a spoke of length more than 2, the effective density of the Delaunay star tends to be quite small. Thus the strategy of the proof is to show that whenever a pentagonal-prism-dipyramid configuration occurs, a neighboring Delaunay star necessarily has effective density considerably and sufficiently less than $\pi/\sqrt{18}$. Of course it is necessary to take into account the fact that there may be several pentagonal-prism-dipyramid Delaunay stars next to the same Delaunay star of low density. It is necessary to study these effects for all stars in an appropriate neighborhood of the pentagonal-prism-dipyramid.

All of these effects may be taken into account by adding two additional terms to the original objective function. One term is proportional to the length of the longest spoke of those shorter than $2\frac{1}{5}$. The other term is proportional to the length of the longest outer edge of those shorter than $2\frac{1}{5}$. We are able to make these correction terms linear in the length rather than some more complicated function of the length because — in the end — only very crude estimates are needed to rule out the possibility of a dense packing based on the pentagonal-prism-dipyramid.

With the pentagonal-prism-dipyramid safely excluded, the numerical evidence shows that there are only two local maxima of remaining interest. They correspond to the Delaunay stars for the face-centered-cubic and hexagonal-close-packings. Thus the numerical evidence may be interpreted as saying that the densest possible packings are those in which almost every packing point v has a Delaunay star $D^*(v)$ close to that of either the face-centered-cubic or hexagonal-close-packing.

Finally to obtain $\pi/\sqrt{18}$ as a bound on density, rather than a numerical approximation to $\pi/\sqrt{18}$, we carry out the required local analysis near the face-centered-cubic and hexagonal-close-pack stars to show that they are local maxima to our objective function and that the effective density predicted by the objective function is indeed $\pi/\sqrt{18}$.

The results we present provide a sketch rather than a complete rigorous mathematical proof in a carefully controlled way.

- Each unfinished step in the proof takes the form

Show that $\sup_K f < C$,

where K is an appropriate compact subspace of the space of Delaunay stars, f is a continuous function and C is an appropriate constant. In each case the data (f, K, C) are given explicitly.

- Each of the functions (f, K) has been studied systematically by numerical methods and in each case we produce a constant $C_0 < C$ such that the numerical maximum of f on K is at most C_0 .

- Each function satisfies the Lipschitz condition $|f(x) - f(y)| \leq M d(x, y)$ on K , so that each step could be established rigorously in finite time by checking that

$$f(x_i) \leq C_0, \quad i = 1, \dots, n,$$

for a suitable constant C_0 and suitable finite subset $\{x_i\} \subseteq K$. Here d is a metric on K .

Consequently, the results of this paper demonstrate numerically that no sphere packing in three dimensions has density exceeding $\pi/\sqrt{18}$. For the physicist, chemist and numerical analyst these results provide evidence for a fact long believed but never justified. For the mathematician, these results reduce the sphere packing problem to one that is mathematically trivial, but certainly not devoid of interest. The optimization problems we give are of the same nature and level of complexity as the problem of minimizing the volume of a Voronoi cell. This problem is not solved but has for some time been recognized as tractable. Thus I hope these results will give the needed encouragement to mathematicians to replace each of these optimization problems by a rigorous proof to achieve the complete solution of this outstanding problem of mathematics.

The remainder of this introduction gives an overview of a different approach to the sphere packing problem, due to Fejes Tóth, through Voronoi cells. The Delaunay star approach and the Voronoi cell approach are roughly dual to each other. As explained above, the ratio of the volume of a sphere to the smallest possible Voronoi cell is a bound on the density of sphere packings. The primary results of Fejes Tóth [2,3] on packings in three dimensions may be summarized as follows.

(1) [3, V.4] The volume V_n of a polyhedron with n faces and containing a unit sphere satisfies

$$V_n \geq (n-2)(3 \tan^2 \omega_n - 1) \sin(2\omega_n), \quad \omega_n = \frac{\pi n}{6(n-2)},$$

and if equality holds, the polyhedron is regular. Fejes Tóth gives an elegant two-paragraph proof of this inequality. This inequality immediately implies that any Voronoi cell with $n \leq 12$ faces has volume at least that of the regular dodecahedron. Here and elsewhere we mean the regular dodecahedron circumscribing the unit sphere.

(2) [2, II.4.5], [3, VII.2] Fix $\mu = -1 + (3(5 - 2\sqrt{5}))^{1/2} = 0.2584\dots$. Consider a convex polyhedron with n faces and containing the unit sphere. Suppose the faces have distances

$d_i = 1 + \epsilon_i$, $\epsilon_i \geq 0$, from the center of the sphere, indexed so that

$$0 \leq \epsilon_1 \leq \epsilon_2 \leq \cdots \leq \epsilon_l < \mu \leq \epsilon_{l+1} \leq \cdots \leq \epsilon_n.$$

If

$$\sum_{i=1}^l \epsilon_i > (l-12)\mu, \quad (*)$$

then the volume of the convex polyhedron exceeds the volume of a regular dodecahedron. Because of Fejes Tóth's truncation procedure, only the faces of distance $1 + \epsilon_i$ less than $1 + \mu$ matter in (*). For $l = 13$ the estimate of $\sum_1^{13} \epsilon_i$ should be viewed as an explicit estimate of the Gregory–Newton problem [1] which asserts that $\sum_1^{13} \epsilon_i > 0$. It was my failure to prove an inequality similar to (*) that led me to develop the new method explained in this paper. A proof of (*) would lead to the dodecahedral bound of $0.754\dots$ on sphere packings.

(3) [2, II.4.5], [3, VII.2] Fejes Tóth then sketched the following two-part approach to proving the bound $\pi/\sqrt{18}$ on sphere packings.

(3a) Show that at most 12 faces of a Voronoi cell come within distance $1 + \mu'$ for some explicit constant $\mu' > 0$.

(3b) For a given Voronoi cell of volume V_0 let V_1, \dots, V_j , $j \leq 12$, be the volumes of the Voronoi cells sharing a face within distance $1 + \mu'$. Show that

$$\frac{1}{12} \{V_1 + \cdots + V_j + (12-j)V_0\} \geq 4\sqrt{2}.$$

He gives some geometrical motivation, without proof, for (3a) and (3b). From (3a), (3b) the packing bound of $\pi/\sqrt{18}$ easily follows. In fact, to relate (3b) to packing densities it is enough to observe that the weighted regions represented by the left-hand side of the formula in (3b) cover space evenly. He concludes in summary, “Obwohl eine exakte Behandlung dieses Minimumproblems recht kompliziert zu sein scheint, kann sie keineswegs als hoffnungslos angesehen werden. Allerdings haben wir zur Lösung des Problems der dichtesten Kugelpackung ein prinzipiell durchführbares konkretes Programm angegeben, wodurch wir der Klärung des Problems einen Schritt nähergekommen sind”.

Hsiang [6,7] has worked to carry out the program of Fejes Tóth, using a different type of truncation, and of course different choices of constants. Despite reports to the contrary, Hsiang does not give a proof of the sphere packing problem. Also, a recent preprint of Muder [9] gives another approach to the problem of finding a Voronoi cell of minimum volume. Other results on packing, including bounds obtained by Rogers, Lindsey and Muder, are discussed in [1].

2. Some inequalities

This section gathers some elementary inequalities together. We let $\|\cdot\|$ be the Euclidean norm on \mathbb{R}^3 . Let $B_r(v)$ be the closed ball of radius r at v , $\partial B_r(v)$ its boundary.

Lemma 2.1. *Suppose that $\gamma_0, \dots, \gamma_n$ are constants such that $\gamma_i \geq \gamma_0$ and that r_1, \dots, r_n are positive constants such that*

$$\sum_{i=1}^n r_i < 1.$$

Set

$$\hat{\gamma}_i = \frac{1}{1+r_i} \gamma_i + \frac{r_i}{1+r_i} \gamma_0, \quad i > 0.$$

Then

$$\gamma_0 + \gamma_1 + \cdots + \gamma_n \leq (n+1) \sup_{1 \leq i \leq n} \hat{\gamma}_i.$$

Proof. Set $\hat{\gamma} = \sup_i \hat{\gamma}_i$. Clearly $\gamma_0 \leq \hat{\gamma}_i \leq \hat{\gamma}$. By definition, $\gamma_i = \hat{\gamma}_i + r_i(\hat{\gamma}_i - \gamma_0)$,

$$\begin{aligned} \gamma_0 + \cdots + \gamma_n &= \left\{ (1 - \sum r_i) \gamma_0 + \sum r_i \hat{\gamma}_i \right\} + \hat{\gamma}_1 + \cdots + \hat{\gamma}_n \\ &\leq \left\{ (1 - \sum r_i) \hat{\gamma} + \sum r_i \hat{\gamma} \right\} + \hat{\gamma} + \cdots + \hat{\gamma} = (n+1) \hat{\gamma}. \quad \square \end{aligned}$$

Lemma 2.2. Let v_1, \dots, v_n be points in \mathbb{R}^3 such that $2 \leq x_i \stackrel{\text{def}}{=} \|v_i\| < 2\sqrt{3}$, and $2 \leq \|v_i - v_j\|$ for all i, j . Set $r_i = \frac{1}{2}(1 - \cos(\arccos(\frac{1}{4}x_i) - \frac{1}{6}\pi))$. Then

$$\sum_{i=1}^n r_i < 1.$$

Proof. Set $a_i = 4\pi r_i = 2\pi(1 - \cos \theta_i)$, $\theta_i = \arccos(\frac{1}{4}x_i) - \frac{1}{6}\pi$. It is enough to interpret the constants a_i as areas of nonoverlapping convex regions on the surface of a unit sphere, for then certainly the total area will be less than 4π . For $v \in \mathbb{R}^3$, $\theta \in [0, \pi]$ let $C(\theta, v)$ be the cone of angle θ :

$$C(\theta, v) = \{w \in \mathbb{R}^3 \mid \|w\| \|v\| \cos \theta \leq w \cdot v\}.$$

Then $2\pi(1 - \cos \theta)$ gives the area of the spherical cap $C(\theta, v) \cap \partial B_1(0)$. Let B_i be the open ball of radius 1 centered at v_i , let $C^+(v_i)$ be the open cone over B_i :

$$C^+(v_i) = \{tw \mid w \in B_i, t > 0\},$$

and let $\bar{C}^+(v_i)$ be its closure. Note that $\bar{C}^+(v_i) = C(\phi_i, v_i)$ for $\phi_i = \arcsin(1/x_i) \leq \frac{1}{6}\pi$. If $x_i = 2$, then $\phi_i(x_i) = \theta_i(x_i)$. For $x_i \in [2, 2\sqrt{3}]$ we have

$$\frac{\partial(\phi_i - \theta_i)}{\partial x_i} = \frac{x_i^4 - 16}{x_i \sqrt{x_i^2 - 1} \sqrt{16 - x_i^2} (x_i \sqrt{x_i^2 - 1} + \sqrt{16 - x_i^2})} \geq 0.$$

Then $\phi_i \geq \theta_i$ and $C(\theta_i, v_i) \subseteq \bar{C}^+(v_i)$. Write $j < i$ if $\|v_j\| \leq \|v_i\|$ and $i \neq j$. Consider the smaller set $\tilde{C}^+(v_i) = C^+(v_i) \setminus \bigcup_{j < i} C^+(v_j)$ of rays which encounter B_i first. By construction the sets $\tilde{C}^+(v_i)$ are disjoint, so the lemma will follow if $C(\theta_i, v_i)$ lies in the closure of $\tilde{C}^+(v_i)$. Set $z = \|v_i - v_j\|$, $x = \|v_i\|$, $y = \|v_j\|$. Assume $j < i$ so that $y \leq x$. Then the angle between v_i and the boundary of $C^+(v_i)$ is

$$\arccos\left(\frac{x^2 + y^2 - z^2}{2xy}\right) - \arcsin\left(\frac{1}{y}\right) \geq \arccos\left(\frac{x^2 + y^2 - 4}{2xy}\right) - \arcsin\left(\frac{1}{y}\right).$$

Thus we are reduced to proving

$$f(x, y) \stackrel{\text{def}}{=} \arccos\left(\frac{x^2 + y^2 - 4}{2xy}\right) - \arcsin\left(\frac{1}{y}\right) - \arccos\left(\frac{1}{4}x\right) + \frac{1}{6}\pi \geq 0.$$

We have

$$\frac{\partial f}{\partial y} = \frac{y(x^2 - y^2)(8 + y^2 - x^2)}{ab(b + a(4 - x^2 + y^2))} = \frac{b - a(4 - x^2 + y^2)}{yab},$$

where

$$a = \sqrt{y^2 - 1}, \quad b = \sqrt{4x^2y^2 - (-4 + x^2 + y^2)^2}.$$

Either $b + a(4 - x^2 + y^2)$ or $b - a(4 - x^2 + y^2)$ is positive, and every other factor is positive on $2 \leq y \leq x \leq 2\sqrt{3}$. So $\partial f / \partial y \geq 0$, which implies $f(x, y) \geq f(x, 2) = 0$. \square

Set

$$r(x) = \frac{1}{2} \left(1 - \cos \left(\arccos \left(\frac{1}{4}x \right) - \frac{1}{6}\pi \right) \right),$$

$$r_+^{a,b}(x) = \frac{r(b) - r(a)}{b - a} (x - a) + r(a), \quad r_-^c(x) = r(c) + (x - c)r'(c).$$

Lemma 2.3. $r_-^c(x) \leq r(x) \leq r_+^{a,b}(x)$ for $2 \leq a \leq x \leq b < 4$, $a \leq c \leq b$.

Proof.

$$r''(x) = \frac{1}{64(1 - \frac{1}{16}x^2)^{3/2}} > 0.$$

By a second derivative test, the curve r lies between its tangent $r_-^c(x)$ and secant $r_+^{a,b}(x)$ approximations. \square

Lemma 2.4. Suppose that γ_0 and γ are negative functions on the interval (a, b) , where $2 \leq a \leq c \leq b \leq 4$. Let r , $r_+^{a,b}$, r_-^c be the functions given above. Then

$$\frac{\gamma + r\gamma_0}{1 + r} \leq \frac{\gamma + r_-^c\gamma_0}{1 + r_+^{a,b}}.$$

Proof. Use the definition of r and the previous lemma. It is best to replace r by $r_+^{a,b}$ first in the denominator. \square

Lemma 2.5. Suppose that γ_0 and γ are linear functions of x on $[a, b]$, $2 \leq a \leq c \leq b \leq 3$. Set

$$f(x) = f(x; a, b, c) = \frac{\gamma + r_-^c\gamma_0}{1 + r_+^{a,b}}.$$

Suppose that γ_0 is a strictly decreasing linear function. Then

$$\sup_{a \leq x \leq b} f = \max(f(a), f(b)).$$

Proof. Since γ_0 , γ , r_- , r_+ are all linear functions, $f(x)$ has the form

$$g(u) = A + Bu + \frac{C}{u},$$

with $u \stackrel{\text{def}}{=} 1 + r_+^{a,b}$ (a linear function of x) for some real constants A, B, C . Then

$$g'(u) = B - \frac{C}{u^2} = 0, \quad \text{when } u = \sqrt{\frac{C}{B}}, \quad \text{provided } BC > 0.$$

The negative square root is discarded because u is positive on the interval.

