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A proof of the Kepler conjecture

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To the memory of László Fejes Tóth

Contents

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Preface

This project would not have been possible without the generous support of many people. I would particularly like to thank Kerri Smith, Sam Ferguson, Sean McLaughlin, Jeff Lagarias, Gabor Fejes Tóth, Robert MacPherson, and the referees for their support of this project. A more comprehensive list of those who contributed to this project in various ways appears in [Hal06b].

1. The top-level structure of the proof

This chapter describes the structure of the proof of the Kepler conjecture.

1.1. *Statement of theorems.*

THEOREM 1.1 (The Kepler conjecture). *No packing of congruent balls in Euclidean three space has density greater than that of the face-centered cubic packing.*

This density is $\pi/\sqrt{18} \approx 0.74$.

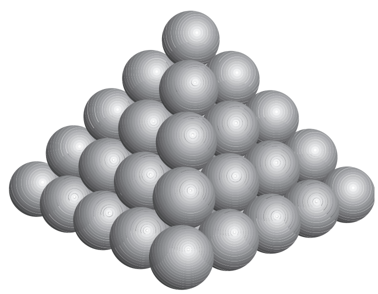

Figure 1.1: The face-centered cubic packing

The proof of this result is presented in this paper. Here, we describe the top-level outline of the proof and give references to the sources of the details of the proof.

An expository account of the proof is contained in [Hal00]. A general reference on sphere packings is [CS98]. A general discussion of the computer algorithms that are used in the proof can be found in [Hal03]. Some speculations on the structure of a second-generation proof can be found in [Hal01]. Details of computer calculations can be found on the internet at [Hal05].

The current paper presents an abridged form of the proof. The full proof appears in [Hal06a]. Samuel P. Ferguson has made important contributions to this proof. His University of Michigan thesis gives the proof of a difficult part of the proof [Fer97]. A key chapter (Chapter 5) of this paper is coauthored with Ferguson.

By a *packing*, we mean an arrangement of congruent balls that are nonoverlapping in the sense that the interiors of the balls are pairwise disjoint. Consider a packing of congruent balls in Euclidean three space. There is no harm in assuming that all the balls have unit radius. The density of a packing does not decrease when balls are added to the packing. Thus, to answer a question about the greatest possible density we may add nonoverlapping balls until there is no room to add further balls. Such a packing will be said to be *saturated*.

Let Λ be the set of centers of the balls in a saturated packing. Our choice of radius for the balls implies that any two points in Λ have distance at least 2 from each other. We call the points of Λ *vertices*. Let $B(x,r)$ denote the closed ball in Euclidean three space at center x and radius r. Let $\delta(x,r,\Lambda)$ be the finite density, defined as the ratio of the volume of $B(x,r,\Lambda)$ to the volume of $B(x,r)$, where $B(x,r,\Lambda)$ is defined as the intersection with $B(x,r)$ of the union of all balls in the packing. Set $\Lambda(x,r) = \Lambda \cap B(x,r)$.

Recall that the Voronoi cell $\Omega(v) = \Omega(v,\Lambda)$ around a vertex $v \in \Lambda$ is the set of points closer to v than to any other ball center. The volume of each Voronoi cell in the face-centered cubic packing is $\sqrt{32}$. This is also the volume of each Voronoi cell in the hexagonal-close packing.

Definition 1.2. Let $A : \Lambda \to \mathbb{R}$ be a function. We say that A is *negligible* if there is a constant C_1 such that for all $r \geq 1$ and all $x \in \mathbb{R}^3$,

$$\sum_{v \in \Lambda(x,r)} A(v) \leq C_1 r^2.$$

We say that the function $A : \Lambda \to \mathbb{R}$ is *fcc-compatible* if for all $v \in \Lambda$ we have the inequality

$$\sqrt{32} \leq \mathrm{vol}(\Omega(v)) + A(v).$$

The value $\mathrm{vol}(\Omega(v)) + A(v)$ may be interpreted as a *corrected* volume of the Voronoi cell. Fcc-compatibility asserts that the corrected volume of the Voronoi cell is always at least the volume of the Voronoi cells in the face-centered cubic and hexagonal-close packings.

Lemma 1.3. *If there exists a negligible* fcc-*compatible function* $A : \Lambda \to \mathbb{R}$ *for a saturated packing* Λ, *then there exists a constant* C *such that for all* $r \geq 1$ *and all* $x \in \mathbb{R}^3$,

$$\delta(x,r,\Lambda) \leq \pi/\sqrt{18} + C/r.$$

The constant C *depends on* Λ *only through the constant* C_1.

Proof. The numerator $\mathrm{vol}\, B(x,r,\Lambda)$ of $\delta(x,r,\Lambda)$ is at most the product of the volume of a ball $4\pi/3$ with the number $|\Lambda(x,r+1)|$ of balls intersecting $B(x,r)$. Hence

$$\mathrm{vol}\, B(x,r,\Lambda) \leq |\Lambda(x,r+1)| 4\pi/3. \tag{1.1}$$

In a saturated packing each Voronoi cell is contained in a ball of radius 2 centered at the *center* of the cell. The volume of the ball $B(x, r+3)$ is at least the combined volume of Voronoi cells whose center lies in the ball $B(x, r+1)$. This observation, combined with fcc-compatibility and negligibility, gives

$$\begin{aligned}\sqrt{32}|\Lambda(x,r+1)| &\le \sum_{v\in\Lambda(x,r+1)} (A(v) + \mathrm{vol}(\Omega(v)))\\ &\le C_1(r+1)^2 + \mathrm{vol}\, B(x, r+3)\\ &\le C_1(r+1)^2 + (1+3/r)^3 \mathrm{vol}\, B(x,r).\end{aligned} \tag{1.2}$$

Recall that $\delta(x, r, \Lambda) = \mathrm{vol}\, B(x, r, \Lambda)/\mathrm{vol}\, B(x, r)$. Divide Inequality 1.1 through by $\mathrm{vol}\, B(x, r)$. Use Inequality 1.2 to eliminate $|\Lambda(x, r+1)|$ from the resulting inequality. This gives

$$\delta(x, r, \Lambda) \le \frac{\pi}{\sqrt{18}}(1+3/r)^3 + C_1 \frac{(r+1)^2}{r^3\sqrt{32}}.$$

The result follows for an appropriately chosen constant C. □

An analysis of the preceding proof shows that fcc-compatibility leads to the particular value $\pi/\sqrt{18}$ in the statement of Lemma 1.3. If fcc-compatibility were to be dropped from the hypotheses, any negligible function A would still lead to an upper bound $4\pi/(3L)$ on the density of a packing, expressed as a function of a lower bound L on all $\mathrm{vol}\,\Omega(v) + A(v)$.

Remark 1.4. We take the precise meaning of the Kepler conjecture to be a bound on the essential supremum of the function $\delta(x, r, \Lambda)$ as r tends to infinity. Lemma 1.3 implies that the essential supremum of $\delta(x, r, \Lambda)$ is bounded above by $\pi/\sqrt{18}$, provided a negligible fcc-compatible function can be found. The strategy will be to define a negligible function, and then to solve an optimization problem in finitely many variables to establish that it is fcc-compatible.

Chapter 4 defines a compact topological space DS (the space of decomposition stars 4.2) and a continuous function σ on that space, which is directly related to packings.

If Λ is a saturated packing, then there is a geometric object $D(v, \Lambda)$ constructed around each vertex $v \in \Lambda$. $D(v, \Lambda)$ depends on Λ only through the vertices in Λ that are at most a constant distance away from v. That constant is independent of v and Λ. The objects $D(v, \Lambda)$ are called *decomposition stars*, and the space of all decomposition stars is precisely DS. Section 4.2 shows that the data in a decomposition star are sufficient to determine a Voronoi cell $\Omega(D)$ for each $D \in \mathrm{DS}$. The same section shows that the Voronoi cell attached to D is related to the Voronoi cell of v in the packing by relation

$$\mathrm{vol}\,\Omega(v) = \mathrm{vol}\,\Omega(D(v, \Lambda)).$$

Chapter 5 defines a continuous real-valued function $A_0 : \mathrm{DS} \to \mathbb{R}$ that assigns a "weight" to each decomposition star. The topological space DS embeds into a finite dimensional Euclidean space. The reduction from an infinite dimensional to a finite dimensional problem is accomplished by the following results.

THEOREM 1.5. *For each saturated packing* Λ, *and each* $v \in \Lambda$, *there is a decomposition star* $D(v, \Lambda) \in \mathrm{DS}$ *such that the function* $A : \Lambda \to \mathbb{R}$ *defined by*

$$A(v) = A_0(D(v, \Lambda))$$

is negligible for Λ.

This is proved as Theorem 5.11. The main object of the proof is then to show that the function A is fcc-compatible. This is implied by the inequality (in a finite number of variables)

$$\sqrt{32} \le \operatorname{vol}\Omega(D) + A_0(D), \tag{1.3}$$

for all $D \in \mathrm{DS}$.

In the proof it is convenient to reframe this optimization problem by composing it with a linear function. The resulting continuous function $\sigma : \mathrm{DS} \to \mathbb{R}$ is called the *scoring function*, or *score*.

Let δ_{tet} be the packing density of a regular tetrahedron. That is, let S be a regular tetrahedron of edge length 2. Let B be the part of S that lies within distance 1 of some vertex. Then δ_{tet} is the ratio of the volume of B to the volume of S. We have $\delta_{\mathrm{tet}} = \sqrt{8}\arctan(\sqrt{2}/5)$.

Let δ_{oct} be the packing density of a regular octahedron of edge length 2, again constructed as the ratio of the volume of points within distance 1 of a vertex to the volume of the octahedron.

The density of the face-centered cubic packing is a weighted average of these two ratios

$$\frac{\pi}{\sqrt{18}} = \frac{\delta_{\mathrm{tet}}}{3} + \frac{2\delta_{\mathrm{oct}}}{3}.$$

This determines the exact value of δ_{oct} in terms of δ_{tet}. We have $\delta_{\mathrm{oct}} \approx 0.72$.

In terms of these quantities,

$$\sigma(D) = -4\delta_{\mathrm{oct}}(\operatorname{vol}(\Omega(D)) + A_0(D)) + \frac{16\pi}{3}. \tag{1.4}$$

Definition 1.6. We define the constant

$$\mathrm{pt} = 4\arctan(\sqrt{2}/5) - \pi/3.$$

Its value is approximately $\mathrm{pt} \approx 0.05537$. Equivalent expressions for pt are

$$\mathrm{pt} = \sqrt{2}\delta_{\mathrm{tet}} - \frac{\pi}{3} = -2(\sqrt{2}\delta_{\mathrm{oct}} - \frac{\pi}{3}).$$

In terms of the scoring function σ, the optimization problem in a finite number of variables (Inequality 1.3) takes the following form. The proof of this inequality is a central concern in this paper.

THEOREM 1.7 (Finite dimensional reduction). *The maximum of σ on the topological space* DS *of all decomposition stars is the constant* $8\,\mathrm{pt} \approx 0.442989$.

Remark 1.8. The Kepler conjecture is an optimization problem in an infinite number of variables (the coordinates of the points of Λ). The maximization of σ on DS is an optimization problem in a finite number of variables. Theorem 1.7 may be viewed as a finite-dimensional reduction of the Kepler conjecture.

Let $t_0 = 1.255$ ($2t_0 = 2.51$). This is a parameter that is used for truncation throughout this paper.