Thus f has at most one critical point in the interval (a, b) . Extend f to a rational function on \mathbb{R} . The pole of $f(x)$ is larger than b . As x tends to infinity, $f(x)$ is asymptotic to $K\gamma_0$, where

$$K = \frac{(a-b)r'(c)}{r(a)-r(b)}.$$

Since $r'(x)$ is increasing, $r'(c) \leq r'(3) < 0$. Also $(r(a)-r(b))/(a-b) \leq r'(b) \leq r'(3) < 0$. So $K > 0$. Thus $f(x)$ tends to $+\infty$ as $x \rightarrow -\infty$. It follows that the critical point in the interval (a, b) — if it exists — yields a local minimum. Therefore the maximum occurs at an endpoint of the interval. \square

3. Some packing bounds

Recall from [5] that a Delaunay star, or simply star, is the union of all Delaunay simplices in \mathbb{R}^3 sharing a common vertex v_0 , called the *center* of the star. The space of all Delaunay stars is compact with respect to a natural topology. When we consider a Delaunay star D^* as a point in an abstract topological space, we call its *geometric realization* a realization of the star as a union of simplices in \mathbb{R}^3 in such a way that its center v_0 is the origin in \mathbb{R}^3 . Such a realization is unique up to orthogonal transformation. However, when we consider a Delaunay star $D^* = D^*(v)$, associated to a concrete packing point $v \in \Lambda$ of a saturated packing Λ , we take its geometric realization to be the natural one centered at v with vertices lying in Λ . To give uniform notation, we let D_{CPS}^* denote any Delaunay star arising from the Delaunay decompositions of the face-centered-cubic or hexagonal-close-packings, and call them *close-packing stars*.

A *vertex* of a Delaunay star is defined to be a vertex, other than the center, of any of its constituent Delaunay simplices. An *edge* of a Delaunay star is defined to be an edge of any of its constituent simplices, provided both endpoints are vertices of the star — not the center. A *spoke* of a Delaunay star is defined as an edge of a constituent Delaunay star which has the center v_0 as one of its endpoints. Note that every Delaunay simplex belongs to four Delaunay stars, and a given edge of the simplex will be a spoke with respect to two of the stars and an edge with respect to the others.

In [5], the function $D^* \rightarrow \Gamma_0(D^*) = -\delta_{\text{oct}} \text{vol}(D^*) + \sigma(D^*)$, defined on the space of Delaunay stars, was defined. We have

$$\delta_{\text{oct}} = \frac{-3\pi + 12\arccos(1/\sqrt{3})}{\sqrt{8}},$$

$\text{vol}(D^*)$ = the volume of the Delaunay star,

$$\sigma(D^*) = \text{the volume of the spheres inside } D^* = \frac{4}{3}\pi + \sum_{i=1}^n \text{vol}(D^* \cap B_1(v_i)),$$

where v_1, \dots, v_n are the vertices of a geometric realization of D^* . We call $\Gamma_0(D^*)$ the *compression* of a Delaunay star. It is negative for Delaunay stars of density σ/vol less than the threshold δ_{oct} . For two stars of equal density above the threshold, the star of greater volume has greater compression. It is shown below that a bound on the density of sphere packings is given in terms of a linear fractional transformation of the compression.

As discussed in the introduction, the bound based on compression is not $\pi/\sqrt{18}$ but higher. We are forced to modify our definition and define a small perturbation of the function Γ_0 which will depend on three small parameters $\lambda_{\text{sp}}, \lambda_{\text{edge}}, \theta$ in \mathbb{R} . The perturbation used below may seem quite arbitrary; perhaps a short explanation will prove helpful. The bound given by compression is higher than $\pi/\sqrt{18}$ because of a spurious local maximum D_{PPDP}^* discussed below. As a first approximation, the correction term, which we call T for the moment, should have the following properties.

(1) T should be a function depending only on D^* , not on the surrounding Delaunay stars of a saturated packing.

(2) T should be sufficiently small at the spurious local maximum, so that the modified compression $\Gamma_0(D_{\text{PPDP}}^*) + T(D_{\text{PPDP}}^*)$ is less than the modified compression at a close-packing star D_{CPS}^* .

(3) T should be sufficiently small or well-behaved, so that no new spurious global maximum to the modified compression is introduced.

(4) T (or T plus a constant) should have a vanishingly small average when averaged over all Delaunay stars in an extremely large region of space.

Property (4) allows one to relate the modified compression $\Gamma_0 + T$ to the density of sphere packings. Many such correction terms could be constructed, perhaps far simpler than the one I introduce. I add one term proportional to the volume of the Voronoi cell dual to the Delaunay star. This term is perhaps completely unnecessary but it helped to sharpen the numerical results, so I retained it. Another correction term depends only on the lengths of the edges and spokes of the star D^* . In our case, it will not actually be necessary for us to verify formally these four properties, stated here only for motivation. Theorem 7.1 shows the precise relation of our compression to the bound $\pi/\sqrt{18}$.

The length of the longest spoke, among those of length at most $2\frac{1}{5}$, will be called the *spoke length* of a star. Similarly, the length of the longest edge, among those of length at most $2\frac{1}{5}$, will be called the *edge length* of a star. Since we are interested in discouraging Delaunay stars such as D_{PPDP}^* with positive edge length, we add a correction term which is a negative scalar times the edge length. Edges for one star are spokes for another, so by adding a positive scalar times the spoke length in a careful way the corrections will cancel sufficiently, when averaged over Delaunay stars in a large region of space, to obtain a packing bound.

Now let us give a more rigorous treatment of this discussion. The compact spaces K of the introduction are all subspaces of the space of abstract Delaunay stars Del^* defined in [5]. We adopt without further notice the terminology of [5]. We define a function on the space of Delaunay stars which depends linearly on three parameters $\lambda_{\text{sp}}, \lambda_{\text{edge}}, \theta$. Set

$$\begin{aligned} \Gamma(D^*, \lambda_{\text{sp}}, \lambda_{\text{edge}}, \theta) = & -\delta_{\text{oct}} \text{vol}(D^*) + \sigma(D^*) + \lambda_{\text{sp}} L_{\text{sp}}(D^*) \\ & + \lambda_{\text{edge}} L_{\text{edge}}(D^*) + \theta \Theta(D^*), \end{aligned}$$

where Θ , L_{sp} and L_{edge} are the following functions of a Delaunay star D^* .

Let $\Theta(D^*)$ be the volume of the Voronoi cell dual to D^* . Define the spoke-indexing set by

$$I_{\text{sp}}(D^*) = \{i \mid 2 \leq \|v_i(D^*)\| \leq 2\frac{1}{5}\} \subseteq \{1, \dots, n(D^*)\}.$$

Here the vertices of D^* are $v_i(D^*)$, $i = 1, \dots, n(D^*)$. Define the spoke length by

$$L_{\text{sp}}(D^*) = \begin{cases} \sup_{i \in I_{\text{sp}}} \|v_i(D^*)\|, & \text{if } I_{\text{sp}}(D^*) \neq \emptyset, \\ 2, & \text{if } I_{\text{sp}}(D^*) = \emptyset. \end{cases}$$

Define the edge-indexing set by

$$I_{\text{edge}}(D^*) = \{(i, j) \mid 2 \leq \|v_i(D^*) - v_j(D^*)\| \leq 2\frac{1}{5}, i, j \in I_{\text{sp}}\} \subseteq \{1, \dots, n(D^*)\}^2.$$

Define the edge length by

$$L_{\text{edge}}(D^*) = \begin{cases} \sup_{(i,j) \in I_{\text{edge}}} \|v_i(D^*) - v_j(D^*)\|, & \text{if } I_{\text{edge}}(D^*) \neq \emptyset, \\ 2, & \text{if } I_{\text{edge}}(D^*) = \emptyset. \end{cases}$$

By definition, $L_{\text{sp}}, L_{\text{edge}} \in [2, 2\frac{1}{5}]$. The functions f of the introduction are all equal to Γ for appropriate choices of parameters $\theta, \lambda_{\text{edge}}, \lambda_{\text{sp}}$. Define the compression by

$$\Gamma_\theta(D^*) = \Gamma(D^*, 0, 0, \theta).$$

We define

$$\rho_\theta(x) = \frac{\delta_{\text{oct}} - \frac{1}{4}\theta}{(1 - 3x/(16\pi))}.$$

We often omit the subscript θ and write $\Gamma(D^*)$, $\rho(x)$ when the context is clear. $\rho_\theta \Gamma_\theta$ is called the *effective density* for reasons made clear by the following lemma. In this paper $\rho_\theta \Gamma_\theta$ is always to be understood as a composition, not as a product. ρ_θ is the linear fractional transformation which converts the compression Γ_θ of a Delaunay star to a packing bound.

Lemma 3.1. *Suppose that Λ is a saturated packing such that for sufficiently large balls $B_M(0)$ of volume $V = \frac{4}{3}\pi M^3$ we have (using Landau's notation)*

$$\sum_{v \in \Lambda \cap B_M(0)} \Gamma_\theta(D^*(v)) \leq |\Lambda \cap B_M(0)| A + o(V),$$

with $A < \frac{16}{3}\pi$. Then the density of the packing Λ is at most $\rho_\theta(A)$.

Proof. By definition,

$$-\delta_{\text{oct}} \text{vol}(D^*) + \sigma(D^*) + \theta \Theta(D^*) = \Gamma_\theta(D^*).$$

Sum over the points in $\Lambda \cap B_M(0)$ to obtain

$$-4\delta_{\text{oct}}V + \frac{16}{3}\pi N + \theta V = \sum \Gamma_\theta(D^*) + o(V) \leq NA + o(V),$$

where $N = |\Lambda \cap B_M(0)|$. Divide by V and take the limit using the definition of density

$$\frac{4\pi N}{3V} = \delta + o(1),$$

to obtain

$$-4\delta_{\text{oct}} + 4\delta + \theta \leq \frac{A\delta 3}{4\pi}.$$

Solving for the density δ of the packing A : $\delta \leq \rho(A)$. Actually the density δ is defined as $\limsup \frac{4}{3}\pi N/V$, so that we should restrict M to lie in an appropriate unbounded subset of \mathbb{R}_+ . But this has no bearing on our argument. \square

If we take the limit of $\rho_\theta(\Gamma_\theta(D^*))$ as $\theta \rightarrow -\infty$, we obtain

$$\rho_{-\infty}\Gamma_{-\infty} = \frac{4\pi}{3\Theta}.$$

This is the effective density function for the classical approach to sphere packings based on Voronoi cells discussed in the introduction. On the other hand, $\rho_0\Gamma_0$ is the effective density function for the “pure” Delaunay approach which is studied in [5]. Any effective density is a weighted harmonic average of the effective densities of Voronoi and Delaunay.

Lemma 3.2.

$$\frac{1}{\rho_\theta\Gamma_\theta} = \frac{1-\lambda}{\rho_0\Gamma_0} + \frac{\lambda}{\rho_{-\infty}\Gamma_{-\infty}},$$

where $\lambda = -\theta/(4\delta_{\text{oct}} - \theta)$. In particular, if $\theta < 0$, $\rho_\theta\Gamma_\theta$ lies between $\rho_0\Gamma_0$ and $\rho_{-\infty}\Gamma_{-\infty}$.

Remark 3.3. The choice of $\theta = -\frac{12}{7}\delta_{\text{oct}}$ used in some sections of this paper is obtained by setting (somewhat arbitrarily) $\lambda = \frac{3}{10}$, $1-\lambda = \frac{7}{10}$. I imagine that other choices would work just as well provided that, for instance, $\rho_\theta\Gamma_\theta(D_{\text{icos}}^*)$ (the effective density of the regular icosahedron with dual dodecahedral Voronoi cell) is kept sufficiently small.

Proof of Lemma 3.2. Use $r_0 = \rho_0(\Gamma_0)$, $r_{-\infty} = \frac{4}{3}\pi/\Theta$, $\lambda = -\theta/(4\delta - \theta)$ to eliminate Γ_0 , Θ and θ from the equation $r_\theta = \rho_\theta(\Gamma_\theta + \theta\Theta)$. \square

Let D_{CPS}^* be any Delaunay star associated to the face-centered-cubic or hexagonal-close-packing.

Corollary 3.4. For any $\theta \neq 4\delta_{\text{oct}}$, we have

$$\rho_\theta(\Gamma_\theta(D_{\text{CPS}}^*)) = \frac{\pi}{\sqrt{18}}.$$

Proof. For $\theta \rightarrow -\infty$ this is immediate from the fact that all the Voronoi cells have the same volume, and the fact that the density of the packing is $\pi/\sqrt{18}$. For $\theta = 0$, this is proved in [5]. The general result follows from Lemma 3.2. \square

4. Patches

A counterexample D_{PPDP}^* shows that some stars have compression higher than the close-packing stars D_{CPS}^* . However, we wish to show that on the average, over a large region of space,

stars can be no more compressed than in the face-centered-cubic and hexagonal-close-packings. Call a Delaunay star *overcompressed* if its compression is greater than the close-packing compression $\Gamma_\theta(D_{\text{CPS}}^*)$, and call it *undercompressed* otherwise. Suppose, throughout this informal discussion, that if D^* is an overcompressed star in a saturated packing, then it is always possible to find a neighboring undercompressed star. This will be formalized below by a map ϕ from the overcompressed stars to undercompressed ones. We will want to claim that a given undercompressed star, together with all the overcompressed ones associated to it by ϕ , will have an average compression less than the close-packing compression $\Gamma_\theta(D_{\text{CPS}}^*)$.

It initially appears that this method will force us to compute averages over a large number of Delaunay stars. This must be avoided. By a careful choice of weights r_i and using Lemma 2.1, we replace the average over a large number of Delaunay stars by a large number of weighted averages between overcompressed stars and their associated undercompressed stars.

If certain conditions are met, we may replace this weighted average by a simple bound. Suppose a given overcompressed star D_+^* has a large edge length. We will arrange the choice of ϕ so that the associated undercompressed star D_-^* has spoke length at least as great as the edge length of D_+^* . We bound the weighted average of two Delaunay stars through two different constrained maximization problems: first maximize the compression of D_+^* subject to a given edge length, and then maximize the compression of D_-^* subject to a given inequality on spoke length. The bound on the weighted average will then be the weighted average of the separate maxima. If this latter weighted average is smaller than the close-packing compression $\Gamma_\theta(D_{\text{CPS}}^*)$, the argument is complete.

A *patch*, defined precisely below, will formalize the discussion of the previous paragraphs. In brief, a patch is a set of Delaunay stars for which all of the assumptions of the previous paragraphs are valid. Theorem 4.2 will assert that if every overcompressed star belongs to a patch, then no packing has density above $\pi/\sqrt{18}$. We define a patch in such a way that undercompressed stars automatically belong to a patch, called the *principal patch*. Let us summarize the assumptions made above. We want an overcompressed star to have an edge in the range $[2, 2\frac{1}{5}]$ (P8). We want the weighted average of the maxima to be less than the close-packing compression (P7). Every overcompressed star should be a neighbor to an undercompressed one (P6). The maximum over all Delaunay stars, constrained by spoke length, should be sufficiently small (P3), (P4). The maximum compression over all overcompressed stars, constrained by edge length, should be sufficiently small (P1). Finally we discourage edge length and encourage spoke length (P5). Notice that (P1) and (P3) may be viewed either as families of constrained maximization problems for Γ_θ or as single maximization problems for a small perturbation of Γ_θ .

Now we turn to the formal definition. Let $\Gamma_{\text{CPS}} = \rho_\theta^{-1}(\pi/\sqrt{18}) = \Gamma_\theta(D_{\text{CPS}}^*)$ be the close-packing compression. Throughout this section θ is taken to be a fixed constant. The subscripts θ on Γ_θ and ρ_θ will be dropped.

Let Del^* be a compact set of Delaunay stars. We say that a compact subset C of Del^* is a *patch* if there exist real numbers λ_{edge} , Γ_{edge} , λ_{sp} , Γ_{sp} , L_{\min} , L_{\max} such that the following conditions hold. The function $r(x)$ is defined in Section 2.

Edge length perturbation bound:

$$\Gamma(D^*) + \lambda_{\text{edge}} L_{\text{edge}}(D^*) \leq \Gamma_{\text{edge}}, \quad \text{on } C. \quad (\text{P1})$$

Edge length range:

$$L_{\min} \leq L_{\text{edge}}(D^*) \leq L_{\max}, \quad \text{on } C. \quad (\text{P2})$$

Spoke length perturbation bounds:

$$\Gamma(D^*) + \lambda_{\text{sp}} L_{\text{sp}}(D^*) \leq \Gamma_{\text{sp}}, \quad \text{on } \{D^* \in \text{Del}^* \mid L_{\min} \leq L_{\text{sp}}(D^*) \leq L_{\max}\}, \quad (\text{P3})$$

$$\Gamma(D^*) + \lambda_{\text{sp}} L_{\max} \leq \Gamma_{\text{sp}}, \quad \text{on } \{D^* \in \text{Del}^* \mid L_{\max} < L_{\text{sp}}(D^*) \leq 2\frac{1}{5}\}. \quad (\text{P4})$$

Relations between constants:

$$\lambda_{\text{edge}} \leq 0 \leq \lambda_{\text{sp}}, \quad (\text{P5})$$

$$\min(\Gamma_{\text{edge}} - \lambda_{\text{edge}} L_{\max}, \Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\min}) \leq \Gamma_{\text{CPS}}. \quad (\text{P6})$$

Relation to weighted averages:

$$\min\left(\Gamma_{\text{edge}} - \lambda_{\text{edge}} x, \frac{(\Gamma_{\text{edge}} - \lambda_{\text{edge}} x) + r(x)(\Gamma_{\text{sp}} - \lambda_{\text{sp}} x)}{1 + r(x)}\right) \leq \Gamma_{\text{CPS}},$$

for $L_{\min} \leq x \leq L_{\max}$. (P7)

$$\text{if } D^* \in C, \Gamma(D^*) > \Gamma_{\text{CPS}}, \quad \text{then } I_{\text{edge}}(D^*) \neq \emptyset. \quad (\text{P8})$$

It is important to note that (P3) and (P4) give conditions on all stars, not just on C . (P1), (P2), (P8) give conditions on C . (P5)–(P7) give conditions on the choice of constants.

Example 4.1 (*principal patch*). Set $C = \{D^* \in \text{Del}^* \mid \Gamma(D^*) \leq \Gamma_{\text{CPS}}\}$, $L_{\min} = \inf_{D^* \in C} L_{\text{edge}}(D^*)$, $L_{\max} = \sup_{D^* \in C} L_{\text{edge}}(D^*)$, $\lambda_{\text{edge}} = \lambda_{\text{sp}} = 0$, $\Gamma_{\text{edge}} = \Gamma_{\text{CPS}}$, $\Gamma_{\text{sp}} = \sup_{D^* \in \text{Del}^*} \Gamma(D^*)$. Then this data defines a patch C called the *principal patch*.

We say that $v \in \Lambda$ is *overcompressed* or *undercompressed*, if the corresponding star $D^*(v)$ is.

Theorem 4.2. *Suppose that every overcompressed Delaunay star belongs to a patch. Then any saturated sphere packing Λ has density at most $\pi/\sqrt{18}$.*

Proof. We choose a map $\phi: \Lambda \rightarrow \Lambda$ as follows. If v is undercompressed, set $\phi(v) = v$. Otherwise, let (i_0, j_0) be vertices in I_{sp} such that $\|v_{i_0}(D^*(v)) - v_{j_0}(D^*(v))\| = L_{\text{edge}}(D^*)$. Such a pair (i_0, j_0) exists by (P8). Then set $\phi(v) = v_{i_0}(D^*(v)) \in \Lambda$. We need a lemma to complete the proof.

Lemma 4.3. *Under the conditions of Theorem 4.2, $v' = \phi(v)$ is undercompressed for all $v \in \Lambda$.*

Proof. If v is undercompressed, then $\phi(v) = v = v'$ and the result follows. Now assume that v is overcompressed. By assumption $D^* = D^*(v)$ belongs to a patch C . We use the constants λ_{sp} , λ_{edge} , Γ_{sp} , Γ_{edge} , etc. defined for this patch. If $\Gamma_{\text{edge}} - \lambda_{\text{edge}} L_{\max} \leq \Gamma_{\text{CPS}}$, then

$$\Gamma(D^*) \leq \Gamma_{\text{edge}} - \lambda_{\text{edge}} L_{\text{edge}}(D^*) \leq \Gamma_{\text{edge}} - \lambda_{\text{edge}} L_{\max} \leq \Gamma_{\text{CPS}},$$

and we have a contradiction. By (P6) we may assume $\Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\min} \leq \Gamma_{\text{CPS}}$. By construction

$L_{\text{edge}}(D^*(v)) = \|v_{i_0}(D^*(v)) - v_{j_0}(D^*(v))\|$ is the length of a spoke of $v' = v_{i_0}(D^*(v))$. So $L_{\text{sp}}(D^*(v')) \geq L_{\text{edge}}(D^*(v)) \geq L_{\min}$. Then by (P3), (P4), which hold for all Delaunay stars,

$$\begin{aligned} \Gamma(D^*(v')) &\leq \begin{cases} \Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\text{sp}}(D^*(v')), & \text{case(P3),} \\ \Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\max}, & \text{case(P4),} \end{cases} \\ &\leq \Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\min} \leq \Gamma_{\text{CPS}}. \quad \square \text{ (Lemma 4.3)} \end{aligned}$$

Now we resume the proof of Theorem 4.2. We have

$$\sum_{v \in \Lambda \cap B_M(0)} \Gamma(D^*(v)) = \sum_{v' \in \phi(\Lambda) \cap B_M(0)} \sum_{v \in \phi^{-1}(v')} \Gamma(D^*(v)) + o(V).$$

In the light of Lemma 3.1, to complete the proof it is enough to show that

$$\sum_{v \in \phi^{-1}(v')} \Gamma(D^*(v)) \leq |\phi^{-1}(v')| \Gamma_{\text{CPS}}.$$

Suppose first that $|\phi^{-1}(v')| = 1$. By the previous lemma, $\{v'\} = \phi^{-1}(v')$. Then v' is undercompressed, and the result follows. If $|\phi^{-1}(v')| > 1$, set $\phi^{-1}(v') = \{v', v_1, \dots, v_n\}$.

Fix i and the constants $\lambda_{\text{sp}}, \Gamma_{\text{sp}}$, etc. for a patch containing v_i . We have $\phi(v_i) \neq v_i$ and (P1) gives

$$\Gamma_{\text{CPS}} < \Gamma(D^*(v_i)) \leq \Gamma_{\text{edge}} - \lambda_{\text{edge}} L_{\text{edge}}(D^*(v_i)) \leq \Gamma_{\text{edge}} - \lambda_{\text{edge}} L_{\max}.$$

So by (P6), $\Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\min} \leq \Gamma_{\text{CPS}}$. The spoke length $L_{\text{sp}}(D^*(v_i))$ does not lie in the interval $[L_{\min}, L_{\max}]$, for otherwise by (P3) we have the contradiction

$$\Gamma_{\text{CPS}} < \Gamma(D^*(v_i)) \leq \Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\text{sp}}(D^*(v_i)) \leq \Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\min} \leq \Gamma_{\text{CPS}}.$$

Similarly $L_{\text{sp}}(D^*(v_i))$ is not in the interval $[L_{\max}, 2\frac{1}{5}]$, for (P4) would then give the contradiction

$$\Gamma_{\text{CPS}} < \Gamma(D^*(v_i)) \leq \Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\max} \leq \Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\min} \leq \Gamma_{\text{CPS}}.$$

Set $x_i = \|v_i - v'\|$. By the definition of the indexing set I_{edge} for the edge length, we have $x_i \leq 2\frac{1}{5}$, and so by the definition of spoke length L_{sp} we also have $x_i \leq L_{\text{sp}}(D^*(v_i))$. Setting $h_i = L_{\text{edge}}(D^*(v_i))$, we have $x_i \leq L_{\text{sp}}(D^*(v_i)) < L_{\min} \leq L_{\text{edge}}(D^*(v_i)) = h_i$. Now as i varies, the vectors $v_i - v'$ and the constants x_i satisfy the conditions of Lemma 2.2 so that $\sum r(x_i) < 1$. But r is decreasing on $[2, 3]$ so $x_i \leq h_i$ gives $\sum r(h_i) \leq \sum r(x_i) < 1$.

Now by Lemma 2.1 we have

$$\begin{aligned} \sum_{v \in \phi^{-1}(v')} \Gamma(D^*(v)) &\leq |\phi^{-1}(v')| \max_i \frac{\Gamma(D^*(v_i)) + r(h_i) \Gamma(D^*(v'))}{1 + r(h_i)}, \\ h_i &= L_{\text{edge}}(D^*(v_i)). \end{aligned}$$

Again we fix v_i and a patch containing v_i and constants for the patch $\lambda_{\text{sp}}, \Gamma_{\text{sp}}$, etc. We drop the subscript i . Notice that the proof of Lemma 4.3 shows that $L_{\text{sp}}(D^*(v')) \geq h$. Also $\Gamma_{\text{edge}} - \lambda_{\text{edge}} h > \Gamma_{\text{CPS}}$, for otherwise (P1) would give $\Gamma(D^*(v)) \leq \Gamma_{\text{CPS}}$, which would imply $\phi(v) = v = v'$. By (P3) and (P4),

$$\Gamma(D^*(v')) \leq \Gamma_{\text{sp}} - \lambda_{\text{sp}} \min(L_{\max}, L_{\text{sp}}(D^*(v'))) \leq \Gamma_{\text{sp}} - \lambda_{\text{sp}} h.$$

So by (P7),

$$\frac{\Gamma(D^*(v)) + r(h)\Gamma(D^*(v'))}{1 + r(h)} \leq \frac{\Gamma_{\text{cdgc}} - \lambda_{\text{cdgc}}h + r(h)(\Gamma_{\text{sp}} - \lambda_{\text{sp}}h)}{1 + r(h)} \leq \Gamma_{\text{CPS}}.$$

□ (Theorem 4.2)

5. The face-centered-cubic and hexagonal-close-packings

Let D_{CPS}^* denote any star arising in the Delaunay decomposition of a face-centered-cubic or hexagonal-close-packing. This section analyzes D_{CPS}^* in more detail. We have already seen that the effective density of these configurations is exactly $\pi/\sqrt{18}$. This section will give a proof of the following theorem.

Theorem 5.1. *If $\theta \leq 0$, then D_{CPS}^* is a local maximum to the effective density function $\rho_\theta \Gamma_\theta$.*

Remark 5.2. Some remarks on the coordinates and analyticity of Γ_θ will be useful. Fix a component of Del_I^* of Del^* , the space of Delaunay stars. By the definition of a component [5], every star has a fixed number of vertices v_1, \dots, v_n and the Delaunay simplicial decomposition is independent of the star in Del_I^* . More precisely, this means that there is an indexing set of triples $I = \{(i, j, k)\} \subseteq \{1, \dots, n\}^3$ with the property that $(0, v_i, v_j, v_k)$ forms a Delaunay simplex if and only if $(i, j, k) \in I$. Then the component embeds into \mathbb{R}^{3n} by sending a star to its vertices (v_1, \dots, v_n) , and this gives coordinates on Del_I^* . Now fix a point $p \in \text{Del}_I^*$ such that $\det(v_i, v_j, v_k) \neq 0$, $\forall (i, j, k) \in I$, and a neighborhood $p \in U \subseteq \mathbb{R}^{3n}$ on which $\|v_i\| > 0$, $i = 1, \dots, n$ and $\det(v_i, v_j, v_k) \neq 0$, $\forall (i, j, k) \in I$. Then Γ_θ extends analytically to U , as is easily seen by checking individual terms. For example, the volume $\text{vol}(D^*)$ is a linear combination of the determinants $\det(v_i, v_j, v_k)$, $(i, j, k) \in I$. (Notice that these determinants, by assumption, have fixed signs on U). The solid angles, used to compute $\sigma(D^*)$, depend analytically on v_i, v_j, v_k whenever $(0, v_i, v_j, v_k)$ are not coplanar. This just expresses the fact that angles in the range $0 < \psi < \pi$ depend analytically on the lengths of the sides of a triangle in either Euclidean or spherical geometry. Finally, the vertices of the Voronoi cell will be points equidistant from the four points $(0, v_i, v_j, v_k)$, $(i, j, k) \in I$. These vertices depend analytically on (v_i, v_j, v_k) when $0, v_i, v_j, v_k$ are not coplanar. In fact, the vertex w equidistant from $(0, v_i, v_j, v_k)$ satisfies the system of equations $\|w - v_l\|^2 = \|w\|^2$ or $w \cdot v_l = \frac{1}{2}v_l^2$, for $l = i, j, k$, a system with determinant $\det(v_i, v_j, v_k)$. Note that on a given component, determined by I , the Voronoi cell has by assumption a fixed combinatorial structure.

Proof of Theorem 5.1. Since $\rho_\theta(x)$ is an increasing function of x , it is enough to consider Γ_θ .

We have proved in [5], that D_{CPS}^* is a local maximum to Γ_0 ($\theta = 0$). The method of proof is to embed a neighborhood of these two stars into Euclidean space of sufficiently high dimension. One finds that the space of Delaunay stars near D_{CPS}^* may be approximated to first order by a cone with vertex D_{CPS}^* defined by the intersection of a finite number of closed half-spaces. We then extend Γ_0 to an analytic function on a Euclidean neighborhood of D_{CPS}^* and give an exact

expression for the gradient of Γ_0 at D_{CPS}^* . We then check that the gradient is strictly negative in the directions leading into the cone of Delaunay stars. See [5] for details.

We begin with the case that D_{CPS}^* has exactly twelve vertices. By Remark 5.2 on analyticity, we may also extend Θ to a function that is analytic in a Euclidean neighborhood of D_{CPS}^* . Our claim will follow if we prove that the gradient of Θ is nonnegative in the directions leading into the cone of Delaunay stars; for then $\Gamma_\theta = \Gamma_0 + \theta\Theta$ with $\theta < 0$ will have a strictly negative gradient in the same directions.

Let T_0 be a regular tetrahedron whose edges have length 2 with one vertex fixed at the origin. Varying the other vertices v_1, v_2, v_3 , we have six local coordinates which determine a tetrahedron T near T_0 (up to rotation). We pick these coordinates to be $x_i = \|v_i\|$, $y_i = \|v_{i-1} - v_{i+1}\|$, $i = 1, 2, 3$ (indices modulo 3). Let $\text{Vor}(D^*)$ be the Voronoi cell attached to D^* so that $\Theta = \text{vol} \circ \text{Vor}$. Set $\Theta_1 = \text{vol}(T \cap \text{Vor}(D^*))$ whenever T coincides with a Delaunay simplex of D^* . Θ_1 is then an analytic function of the local coordinates of T near T_0 . Lemma 5.4(a) shows that at T_0 ,

$$12 \, d\Theta_1 = -\frac{1}{18}\sqrt{2} (dx_1 + dx_2 + dx_3) + \frac{19}{18}\sqrt{2} (dy_1 + dy_2 + dy_3).$$

Set $A_1 = 3 \, \text{vol}(B_1(0) \cap T)$ and consider it an analytic function of the coordinates of T near T_0 . We find by Lemma 5.3(a) that at T_0 ,

$$dA_1 = \frac{1}{6}\sqrt{2} (-dx_1 - dx_2 - dx_3 + dy_1 + dy_2 + dy_3).$$

The condition for T to be a Delaunay simplex includes the conditions $x_i \geq 2$, $y_i \geq 2$, $i = 1, 2, 3$.