Let $U(v, \Lambda)$ be the set of vertices in Λ at nonzero distance at most $2t_0$ from v. From v and a decomposition star $D(v, \Lambda)$ it is possible to recover $U(v, \Lambda)$, which we write as $U(D)$. We can completely characterize the decomposition stars at which the maximum of σ is attained.

THEOREM 1.9. *Let D be a decomposition star at which the function σ :* DS $\to \mathbb{R}$ *attains its maximum. Then the set $U(D)$ of vectors at distance at most $2t_0$ from the center has cardinality* 12. *Up to Euclidean motion, $U(D)$ is one of two arrangements: the kissing arrangement of the* 12 *balls around a central ball in the face-centered cubic packing or the kissing arrangement of* 12 *balls in the hexagonal-close packing.*

There is a complete description of all packings in which every sphere center is surrounded by 12 others in various combinations of these two patterns. All such packings are built from parallel layers of the A_2 lattice. (The A_2 lattice formed by equilateral triangles, is the optimal packing in two dimensions.) See [Hal06b].

1.2. *Basic concepts in the proof.* To prove Theorems 1.1, 1.7, and 1.9, we wish to show that there is no counterexample. In particular, we wish to show that there is no decomposition star D with value $\sigma(D) > 8\,\mathrm{pt}$. We reason by contradiction, assuming the existence of such a decomposition star. With this in mind, we call D a *contravening decomposition star*, if

$$\sigma(D) \geq 8\,\mathrm{pt}.$$

In much of what follows we will tacitly assume that every decomposition star under discussion is a contravening one. Thus, when we say that no decomposition stars exist with a given property, it should be interpreted as saying that no such contravening decomposition stars exist.

To each contravening decomposition star D, we associate a (combinatorial) plane graph $G(D)$. A restrictive list of properties of plane graphs is described in Section 7.3. Any plane graph satisfying these properties is said to be *tame.* All tame plane graphs have been classified. There are several thousand, up to isomorphism. The list appears in [Hal05]. We refer to this list as the *archival list* of plane graphs.

A few of the tame plane graphs are of particular interest. Every decomposition star attached to the face-centered cubic packing gives the same plane graph (up to isomorphism). Call it G_{fcc}. Likewise, every decomposition star attached to the hexagonal-close packing gives the same plane graph G_{hcp}.

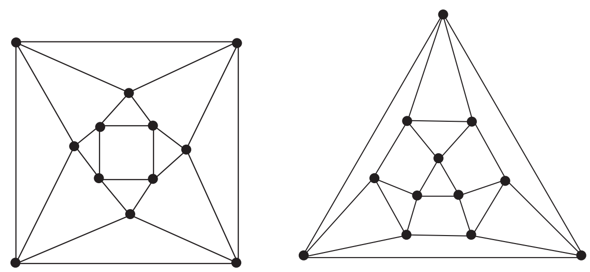

Figure 1.2: The plane graphs G_{fcc} and G_{hcp}

There is one more tame plane graph that is particularly troublesome. It is the graph G_{pent} obtained from the pictured configuration of twelve balls tangent to a given central ball (Figure 1.3). (Place a ball at the north pole, another at the south pole, and then form two pentagonal rings of five balls.) This case requires individualized attention. S. Ferguson proves the following theorem in his thesis [Fer97].

Theorem 1.10 (Ferguson). *There are no contravening decomposition stars D whose associated plane graph is isomorphic to G_{pent}.*

1.3. *Logical skeleton of the proof.* Consider the following six claims. Eventually we will give a proof of all six statements. First, we draw out some of their consequences. The main results (Theorems 1.1, 1.7, and 1.9) all follow from these claims.

Claim 1.11. *If the maximum of the function σ on* DS *is* $8\,\mathrm{pt}$, *then for every saturated packing Λ there exists a negligible* fcc-*compatible function A.*

Claim 1.12. *Let D be a contravening decomposition star. Then its plane graph $G(D)$ is tame.*

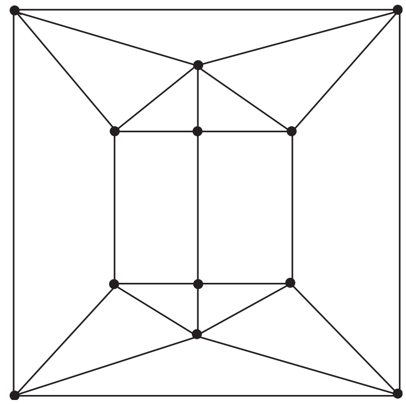

Figure 1.3: The plane graph G_{pent} of the pentahedral prism.

Claim 1.13. *If a plane graph is tame, then it is isomorphic to one of the several thousand plane graphs that appear in the archival list of plane graphs.*

Claim 1.14. *If the plane graph of a contravening decomposition star is isomorphic to one in the archival list of plane graphs, then it is isomorphic to one of the following three plane graphs:* G_{pent}, G_{hcp}, *or* G_{fcc}.

Claim 1.15. *There do not exist any contravening decomposition stars* D *whose associated graph is isomorphic to* G_{pent}.

Claim 1.16. *Contravening decomposition stars exist. If* D *is a contravening decomposition star, and if the plane graph of* D *is isomorphic to* G_{fcc} *or* G_{hcp}, *then* $\sigma(D) = 8\,\text{pt}$. *Moreover, up to Euclidean motion,* $U(D)$ *is the kissing arrangement of the* 12 *balls around a central ball in the face-centered cubic packing or the kissing arrangement of* 12 *balls in the hexagonal-close packing.*

Next, we state some of the consequences of these claims.

Lemma 1.17. *Assume Claims* 1.12, 1.13, 1.14, *and* 1.15. *If* D *is a contravening decomposition star, then its plane graph* $G(D)$ *is isomorphic to* G_{hcp} *or* G_{fcc}.

Proof. Assume that D is a contravening decomposition star. Then its plane graph is tame, and consequently appears on the archival list of plane graphs. Thus, it must be isomorphic to one of G_{fcc}, G_{hcp}, or G_{pent}. The final graph is ruled out by Claim 1.15. □

Lemma 1.18. *Assume Claims* 1.12, 1.13, 1.14, 1.15, *and* 1.16. *Then Theorem* 1.7 *holds.*

Proof. By Claim 1.16 and Lemma 1.17, the value 8 pt lies in the range of the function σ on DS. Assume for a contradiction that there exists a decomposition star $D \in \mathrm{DS}$ that has $\sigma(D) > 8\,\mathrm{pt}$. By definition, this is a contravening star. By Lemma 1.17, its plane graph is isomorphic to G_{hcp} or G_{fcc}. By Claim 1.16, $\sigma(D) = 8\,\mathrm{pt}$, in contradiction with $\sigma(D) > 8\,\mathrm{pt}$. □

LEMMA 1.19. *Assume Claims* 1.12, 1.13, 1.14, 1.15, *and* 1.16. *Then Theorem* 1.9 *holds.*

Proof. By Theorem 1.7, the maximum of σ on DS is 8 pt. Let D be a decomposition star at which the maximum 8 pt is attained. Then D is a contravening star. Lemma 1.17 implies that the plane graph is isomorphic to G_{hcp} or G_{fcc}. The hypotheses of Claim 1.16 are satisfied. The conclusion of Claim 1.16 is the conclusion of Theorem 1.9. □

LEMMA 1.20. *Assume Claims* 1.11–1.16. *Then the Kepler conjecture* (*Theorem* 1.1) *holds.*

Proof. As pointed out in Remark 1.4, the precise meaning of the Kepler conjecture is for every saturated packing Λ, the essential supremum of $\delta(x, r, \Lambda)$ is at most $\pi/\sqrt{18}$.

Let Λ be the set of centers of a saturated packing. Let $A : \Lambda \to \mathbb{R}$ be the negligible, fcc-compatible function provided by Claim 1.11 (and Lemma 1.18). By Lemma 1.3, the function A leads to a constant C such that for all $r \geq 1$ and all $x \in \mathbb{R}^3$, the density $\delta(x, r, \Lambda)$ satisfies

$$\delta(x, r, \Lambda) \leq \pi/\sqrt{18} + C/r.$$

This implies that the essential supremum of $\delta(x, r, \Lambda)$ is at most $\pi/\sqrt{18}$. □

Remark 1.21. One other theorem (Theorem 1.5) was stated without proof in Section 1.1. This result was placed there to motivate the other results. However, it is not an immediate consequence of Claims 1.11–1.16. Its proof appears in Theorem 5.11.

1.4. *Proofs of the central claims.* The previous section showed that the main results in the introduction (Theorems 1.1, 1.7, and 1.9) follow from six claims. This section indicates where each of these claims is proved, and mentions a few facts about the proofs.

Claim 1.11 is proved in Theorem 5.14. Claim 1.12 is proved in Theorem 9.20. Claim 1.13, the classification of tame graphs, is proved in Theorem 8.1. By the classification of such graphs, this reduces the proof of the Kepler conjecture to the analysis of the decomposition stars attached to the finite explicit list of tame plane graphs. We will return to Claim 1.14 in a moment. Claim 1.15 is Ferguson's thesis, cited as Theorem 1.10.

Claim 1.16 is the local optimality of the face-centered cubic and hexagonal close packings. In Chapter 6, the necessary local analysis is carried out to prove Claim 1.16 as Corollary 6.3.

Now we return to Claim 1.14. This claim is proved as Theorem 12.1. The idea of the proof is the following. Let D be a contravening decomposition star with graph $G(D)$. We assume that the graph $G(D)$ is not isomorphic to G_{fcc}, G_{hcp}, G_{pent} and then prove that D is not contravening. This is a case-by-case argument, based on the explicit archival list of plane graphs.

To eliminate these remaining cases, more-or-less generic arguments can be used. A linear program is attached to each tame graph G. The linear program can be viewed as a linear relaxation of the nonlinear optimization problem of maximizing σ over all decomposition stars with a given tame graph G. Because it is obtained by relaxing the constraints on the nonlinear problem, the maximum of the linear problem is an upper bound on the maximum of the original nonlinear problem. Whenever the linear programming maximum is less than 8 pt, it can be concluded that there is no contravening decomposition star with the given tame graph G. This linear programming approach eliminates most tame graphs.

When a single linear program fails to give the desired bound, it is broken into a series of linear programming bounds, by branch and bound techniques. For every tame plane graph G other than G_{hcp}, G_{fcc}, and G_{pent}, we produce a series of linear programs that establish that there is no contravening decomposition star with graph G.

The paper is organized in the following way. Chapters 2 through 5 introduce the basic definitions. Chapter 5 gives a proof of Claim 1.11. Chapter 6 proves Claim 1.16. Chapters 7 through 8 give a proof of Claim 1.13. Chapters 9 through 11 give a proof of Claim 1.12. Chapters 12 through 14 give a proof of Claim 1.14. Claim 1.15 (Ferguson's thesis) is to be published as a separate paper.

2. Construction of the Q-system

It is useful to separate the parts of space of relatively high packing density from the parts of space with relatively low packing density. The Q-system, which is developed in this chapter, is a crude way of marking off the parts of space where the density is potentially high. The Q-system is a collection of simplices whose vertices are points of the packing Λ. The Q-system is reminiscent of the Delaunay decomposition, in the sense of being a collection of simplices with vertices in Λ. In fact, the Q-system is the remnant of an earlier approach to the Kepler conjecture that was based entirely on the Delaunay decomposition (see [Hal93]). However, the Q-system differs from the Delaunay decomposition in crucial respects. The most fundamental difference is that the Q-system, while consisting of nonoverlapping simplices, does not partition all of space.