Let D_0 be half an octahedron, or square pyramid, with apex at the origin and edges of length 2. We consider D_0 as the union of two simplices divided by the plane through the origin and two opposite vertices v_1 and v_3 . Again we may let D be a nearby pair of simplices sharing the face $[0, v_1, v_3]$ with apex at the origin. We let v_1, v_2, v_3, v_4 be the vertices of the configuration. Set $z = \|v_1 - v_3\|$, $y_i = \|v_i - v_{i+1}\|$, $x_i = \|v_i\|$, $i = 1, 2, 3, 4$ (indices modulo 4). As in the preceding paragraph set $\Theta_2 = \text{vol}(D \cap \text{Vor}(D^*))$ for any Delaunay star D^* with two Delaunay stars equal to the two simplices constituting D . Lemma 5.4(b), after accounting for the conflict in notation, gives the differential evaluated at D_0 to be

$$12 \, d\Theta_2 = -\frac{4}{9}\sqrt{2} (dx_1 + dx_2 + dx_3 + dx_4) + \frac{22}{9}\sqrt{2} (dy_1 + dy_2 + dy_3 + dy_4).$$

This statement has combined the results of Lemma 5.4(b) for two simplices S_1, S_2 . Also Lemma 5.4 assumes that the Voronoi vertices w_1, w_2 for S_1, S_2 lie in the cones \hat{S}_1, \hat{S}_2 , respectively. But by the analyticity of this volume (Remark 5.2) the formula holds whenever both w_1 and w_2 lie in the union of the cones $\hat{S}_1 \cup \hat{S}_2$. This always holds for sufficiently small perturbations.

Set $A_2 = 3 \, \text{vol}(B_1(0) \cap D)$, considered as an analytic function near D_0 . Again we find, using Lemma 5.3(b) twice, the partial derivatives at D_0 to be

$$dA_2 = \frac{1}{3}\sqrt{2} (dy_1 + dy_2 + dy_3 + dy_4 - dx_1 - dx_2 - dx_3 - dx_4).$$

Given D^* near D_{CPS}^* , there are eight tetrahedra near T_0 . Let $x_1^j, x_2^j, x_3^j, y_1^j, y_2^j, y_3^j$, $j = 1, \dots, 8$, be the variables given above for each of these. Set $s_1 = \sum_{i,j} (x_i^j - 2)$, $s_2 = \sum_{i,j} (y_i^j - 2)$. Similarly there are six half-octahedra near D_0 . Let $x_1^j, x_2^j, x_3^j, x_4^j, y_1^j, y_2^j, y_3^j, y_4^j, z^j$, $j = 1, \dots, 6$, be the variables given for each of these. Set $s_3 = \sum_{i,j} (x_i^j - 2)$, $s_4 = \sum_{i,j} (y_i^j - 2)$. Then the total of all the A_i 's for these eight tetrahedra and six half-octahedra must be the area of a sphere 4π . This gives, by the differentials above, the first-order condition for s_i infinitesimally small:

$$0 = -\frac{1}{6}\sqrt{2} (s_1 - s_2 + 2s_3 - 2s_4).$$

The change in 12Θ , as infinitesimals s_i vary, is given to first order by

$$\frac{1}{18}\sqrt{2}(-s_1 + 19s_2 - 8s_3 + 44s_4).$$

Our problem then becomes of minimizing this expression subject to the constraints $s_i \geq 0$, and the above linear constraint. Fix $s = s_1 + 2s_3 = s_2 + 2s_4 \geq 0$. Then

$$\min_{s_2 + 2s_4 = s, s_i \geq 0} (19s_2 + 44s_4) = 19s, \quad \max_{s_1 + 2s_3 = s, s_i \geq 0} (s_1 + 8s_3) = 4s;$$

so

$$\frac{1}{18}\sqrt{2}(-s_1 + 19s_2 - 8s_3 + 44s_4) \geq \frac{1}{18}\sqrt{2}(19s - 4s) = \frac{5}{6}\sqrt{2}s.$$

Thus the minimum is zero and this occurs only if $s_i = 0$, $1 \leq i \leq 4$. This completes the proof of Theorem 5.1 in the case that D_{CPS}^* has exactly twelve vertices.

Now we drop the assumption that D_{CPS}^* has exactly twelve vertices. Let D_{CPS}^* be any close-packing star and let D^* be a nearby star. The Voronoi cell of D_{CPS}^* is identical to one just considered. In [5] we had to allow for the possibility of several different types of Delaunay decomposition of a regular octahedron. This is because different decompositions give rise to different Delaunay stars. However, no matter how the Delaunay decomposition for D_{CPS}^* is chosen, the Voronoi cell is the same. In a small neighborhood of D_{CPS}^* the effect of these different choices is at worst to cut off a small tip from an extreme point of the Voronoi cell. Intuitively, this will not affect the volume of a Voronoi cell to the first order. To prove this rigorously it is enough to place every vertex of the small tip in a ball of radius $C|t|$ centered at the center of the octahedron D_0 , where C is a constant and t is a parameter for an infinitesimal deformation of the star, for this shows the volume of the tip to be of third order. This is proved in Lemma 5.5. This completes the proof. \square

The following three lemmas were used in the proof of Theorem 5.1.

Lemma 5.3. *Let A be the solid angle at the origin of a tetrahedron with vertex at the origin and with sides of length $x_1, x_2, x_3, y_1, y_2, y_3$, where x_1, x_2, x_3 are the lengths of sides meeting at the vertex at the origin. Then the differential dA of A , considered as a function of x_i, y_i evaluates to*

$$(a) \quad dA = \frac{1}{6}\sqrt{2}(dy_1 + dy_2 + dy_3 - dx_1 - dx_2 - dx_3),$$

when $x_1 = x_2 = x_3 = y_1 = y_2 = y_3 = 2$, and

$$(b) \quad dA = \frac{1}{3}\sqrt{2}(dy_1 + dy_2 - \frac{1}{2}dx_1 - \frac{1}{2}dx_2 - dx_3),$$

when $x_1 = x_2 = x_3 = y_1 = y_2 = 2$, $y_3 = 2\sqrt{2}$.

Proof. Let x_3 be the length of the edge not incident with the edge of length y_3 . By symmetry $\partial A / \partial x_1$ equals $\partial A / \partial x_2$ and $\partial A / \partial y_1$ equals $\partial A / \partial y_2$ when these derivatives are evaluated at either of the values in (a) or (b). Thus it is enough to consider the case $x = x_1 = x_2$, $y = y_1 = y_2$. In this case the spherical triangle giving the solid angle is isosceles with angles denoted ϕ, ϕ, ψ . The solid angle is $A = 2\phi + \psi - \pi$. If the spherical lengths of the sides of this spherical triangle are denoted t, t, u , then by the spherical law of cosines:

$$\cos \psi = \frac{\cos u - \cos^2 t}{\sin^2 t}, \quad \cos \phi = \frac{\cos t - \cos t \cos u}{\sin t \sin u}.$$

Also by the Euclidean law of cosines, the angles t and u are related to the tetrahedron's edge lengths by

$$y^2 = x^2 + x_3^2 - 2xx_3 \cos t, \quad y_3^2 = 2x^2 - 2x^2 \cos u.$$

We take the differentials of each of these relations:

$$\begin{aligned} dA &= 2 d\phi + d\psi, \\ -\sin \psi d\psi &= \frac{-\sin u du}{\sin^2 t} + \frac{2 \cos t (1 - \cos u) dt}{\sin^3 t}, \\ -\sin \phi d\phi &= \frac{(\cos u - 1) dt}{\sin^2 t \sin u} + \frac{\cos t (1 - \cos u) du}{\sin t \sin^2 u}, \\ y dy &= (x - x_3 \cos t) dx + (x_3 - x \cos t) dx_3 + xx_3 \sin t dt, \\ y_3 dy_3 &= 2x(1 - \cos u) dx + x^2 \sin u du. \end{aligned}$$

In case (a), the data $x = x_1 = x_2 = x_3 = y = y_1 = y_2 = y_3 = 2$ gives $t = u = \frac{1}{3}\pi$, $\cos \psi = \frac{1}{3}$, $\cos \phi = \frac{1}{3}$, so that these differentials evaluate to

$$\begin{aligned} -\frac{2}{3}\sqrt{2} d\psi &= -\frac{2}{3}\sqrt{3} du + \frac{4}{9}\sqrt{3} dt, & -\frac{2}{3}\sqrt{2} d\phi &= -\frac{4}{9}\sqrt{3} dt + \frac{2}{9}\sqrt{3} du, \\ 2 dy &= dx + dx_3 + 2\sqrt{3} dt, & 2 dy_3 &= 2 dx + 2\sqrt{3} du. \end{aligned}$$

We eliminate $d\phi$, $d\psi$, dt , du from these linear relations and use $2dx = dx_1 + dx_2$, $2dy = dy_1 + dy_2$ to obtain (a).

In case (b), the data $x = x_1 = x_2 = x_3 = y = y_1 = y_2 = y_3/\sqrt{2} = 2$ gives $t = \frac{1}{3}\pi$, $u = \frac{1}{2}\pi$, $\cos \psi = -\frac{1}{3}$, $\cos \phi = 1/\sqrt{3}$. The differentials given above evaluate to

$$\begin{aligned} -\frac{2}{3}\sqrt{2} d\psi &= -\frac{4}{3} du + \frac{8}{9}\sqrt{3} dt, & -\frac{1}{3}\sqrt{6} d\phi &= -\frac{4}{3} dt + \frac{1}{3}\sqrt{3} du, \\ 2 dy &= dx + dx_3 + 2\sqrt{3} dt, & 2 dy_3 &= 4 dx + 4 du. \end{aligned}$$

We eliminate $d\phi$, $d\psi$, dt , du from these linear relations to obtain (b). \square

We continue to use the notation from Lemma 5.3, and the initial data for x_i and y_i from part (a) or (b) of the lemma. Pick coordinates so that the vertices of the tetrahedron are v_1, v_2, v_3 and the origin, where the lengths of v_1, v_2 and v_3 are x_1, x_2, x_3 respectively. Assume that the tetrahedron S has a circumcenter w lying in the cone \hat{S} at the origin over S . Complete S to a Delaunay star D^* with S as a constituent simplex, which we assume to be a small neighborhood of a close-packing star D_{CPS}^* . Let B denote the volume of the intersection of the cone \hat{S} with the Voronoi cell attached to D^* .

Lemma 5.4. *Under the conditions above, in case (a) the differential is*

$$12 dB = -\frac{1}{9\sqrt{2}}(dx_1 + dx_2 + dx_3) + \frac{19}{9\sqrt{2}}(dy_1 + dy_2 + dy_3),$$

at $x_1 = x_2 = x_3 = y_1 = y_2 = y_3 = 2$, and in case (b)

$$12 dB = -\frac{2}{9}\sqrt{2}(dx_1 + dx_2 + 2 dx_3) + \frac{22}{9}\sqrt{2}(dy_1 + dy_2),$$

at $x_1 = x_2 = x_3 = y_1 = y_2 = y_3/\sqrt{2} = 2$.

Proof. Under the assumptions above, B is the volume of the convex hull of the points $0, w, \frac{1}{2}v_1, \frac{1}{2}v_2, \frac{1}{2}v_3, v'_1, v'_2, v'_3$ where v'_i is the point in the plane of v_{i+1} and v_{i-1} equidistant from $0, v_{i+1}, v_{i-1}$ (indices modulo 3). So B is the sum of six determinants: $12B = \sum_{(a,b,c)} \det(a, b, c)$,

$$(a, b, c) = (v_1, v'_3, w), (v'_3, v_2, w), (v_2, v'_1, w), (v'_1, v_3, w), (v_3, v'_2, w), (v'_2, v_1, w).$$

We take care to orient the vectors so that all determinants are nonnegative.

We have $x_i^2 = \|v_i\|^2$, $y_i^2 = \|v_{i-1} - v_{i+1}\|^2$. The vertex w satisfies $\|w - v_i\|^2 = \|w\|^2$ or $2w \cdot v_i = \|v_i\|^2$. The planar circumcenter v'_i satisfies $\det(v'_i, v_{i-1}, v_{i+1}) = 0$, and $2v_i \cdot v_{i\pm 1} = \|v_{i\pm 1}\|^2$. Taking differentials of these relations we obtain for $i = 1, 2, 3$:

$$12 \, dB = \sum (\det(da, b, c) + \det(a, db, c) + \det(a, b, dc)), \quad (a, b, c) \text{ as above,} \quad (1)$$

$$x_i \, dx_i = v_i \cdot dv_i, \quad y_i \, dy_i = (v_{i-1} - v_{i+1}) \cdot (dv_{i-1} - dv_{i+1}), \quad (2)$$

$$dw \cdot v_i = (v_i - w) \cdot dv_i, \quad dv'_i \cdot v_{i\pm 1} = (v_{i\pm 1} - v'_i) \cdot dv_{i\pm 1}, \quad (3)$$

$$0 = \det(dv'_i, v_{i+1}, v_{i+2}) + \det(v'_i, dv_{i+1}, v_{i+2}) + \det(v'_i, v_{i+1}, dv_{i+2}). \quad (4)$$

Evaluating at (a) $x_i = y_i = 2$ we may take (fixing a choice of v_1, v_2, v_3)

$$\begin{aligned} v_1 &= \left(\frac{2\sqrt{2}}{\sqrt{3}}, \frac{2}{\sqrt{3}}, 0 \right), & v_2 &= \left(\frac{2\sqrt{2}}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, 1 \right), & v_3 &= \left(\frac{2\sqrt{2}}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, -1 \right), \\ v'_1 &= \left(\frac{4}{9}\sqrt{6}, -\frac{2}{9}\sqrt{3}, 0 \right), & v'_2 &= \left(\frac{4}{9}\sqrt{6}, \frac{1}{9}\sqrt{3}, -\frac{1}{3} \right), & v'_3 &= \left(\frac{4}{9}\sqrt{6}, \frac{1}{9}\sqrt{3}, \frac{1}{3} \right), \\ w &= \left(\frac{1}{2}\sqrt{6}, 0, 0 \right). \end{aligned}$$

Expand the determinants (1) using these values for v_i, v'_i, w :

$$\begin{aligned} 12 \, dB &= \left(0, \frac{\sqrt{2}}{\sqrt{3}}, 0 \right) \cdot dv_1 + \left(0, -\frac{\sqrt{2}}{2\sqrt{3}}, \frac{1}{2}\sqrt{2} \right) \cdot dv_2 + \left(0, -\frac{\sqrt{2}}{2\sqrt{3}}, -\frac{1}{2}\sqrt{2} \right) \cdot dv_3 \\ &\quad + \left(0, -\frac{3\sqrt{2}}{\sqrt{3}}, 0 \right) \cdot dv'_1 + \left(0, \frac{3\sqrt{2}}{2\sqrt{3}}, -\frac{3}{2}\sqrt{2} \right) \cdot dv'_2 + \left(0, \frac{3\sqrt{2}}{2\sqrt{3}}, \frac{3}{2}\sqrt{2} \right) \cdot dv'_3 \\ &\quad + \left(\frac{4}{\sqrt{3}}, 0, 0 \right) \cdot dw. \end{aligned}$$

Using (3) and (4) to eliminate dv'_i, dw we obtain

$$\begin{aligned} 12 \, dB &= \frac{1}{9\sqrt{6}} ((-\sqrt{2}, 56, 0) \cdot dv_1 + (-\sqrt{2}, -28, 28\sqrt{3}) \cdot dv_2 \\ &\quad + (-\sqrt{2}, -28, -28\sqrt{3}) \cdot dv_3) \\ &= \frac{1}{18\sqrt{2}} ((-v_1 - 19(v_2 - v_1) - 19(v_3 - v_1)) \cdot dv_1 \\ &\quad + (-v_2 - 19(v_3 - v_2) - 19(v_1 - v_2)) \cdot dv_2 \\ &\quad + (-v_3 - 19(v_1 - v_3) - 19(v_2 - v_3)) \cdot dv_3) \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{18\sqrt{2}} \left(-(v_1 \cdot dv_1 + v_2 \cdot dv_2 + v_3 \cdot dv_3) \right. \\
&\quad \left. + 19((v_1 - v_2) \cdot (dv_1 - dv_2) + (v_2 - v_3) \cdot (dv_2 - dv_3) \right. \\
&\quad \left. + (dv_1 - dv_3) \cdot (dv_1 - dv_3)) \right) \\
&= \frac{1}{18\sqrt{2}} (-2(dx_1 + dx_2 + dx_3) + 38(dy_1 + dy_2 + dy_3)).
\end{aligned}$$

For part (b) we may take (again fixing a choice of v_1, v_2, v_3)

$$\begin{aligned}
v_1 &= (\sqrt{2}, -\sqrt{2}, 0), & v_2 &= (\sqrt{2}, \sqrt{2}, 0), & v_3 &= (\sqrt{2}, 0, \sqrt{2}), \\
v'_1 &= \left(\frac{2}{3}\sqrt{2}, \frac{1}{3}\sqrt{2}, \frac{1}{3}\sqrt{2}\right), & v'_2 &= \left(\frac{2}{3}\sqrt{2}, -\frac{1}{3}\sqrt{2}, \frac{1}{3}\sqrt{2}\right), & v'_3 &= (\sqrt{2}, 0, 0), \\
w &= (\sqrt{2}, 0, 0).
\end{aligned}$$

Expand the determinants (1) using these values for v_i, v'_i, w :

$$\begin{aligned}
12 \, dB &= \frac{1}{3}((0, -2, -2) \cdot dv_1 + (0, 2, -2) \cdot dv_2 + (0, 0, 4) \cdot dv_3 \\
&\quad + (0, 6, 6) \cdot dv'_1 + (0, -6, 6) \cdot dv'_2 + (0, 0, -12) \cdot dv'_3 + (8, 0, 4) \cdot dw).
\end{aligned}$$

Using (3) and (4) to eliminate dv'_i, dw we obtain

$$\begin{aligned}
12 \, dB &= -\frac{2}{9}((1, 10, 11) \cdot dv_1 + (1, -10, 11) \cdot dv_2 + (2, 0, -20) \cdot dv_3) \\
&= -\frac{2}{9\sqrt{2}}((v_1 + 11(v_3 - v_1)) \cdot dv_1 + (v_2 + 11(v_3 - v_2)) \cdot dv_2 \\
&\quad + (2v_3 + 11(v_1 - v_3) + 11(v_2 - v_3)) \cdot dv_3) \\
&= -\frac{2}{9\sqrt{2}}((v_1 \cdot dv_1 + v_2 \cdot dv_2 + 2v_3 \cdot dv_3) \\
&\quad - 11((v_1 - v_3) \cdot (dv_1 - dv_3) + (v_2 - v_3) \cdot (dv_2 - dv_3))) \\
&= -\frac{4}{9\sqrt{2}}(dx_1 + dx_2 + 2 \, dx_3) + \frac{44}{9\sqrt{2}}(dy_1 + dy_2). \quad \square
\end{aligned}$$

Lemma 5.5. Consider the octahedron with center $w = (\sqrt{2}, 0, 0)$, vertices at the origin and

$$\begin{aligned}
v_1 &= (\sqrt{2}, \sqrt{2}, 0), & v_2 &= (\sqrt{2}, 0, \sqrt{2}), & v_3 &= (\sqrt{2}, -\sqrt{2}, 0), \\
v_4 &= (\sqrt{2}, 0, -\sqrt{2}), & v_5 &= (2\sqrt{2}, 0, 0).
\end{aligned}$$

Let $v_i(t)$ be a small analytic deformation of the vertices with $v_i(0) = v_i$. Fix a Delaunay decomposition of the octahedron. Assume $v_i(t)$ gives combinatorially the same Delaunay decomposition for all sufficiently small t . To each simplex S of the decomposition with vertex at 0, we associate a point $w_S(t)$ equidistant from the four vertices of S .

Then there is a constant C such that $\|w_S(t) - (\sqrt{2}, 0, 0)\| \leq C|t|$ for t sufficiently small.

Proof. Note that the point $(\sqrt{2}, 0, 0)$ is equidistant from all the vertices v_i and 0. As t varies, the point equidistant from the four vertices $(0, v_i, v_j, v_k)$ depends analytically on v_i, v_j, v_k when

$\det(v_i, v_j, v_k) \neq 0$ (Remark 5.2), so that the result is immediate by analyticity when $\det(v_i, v_j, v_k) \neq 0$. The only two simplices with vertex at 0 and determinant zero at $t = 0$ are $(0, v_1, v_3, v_5)$ and $(0, v_2, v_4, v_5)$. These cases are identical (up to reshuffling indices), so it is enough to treat $(0, v_1, v_3, v_5)$. The Delaunay decomposition of the octahedron is then by the discussion of [5] either

$$S_1 = (0, v_1, v_3, v_5), (0, v_1, v_2, v_3), (0, v_3, v_4, v_5), (0, v_1, v_4, v_5), (v_1, v_2, v_3, v_5)$$

or

$$S_1 = (0, v_1, v_3, v_5), (0, v_1, v_4, v_3), (0, v_3, v_2, v_5), (0, v_1, v_2, v_5), (v_1, v_4, v_3, v_5).$$

These cases are symmetrical by swapping v_2 and v_4 , so we treat only the first case. There are four simplices with 0 as a vertex. The determinant is nonzero for small t for all but S_1 , so $w_S(t)$ varies analytically for $S \neq S_1$.

For S_1 we argue as follows. Compose the vectors $v_i(t)$ with an analytic special orthogonal transformation T_t with the properties (1) T_0 is the identity transformation, (2) $T_t v_1(t)$ and $T_t v_3(t)$ lie in the plane $z = 0$, and (3) the circumcenter of $(0, T_t v_1(t), T_t v_3(t))$ in the plane $z = 0$ lies on the x -axis. Since these properties hold for $t = 0$, there clearly exists such an analytic family T_t . Since T_t is analytic, the conclusion of the lemma will hold for $T_t v_i(t)$ and $T_t w_{S_1}(t)$ if and only if it holds for $v_i(t)$ and $w_{S_1}(t)$. Thus we may assume from the outset without loss of generality that $v_1(t)$ and $v_3(t)$ lie in the plane $z = 0$ and the axis of points equidistant from $(0, v_1(t), v_3(t))$ has the form $\{(r(t), 0, z)\}$ for some analytic function $r(t)$ with $r(0) = \sqrt{2}$. Hence $w_{S_1}(t) = (r(t), 0, f(t))$ for some function $f(t)$ which is not assumed to be analytic. Write $v_i(t) = (x_i(t), y_i(t), z_i(t))$.

By the definition of the Delaunay decomposition,

$$\|w_{S_1}(t) - v_i(t)\|^2 \geq \|w_{S_1}(t)\|^2,$$

or equivalently

$$x_i^2 + y_i^2 + z_i^2 \geq 2x_i r + 2z_i f.$$

Using $z_2(0) = \sqrt{2} > 0$ and $z_4(0) = -\sqrt{2} < 0$ we obtain for small t :

$$\frac{x_2^2 + y_2^2 + z_2^2 - 2x_2 r}{2z_2} \geq f \geq \frac{x_4^2 + y_4^2 + z_4^2 - 2x_4 r}{2z_4}.$$

z_2, z_4 are bounded away from zero for small t , and the outer terms of this inequality are analytic. At $t = 0$, $(x_2, y_2, z_2) = (\sqrt{2}, 0, \sqrt{2})$, $(x_4, y_4, z_4) = (\sqrt{2}, 0, -\sqrt{2})$, $r = \sqrt{2}$, so that for $t = 0$ the outer terms vanish. Hence for small t , $|f| \leq C_1 |t|$ for some C_1 . The conclusion of the lemma now easily follows. \square

6. Analysis of pentagonal-prism-dipyramids

We begin with a lemma from classical spherical geometry.

Lemma 6.1. *The spherical n -gon of a given spherical perimeter $< 2\pi$ attains its maximum when it is regular.*

Proof. We begin with the case of a triangle of a given perimeter. It is enough to show that for a given base and perimeter the area is maximized by an isosceles triangle constructed on the given base. Let A and B be the endpoints of the base, and C be the remaining vertex of the triangle. Let l be the perpendicular bisector to AB . Holding A and B fixed, the locus of points C giving ABC fixed area is a small circle whose center lies on l [10]. Let G be a great circle with pole on l . A simple optimization problem shows that the point C on G which minimizes the sum of the distances $AC + CB$ lies on l . The result easily follows.

By considering a triangulation of a regular n -gon, we may apply this result to pairs of adjacent sides to show that the area of an n -gon is maximized for some polygon with sides of equal length. A lemma in [4] shows that the area of an n -gon with equal sides is given by the equal angle configurations. \square

We define a PPDP (pentagonal-prism-dipyramid) to be a Delaunay star for which the following holds. The Delaunay star has at least twelve vertices and twelve may be selected so that there exists an ordering of the vertices $v_i(D^*)$ such that $\|v_i\| \leq 2\frac{1}{5}$ for all $i \leq 12$ and $\|v_i - v_j\| \leq 2\frac{1}{5}$ for $(i, j) \in S$ where S is the set of pairs

$$\begin{aligned} &\{(1, 2), (1, 3), (1, 4), (1, 5), (1, 6), (2, 3), (3, 4), (4, 5), (5, 6), (6, 2), (7, 8), \\ &(8, 9), (9, 10), (10, 11), (11, 7), (2, 7), (3, 8), (4, 9), (5, 10), (6, 11), \\ &(7, 12), (8, 12), (9, 12), (10, 12), (11, 12)\}. \end{aligned}$$

Its shape is described in the introduction.

Lemma 6.2. *Let D^* be a PPDP. Then at least one of the edges $\|v_i - v_j\|$, $(i, j) \in S$, has length at least*

$$h = \frac{4 \sin(\frac{1}{5}\pi)}{\sqrt{1 + \sin^2(\frac{1}{5}\pi)}}.$$

Proof. Suppose for a contradiction that all edges in S have length strictly less than h . This allows us to assume that the angle between v_i and v_j is less than ψ for all $(i, j) \in S$, where $\psi = 2 \arcsin(\frac{1}{4}h)$ is the angle formed by two vectors of length 2 separated by distance h . To contradict this we consider the projection of all vectors to the unit sphere, replacing the segments between v_i and v_j by spherical geodesics on the unit sphere. The ten tetrahedra determined by the edges of S cut out two spherical pentagons (around vertices 1 and 12) on the surface of the unit sphere of perimeters $P_1, P_2 < 5\psi$. The five quadrilateral faces of the prism cut out five spherical quadrilaterals on the unit sphere of spherical perimeters $Q_1, \dots, Q_5 < 4\psi$. These regions cover the sphere, so they have total area 4π . A quadrilateral or pentagon of given perimeter has maximum area when it is regular (Lemma 6.1) so we have

$$4\pi < 2 \text{Pent}_\psi + 5 \text{Quad}_\psi,$$

where Pent_ψ and Quad_ψ are the areas of regular spherical pentagons and squares of edge ψ .

Consider the PPDP, symmetric with respect to the x -axis, with vertices

$$\begin{aligned} v_1 &= (4 \cos t, 0, 0), & v_{12} &= -v_1, & v_i &= v_{i-5} - v_1, & \text{for } 7 \leq i \leq 11, \\ v_k &= (2 \cos t, 2 \sin t \cos(\frac{2}{5}\pi k), 2 \sin t \sin(\frac{2}{5}\pi k)), & 2 \leq k \leq 6. \end{aligned}$$

The edges S cut the surface of the sphere into two regular pentagons and five rectangles. The sides of the rectangle have Euclidean lengths $4 \cos t$ and $4 \sin t \sin(\frac{1}{5}\pi)$. If we select t so that these are equal, then the sides have length h . This shows that

$$2 \text{Pent}_\psi + 5 \text{Quad}_\psi = 4\pi.$$

This is a contradiction. \square

In the remainder of this section we carry out the optimization of Γ_θ for a particular choice of θ over a certain five-dimensional subspace of the space of Delaunay stars. We show particular interest in this five-dimensional space because of certain numerical results we have obtained. While seeking a numerical maximum to $\Gamma_\theta(D^*) + \lambda_{\text{edge}} L_{\text{edge}}(D^*)$ on the space of PPDPs, we found very rapid convergence to points in this five-dimensional space. However, once the points reached this space, progress towards a local maximum often became quite slow. In fact, in early versions of our computer program, our method failed to find a numerical maximum at all. Thus it seemed advisable to carry out an exact maximization over this five-dimensional space. As a result we find an analytic expression for a curve that may be conjectured to be the maximum of $\Gamma_\theta(D^*)$ considered as a function of $L_{\text{edge}}(D^*)$.

We define a *wedge* $W(\psi)$ to be the convex hull of six points $w_1 = (2, 0, 0)$, $w_2 = (1, x, y)$, $w_3 = (1, x, -y)$, $w_4 = (-1, x, y)$, $w_5 = (-1, x, -y)$, $w_6 = (-2, 0, 0)$, where $x = \sqrt{3} \cos \psi$ and $y = \sqrt{3} \sin \psi$. We always assume that $\|w_2 - w_3\| \geq 2$, so that $\psi \geq \psi_{\min} = \arcsin(1/\sqrt{3})$. When ψ_1, \dots, ψ_5 satisfy $\psi_i \geq \psi_{\min}$, $\psi_1 + \dots + \psi_5 = \pi$, wedges congruent to $W(\psi_1), \dots, W(\psi_5)$ may be assembled along the edge $w_1 w_6$ to form a Delaunay star with twelve vertices. This Delaunay star will always be a PPDP. Also $L_{\text{edge}}(D^*) = \max_i 2\sqrt{3} \sin \psi_i$.

For stars constructed in this manner we break the function Γ_θ into the sum of five terms according to the contribution of each wedge $W(\psi_i)$. First note that Γ_θ is a linear combination of volumes: the volume of the star, the volume of the Voronoi cell and the volume of that part of the Delaunay stars lying in balls of unit radius at the vertices. Each of these volumes is a sum of five volumes, each of the five volumes being that part of the volume lying inside the appropriate infinite wedge-shaped region of angle ψ_i . The volumes within a wedge i depend only on the wedge $W(\psi_i)$ and not on the other vertices in the star. Hence we write

$$\Gamma_\theta(D^*) = \sum_{i=1}^5 \Gamma W_\theta(\psi_i),$$

for appropriate functions ΓW_θ of a single variable. By construction ΓW_θ has the form

$$\Gamma W_\theta(\psi) = -\delta_{\text{oct}} \text{vol}_W(\psi) + \sigma_W(\psi) + \theta \Theta_W(\psi),$$

for functions $\text{vol}_W(\psi)$, $\sigma_W(\psi)$, $\Theta_W(\psi)$ described but not named above.