This chapter defines the set of simplices in the Q-system and proves that they do not overlap. In order to prove this, we develop a long series of lemmas that study the geometry of intersections of various edges and simplices. At the end of this chapter, we give the proof that the simplices in the Q-system do not overlap.

2.1. *Description of the Q-system.* Fix a packing of balls of radius 1. We identify the packing with the set Λ of its centers. A packing is thus a subset Λ of $\mathbb{R}^3$ such that for all $v, w \in \Lambda$, $|v - w| < 2$ implies $v = w$. The centers of the balls are called *vertices*. The term 'vertex' will be reserved for this technical usage. A packing is said to be *saturated* if for every $x \in \mathbb{R}^3$, there is some $v \in \Lambda$ such that $|x - v| < 2$. Any packing is a subset of a saturated packing. We assume that Λ is saturated. The set Λ is countably infinite.

Definition 2.1. We define the *truncation parameter* to be the constant $t_0 = 1.255$. It is used throughout. Informal arguments that led to this choice of constant are described in [Hal06a].

Precise constructions that rely on the truncation parameter t_0 will appear below. We will regularly intersect Voronoi cells with balls of radius t_0 to obtain lower bounds on their volumes. We will regularly disregard vertices of the packing that lie at distance greater than $2t_0$ from a fixed $v \in \Lambda$ to obtain a finite subset of Λ (a finite cluster of balls in the packing) that is easier to analyze than the full packing Λ.

The truncation parameter is the first of many decimal constants that appear. Each decimal constant is an exact rational value, e.g. $2t_0 = 251/100$. They are not to be regarded as approximations of some other value.

Definition 2.2. A *quasi-regular* triangle is a set $T \subset \Lambda$ of three vertices such that if $v, w \in T$ then $|w - v| \leq 2t_0$.

Definition 2.3. A simplex is a set of four vertices. A *quasi-regular* tetrahedron is a simplex S such that if $v, w \in S$ then $|w - v| \leq 2t_0$. A *quarter* is a simplex whose edge lengths $y_1, \ldots, y_6$ can be ordered to satisfy $2t_0 \leq y_1 \leq \sqrt{8}$, $2 \leq y_i \leq 2t_0$, $i = 2, \ldots, 6$. If a quarter satisfies the strict inequalities $2t_0 < y_1 < \sqrt{8}$, then we say that it is a strict quarter. We call the longest edge $\{v, w\}$ of a quarter its *diagonal*. When the quarter is strict, we also say that its diagonal is strict. When the quarter has a distinguished vertex, the quarter is *upright* if the distinguished vertex is an endpoint of the diagonal, and *flat* otherwise.

At times, we identify a simplex with its convex hull. We will say, for example, that the circumcenter of a simplex is contained in the simplex to mean that the circumcenter is contained in the convex hull of the four vertices.

Similar remarks apply to triangles, quasi-regular tetrahedra, quarters, and so forth. We will write $|S|$ for the convex hull of S when we wish to be explicit about the distinction between $|S|$ and its set of extreme points.

When we wish to give an order on an edge, triangle, simplex, etc. we present the object as an ordered tuple rather than a set. Thus, we refer to both $(v_1, \ldots, v_4)$ and $\{v_1, \ldots, v_4\}$ as simplices, depending on the needs of the given context.

Definition 2.4. Two manifolds with boundary *overlap* if their interiors intersect.

Definition 2.5. A set O of six vertices is called a *quartered octahedron*, if there are four pairwise nonoverlapping strict quarters $S_1, \ldots, S_4$ all having the same diagonal, such that O is the union of the four sets S_i of four vertices. (It follows easily that the strict quarters S_i can be given a cyclic order with respect to which each strict quarter S_i has a face in common with the next, so that a quartered octahedron is literally a octahedron that has been partitioned into four quarters.)

Remark 2.6. A quartered octahedron may have more than one diagonal of length less than $\sqrt{8}$, so its decomposition into four strict quarters need not be unique. The choice of diagonal has no particular importance. Nevertheless, to make things canonical, we pick the diagonal of length less than $\sqrt{8}$ with an endpoint of smallest possible value with respect to the lexicographical ordering on coordinates; that is, with respect to the ordering $(y_1, y_2, y_3) < (y'_1, y'_2, y'_3)$, if $y_i = y'_i$, for $i = 1, \ldots, k$, and $y_{k+1} < y'_{k+1}$. This selection rule for diagonals is fully translation invariant in the sense that if one octahedron is a translate of another (whether or not they belong to the same saturated packing), then the selected diagonal of one is a translate of the selected diagonal of the other.

Definition 2.7. If $\{v_1, v_2\}$ is an edge of length between $2t_0$ and $\sqrt{8}$, we say that a vertex v $(\neq v_1, v_2)$ is an *anchor* of $\{v_1, v_2\}$ if its distances to v_1 and v_2 are at most $2t_0$.

The two vertices of a quarter that are not on the diagonal are anchors of the diagonal, and the diagonal may have other anchors as well.

Definition 2.8. Let $\mathcal{Q}$ be the set of quasi-regular tetrahedra and strict quarters, enumerated as follows. This set is called the Q-system. It is canonically associated with a saturated packing Λ. (The Q stands for quarters and quasi-regular tetrahedra.)

1. All quasi-regular tetrahedra.

2. Every strict quarter such that none of the quarters along its diagonal overlaps any other quasi-regular tetrahedron or strict quarter.

3. Every strict quarter whose diagonal has four or more anchors, as long as there are not exactly four anchors arranged as a quartered octahedron.

4. The fixed choice of four strict quarters in each quartered octahedron.

5. Every strict quarter $\{v_1, v_2, v_3, v_4\}$ whose diagonal $\{v_1, v_3\}$ has exactly three anchors v_2, v_4, v_5 provided that the following hold (for some choice of indexing). (a) $\{v_2, v_5\}$ is a strict diagonal with exactly three anchors: v_1, v_3, v_4. (b) $d_{24}+d_{25} > \pi$, where d_{24} is the dihedral angle of the simplex $\{v_1, v_3, v_2, v_4\}$ along the edge $\{v_1, v_3\}$ and d_{25} is the dihedral angle of the simplex $\{v_1, v_3, v_2, v_5\}$ along the edge $\{v_1, v_3\}$.

No other quasi-regular tetrahedra or strict quarters are included in the Q-system $\mathcal{Q}$.

The following theorem is the main result of this chapter.

THEOREM 2.9. *For every saturated packing, there exists a uniquely determined Q-system. Distinct simplices in the Q-system have disjoint interiors.*

While proving the theorem, we give a complete classification of the various ways in which one quasi-regular tetrahedron or strict quarter can overlap another.

Having completed our primary purpose of showing that the simplices in the Q-system do not overlap, we state the following small lemma. It is an immediate consequence of the definitions, but is nonetheless useful in the chapters that follow.

LEMMA 2.10. *If one quarter along a diagonal lies in the Q-system, then all quarters along the diagonal lie in the Q-system.*

Proof. This is true by construction. Each of the defining properties of a quarter in the Q-system is true for one quarter along a diagonal if and only if it is true of all quarters along the diagonal. $\square$

2.2. *Geometric considerations.*

Remark 2.11. The primary definitions and constructions of this paper are translation invariant. That is, if $\lambda \in \mathbb{R}^3$ and Λ is a saturated packing, then $\lambda + \Lambda$ is a saturated packing. If $A : \Lambda \to \mathbb{R}$ is a negligible fcc-compatible function for Λ, then $\lambda + v \mapsto A(v)$ is a negligible fcc-compatible function for $\lambda+\Lambda$. If $\mathcal{Q}$ is the Q-system of Λ, then $\lambda+\mathcal{Q}$ is the Q-system of $\lambda+\Lambda$. Because of general translational invariance, when we fix our attention on a particular $v \in \Lambda$, we will often assume (without loss of generality) that the coordinate system is fixed in such a way that v lies at the origin.

Our simplices are generally assumed to come labeled with a distinguished vertex, fixed at the origin. (The origin will always be at a vertex of the packing.) We number the edges of each simplex $1, \ldots, 6$, so that edges 1, 2, and 3 meet at the origin, and the edges i and $i+3$ are opposite, for $i = 1, 2, 3$. (See Figure 2.1.) $S(y_1, y_2, \ldots, y_6)$ denotes a simplex whose edges have lengths y_i, indexed in this way. We refer to the endpoints away from the origin of the first, second, and third edges as the first, second, and third vertices.

Definition 2.12. In general, let $\mathrm{dih}(S)$ be the dihedral angle of a simplex S along its first edge. When we write a simplex in terms of its vertices (w_1, w_2, w_3, w_4), then $\{w_1, w_2\}$ is understood to be the first edge.

Definition 2.13. We define the *radial projection* of a set X to be the radial projection $x \mapsto x/|x|$ of $X \setminus 0$ to the unit sphere centered at the origin. We say the two sets *cross* if their radial projections to the unit sphere overlap.

Definition 2.14. If S and S' are nonoverlapping simplices with a shared face F, we define $\mathcal{E}(S, S')$ as the distance between the two vertices (one on S and the other on S') that do not lie on F. We may express this as a function

$$\mathcal{E}(S, S') = \mathcal{E}(S(y_1, \ldots, y_6), y_1', y_2', y_3')$$

of nine variables, where $S = S(y_1, \ldots, y_6)$ and $S' = S(y_1', y_2', y_3', y_4, y_5, y_6)$, positioned so that S and S' are nonoverlapping simplices with a shared face F of edge-lengths (y_4, y_5, y_6). The function of nine variables is defined only for values (y_i, y_i') for which the simplices S and S' exist (Figure 2.1).

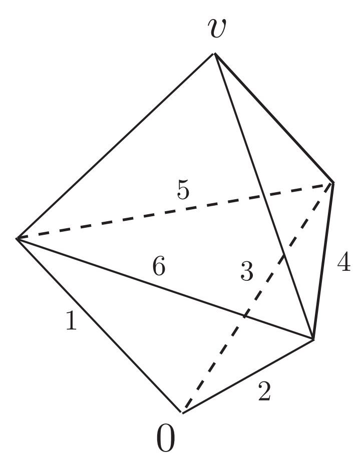

Figure 2.1: $\mathcal{E}$ measures the distance between the vertices at 0 and v. The standard indexing of the edges of a simplex is marked on the lower simplex.

Several lemmas in this paper rely on calculations of lower bounds to the function $\mathcal{E}$ in the special case when the edge between the vertices 0 and v passes through the shared face F. If intervals containing $y_1, \ldots, y_6, y_1', y_2', y_3'$ are given, then lower bounds on $\mathcal{E}$ over that domain are generally easy to obtain. Detailed examples of calculations of the lower bound of this function can be found in [Hal97a, §4].