Lemma 6.3. *Set $c = \cos \psi$, $s = \sin \psi$. Then*

$$\text{vol}_W(\psi) = 8cs,$$

$$\sigma_W(\psi) = \frac{1}{3} \left(8 \arctan \left(\frac{cs}{2-s^2} \right) + 4 \arctan \left(\frac{s}{2c} \right) + 8 \arctan \left(\frac{c}{\sqrt{3} + 2s} \right) + 8 \arctan \left(\frac{c}{\sqrt{3} + s} \right) \right),$$

$$\Theta_W(\psi) = \frac{14s}{9c}.$$

Proof. Let w, w' denote the circumcenters of the simplices with vertices $(0, w_1, w_2, w_3)$ and $(0, w_2, w_3, w_4)$, respectively. Let $w'_3, w'_2, w'_1, w''_3, w'_5$ be the planar circumcenters for the triangles $(0, w_1, w_2)$, $(0, w_1, w_3)$, $(0, w_2, w_3)$, $(0, w_2, w_4)$, $(0, w_3, w_4)$, respectively. Then as in Section 5, $6\Theta_W = \sum_{(a,b,c)} |\det(a, b, c)|$,

$$\begin{aligned} (a, b, c) = & (w_2, w'_3, w'), (w'_3, w_4, w'), (w_4, w'_5, w'), (w'_5, w_3, w'), (w_3, w'_1, w'), \\ & (w'_1, w_2, w'), \\ & (w_1, w'_3, w), (w'_3, w_2, w), (w_2, w'_1, w), (w'_1, w_3, w), (w_3, w'_2, w), \\ & (w'_2, w_1, w), \end{aligned}$$

$$\text{vol}_W = \frac{1}{3} (|\det(w_1, w_2, w_3)| + |\det(w_2, w_3, w_4)|).$$

By [8, pp. 331–359] the solid angle \mathcal{L} formed by vectors v_1, v_2, v_3 is given by

$$\tan\left(\frac{1}{2}\mathcal{L}(v_1, v_2, v_3)\right) = \frac{|\det(v_1, v_2, v_3)|}{xyz + xv_2 \cdot v_3 + yv_1 \cdot v_3 + zv_1 \cdot v_2},$$

$$x = \|v_1\|, \quad y = \|v_2\|, \quad z = \|v_3\|.$$

The solid angle at the origin is 4ψ , at w_1 or w_6 it is $\mathcal{L}(w_3 - w_1, w_2 - w_1, -w_1)$, at w_2, w_3, w_4 or w_5 it is $\mathcal{L}(w_5 - w_3, w_2 - w_3, w_1 - w_3)$, hence the volume σ_W is

$$\sigma_W = \frac{1}{3} (2\mathcal{L}(w_3 - w_1, w_2 - w_1, -w_1) + 4\mathcal{L}(w_5 - w_3, w_2 - w_3, w_1 - w_3) + 4\psi).$$

Expanding the determinants gives the result. \square

Lemma 6.4. *If $\theta = -\frac{12}{7}\delta_{\text{oct}}$, then*

$$\frac{d^2 \Gamma W_\theta(\psi)}{d\psi^2}$$

is positive on the interval $\psi_{\min} \leq \psi \leq \pi - 4\psi_{\min}$.

Proof. Set $u = \sin \psi$. Define ΓU_θ by the relation $\Gamma U_\theta(u) = \Gamma W_\theta(\psi)$ for $0 \leq u \leq 1$. We have

$$\frac{d^2 \Gamma W_\theta(\psi)}{d\psi^2} = \frac{d^2 \Gamma U_\theta(u)}{du^2} (1 - u^2) - \frac{d \Gamma U_\theta(u)}{du} u.$$

Using this expression for the second derivative, Mathematica shows that $\Gamma W_\theta''(\psi)$ is the product of a polynomial $P_\theta(u)$ of degree 15 and the factor

$$\frac{4}{3(1 - u^2)^{3/2} (-4 + 3u^2)^2 (2 + \sqrt{3}u)^6}.$$

Since $\psi_{\min} \leq \psi \leq \pi - 4\psi_{\min}$ we have $1/\sqrt{3} \leq u \leq \sin(4 \arcsin(1/\sqrt{3})) = \frac{4}{9}\sqrt{2}$.

If we have $P_\theta(u) = \sum a_i u^i$ where $u_0 \leq u \leq u_1$, then setting $I = \{i \mid a_i > 0\}$, $J = \{j \mid a_j < 0\}$,

$$P_\theta(u) = \sum_I a_i u^i + \sum_J a_j u^j \geq \sum_I a_i u_0^i + \sum_J a_j u_1^j \stackrel{\text{def}}{=} P_{u_0, u_1}.$$

Subdividing the interval $(1/\sqrt{3}, \frac{4}{9}\sqrt{2})$ into subintervals

$$(x_i, x_{i+1}) = \left(\frac{1}{\sqrt{3}} + \frac{1}{100}i, \frac{1}{\sqrt{3}} + \frac{1}{100}(i+1) \right),$$

we easily check that the constants $P_{(x_i, x_{i+1})}$ are positive. So $P_\theta(u)$ and thus $\Gamma W_\theta''(\psi)$ are positive on this interval. \square

Theorem 6.5. Set $\theta = -\frac{12}{7}\delta_{\text{oct}}$. Define $\chi_i = (\pi - i\psi_{\min})/(5-i)$, $i = 0, 1, 2, 3, 4$. Let ψ_{\max} and t be constants satisfying $\chi_t \leq \psi_{\max} \leq \chi_{t+1}$. The maximum of $\sum_{i=1}^5 \Gamma W_\theta(\psi_i)$ subject to the constraints $\psi_{\min} \leq \psi_i \leq \psi_{\max}$, $\psi_1 + \dots + \psi_5 = \pi$ is

$$\hat{\Gamma} W_\theta(\psi_{\max}) \stackrel{\text{def}}{=} t \Gamma W_\theta(\psi_{\min}) + (4-t) \Gamma W_\theta(\psi_{\max}) + \Gamma W_\theta(\pi - (4-t)\psi_{\max} - t\psi_{\min}).$$

Proof. Since the second derivative is positive, we maximize the sum when at most one of the ψ_i is different from ψ_{\min} , ψ_{\max} . The result follows easily. \square

We let D_{PPDP}^* be the PPDP determined by five wedges of angles ψ_{\min} , ψ_{\min} , ψ_{\min} , ψ_{\min} and $\pi - 4\psi_{\min}$. This star gives the global maximum to the effective density function over the five-dimensional space considered above. The star D_{PPDP}^* and the family of stars D_{CPS}^* are without question the most important stars for the understanding of dense packings in three dimensions. The following lemma gives us an exact formula for the effective density of D_{PPDP}^* .

Lemma 6.6.

$$\Gamma_0(D_{\text{PPDP}}^*) = \frac{814}{27}\pi + \frac{4}{3} \sum_{i=1}^6 \arccos(a_i) - \frac{3040}{27} \arccos\left(\frac{1}{\sqrt{3}}\right) + 4 \arccos\left(\frac{4\sqrt{3}}{3\sqrt{38}}\right),$$

$$\Theta(D_{\text{PPDP}}^*) = 4\sqrt{2},$$

where $a_1 = \frac{17}{81}$, $a_2 = \frac{11}{38}$, $a_3 = 8/(9\sqrt{2})$, $a_4 = 3\sqrt{3}/(2\sqrt{19})$, $a_5 = 7\sqrt{3}/(3\sqrt{59})$, $a_6 = 28/\sqrt{2242}$.

Remark 6.7. As far as I know it is a complete coincidence that $\Theta(D_{\text{PPDP}}^*) = \Theta(D_{\text{CPS}}^*)$.

Proof of Lemma 6.6. Use the explicit formulas of Lemma 6.3,

$$\Gamma_0(D_{\text{PPDP}}^*) = -4\delta_{\text{oct}} \text{vol}_W(\psi_{\min}) - \delta_{\text{oct}} \text{vol}_W(\pi - 4\psi_{\min}) + 4\sigma_W(\psi_{\min}) + \sigma_W(\pi - 4\psi_{\min}),$$

$$\Theta(D_{\text{PPDP}}^*) = 4\Theta_W(\psi_{\min}) + \Theta_W(\pi - 4\psi_{\min}),$$

together with some trigonometric identities. \square

7. Summary of analytic results

In this section $\theta = -\frac{12}{7}\delta_{\text{oct}}$. We also fix the constants $\Gamma_{\text{CPS}} = \rho_\theta^{-1}(\pi/\sqrt{18})$, $L_{\min} = 4s/\sqrt{1+s^2}$, $s = \sin(\frac{1}{5}\pi)$, $L_{\max} = \frac{8}{9}\sqrt{6}$, $\lambda_{\text{edge}} = -0.068287$, $\Gamma_{\text{edge}} = -6.68563$, $\lambda_{\text{sp}} = 1.26566$, $\Gamma_{\text{sp}} = -3.9937$, $\Gamma'_{\text{edge}} = -6.537252$, $\Gamma'_{\text{sp}} = -6.749453$. These are exact rational values for λ_{edge} , Γ_{edge} , λ_{sp} , Γ_{sp} , Γ'_{edge} , Γ'_{sp} , not approximations.

Consider the following statements.

- (I) If D^* is a PPDP and if $L_{\text{edge}}(D^*) \leq L_{\text{max}}$, then $\Gamma_\theta(D^*) + \lambda_{\text{edge}} L_{\text{edge}}(D^*) < \Gamma_{\text{edge}}$.
- (II) If D^* is a PPDP and if $L_{\text{max}} \leq L_{\text{edge}}(D^*)$, then $\Gamma_\theta(D^*) < \Gamma'_{\text{edge}}$.
- (III) If D^* is a Delaunay star for which $L_{\text{min}} \leq L_{\text{sp}}(D^*) \leq L_{\text{max}}$, then $\Gamma_\theta(D^*) + \lambda_{\text{sp}} L_{\text{sp}}(D^*) < \Gamma_{\text{sp}}$.
- (IV) If D^* is a Delaunay star for which $L_{\text{max}} \leq L_{\text{sp}}(D^*) \leq \frac{11}{5}$, then $\Gamma_\theta(D^*) < \Gamma'_{\text{sp}}$.
- (V) Fix any neighborhood U_{CPS} in the space Del^* of Delaunay stars containing all stars D_{CPS}^* associated to face-centered-cubic or hexagonal-close-packings. If D^* is not a PPDP and if D^* does not lie in U_{CPS} , then $\rho_\theta \Gamma_\theta(D^*) < \pi/\sqrt{18}$.

Section 9 will give strong numerical evidence that all five of these statements are true. They could all be verified rigorously by a finite computer program. We could have selected a much simpler set of constants, but prefer to keep constants that would make statements (I)–(V) more easily satisfied. The constants were found by experimentation. There was considerable freedom in their selection.

Theorem 7.1. *If the statements (I)–(V) are all true, then no sphere packing has density exceeding $\pi/\sqrt{18}$.*

Proof. Fix U_{CPS} small enough so that $\rho_\theta \Gamma_\theta(D^*) \leq \pi/\sqrt{18}$ on U_{CPS} . This is possible by Theorem 5.1. By (V) the principal patch covers every star which is not a PPDP. On the set of all PPDPs, $L_{\text{min}} \leq L_{\text{edge}}(D^*) \leq \frac{11}{5}$ (Lemma 6.2). Let us verify that the set of PPDPs with $L_{\text{edge}}(D^*) \leq L_{\text{max}}$ is a patch using the unprimed constants above. Axiom (P1) is statement (I); (P2) holds by definition; (P3) is statement (III); (P4) follows from (IV) and $\Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\text{max}} \geq \Gamma'_{\text{sp}}$; (P5) is obvious; (P6) follows by evaluating the constant $\Gamma_{\text{sp}} - \lambda_{\text{sp}} L_{\text{min}} - \Gamma_{\text{CPS}}$; (P8) holds because $I_{\text{edge}} \neq \emptyset$ for PPDPs.

Consider (P7). Divide the interval $(L_{\text{min}}, L_{\text{max}})$ into intervals (x_i, x_{i+1}) with $x_i = L_{\text{min}} + 0.01i$, $i \leq 15$, $x_{16} = L_{\text{max}}$. Then evaluate the function $f(x; a, b, c)$ of Lemma 2.5:

$$f(x_i; x_i, x_{i+1}, x_i) - \Gamma_{\text{CPS}}, \quad f(x_{i+1}; x_i, x_{i+1}, x_i) - \Gamma_{\text{CPS}}, \quad i \leq 15,$$

use the bound of Lemma 2.5, and check that they all take negative values.

Now we turn to the PPDPs such that $L_{\text{max}} \leq L_{\text{edge}}(D^*) \leq \frac{11}{5}$. We need to verify the patch axioms (P^*) are satisfied for the following data (with primes)

$$(\lambda'_{\text{edge}}, \Gamma'_{\text{edge}}, \lambda'_{\text{sp}}, \Gamma'_{\text{sp}}, L'_{\text{min}}, L'_{\text{max}}) = (0, \Gamma'_{\text{edge}}, 0, \Gamma'_{\text{sp}}, L_{\text{max}}, \frac{11}{5}).$$

(P1) is assumption (II); (P2) holds by definition; (P3) is assumption (IV); (P4) is vacuous; (P5) is trivial; (P6) follows since $\Gamma'_{\text{sp}} - \lambda'_{\text{sp}} L'_{\text{min}} = \Gamma'_{\text{sp}} < \Gamma_{\text{CPS}}$; (P8) holds because $I_{\text{edge}} \neq \emptyset$ for PPDPs; (P7) remains to be seen. Now

$$\frac{\Gamma'_{\text{edge}} - \lambda'_{\text{edge}} x + r(x)(\Gamma'_{\text{sp}} - \lambda'_{\text{sp}} x)}{1 + r(x)} = \frac{\Gamma'_{\text{edge}} + r(x)\Gamma'_{\text{sp}}}{1 + r(x)}.$$

Since $\Gamma'_{\text{edge}} > \Gamma'_{\text{sp}}$, $(\Gamma'_{\text{edge}} + r(x)\Gamma'_{\text{sp}})/(1 + r(x))$ is maximized when $r(x)$ is minimized. As we see from Section 2, $r'(x) < 0$ on $(2, 3)$, so $r(x) \geq r(L'_{\text{max}})$. So

$$\frac{\Gamma'_{\text{edge}} + r(x)\Gamma'_{\text{sp}}}{1 + r(x)} \leq \frac{\Gamma'_{\text{edge}} + r(L'_{\text{max}})\Gamma'_{\text{sp}}}{1 + r(L'_{\text{max}})}.$$

Evaluating this constant we find it is less than Γ_{CPS} . So (P7) holds. The theorem now follows from Theorem 4.2. \square

We say that a subset X of a packing Λ is *replete* if

$$\limsup_{r \rightarrow \infty} \frac{|X \cap B_r(0)|}{|\Lambda \cap B_r(0)|} = 1.$$

We use \limsup rather than \liminf because we have defined the density by \limsup rather than \liminf . Again we remind the reader that for notational convenience throughout this paper we let D_{CPS}^* denote any star associated to either the face-centered-cubic or hexagonal-close-packing.

Theorem 7.2. *Suppose that the statements (I)–(V) are all true. Suppose that Λ is a sphere packing with density $\pi/\sqrt{18}$. Then for every open neighborhood U_{CPS} containing all the stars D_{CPS}^* , the set of packing points with stars in U_{CPS} is replete. Conversely, any packing with this property has density $\pi/\sqrt{18}$.*

Proof. This is a straightforward δ - ϵ argument. We use the fact that the maximum of Γ_θ or of a suitable average of $\Gamma_\theta(D^*)$'s will be bounded away from $\rho_\theta^{-1}(\pi/\sqrt{18})$ on any compact set that does not contain the stars D_{CPS}^* . Note that an average of $\Gamma_\theta(D^*)$'s is required to dismiss PPDPs. \square

8. Description of the sphere packing algorithm

This section describes in general terms an algorithm we have developed to find local maxima to Γ_θ . In the next section we will refer to an application of this algorithm as *flowing* to a local maximum.