To work one example, we suppose we are asked to give a lower bound on $\mathcal{E}$ when the simplex $S = S(y_1, \ldots, y_6)$ satisfies $y_i \ge 2$ and $y_4, y_5, y_6 \le 2t_0$ and $S' = S(y_1', y_2', y_3', y_4, y_5, y_6)$ satisfies $y_i' \ge 2$, for $i = 1, \ldots, 3$. Assume that the edge $\{0, v\}$ passes through the face shared between S and S', and that $|v| < \sqrt{8}$, where v is the vertex of S' that is not on S. We claim that any pair S, S' can be deformed by moving one vertex at a time until S is deformed into $S(2,2,2,2t_0,2t_0,2t_0)$ and S' is deformed into $S(2,2,2,2t_0,2t_0,2t_0)$. Moreover, these deformations preserve the constraints (including that $\{0, v\}$ passes through the shared face), and are non-increasing in $|v|$. From the existence of this deformation, it follows that the original $|v|$ satisfies

$$|v| \ge \mathcal{E}(S(2,2,2,2t_0,2t_0,2t_0), 2, 2, 2).$$

We produce the deformation in this case as follows. We define the *pivot* of a vertex v with respect to two other vertices $\{v_1, v_2\}$ as the circular motion of v held at a fixed distance from v_1 and v_2, leaving all other vertices fixed. The *axis* of the pivot is the line through the two fixed vertices. Each pivot of a vertex can move in two directions. Let the vertices of S be $\{0, v_1, v_2, v_3\}$, labeled so that $|v_i| = y_i$. Let $S' = \{v, v_1, v_2, v_3\}$. We pivot v_1 around the axis through 0 and v_2. By choice of a suitable direction for the pivot, v_1 moves away from v and v_3. Its distance to 0 and v_2 remains fixed. We continue with this circular motion until $|v_1 - v_3|$ achieves its upper bound or the segment $\{v_1, v_3\}$ intersects the segment $\{0, v\}$ (which threatens the constraint that the segment $\{0, v\}$ must pass through the common face). (We leave it as an exercise[1] to check that the second possibility cannot occur because of the edge length upper bounds on both diagonals of $\sqrt{8}$. That is, there does not exist a convex planar quadrilateral with sides at least 2 and diagonals less than $\sqrt{8}$.) Thus, $|v_1 - v_3|$ attains its constrained upper bound $2t_0$. Similar pivots to v_2 and v_3 increase the lengths $|v_1 - v_2|$, $|v_2 - v_3|$, and $|v_3 - v_1|$ to $2t_0$. Similarly, v may be pivoted around the axis through v_1 and v_2 so as to decrease the distance to v_3 and 0 until the lower bound of 2 on $|v - v_3|$ is attained. Further pivots reduce all remaining edge lengths to 2. In this way, we obtain a rigid figure realizing the absolute lower bound of $|v|$. A calculation with explicit coordinates gives $|v| > 2.75$.

[1]Compare Lemma 2.21.

Because lower bounds are generally easily determined from a series of pivots through arguments such as this one, we will state them without proof. We will state that these bounds were obtained by *geometric considerations*, to indicate that the bounds were obtained by the deformation arguments of this paragraph.

2.3. *Incidence relations.*

LEMMA 2.15. *Let v, v_1, v_2, v_3, and v_4 be distinct points in $\mathbb{R}^3$ with pairwise distances at least 2. Suppose that $|v_i - v_j| \le 2t_0$ for $i \ne j$ and $\{i, j\} \ne \{1, 4\}$. Then v does not lie in the convex hull of $\{v_1, v_2, v_3, v_4\}$.*

Proof. This lemma is proved in [Hal97a, Lemma 3.5]. □

LEMMA 2.16. *Let S be a simplex whose edges have length between 2 and $2\sqrt{2}$. Suppose that v has distance at least 2 from each of the vertices of S. Then v does not lie in the convex hull of S.*

Proof. Assume for a contradiction that v lies in the convex hull of S. Place a unit sphere around v. The simplex S partitions the unit sphere into four spherical triangles, where each triangle is the intersection of the unit sphere with the cone over a face of S, centered at v. By the constraints on the lengths of edges, the arclength of each edge of the spherical triangle is at most $\pi/2$. ($\pi/2$ is attained when v has distance 2 to two of the vertices, and these two vertices have distance $2\sqrt{2}$ between them.) A spherical triangle with edges of arclength at most $\pi/2$ has area at most $\pi/2$. In fact, any such spherical triangle can be placed inside an octant of the unit sphere, and each octant has area $\pi/2$. This partitions the sphere of area 4π into four regions of area at most $\pi/2$. This is absurd. □

COROLLARY 2.17. *No vertex of the packing is contained in the convex hull of a quasi-regular tetrahedron or quarter* (*other than the vertices of the simplex*).

Proof. The corollary is immediate. □

Definition 2.18. Let $v_1, v_2, w_1, w_2, w_3 \in \Lambda$ be distinct. We say that an edge $\{v_1, v_2\}$ *passes through* the triangle $\{w_1, w_2, w_3\}$ if the convex hull of $\{v_1, v_2\}$ meets some point of the convex hull of $\{w_1, w_2, w_3\}$ and if that point of intersection is not any of the extreme points v_1, v_2, w_1, w_2, w_3.

LEMMA 2.19. *An edge of length $2t_0$ or less cannot pass through a triangle whose edges have lengths $2t_0$, $2t_0$, and $\sqrt{8}$ or less.*

Proof. The distance between each pair of vertices is at least 2. Geometric considerations show that the edge has length at least

$$\mathcal{E}(S(2,2,2,2t_0,2t_0,\sqrt{8}),2,2,2) > 2t_0. \qquad \square$$

Definition 2.20. Let $\eta(x,y,z)$ denote the circumradius of a triangle with edge-lengths x, y, and z.

LEMMA 2.21. *Suppose that the circumradius of* $\{v_1,v_2,v_3\}$ *is less than* $\sqrt{2}$. *Then an edge* $\{w_1,w_2\}\subset\Lambda$ *of length at most* $\sqrt{8}$ *cannot pass through the face.*

Proof. Assume for a contradiction that $\{w_1,w_2\}$ passes through the triangle $\{v_1,v_2,v_3\}$. By geometric considerations, the minimal length for $\{w_1,w_2\}$ occurs when $|w_i - v_j| = 2$, for $i = 1,2$, $j = 1,2,3$. This distance constraint places the circumscribing circle of $\{v_1,v_2,v_3\}$ on the sphere of radius 2 centered at w_1 (resp. w_2). If $r < \sqrt{2}$ is the circumradius of $\{v_1,v_2,v_3\}$, then for this extremal configuration we have the contradiction

$$\sqrt{8} \geq |w_1 - w_2| = 2\sqrt{4-r^2} > \sqrt{8}. \qquad \square$$

LEMMA 2.22. *If an edge of length at most* $\sqrt{8}$ *passes through a quasi-regular triangle, then each of the two endpoints of the edge is at most* 2.2 *away from each of the vertices of the triangle* (*see Figure* 2.2).

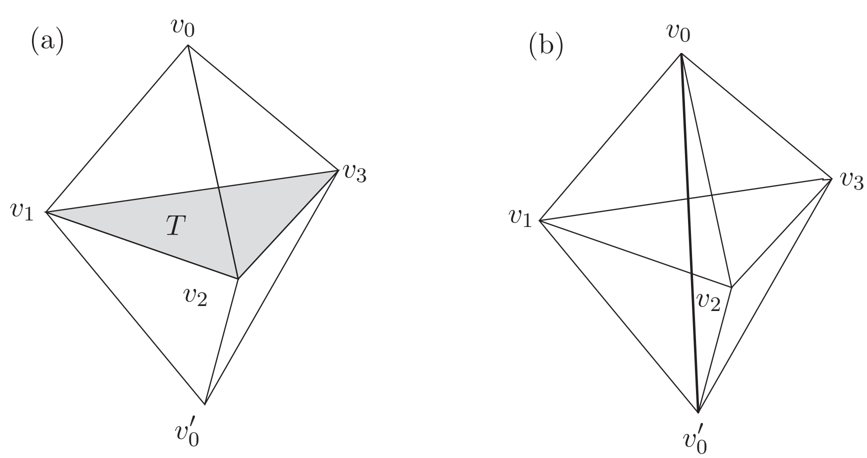

Figure 2.2: Frame (a) depicts two quasi-regular tetrahedra that share a face. The same convex body may also be viewed as three quarters that share a diagonal, as in Frame (b).

Proof. Let the diagonal edge be $\{v_0, v_0'\}$ and the vertices of the face be $\{v_1, v_2, v_3\}$. If $|v_i - v_0| > 2.2$ or $|v_i - v_0'| > 2.2$ for some $i > 0$, then geometric considerations give the contradiction

$$|v_0 - v_0'| \geq \mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 2t_0), 2, 2, 2.2) > \sqrt{8}. \qquad \square$$

LEMMA 2.23. *Suppose S and S' are quasi-regular tetrahedra that share a face. Suppose that the edge e between the two vertices that are not shared has length at most $\sqrt{8}$. Then the convex hull of S and S' consists of three quarters with diagonal e. No other quarter overlaps S or S'.*

Proof. Suppose that S and S' are adjacent quasi-regular tetrahedra with a common face F. By the Lemma 2.22, each of the six external faces of this pair of quasi-regular tetrahedra has circumradius at most $\eta(2.2, 2.2, 2t_0) < \sqrt{2}$. A diagonal of a quarter cannot pass through a face of this size by Lemma 2.21. This implies that no other quarter overlaps these quasi-regular tetrahedra. $\square$

LEMMA 2.24. *Suppose an edge $\{w_1, w_2\}$ of length at most $\sqrt{8}$ passes through the face formed by a diagonal $\{v_1, v_2\}$ and one of its anchors. Then w_1 and w_2 are also anchors of $\{v_1, v_2\}$.*

Proof. This follows from the inequality

$$\mathcal{E}(S(2, 2, 2, \sqrt{8}, 2t_0, 2t_0), 2, 2, 2t_0) > \sqrt{8}$$

and geometric considerations. $\square$

Definition 2.25. Let Λ be a saturated packing. Assume that the coordinate system is fixed in such a way that the origin is a vertex of the packing. The *height* of a vertex is its distance from the origin.

Definition 2.26. We say that a vertex is *enclosed* over a figure if it lies in the interior of the cone at the origin generated by the figure.

Definition 2.27. An *adjacent pair of quarters* consists of two quarters sharing a face along a common diagonal. The common vertex that does not lie on the diagonal is called the *base point* of the adjacent pair. (When one of the quarters comes with a marked distinguished vertex, we do *not* assume that this marked vertex coincides with the base point of the pair.) The other four vertices are called the *corners* of the configuration.

Definition 2.28. If the two corners, v and w, that do not lie on the diagonal satisfy $|w - v| < \sqrt{8}$, then the base point and four corners can be considered as an adjacent pair in a second way, where $\{v, w\}$ functions as the diagonal. In this case we say that the original diagonal and the diagonal $\{v, w\}$ are *conflicting diagonals.*

Definition 2.29. A quarter is said to be *isolated* if it is not part of an adjacent pair. Two isolated quarters that overlap are said to form an *isolated pair*.

LEMMA 2.30. *Suppose that there exist four nonzero vertices* $v_1, \ldots, v_4$ *of height at most* $2t_0$ (*that is,* $|v_i| \le 2t_0$) *forming a skew quadrilateral. Suppose that the diagonals* $\{v_1, v_3\}$ *and* $\{v_2, v_4\}$ *have lengths between* $2t_0$ *and* $\sqrt{8}$. *Suppose the diagonals* $\{v_1, v_3\}$ *and* $\{v_2, v_4\}$ *cross. Then the four vertices are the corners of an adjacent pair of quarters with base point at the origin.*

Proof. Set $d_1 = |v_1 - v_3|$ and $d_2 = |v_2 - v_4|$. By hypothesis, d_1 and d_2 are at most $\sqrt{8}$. If $|v_1 - v_2| > 2t_0$, geometric considerations give the contradiction

$$\max(d_1, d_2) \ge \mathcal{E}(S(2t_0, 2, 2, 2t_0, \sqrt{8}, 2t_0), 2, 2, 2) > \sqrt{8} \ge \max(d_1, d_2).$$

Thus, $\{0, v_1, v_2\}$ is a quasi-regular triangle, as are $\{0, v_2, v_3\}$, $\{0, v_3, v_4\}$, and $\{0, v_4, v_1\}$ by symmetry. □

LEMMA 2.31. *If, under the same hypotheses as Lemma* 2.30, *there is a vertex* w *of height at most* $\sqrt{8}$ *enclosed over the adjacent pair of quarters, then* $\{0, v_1, \ldots, v_4, w\}$ *is a quartered octahedron.*

Proof. If the enclosed w lies over say $\{0, v_1, v_2, v_3\}$, then $|w - v_1|$, $|w - v_3| \le 2t_0$ (Lemma 2.24), where $\{v_1, v_3\}$ is a diagonal. Similarly, the distance from w to the other two corners is at most $2t_0$. □

LEMMA 2.32. *Let* v_1 *and* v_2 *be anchors of* $\{0, w\}$ *with* $2t_0 \le |w| \le \sqrt{8}$. *If an edge* $\{v_3, v_4\}$ *passes through both faces,* $\{0, w, v_1\}$ *and* $\{0, w, v_2\}$, *then* $|v_3 - v_4| > \sqrt{8}$.

Proof. Suppose the figure exists with $|v_3 - v_4| \le \sqrt{8}$. Label vertices so v_3 lies on the same side of the figure as v_1. Contract $\{v_3, v_4\}$ by moving v_3 and v_4 until $\{v_i, u\}$ has length 2, for $u = 0, w, v_{i-2}$, and $i = 3, 4$. Pivot w away from v_3 and v_4 around the axis $\{v_1, v_2\}$ until $|w| = \sqrt{8}$. Contract $\{v_3, v_4\}$ again. By stretching $\{v_1, v_2\}$, we obtain a square of edge two and vertices $\{0, v_3, w, v_4\}$. Short calculations based on explicit formulas for the dihedral angle and its partial derivatives give

$$\mathrm{dih}(S(\sqrt{8}, 2, y_3, 2, y_5, 2)) > 1.075, \quad y_3, y_5 \in [2, 2t_0], \tag{2.1}$$

$$\mathrm{dih}(S(\sqrt{8}, y_2, y_3, 2, y_5, y_6)) > 1, \quad y_2, y_3, y_5, y_6 \in [2, 2t_0]. \tag{2.2}$$

Then

$$\pi \ge \mathrm{dih}(0, w, v_3, v_1) + \mathrm{dih}(0, w, v_1, v_2) + \mathrm{dih}(0, w, v_2, v_4) > 1.075 + 1 + 1.075 > \pi.$$

Therefore, the figure does not exist. □

LEMMA 2.33. *Two vertices w, w' of height at most $\sqrt{8}$ cannot be enclosed over a triangle $\{v_1, v_2, v_3\}$ satisfying $|v_1 - v_2| \le \sqrt{8}$, $|v_1 - v_3| \le 2t_0$, and $|v_2 - v_3| \le 2t_0$.*

Proof. For a contradiction, assume the figure exists. The long edge $\{v_1, v_2\}$ must have length at least $2t_0$ by Lemma 2.22. This diagonal has anchors $\{0, v_3, w, w'\}$. Assume that the cyclic order of vertices around the line $\{v_1, v_2\}$ is $0, v_3, w, w'$. We see that $\{v_1, w\}$ is too short to pass through $\{0, v_2, w'\}$, and w is not inside the simplex $\{0, v_1, v_2, w'\}$. Thus, the projections of the edges $\{v_2, w\}$ and $\{0, w'\}$ to the unit sphere at v_1 must intersect. It follows that $\{0, w'\}$ passes through $\{v_1, v_2, w\}$, or $\{v_2, w\}$ passes through $\{v_1, 0, w'\}$. But $\{v_2, w\}$ is too short to pass through $\{v_1, 0, w'\}$. Thus, $\{0, w'\}$ passes through both $\{v_1, v_2, w\}$ and $\{v_1, v_2, v_3\}$. Lemma 2.32 gives the contradiction $|w'| > \sqrt{8}$. □

LEMMA 2.34. *Let v_1, v_2, v_3 be anchors of $\{0, w\}$, where $2t_0 \le |w| \le \sqrt{8}$, $|v_1 - v_3| \le \sqrt{8}$, and the edge $\{v_1, v_3\}$ passes through the face $\{0, w, v_2\}$. Then $\min(|v_1 - v_2|, |v_2 - v_3|) \le 2t_0$. Furthermore, if the minimum is $2t_0$, then $|v_1 - v_2| = |v_2 - v_3| = 2t_0$.*

Proof. Assume $\min \ge 2t_0$. As in the proof of Lemma 2.32, we may assume that $(0, v_1, w, v_3)$ is a square. We may also assume, without loss of generality, that $|w - v_2| = |v_2| = 2t_0$. This forces $|v_2 - v_i| = 2t_0$, for $i = 1, 3$. This is rigid, and is the unique figure that satisfies the constraints. The lemma follows. □

2.4. *Overlap of simplices.* This section gives a proof of Theorem 2.9 (simplices in the Q-system do not overlap). This is accomplished in a series of lemmas. The first of these treats quasi-regular tetrahedra.

LEMMA 2.35. *A quasi-regular tetrahedron does not overlap any other simplex in the Q-system.*

Proof. Edges of quasi-regular tetrahedra are too short to pass through the face of another quasi-regular tetrahedron or quarter (Lemma 2.19). If a diagonal of a strict quarter passes through the face of a quasi-regular tetrahedron, then Lemma 2.23 shows that the strict quarter is one of three joined along a common diagonal. This is not one of the enumerated types of strict quarter in the Q-system. □

LEMMA 2.36. *A quarter in the Q-system that is part of a quartered octahedron does not overlap any other simplex in the Q-system.*

Proof. By construction, the quarters that lie along a different diagonal of the octahedron do not belong to the Q-system. Edges of length at most $2t_0$ are too short to pass through an external face of the octahedron (Lemma 2.19).

A diagonal of a strict quarter cannot pass through an external face either, because of Lemma 2.22. □

LEMMA 2.37. *Let Q be a strict quarter that is part of an adjacent pair. Assume that Q is not part of a quartered octahedron. If Q belongs to the Q-system, then it does not overlap any other simplex in the Q-system.*

The proof of this lemma will give valuable details about how one strict quarter overlaps another.

Proof. Fix the origin at the base point of an adjacent pair of quarters. We investigate the local geometry when another quarter overlaps one of them. (This happens, for example, when there is a conflicting diagonal in the sense of Definition 2.27.)

Label the base point of the pair of quarters v_0, and the four corners v_1, v_2, v_3, v_4, with $\{v_1, v_3\}$ the common diagonal. Assume that $|v_1 - v_3| < \sqrt{8}$.

If two quarters overlap then a face on one of them overlaps a face on the other. By Lemmas 2.33 and 2.32, we actually have that some edge (in fact the diagonal) of each passes through a face of the other. This edge cannot exit through another face by Lemma 2.32 and it cannot end inside the simplex by Corollary 2.17. Thus, it must end at a vertex of the other simplex. We break the proof into cases according to which vertex of the simplex it terminates at. In Case 1, the edge has the base point as an endpoint. In Case 2, the edge has a corner as an endpoint.

Case 1. The edge $\{0, w\}$ passes through the triangle $\{v_1, v_2, v_3\}$, where $\{0, w\}$ is a diagonal of a strict quarter.

Lemma 2.24 implies that v_1 and v_3 are anchors of $\{0, w\}$. The only other possible anchors of $\{0, w\}$ are v_2 or v_4, for otherwise an edge of length at most $2t_0$ passes through a face formed by $\{0, w\}$ and one of its anchors. If both v_2 and v_4 are anchors, then we have a quartered octahedron, which has been excluded by the hypotheses of the lemma. Otherwise, $\{0, w\}$ has at most 3 anchors: v_1, v_3, and either v_2 or v_4. In fact, it must have exactly three anchors, for otherwise there is no quarter along the edge $\{0, w\}$. So there are exactly two quarters along the edge $\{0, w\}$. There are at least four anchors along $\{v_1, v_3\}$: 0, w, v_2, and v_4. The quarters along the diagonal $\{v_1, v_3\}$ lie in the Q-system. (None of these quarters is isolated.) The other two quarters, along the diagonal $\{0, w\}$, are not in the Q-system. They form an adjacent pair of quarters (with base point v_4 or v_2) that has conflicting diagonals, $\{0, w\}$ and $\{v_1, v_3\}$, of length at most $\sqrt{8}$.

Case 2. $\{v_2, v_4\}$ is a diagonal of length less than $\sqrt{8}$ (conflicting with $\{v_1, v_3\}$).

(Note that if an edge of a quarter passes through the shared face of an adjacent pair of quarters, then that edge must be $\{v_2, v_4\}$, so that Case 1 and Case 2 are exhaustive.) The two diagonals $\{v_1, v_3\}$ and $\{v_2, v_4\}$ do not overlap. By symmetry, we may assume that $\{v_2, v_4\}$ passes through the face $\{0, v_1, v_3\}$. Assume (for a contradiction) that both diagonals have an anchor other than 0 and the corners v_i. Let the anchor of $\{v_2, v_4\}$ be denoted v_{24} and that of $\{v_1, v_3\}$ be v_{13}. Assume the figure is not a quartered octahedron, so that $v_{13} \neq v_{24}$. By Lemma 2.19, it is impossible to draw the edges $\{v_1, v_{13}\}$ and $\{v_{13}, v_3\}$ between v_1 and v_3. In fact, if the edges pass outside the quadrilateral $\{0, v_2, v_{24}, v_4\}$, one of the edges of length at most $2t_0$ (that is, $\{0, v_2\}$, $\{v_2, v_{24}\}$, $\{v_{24}, v_4\}$, or $\{v_4, 0\}$) violates the lemma applied to the face $\{v_1, v_3, v_{13}\}$. If they pass inside the quadrilateral, one of the edges $\{v_1, v_{13}\}$, $\{v_{13}, v_3\}$ violates the lemma applied to the face $\{0, v_2, v_4\}$ or $\{v_{24}, v_2, v_4\}$. We conclude that at most one of the two diagonals has additional anchors.

If neither of the two diagonals has more than three anchors, we have nothing more than two overlapping adjacent pairs of quarters along conflicting diagonals. The two quarters along the lower edge $\{v_2, v_4\}$ lie in the Q-system. Another way of expressing this "lower-edge" condition is to require that the two adjacent quarters Q_1 and Q_2 satisfy $\mathrm{dih}(Q_1) + \mathrm{dih}(Q_2) > \pi$, when the dihedral angles are measured along the diagonal. The pair (Q_1', Q_2') along the upper edge will have $\mathrm{dih}(Q_1') + \mathrm{dih}(Q_2') < \pi$.

If there is a diagonal with more than three anchors, the quarters along the diagonal with more than three anchors lie in the Q-system. Any additional quarters along the diagonal $\{v_2, v_4\}$ belong to an adjacent pair. Any additional quarters along the diagonal $\{v_1, v_3\}$ cannot intersect the adjacent pair along $\{v_2, v_4\}$. Thus, every quarter intersecting an adjacent pair also belongs to an adjacent pair.

In both possibilities of Case 2, the two quarters left out of the Q-system correspond to a conflicting diagonal. □

Remark 2.38. We have seen in the proof of Lemma 2.37 that if a strict quarter Q overlaps a strict quarter that is part of an adjacent pair, then Q is also part of an adjacent pair. Thus, if an isolated strict quarter overlaps another strict quarter, then both strict quarters are necessarily isolated.