Given an initial star, our algorithm uses a gradient method to search for a local maximum to $\Gamma_\theta(D^*)$ on the space of Delaunay stars Del^* . The optimization is made more complicated by the disconnectedness of the space of Delaunay stars, and by the tendency of local maxima to lie on strata of high codimension on the boundary of Del^* . However, these difficulties can be overcome.

A rough picture of the boundary of Del^* is as follows. Boundary points corresponds to configurations in which one or more pairs of spheres are tangent. Such boundary points fall into strata according to the number of pairs of tangent spheres. In the simplest case of one pair of tangent spheres the neighborhood of such a boundary point locally resembles a product of an affine space with the exterior of a solid ball. This property of local concavity near the boundary along strata of a given dimension also holds for strata of smaller dimensions. This property of local concavity is extremely convenient, for a small displacement tangent to a stratum always leads into the interior of Del^* . Locally we consider Del^* as embedded in Euclidean space of sufficiently high dimension as a manifold with stratified boundary.

A typical step in the initial stages of the algorithm goes as follows. If the point lies in the interior of a component, then we compute the gradient and take a step in the direction of

greatest increase. However, if the point p lies on the boundary, we constrain the motion of the small step to be tangent to the stratum on which p lies. Without such a constraint a step in the direction of the gradient would often lead outside of Del^* . A basis for the tangent space is found by Gaussian elimination.

At late stages of the algorithm, if p is a point on the boundary, we relax the condition that the step be tangent to the boundary. We approximate Del^* at p by a cone with vertex p bounded by finitely many hyperplanes. As always we are viewing Del^* as locally embedded in Euclidean space, and extend the function Γ_θ to a Euclidean neighborhood of p . We then solve the linear programming problem of maximizing the gradient at p subject to the linear inequalities which locally define Del^* inside Euclidean space. We then take a small step in the direction obtained as the solution to this linear programming problem. Thus at late stages in the algorithm a separate linear programming problem potentially has to be solved at every step. A number of conditions tell us when to switch from Gaussian elimination to linear programming including insufficient improvements in the function Γ_θ , arriving at a stratum of dimension zero, or simply taking sufficiently many steps. Finally when one reaches a stage when no further improvement is found (or when our computer resources have been exhausted), the algorithm terminates.

The disconnectedness of Del^* is dealt with by placing a weaker topology on Del^* . The topology we placed on Del^* makes Del^* a disconnected compact space. This topology, however, is perhaps not the most natural topology for Del^* . A more natural topology would make Del^* into a non-Hausdorff space. The space of Voronoi cells arising from saturated packings is a compact Hausdorff space in a natural way. We have a projection map from Delaunay stars to Voronoi cells. Pulling open sets back by this projection map gives a non-Hausdorff topology on Del^* . This topology will become relevant as we discuss two other types of boundary points.

In addition to boundary points arising from the tangency of spheres, two other types of boundary points can be identified. When the configuration approaches one of these other boundary points special actions are taken. To introduce some terminology, we let S be a set of packing points — usually those associated to a fixed Delaunay star. We call a *hole* a point in Euclidean three-space whose distance to S is a local maximum. Equivalently it is a vertex of a Voronoi cell. Such a point is equidistant to four or more points of S . If a hole h is equidistant to five or more nearest packing points, we say that h is a *degenerate hole*. If a hole has distance 2 or more from S , then we say that S is *unsaturated*.

One type of boundary point corresponds to a configuration that has become unsaturated. Our remedy to this situation is simple. Add another packing point at a random position near the hole h causing the unsaturation.

The other type of boundary point corresponds to configurations with a degenerate hole. For such configurations the Delaunay decomposition is not unique. Several Delaunay stars may have the same Voronoi cell and hence the same non-Hausdorff neighborhoods. Each of these points lies in a different component of Del^* with respect to the Hausdorff topology. In brief, the boundary points corresponding to degenerate holes cease to be boundary points when viewed from the non-Hausdorff topology. Thus we may take a small non-Hausdorff step in the direction given us by the gradient, although this may land us in a different component for the Hausdorff topology.

The picture is actually somewhat more complicated than this because the function Γ_θ is not

continuous with respect to the non-Hausdorff topology. From the non-Hausdorff point of view we are seeking to maximize a discontinuous function. Thus a small non-Hausdorff step may bring significant gains in Γ_θ , or may cause a large drop in Γ_θ . If the small non-Hausdorff step brings significant gains, we silently accept the windfall and move on. If the step would cause Γ_θ to drop, we move up to the discontinuity, then along the “fissure of degeneracy”, the locus of configurations with a given degenerate hole, until we come to the point where we may improve Γ_θ by moving away again from the fissure.

In practice, we are forced to navigate along such fissures quite often in the final stages of the algorithm. In fact, multiply degenerate situations frequently arise. Notice that the regular octahedron occurring in the D_{CPS}^* and D_{PPDP}^* stars gives a degenerate hole. With respect to the non-Hausdorff topology octahedra in a small neighborhood of the regular octahedron of edge 2 give rise to a continuous but nondifferentiable ridge. One may slowly increase the function Γ_θ by slowly moving along the ridge, but following a naive gradient approach the algorithm would tend to hop incessantly back and forth in small steps across the ridge rather than along the ridge.

Our algorithm takes all of these effects into account, and in the end we are able to amass evidence in support of our statements...

9. Numerical evidence

This section discusses the numerical evidence in support of statements (I)–(V) of Section 7. As we will see, the numerical evidence strongly supports these statements. In fact the evidence indicates that these inequalities all hold by a considerable margin. This large margin may be interpreted as meaning that no sphere packing comes close to achieving the density of the face-centered-cubic or hexagonal-close-packings unless of course sufficiently many of the Delaunay stars of the packing are sufficiently close to one of the stars D_{CPS}^* . The evidence will come by applying the algorithm described in the previous section repeatedly to various randomly generated Delaunay stars, and studying the resulting local maxima. We use the constants defined at the beginning of Section 7.

Numerical Finding 9.1. *The only Delaunay stars with $\rho_0 \Gamma_0(D^*) \geq 0.740$ lie in a neighborhood of some D_{CPS}^* or lie in the set of PPDPs. The global maximum of $\Gamma_0(D^*)$ is attained for $D^* = D_{\text{PPDP}}^*$ and gives a bound on any sphere packing in three dimensions of $0.740873\dots$. An exact value for this constant is given by $\rho_0 \Gamma_0(D_{\text{PPDP}}^*)$ where $\Gamma_0(D_{\text{PPDP}}^*)$ is given in Lemma 6.6.*

Table 9.1

Density	p_1	p_2	p_3	p_4	h_1	f_1	Total
$0.7400 < x < 0.7402$			1	2	1	2	6
$0.7402 < x < 0.7404$		1	1	5	7	1	15
$0.7404 < x < 0.7406$		2	2		3	2	9
$0.7406 < x < 0.7408$	14	8	7				29
$0.7408 < x < 0.7409$	2	1					3
$0.7409 < x$							0

Evidence. 311 randomly generated initial Delaunay stars are generated and each is allowed to flow to a local maximum. Of the 311 resulting terminal configurations 62 had effective density over 0.740. All of these without exception is either a PPDP, or a star in a small neighborhood of some D_{CPS}^* . Of these 62 configurations 11 lie in a neighborhood of the hexagonal-close-packing star, 5 are in a neighborhood of the face-centered-cubic star, and the remaining 46 are in a neighborhood of D_{PPDP}^* . Table 9.1 shows the correlation between the effective density of such a star and its nearness to a face-centered-cubic star (FCC), hexagonal-close-packing star (HCP), or D_{PPDP}^* .

The columns have the following interpretations. Let v_1, \dots, v_{12} be the vertices of the star. Set

$$d(D^*) = \sum_{i=1}^{12} \|v_i\|^2 - 48 + \sum_{p=1}^n \|v_{i_p} - v_{j_p}\|^2 - 4n.$$

Here n is 24 for stars near FCC or HCP but 23 for PPDPs. The second sum runs over the edges that have length 2 for FCC, HCP or D_{PPDP}^* . Then $\text{PPDP}(x)$, $\text{HCP}(x)$, or $\text{FCC}(x)$ will be the stars near D_{PPDP}^* , HCP or FCC with $d(D^*) < x$:

$$\begin{aligned} p_1 &= \text{PPDP}(0.0025), \quad p_2 = \text{PPDP}(0.01) \setminus \text{PPDP}(0.0025), \\ p_3 &= \text{PPDP}(0.22) \setminus \text{PPDP}(0.01), \quad p_4 = \text{PPDP}(\infty) \setminus \text{PPDP}(0.22), \\ h_1 &= \text{HCP}(0.011), \quad f_1 = \text{FCC}(0.007). \quad \square \end{aligned}$$

Remark 9.2. This numerical study was the first one completed (June 1990). It is this study that first showed that an approach based on the Delaunay decomposition will give a very good bound on the density of sphere packings, but that various correction terms are necessary before one is to arrive at a bound of $\pi/\sqrt{18}$. The other numerical studies will take $\theta = -\frac{12}{7}\delta_{\text{oct}}$. Since the optimization of Γ_θ may be viewed as a perturbation of Γ_0 , and since the solutions to Γ_θ are corner solutions rather than interior points, the global maximum will not change for sufficiently small perturbations θ . Not only are these points corner solutions but they lie on strata of dimension zero on the boundary. Even more they lie at overdetermined zero-dimensional strata since they are defined by 35 or 36 equations in a 33-dimensional space.

Now set $\theta = -\frac{12}{7}\delta_{\text{oct}}$.

Numerical Finding 9.3. If D^* is a Delaunay star such that $\rho_\theta \Gamma_\theta(D^*) > 0.74048$, then D^* is a PPDP or lies in a small neighborhood of some D_{CPS}^* . The global maximum of Γ_θ on the space of Delaunay stars is given by $\rho_\theta \Gamma_\theta(D_{\text{PPDP}}^*) = 0.740755 \dots$.

Remark 9.4. An exact value for $\Gamma_\theta(D_{\text{PPDP}}^*)$ is easily given by Lemma 6.6.

Evidence. We generate an additional 105 Delaunay stars and let them flow to a local maximum. We let a_i be the 105 values for $\rho_\theta \Gamma_\theta$ so obtained. For all 105 terminal Delaunay stars the number of vertices $n(D^*)$ is 10, 11 or 12. Figure 9.3(a) shows the approximate delta function

$$f_{105}(x) = \sum_{i=1}^{105} \frac{1}{1 + T(x - a_i)^2}, \quad T = 500,000,$$

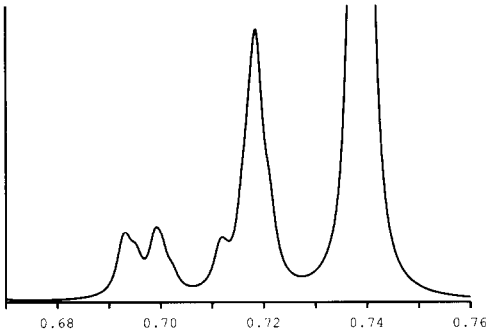


Fig. 9.3(a). All data.

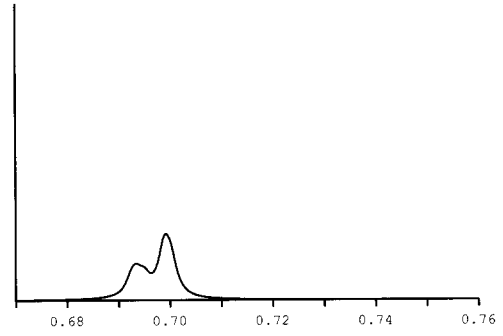


Fig. 9.3(b). 10 spheres.

over the interval $0.67 \leq x \leq 0.76$. (The truncated region in Figs. 9.3(a) and 9.3(d) will be shown at higher resolution below.) We interpret the three major humps as corresponding to the maximum of $\Gamma(D^*)$ when the number of vertices is given by $n(D^*) = 10, 11$ or 12 , respectively. To support this claim we write the function f_{105} as the sum of three terms $f_{105}^n = \sum_{i=1, n(D^*)=n}(\dots)$ and plot them separately in Figs. 9.3(b)–9.3(d).

To continue our analysis of the best of the 105 stars obtained by our gradient method, we plot the smoothed data with higher resolution in the interval $0.735 \leq x \leq 0.741$. We smooth the data using the function obtained from f_{105} by replacing 500,000 by 250,000,000. Call this function g_{105} . The resulting curve is shown in Fig. 9.3(e). We claim that the highest peak to the right in this plot is formed by the PPDPs. The neighboring peak just to its left is formed by the stars near some D_{CPS}^* . To check this claim we resolve g_{105} into the sum of three pieces:

$$g_{105} = g_{105, \text{PPDP}} + g_{105, \text{CPS}} + g_{105, \text{other}},$$

by separating out those stars that lie in a small neighborhood of D_{PPDP}^* , or some D_{CPS}^* . These neighborhoods are defined by a cutoff of $2\frac{1}{5}$ similar to the definition of PPDPs. The resulting data is shown in Figs. 9.3(f)–9.3(h).

In all there are 15 stars near D_{PPDP}^* , 11 near some D_{CPS}^* and 79 others. Of those near D_{PPDP}^* the greatest effective density is 0.750755. Of those near some D_{CPS}^* the greatest effective density is 0.74048. Of those not near any of these fixed stars the greatest effective density is 0.739.

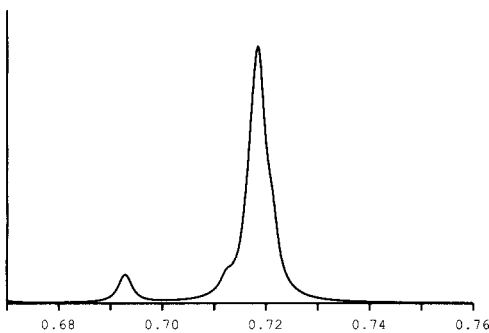


Fig. 9.3(c). 11 spheres.

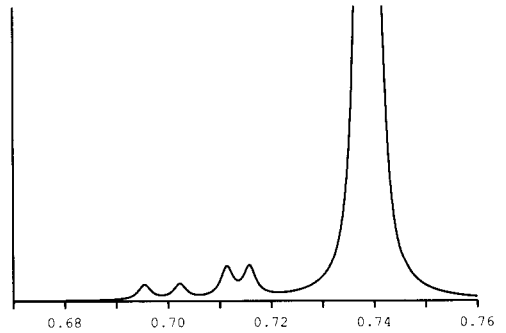


Fig. 9.3(d). 12 spheres.

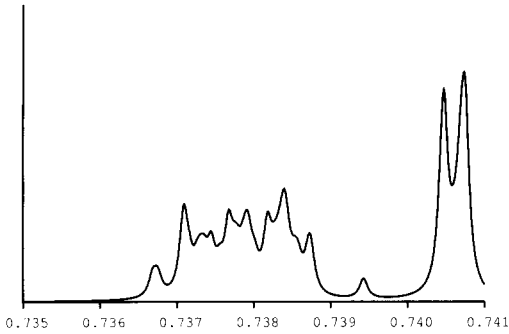


Fig. 9.3(c). All data.

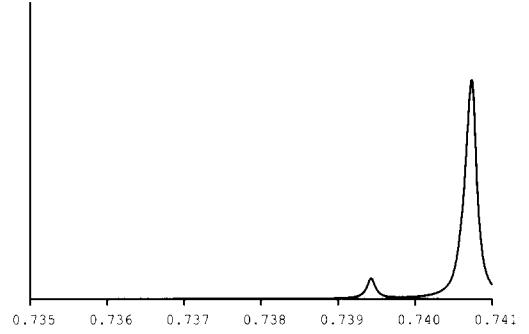


Fig. 9.3(f). PPDP.

It appears that there are many local maxima in the interval $(0.736, 0.740)$. I have analyzed an assortment of them. They tend to be made up of twelve vertices at distance 2 from the central sphere. The simplices tend to form clusters of up to ten regular tetrahedra, together with a couple of square pyramids. However, this local structure of tetrahedra and pyramids lacks any global coherence over the full star. \square

This data supports statement (II). In fact it supports the much stronger statement: the global numerical maximum of $\Gamma_\theta(D^*)$ over all Delaunay stars is equal to

$$\Gamma_\theta(D_{\text{PPDP}}^*) = \rho_\theta^{-1}(0.740755\dots) = -6.53931\dots < \Gamma'_{\text{edge}}.$$

This data supports statement (V). In fact the largest value of $\rho_\theta \Gamma_\theta(D^*)$ of the 105 Delaunay stars after removing those near some D_{CPS}^* or D_{PPDP}^* is $0.739 < \pi/\sqrt{18}$.

I have also carried out some numerical studies to check that Γ_θ drops rather quickly on the space of PPDPs as $L_{\text{edge}}(D^*)$ increases beyond L_{max} , so that by the time $L_{\text{edge}}(D^*)$ reaches $\frac{11}{5}$ (the boundary of the set of PPDPs), the effective density is well below $\pi/\sqrt{18}$.

Because the Delaunay decomposition of the regular octahedron is not unique, there are several stars D_{CPS}^* . Vertices may be added at appropriate points at distance $2\sqrt{2}$ from the center of the star. This does not affect the density. Similarly there are stars other than D_{PPDP}^* that have the same effective density as D_{PPDP}^* . They are obtained by adding vertices to D_{PPDP}^*

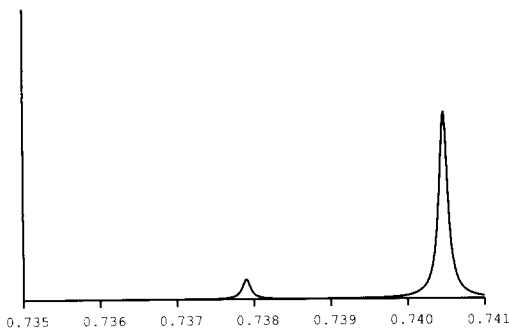


Fig. 9.3(g). FCC/HCP.

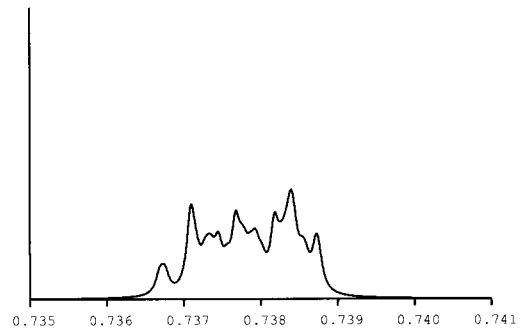


Fig. 9.3(h). Not FCC/HCP/PPDP.

at distance $2\sqrt{2}$ from the center of the star at points that would form a regular octahedron. (There are four such points.) There is a fifth point (or rather region) where a vertex can be added to D_{PPDP}^* to obtain another star. There are four vertices (say v_2, v_3, v_7, v_8) which are characterized as the closest vertices to the deepest hole of D_{PPDP}^* . One may place an additional vertex at distance 2 from all of these to obtain a new star. A corner of volume

$$\frac{2000}{1973727}\sqrt{2}$$

is cut from the Voronoi cell. One may check that adding this additional vertex causes Γ_θ to decrease.

A function $\hat{I}W_\theta(\psi)$ is defined in Theorem 6.5. Write $\hat{I}(h)$ for $\hat{I}W_\theta(\arcsin(h/\sqrt{12}))$, and $\hat{\chi}_i = \sqrt{12} \sin \chi_i$, $i = 0, 1, 2, 3, 4$.

Numerical Finding 9.5. For $\hat{\chi}_0 \leq h \leq L_{\max}$, the maximum of $\Gamma_\theta(D^*)$ over the set of PPDPs with $L_{\text{edge}}(D^*) = h$ is given by $\hat{I}(h)$. The maximum of $\Gamma_\theta(D^*) + \lambda_{\text{edge}} L_{\text{edge}}(D^*)$ over the same set is given by $\hat{I}(\hat{\chi}_3) + \lambda_{\text{edge}} \hat{\chi}_3$.

Evidence. We generate random PPDPs with $\|v_i\|$ near 2 subject to the constraint that h be at most L_{\max} . We then let the PPDP flow to a local maximum subject to the constraint that $L_{\text{edge}}(D^*)$ remain constant throughout the flow. The data for 432 such trials is shown in Fig. 9.5. The points in Fig. 9.5 are the 432 pairs $(L_{\text{edge}}(D^*), \Gamma_\theta(D^*))$. The two vertical lines mark L_{\min} and L_{\max} , the horizontal line marks $\rho_\theta^{-1}(\pi/\sqrt{18})$. Points below this horizontal line lie in the principal patch and are of no concern to us. The line of positive slope is the line

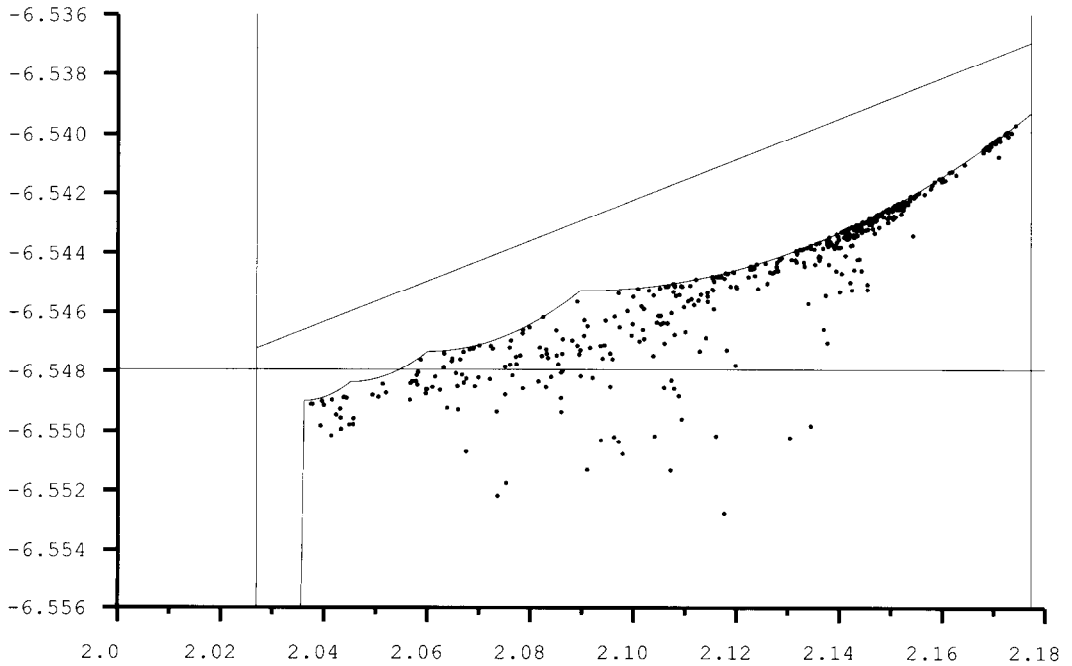


Fig. 9.5. PPDPs and $\Gamma_\theta(D^*)$.

$-\lambda_{\text{edge}}x + \Gamma_{\text{edge}}$. The piecewise analytic curve shown near the upper envelope of the 432 points is the graph of $\hat{\Gamma}$. The evidence, as seen from this plot, then indicates that the curve $\hat{\Gamma}$ is the upper envelope for the points $(L_{\text{edge}}(D^*), \Gamma_{\theta}(D^*))$.

If the results of the first part of 9.5 hold, then for $2\sqrt{3} \sin \frac{1}{5}\pi \leq h = L_{\text{edge}}(D^*) \leq \frac{8}{9}\sqrt{6}$:

$$\Gamma_{\theta}(D^*) + \lambda_{\text{edge}}L_{\text{edge}}(D^*) \leq \hat{\Gamma}(h) + \lambda_{\text{edge}}h.$$

An upper bound for the curve $\hat{\Gamma}(h)$ is given by the piecewise linear curve which connects the points $p_i = (\hat{\chi}_i, \hat{\Gamma}(\hat{\chi}_i))$, $i = 0, 1, 2, 3, 4$. The linear segments between p_i and p_{i+1} , $i = 0, 1, 2$, may be shown to have slope greater than $-\lambda_{\text{edge}}$ while the slope of the linear segment between p_3 and p_4 has slope slightly less than $-\lambda_{\text{edge}}$, so an upper bound on $\Gamma_{\theta}(D^*) + \lambda_{\text{edge}}L_{\text{edge}}(D^*)$ is given by a Delaunay star D^* satisfying $(L_{\text{edge}}(D^*), \Gamma_{\theta}(D^*)) = p_3$. This is the second part of 9.5. \square

We have also indicated in Fig. 9.5 a nearly vertical segment that gives a rough estimate of an upper bound on the graph $(L_{\text{edge}}(D^*), \Gamma_{\theta}(D^*))$ on the interval $[L_{\min}, \hat{\chi}_0]$. Such stars lie in a small neighborhood of the PPDP of Lemma 6.2. Call it D_m^* . A Mathematica computation shows that $\Gamma_{\theta}(D_m^*) = -6.6576\dots$. The nearly vertical segment is formed by joining the points $(L_{\min}, \Gamma_{\theta}(D_m^*))$ and $(\hat{\chi}_0, \hat{\Gamma}(\hat{\chi}_0))$ with a line. It shows how rapidly Γ_{θ} would rise as a function of $L_{\text{edge}}(D^*)$ if Γ_{θ} were linear on this interval.

The conclusions of 9.5 clearly support statement (I) of Section 7. The gap in Fig. 9.5 between the upper bound line $-\lambda_{\text{edge}}x + \Gamma_{\text{edge}}$ and $\hat{\Gamma}(x)$ gives us a considerable margin for error.

Numerical Finding 9.6. *Let D^* be a Delaunay star satisfying $L_{\min} \leq L_{\text{sp}}(D^*) \leq L_{\max}$. Then $\Gamma_{\theta}(D^*(x)) + \lambda_{\text{sp}}L_{\text{sp}}(D^*) \leq -4.02$. Let D^* be a Delaunay star satisfying $L_{\max} \leq L_{\text{sp}}(D^*) \leq \frac{11}{5}$. Then $\Gamma_{\theta}(D^*) \leq -6.85$.*

Evidence. We generate 575 random Delaunay stars subject to the condition that $L_{\text{sp}}(D^*)$ fall in the interval $[2, \frac{11}{5}]$. We then let them flow to a local maximum subject to the condition that $L_{\text{sp}}(D^*)$ remain constant throughout the flow. The data

$$(L_{\text{sp}}(D^*), \Gamma_{\theta}(D^*))$$

is plotted in Fig. 9.6(a). It is the upper envelope of these points that concerns us.

We notice that there are a couple of points that lie slightly above the others near them. Analyzing the Delaunay stars that give rise to these points, we find that they are PPDPs (as expected) and that it is the apex of the pyramid (v_1 or v_{12} in the notation of Section 6) that has distance $L_{\text{sp}}(D^*)$ from the center. We generate 480 additional PPDPs by taking D_{PPDP}^* and lifting the apex vertex v_1 to a random height $L_{\text{sp}}(D^*)$ from the center of the star. We then let these points flow to a local maximum subject to the condition that $L_{\text{sp}}(D^*)$ remain constant throughout the flow. The data $(L_{\text{sp}}(D^*), \Gamma_{\theta}(D^*))$ is plotted in Fig. 9.6(b). Again it is the upper envelope of these points that concerns us. Of the $480 + 575$ stars for which $L_{\text{edge}}(D^*)$ lies in the interval $[L_{\max}, \frac{11}{5}]$ the maximum of $\Gamma_{\theta}(D^*)$ is -6.90571 . This is less than the bound given in 9.6. Of the $480 + 575$ stars for which $L_{\text{edge}}(D^*)$ lies in the interval $[L_{\min}, L_{\max}]$ the maximum of $\Gamma_{\theta}(D^*) + \lambda_{\text{sp}}L_{\text{sp}}(D^*)$ is -4.03206 . This is less than the bound given in 9.6, which in turn is less than the bound given in Section 7. \square

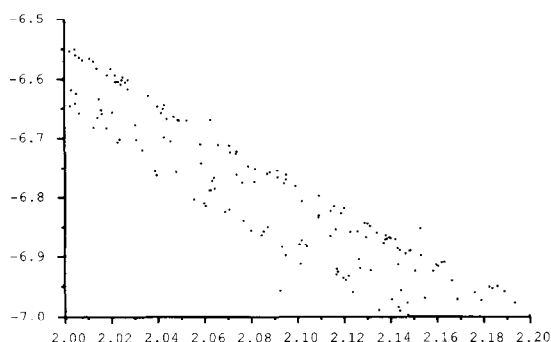


Fig. 9.6(a). All Delaunay stars.

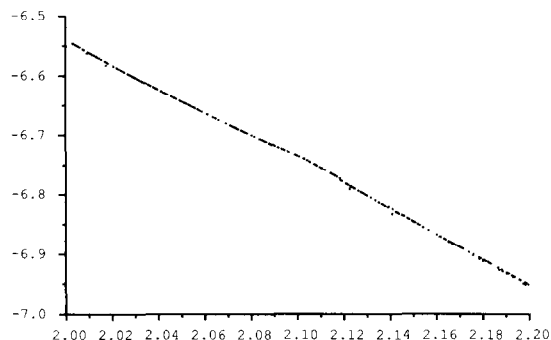


Fig. 9.6(b). PPDs.

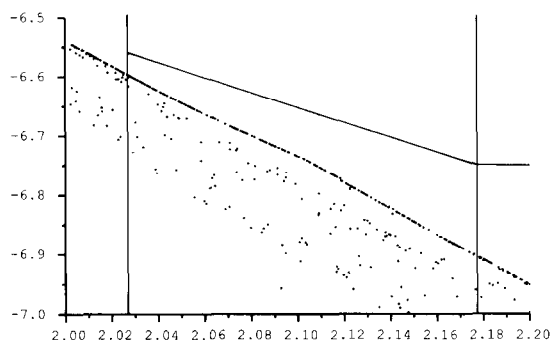


Fig. 9.6(c). Numerical bounds.

The bounds given by statements (III) and (IV) of Section 7 are two line segments on the intervals (L_{\min}, L_{\max}) , $(L_{\max}, \frac{11}{5})$ plotted in Fig. 9.6(c). Again we see that the statements are numerically valid even when we leave a considerable margin for error.

This completes our discussion of the numerical evidence. The reader who wishes to replace the numerical evidence by rigorous proof would probably find it easiest to begin with the statements concerning the set of PPDs.

Appendix

In this Appendix we indicate the dependence of our results on computer calculation. The following results relied on Mathematica.

(1) The determinants of Lemmas 5.4 and 6.3, as well as the proofs of Lemmas 6.4 and 6.6. In Lemma 6.4 we found the second derivative of an explicit function and required the use of a high-precision calculator. The main conclusions of the paper do not rely on Section 6.

(2) Evaluation of constants in Section 7. Here we could have used any high-precision calculator.

A computer was freely used in the processing and evaluation of data in Section 9. In Section 5, we also rely on a result of [5], which was established using Mathematica. The computer code for this result has been carefully checked.

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