LEMMA 2.39. *If an isolated strict quarter Q overlaps another strict quarter, then the diagonal of Q has exactly three anchors.*

The proof of the lemma will give detailed information about the geometrical configuration that is obtained when an isolated quarter overlaps another strict quarter.

Proof. Assume that there are two strict quarters Q_1 and Q_2 that overlap. Following Remark 2.38, assume that neither is adjacent to another quarter.

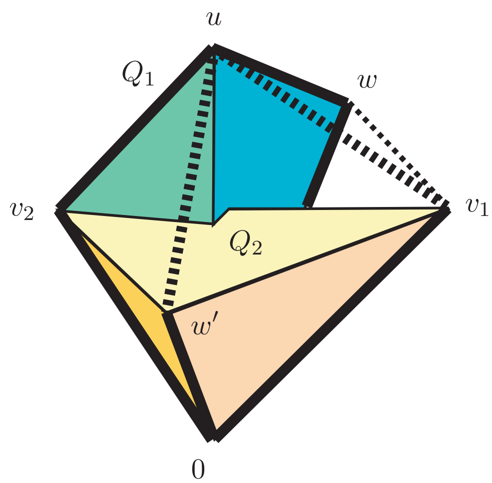

Figure 2.3: An isolated pair. The isolated pair consists of two simplices $Q_1 = \{0, u, w, v_2\}$ and $Q_2 = \{0, w', v_1, v_2\}$. The six extremal vertices form an octahedron. This is not a quartered octahedron because the edges $\{u, w'\}$ and $\{w, v_1\}$ have length greater than $2t_0$.

Let $\{0, u\}$ and $\{v_1, v_2\}$ be the diagonals of Q_1 and Q_2. Suppose the diagonal $\{v_1, v_2\}$ passes through a face $\{0, u, w\}$ of Q_1. By Lemma 2.24, v_1 and v_2 are anchors of $\{0, u\}$. Again, either the length of $\{v_1, w\}$ is at most $2t_0$ or the length of $\{v_2, w\}$ is at most $2t_0$, say $\{w, v_2\}$ (by Lemma 2.34). It follows that $Q_1 = \{0, u, w, v_2\}$ and $|v_1 - w| \geq 2t_0$. (Q_1 is not adjacent to another quarter.) So w is not an anchor of $\{v_1, v_2\}$.

Let $\{v_1, v_2, w'\}$ be a face of Q_2 with $w' \neq 0, u$. If $\{v_1, w', v_2\}$ does not link $\{0, u, w\}$, then $\{v_1, w'\}$ or $\{v_2, w'\}$ passes through the face $\{0, u, w\}$, which is impossible by Lemma 2.19. So $\{v_1, v_2, w'\}$ links $\{0, u, w\}$ and an edge of $\{0, u, w\}$ passes through the face $\{v_1, v_2, w'\}$. It is not the edge $\{u, w\}$ or $\{0, w\}$, for they are too short by Lemma 2.19. So $\{0, u\}$ passes through $\{w', v_1, v_2\}$. The only anchors of $\{v_1, v_2\}$ (other than w') are u and 0 (by Lemma 2.32). Either $\{u, w'\}$ or $\{w', 0\}$ has length at most $2t_0$ by Lemma 2.34, but not both, because this would create a quarter adjacent to Q_2. By symmetry, $Q_2 = \{v_1, v_2, w', 0\}$ and the length of $\{u, w'\}$ is greater than $2t_0$. By symmetry, $\{0, u\}$ has no other anchors either. This determines the local geometry when there are two quarters that intersect without belonging to an adjacent pair of quarters (see Figure 2.3). It follows that the two quarters form an isolated pair. □

Isolated quarters that overlap another strict quarter do not belong to the Q-system.

We conclude with the proof of the main theorem of the chapter.

Proof of Theorem 2.9. The rules defining the Q-system specify a uniquely determined set of simplices. The proof that they do not overlap is established by the preceding series of lemmas. Lemma 2.35 shows that quasi-regular tetrahedra do not overlap other simplices in the Q-system. Lemma 2.36 shows that the quarters in quartered octahedra are well-behaved. Lemma 2.37 shows that other quarters in adjacent pairs do not overlap other simplices in the Q-system. Finally, we treat isolated quarters in Lemma 2.39. These cases cover all possibilities since every simplex in the Q-system is a quasi-regular tetrahedron or strict quarter, and every strict quarter is either part of an adjacent pair or isolated. □

3. V-cells

In the proof of the Kepler conjecture we make use of two quite different structures in space. The first structure is the Q-system, which was defined in the previous chapter. It is inspired by the Delaunay decomposition of space and consists of a nonoverlapping collection of simplices that have their vertices at the points of Λ. Historically, the construction of the nonoverlapping simplices of the Q-system grew out of a detailed investigation of the Delaunay decomposition.

The second structure is inspired by the Voronoi decomposition of space. In the Voronoi decomposition, the vertices of Λ are the centers of the cells. It is well known that the Voronoi decomposition and Delaunay decomposition are dual to one another. Our modification of Voronoi cells will be called V-cells.

In general, it is not true that a Delaunay simplex is contained in the union of the Voronoi cells at its four vertices. This incompatibility of structures adds a few complications to Rogers's elegant proof of a sphere packing bound [Rog58]. In this chapter, we show that V-cells are compatible with the Q-system in the sense that each simplex in the Q-system is contained in the union of the V-cells at its four vertices (Lemma 3.28). A second compatibility result between these two structures is proved in Lemma 3.29.

The purpose of this chapter is to define V-cells and to prove the compatibility results just mentioned. In the proof of the Kepler conjecture it will be important to keep both structures (the Q-system and the V-cells) continually at hand. We will frequently jump back and forth between these dual descriptions of space in the course of the proof. In Chapter 4, we define a geometric object (called the decomposition star) around a vertex that encodes both structures. The decomposition star will become our primary object of analysis.

3.1. *V-cells.*

Definition 3.1. The Voronoi cell $\Omega(v)$ around a vertex $v \in \Lambda$ is the set of points closer to v than to any other vertex.

Definition 3.2. We construct a set of triangles $\mathcal{B}$ in the packing. The triangles in this set will be called *barriers*. A triangle $\{v_1, v_2, v_3\}$ with vertices in the packing belongs to $\mathcal{B}$ if and only if one or more of the following properties hold.

1. The triangle is a quasi-regular, or

2. The triangle is a face of a simplex in the Q-system.

LEMMA 3.3. *No two barriers overlap; that is, no two open triangular regions of* $\mathcal{B}$ *intersect.*

Proof. If there is overlap, an edge $\{w_1, w_2\}$ of one triangle passes through the interior of another $\{v_1, v_2, v_3\}$. Since $|w_1 - w_2| < \sqrt{8}$, we have that the circumradius of $\{v_1, v_2, v_3\}$ is at least $\sqrt{2}$ by Lemma 2.21 and that the length $|w_1 - w_2|$ is greater than $2t_0$ by Lemma 2.19. If the edge $\{w_1, w_2\}$ belongs to a simplex in the Q-system, the simplex must be a strict quarter. If $\{v_1, v_2, v_3\}$ has edge lengths at most $2t_0$, then Lemma 2.22 implies that $|w_i - v_j| \le 2.2$ for $i = 1, 2$ and $j = 1, 2, 3$. The simplices $\{v_1, v_2, v_3, w_1\}$ and $\{v_1, v_2, v_3, w_2\}$ form a pair of quasi-regular tetrahedra. We conclude that $\{v_1, v_2, v_3\}$ is a face of a quarter in the Q-system. Since, the simplices in the Q-system do not overlap, the edge $\{w_1, w_2\}$ does not belong to a simplex in the Q-system. The result follows. □

Definition 3.4. We say that a point y is *obstructed* at $x \in \mathbb{R}^3$ if the line segment from x to y passes through the interior of a triangular region in $\mathcal{B}$. Otherwise, y is unobstructed at x. The 'obstruction' relation between x and y is clearly symmetric.

For each $w \in \Lambda$, let I_w be the cube of side 4, with edges parallel to the coordinate axes, centered at w. Thus,

$$I_0 = \{(y_1, y_2, y_3) : |y_i| \le 2, \quad i = 1, 2, 3\}.$$

I_w has diameter $4\sqrt{3}$ and $I_w \subset B(w, 2\sqrt{3})$. Let $\mathbb{R}^{3\prime}$ be the subset of $x \in \mathbb{R}^3$ for which x is not equidistant from any two $v, w \in \Lambda(x, 2\sqrt{3}) = B(x, 2\sqrt{3}) \cap \Lambda$. The subset $\mathbb{R}^{3\prime}$ is dense in $\mathbb{R}^3$, and is obtained locally around a point x by removing finitely many planes (perpendicular bisectors of $\{v, w\}$, for $v, w \in B(x, 2\sqrt{3})$). For $x \in \mathbb{R}^{3\prime}$, the vertices of $\Lambda(x, 2\sqrt{3})$ can be strictly ordered by their distance to x.

Definition 3.5. Let Λ be a saturated packing. We define a map $\phi : \mathbb{R}^{3\prime} \to \Lambda$ such that the image of x lies in $\Lambda(x, 2\sqrt{3})$. If $x \in \mathbb{R}^{3\prime}$, let

$$\Lambda_x = \{w \in \Lambda : x \in I_w \text{ and } w \text{ is unobstructed at } x\}.$$

If $\Lambda_x = \emptyset$, then let $\phi(x)$ be the vertex of $\Lambda(x, 2\sqrt{3})$ closest to x. (Since Λ is saturated, $\Lambda(x, 2\sqrt{3})$ is nonempty.) If Λ_x is nonempty, then let $\phi(x)$ be the vertex of Λ_x closest to x.

Definition 3.6. For $v \in \Lambda$, let $\mathrm{VC}(v)$ be defined as the closure of $\phi^{-1}(v)$ in $\mathbb{R}^3$. We call it the *V-cell* at v.

Remark 3.7. In a saturated packing, the Voronoi cell at v will be contained in a ball centered at v of radius 2. Hence I_v contains the Voronoi cell at v. By construction, the V-cell at v is confined to the cube I_v. The cubes I_v were introduced into the definition of ϕ with the express purpose of forcing V-cells to be reasonably small. Had the cubes been omitted from the construction, we would have been drawn to frivolous questions such as whether the closest unobstructed vertex to some $x \in \mathbb{R}^3$ might be located in a remote region of the packing.

The set of V-cells is our promised decomposition of space.

LEMMA 3.8. *V-cells cover space. The interiors of distinct V-cells are disjoint. Each V-cell is the closure of its interior.*

Proof. The sets $\phi^{-1}(v)$, for $v \in \Lambda$, cover $\mathbb{R}^{3\prime}$. Their closures cover $\mathbb{R}^3$. The other statements in the lemma will follow from the fact that a V-cell is a union of finitely many nonoverlapping, closed, convex polyhedra. This is proved below in Lemma 3.9. □

LEMMA 3.9. *Each V-cell is a finite union of nonoverlapping convex polyhedra.*

Proof. During this proof, we ignore sets of measure zero in $\mathbb{R}^3$ such as finite unions of planes. Thus, we present the proof as if each point belongs to exactly one Voronoi cell, although this fails on an inconsequential set of measure zero in $\mathbb{R}^3$.

It is enough to show that if $E \subset \mathbb{R}^3$ is an arbitrary unit cube, then the V-cell decomposition of space within E consists of finite unions of nonoverlapping convex polyhedra. Let X_E be the set of $w \in \Lambda$ such that I_w meets E. Included in X_E is the set of w whose Voronoi cells cover E. The rules for V-cells assign $x \in E$ to the V-cell centered at some $w \in X_E$.

Let d be an upper bound on the distance between a vertex in X_E and a point of E. By the pythagorean theorem, we may take $d = (1+2)\sqrt{3}$. Let B_E be the set of barriers with a vertex at most distance d from some point in E.

For each pair $\{u, v\}$ of distinct vertices of X_E, draw the perpendicular bisecting plane of $\{u, v\}$. Draw the plane through each barrier in B_E. Draw the plane through each triple $\{u, v, w\}$, where $u \in X_E$ and $\{v, w\}$ are two of the vertices of a barrier in B_E. These finitely many planes partition E into finitely many convex polyhedra. The ranking of distances from x to the points of X_E is constant for all x in the interior of any fixed polyhedron. The set of $w \in X_E$ that are obstructed at x is constant on the interior of any fixed polyhedron. Thus, by the rules of construction of V-cells, for each of these convex polyhedra, there is a V-cell that contains it. The result follows. □

Remark 3.10. A number of readers of the first version of this manuscript presumed that V-cells were necessarily star-convex, in large part because of the inapt name *'decomposition star'* for a closely related object. The geometry of a V-cell is significantly more complex than that of a Voronoi cell. Nowhere do we make a general claim that all V-cells are convex, star-convex, or even connected. In Figure 3.1, we depict a hypothetical case in which the V-cell at v is potentially disconnected. (This figure is merely hypothetical, because I have not checked whether it is possible to satisfy all the metric constraints needed for it to exist.) The shaded triangle represents a barrier. The point x is obstructed by the shaded barrier at w. If x and y lie closer to w than to v, if v is the closest unobstructed vertex to x, if w is the closest unobstructed vertex to y, if x, y, and z are all unobstructed at v, and if z lies closer to v than to w, then it follows that x and z lie in the V-cell at v, but that the intervening point y does not. Thus, if all of these conditions are satisfied, the V-cell at v is not star-shaped at v.

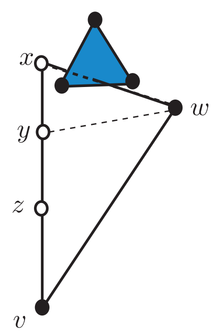

Figure 3.1: A hypothetical arrangement that leads to a nonconvex V-cell at v.

Remark 3.11. Although we have not made a detailed investigation of the subtleties of the geometry of V-cells, we face a practical need to give explicit lower bounds on the volume of V-cells. Possible geometric pathologies are avoided in the proof by the use of truncation. (To obtain lower bounds on the volume of V-cells, parts of the V-cell can be discarded.) For example, Lemma 3.23 shows that inside $B(v, t_0)$, the V-cell and the Voronoi cell are equal.

In general, truncation will discard points x of V-cells where $\Lambda_x = \emptyset$. These estimates also discard points of the V-cell that are not part of a star-shaped subset of the V-cell. (This star-shaped region is not made explicit in this paper. It is discussed in detail in [Hal06a].)

Truncation will be justified later in Lemma 5.18, which shows that the term involving the volume of V-cells in the scoring function σ has a negative coefficient, so that by decreasing the volume through truncation, we obtain an upper bound on the function σ.

3.2. *Orientation.* We introduce the concept of the orientation of a simplex and study its basic properties. The orientation of a simplex will be used to establish various compatibilities between V-cells.

Definition 3.12. We say that the *orientation* of the face of a simplex is *negative* if the plane through that face separates the circumcenter of the simplex from the vertex of the simplex that does not lie on the face. The orientation is positive if the circumcenter and the vertex lie on the same side of the plane. The orientation is zero if the circumcenter lies in the plane.

LEMMA 3.13. *At most one face of a quarter Q has negative orientation.*

Proof. The proof applies to any simplex with nonobtuse faces. (All faces of a quarter are acute.) Fix an edge and project Q orthogonally to a triangle in a plane perpendicular to that edge. The faces F_1 and F_2 of Q along the edge project to edges e_1 and e_2 of the triangular projection of Q. The line equidistant from the three vertices of F_i projects to a line perpendicular to e_i, for $i = 1, 2$. These two perpendiculars intersect at the projection of the circumcenter of Q. If the faces of Q are nonobtuse, the perpendiculars pass through the segments e_1 and e_2 respectively; and the two faces F_1 and F_2 cannot both be negatively oriented. □

Definition 3.14. Define the polynomial χ by

$$\begin{aligned}\chi(x_1,\ldots,x_6) &= x_1x_4x_5 + x_1x_6x_4 + x_2x_6x_5 + x_2x_4x_5 + x_5x_3x_6 \\ &\quad + x_3x_4x_6 - 2x_5x_6x_4 - x_1x_4^2 - x_2x_5^2 - x_3x_6^2.\end{aligned}$$

In applications of χ, we have $x_i = y_i^2$, where $(y_1,\ldots,y_6)$ are the lengths of the edges of a simplex.

LEMMA 3.15. *A simplex $S(y_1,\ldots,y_6)$ has negative orientation along the face indexed by* $(4,5,6)$ *if and only if* $\chi(y_1^2,\ldots,y_6^2) < 0$.

Proof. (This lemma is asserted without proof in [Hal97a].) Let $x_i = y_i^2$. Represent the simplex as $S = \{0, v_1, v_2, v_3\}$, where $\{0, v_i\}$ is the ith edge. Write $n = (v_1 - v_3) \times (v_2 - v_3)$, a normal to the plane $\{v_1, v_2, v_3\}$. Let c be the circumcenter of S. We can solve for a unique $t \in \mathbb{R}$ such that $c + t\, n$ lies in the plane $\{v_1, v_2, v_3\}$. The sign of t gives the orientation of the face $\{v_1, v_2, v_3\}$. We find by direct calculation that

$$t = \frac{\chi(x_1, \ldots, x_6)}{\sqrt{\Delta(x_1, \ldots, x_6)}u(x_4, x_5, x_6)},$$

where the terms Δ and u in the denominator are positive whenever $x_i = y_i^2$, where $(y_1, \ldots, y_6)$ are the lengths of edges of a simplex (see [Hal97a, §8.1]). Thus, t and χ have the same sign. The result follows. □

Lemma 3.16. *Let F be a set of three vertices. Assume that one edge between pairs of vertices has length between $2t_0$ and $\sqrt{8}$ and that the other two edges have length at most $2t_0$. Let v be any vertex not on Q. If the simplex (F, v) has negative orientation along F, then it is a quarter.*

Proof. The orientation of F is determined by the sign of the function χ (see Lemma 3.15). The face F is an acute or right triangle. Note that $\partial\chi/\partial x_1 = x_4(-x_4 + x_5 + x_6)$. By the law of cosines, $-x_4 + x_5 + x_6 \geq 0$ for an acute triangle. Thus, we have monotonicity in the variable x_1, and the same is true of x_2, and x_3. Also, χ is quadratic with negative leading coefficient in each of the variables x_4, x_5, x_6. Thus, to check positivity, when any of the lengths is greater than $2t_0$, it is enough to evaluate

$$\chi(2^2, 2^2, 4t_0^2, x^2, y^2, z^2), \quad \chi(2^2, 4t_0^2, 2^2, x^2, y^2, z^2), \quad \chi(4t_0^2, 2^2, 2^2, x^2, y^2, z^2),$$

for $x \in [2, 2t_0]$, $y \in [2, t_0]$, and $z \in [2t_0, \sqrt{8}]$, and verify that these values are nonnegative. (The minimum, which must be attained at a corner of the domain, is 0.) □

Lemma 3.17. *Let $\{v_1, v_2, v_3\}$ be a quasi-regular triangle. Let v be any other vertex. If the simplex $S = \{v, v_1, v_2, v_3\}$ has negative orientation along $\{v_1, v_2, v_3\}$, then S is a quasi-regular tetrahedron and $|v - v_i| < 2t_0$.*

Proof. The proof is similar to the proof of Lemma 3.16. It comes down to checking that

$$\chi(2^2, 2^2, 4t_0^2, x^2, y^2, z^2) > 0,$$

for $x, y, z \in [2, 2t_0]$. □

Lemma 3.18. *If a face of a simplex has circumradius less than $\sqrt{2}$, then the orientation is positive along that face.*

Proof. If the face has circumradius less than $\sqrt{2}$, by monotonicity

$$\chi(y_1^2, \ldots, y_6^2) \geq \chi(4, 4, 4, y_4^2, y_5^2, y_6^2) = 2y_4^2y_5^2y_6^2(2/\eta(y_4, y_5, y_6)^2 - 1) > 0.$$

(Here y_i are the edge-lengths of the simplex.) □

3.3. *Interaction of V-cells with the Q-system.* We study the structure of one V-cell, which we take to be the V-cell at the origin $v = 0$. Let $\mathcal{Q}$ be the set of simplices in the Q-system. For $v \in \Lambda$, let $\mathcal{Q}_v$ be the subset of those with a vertex at v.

LEMMA 3.19. *If x lies in the* (*open*) *Voronoi cell at the origin, but not in the V-cell at the origin, then there exists a simplex $Q \in \mathcal{Q}_0$, such that x lies in the cone* (*at* 0) *over Q. Moreover, x does not lie in the interior of Q.*

Proof. If x lies in the open Voronoi cell at the origin, then the segment $\{t\,x : 0 \le t \le 1\}$ lies in the Voronoi cell as well. By the definition of V-cell, there is a barrier $\{v_1, v_2, v_3\}$ that the segment passes through. If the simplex $Q = \{0, v_1, v_2, v_3\}$ were to have positive orientation with respect to the face $\{v_1, v_2, v_3\}$, then the circumcenter of $\{0, v_1, v_2, v_3\}$ would lie on the same side of the plane $\{v_1, v_2, v_3\}$ as 0, forcing the intersection of the Voronoi cell with the cone over Q to lie in this same half space. But, by assumption, x is a point of the Voronoi cell in the opposing half space. Hence, the simplex Q has negative orientation along $\{v_1, v_2, v_3\}$.

By construction, the barriers are acute or right triangles. The function χ (which gives the sign of the orientations of faces) is monotonic in x_1, x_2, x_3 when these come from simplices (see the proof of Lemma 3.16). We consider the implications of negative orientation for each kind of barrier. If the barrier is a quasi-regular triangle, then Lemma 3.17 gives that Q is a quasi-regular tetrahedron when $\chi < 0$. If the barrier is a face of a flat quarter in the Q-system, then Lemma 3.16 gives that Q is a flat-quarter in the Q-system as well. Hence $Q \in \mathcal{Q}_0$.

The rest is clear. □

LEMMA 3.20. *If x lies in the open ball of radius $\sqrt{2}$ at the origin, and if x is not in the closed cone over any simplex in $\mathcal{Q}_0$, then the origin is unobstructed at x.*

Proof. Assume for a contradiction that the origin is obstructed by the barrier $T = \{u, v, w\}$ at x, and $\{0, u, v, w\}$ is not in $\mathcal{Q}_0$. We show that every point in the convex hull of T has distance at least $\sqrt{2}$ from the origin. Since T is a barrier, each edge $\{u, v\}$ has length at most $\sqrt{8}$. Moreover, the heights $|u|$ and $|v|$ are at least 2, so that every point along each edge of T has distance at least $\sqrt{2}$ from the origin. Suppose that the closest point to the origin in the convex hull of T is an interior point p. Reflect the origin through the plane of T to get w'. The assumptions imply that the edge $\{0, w'\}$ passes through the barrier T and has length less than $\sqrt{8}$. If the barrier T is a quasi-regular triangle, then Lemma 2.22 implies that $\{0, u, v, w\}$ is a quasi-regular tetrahedron in $\mathcal{Q}_0$, which is contrary to the hypothesis. Hence T is the face of a quarter in $\mathcal{Q}_0$. By

Lemma 2.34, one of the simplices $\{0, u, v, w\}$ or $\{w', u, v, w\}$ is a quarter. Since these are mirror images, both are quarters. Hence $\{0, u, v, w\}$ is a quarter and it is in the Q-system by Lemma 2.10. This contradicts the hypothesis of the lemma. □

The following corollary is a V-cell analogue of a standard fact about Voronoi cells.

COROLLARY 3.21. *The V-cell at the origin contains the open unit ball at the origin.*

Proof. Let x lie in the open unit ball at the origin. If it is not in the cone over any simplex, then the origin is unobstructed by the lemma, and the origin is the closest point of Λ. Hence $x \in \mathrm{VC}(0)$. A point in the cone over a simplex $\{0, v_1, v_2, v_3\} \in \mathcal{Q}_0$ lies in $\mathrm{VC}(0)$ if and only if it lies in the set bounded by the perpendicular bisectors of v_i and the plane through $\{v_1, v_2, v_3\}$. The bisectors pose no problem. It is elementary to check that every point of the convex hull of $\{v_1, v_2, v_3\}$ has distance at least 1 from the origin. (Apply the reflection principle as in the proof of Lemma 3.20 and invoke Lemma 2.19.) □

LEMMA 3.22. *If $x \in B(v, t_0)$, then x is unobstructed at v.*

Proof. For a contradiction, supposed that the barrier T obstructs x from the v. As in the proof of Lemma 3.20, we find that every edge of T has distance at least $\sqrt{2}$ from the v. We may assume that the point of T that is closest to the origin is an interior point. Let w be the reflection of v through T. By Lemma 2.19, we have $|v - w| > 2t_0$. This implies that every point of T has distance at least t_0 from v. Thus T cannot obstruct $x \in B(0, t_0)$ from v. □

LEMMA 3.23. *Inside the ball of radius t_0 at the origin, the V-cell and Voronoi cell coincide*:

$$B(0, t_0) \cap \mathrm{VC}(0) = B(0, t_0) \cap \Omega(0).$$

Proof. Let $x \in B(0, t_0) \cap \mathrm{VC}(0) \cap \Omega(v)$, where $v \neq 0$. By Lemma 3.22, the origin is unobstructed at x. Thus, $|x - v| \leq |x| \leq t_0$. By Lemma 3.22 again, v is unobstructed at x, so that $x \in \mathrm{VC}(v)$, contrary to the assumption $x \in \mathrm{VC}(0)$. Thus $B(0, t_0) \cap \mathrm{VC}(0) \subset \Omega(0)$. Similarly, if $x \in B(0, t_0) \cap \Omega(0)$, then x is unobstructed at the origin, and $x \in \mathrm{VC}(0)$. □

Definition 3.24. For every pair of vertices v_1, v_2 such that $\{0, v_1, v_2\}$ is a quasi-regular triangle, draw a geodesic arc on the unit sphere with endpoints at the radial projections of v_1 and v_2. These arcs break the unit sphere into regions called *standard regions*, as follows. Take the complement of the union of arcs inside the unit sphere. The closure of a connected component of this complement is a standard region. We say that the standard region is triangular if it is bounded by three geodesic arcs, and say that it is non-triangular otherwise.

LEMMA 3.25. *Let v_1, v_2, v_3, and v_4 be distinct vertices such that $|v_i| \le 2t_0$ for $i = 1, 2, 3, 4$ and $|v_1 - v_3|, |v_2 - v_4| \le 2t_0$. Then the edges $\{v_1, v_3\}$ and $\{v_2, v_4\}$ do not cross. In particular, the arcs of Definition* 3.24 *do not meet except at endpoints.*

Proof. Exchanging $(1, 3)$ with $(2, 4)$ if necessary, we may assume for a contradiction that the edge $\{v_1, v_3\}$ passes through the face $\{0, v_2, v_4\}$. Geometric considerations lead immediately to a contradiction

$$2t_0 < \mathcal{E}(2, 2, 2, 2t_0, 2t_0, 2t_0, 2, 2, 2) \le |v_1 - v_3| \le 2t_0. \qquad \square$$

LEMMA 3.26. *Each simplex in the Q-system with a vertex at the origin lies entirely in the closed cone over some standard region R.*

Proof. Assume for a contradiction that $Q = \{0, v_1, v_2, v_3\}$ with v_1 in the open cone over R_1 and with v_2 in the open cone over R_2. Then $\{0, v_1, v_2\}$ and $\{0, w_1, w_2\}$ (a wall between R_1 and R_2) overlap; this is contrary to Lemma 3.3. $\square$

Remark 3.27. The next two lemmas help to determine which V-cell a given point x belongs to. If x lies in the open cone over a simplex Q_0 in $\mathcal{Q}$, then Lemma 3.28 describes the V-cell decomposition inside Q; beyond Q the origin is obstructed by a face of Q, so that such x do not lie in the V-cell at 0. If x does not lie in the open cone over a simplex in $\mathcal{Q}$, but lies in the open cone over a standard region R, then Lemma 3.29 describes the V-cell. It states in particular, that for unobstructed x, it can be determined whether x belongs to the V-cell at the origin by considering only the vertices w that lie in the closed cone over R (the standard region containing the radial projection of x). In this sense, the intersection of a V-cell with the open cone over R is *local* to the cone over R.

LEMMA 3.28. *If x lies in the interior of a simplex $Q \in \mathcal{Q}$, and if it does not lie on the perpendicular bisector of any edge of Q, then it lies in the V-cell of the closest vertex of Q.*

Proof. The segment to any other vertex v crosses a face of the simplex. Such faces are barriers so that v is obstructed at x. Thus, the vertices of Q are the only vertices that are not obstructed at x. $\square$

Let $\mathcal{B}'_0$ be the set of triangles T such that one of the following holds:

- T is a barrier at the origin, or

- $T = \{0, v, w\}$ consists of a diagonal of a quarter in the Q-system together with one of its anchors.

LEMMA 3.29 (Decoupling Lemma). *Let $x \in I_0$, the cube of side 4 centered at the origin parallel to coordinate axes. Assume that the closed segment $\{x, w\}$ intersects the closed 2-dimensional cone with center 0 over $F = \{0, v_1, v_2\}$, where $F \in \mathcal{B}'_0$. Assume that the origin is not obstructed at x. Assume that x is closer to the origin than to both v_1 and v_2. Then $x \notin \mathrm{VC}(w)$.*

Remark 3.30. The Decoupling Lemma is a crucial result. It permits estimates of the scoring function in Chapter 5 to be made separately for each standard region. The estimates for separate standard regions are far easier to come by than estimates for the score of the full decomposition star. Eventually, the separate estimates for each standard will be reassembled with linear programming techniques in Chapter 12.

Proof. (This proof is a minor adaptation of [Hal97b, Lemma 2.2].) Assume for a contradiction that x lies in $\mathrm{VC}(w)$. In particular, we assume that w is not obstructed at x. Since the origin is not obstructed at x, w must be closer to x than x is to the origin: $x \cdot w \geq w \cdot w/2$. The line segment from x to w intersects the closed cone $C(F)$ of the triangle $F = \{0, v_1, v_2\}$.

Consider the set X containing x and bounded by the planes H_1 through $\{0, v_1, w\}$, H_2 through $\{0, v_2, w\}$, H_3 through $\{0, v_1, v_2\}$, $H_4 = \{x : x \cdot v_1 = v_1 \cdot v_1/2\}$, and $H_5 = \{x : x \cdot v_2 = v_2 \cdot v_2/2\}$. The planes H_4 and H_5 contain the faces of the Voronoi cell at 0 defined by the vertices v_1 and v_2. The plane H_3 contains the triangle F. The planes H_1 and H_2 bound the set containing points, such as x, that can be connected to w by a segment that passes through $C(F)$.

Let $P = \{x : x \cdot w > w \cdot w/2\}$. The choice of w implies that $X \cap P$ is nonempty. We leave it as an exercise to check that $X \cap P$ is bounded. If the intersection of a bounded polyhedron with a half-space is nonempty, then some vertex of the polyhedron lies in the half-space. Thus, some vertex of X lies in P.

We claim that the vertex of X lying in P cannot lie on H_1. To see this, pick coordinates (x_1, x_2) on the plane H_1 with origin $v_0 = 0$ so that $v_1 = (0, z)$ (with $z > 0$) and $X \cap H_1 \subset X' := \{(x_1, x_2) : x_1 \geq 0,\ x_2 \leq z/2\}$. See Figure 3.2. If the quadrant X' meets P, then the point $v_1/2$ lies in P. This is impossible, because every point between 0 and v_1 lies in the Voronoi cell at 0 or v_1, and not in the Voronoi cell of w. (Recall that for every vertex v_1 on a barrier at the origin, $|v_1| < \sqrt{8}$.)

Similarly, the vertex of X in P cannot lie on H_2. Thus, the vertex must be the unique vertex of X that is not on H_1 or H_2, namely, the point of intersection of H_3, H_4, and H_5. This point is the circumcenter c of the face F.

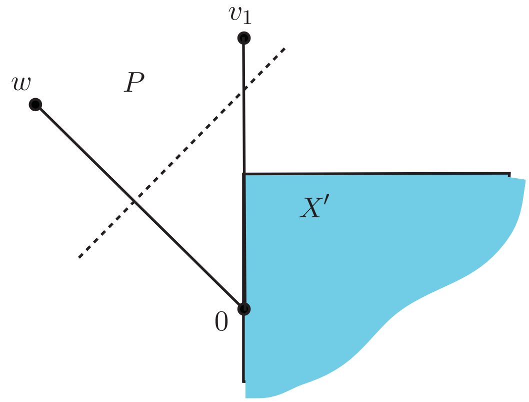

Figure 3.2: The perpendicular bisector to $\{0, w\}$ (dashed line) cannot meet the quadrant X' (shaded).

We conclude that the polyhedron $X_0 := X \cap P$ contains c. Since $c \in X_0$, the simplex $S = \{w, v_1, v_2, 0\}$ has nonpositive orientation along the face $\{0, v_1, v_2\}$. By Lemmas 3.16 and 3.17, the simplex S lies in $\mathcal{Q}_0$.

Let c be the circumcenter of the triangle $F = \{0, v_1, v_2\}$ and let c_2 be the circumcenter of the simplex $\{0, v_1, v_2, w\}$. Let C be the convex hull of $\{0, v_1/2, v_2/2, c, c_2\}$. The set C contains the set of points separated from w by the half-plane H_3, closer to w than to 0, and closer to 0 than to both v_1 and v_2. The point x lies in this convex hull C. Since this convex hull is nonempty, the simplex S has negative orientation along the face $\{0, v_1, v_2\}$.

By assumption, w is not obstructed at x. Hence the segment from w to x does not pass through the face $\{0, v_1, v_2\}$. The set C' of points $y \in C$ such that the segment from w to y does not pass through the face $\{0, v_1, v_2\}$ is thus nonempty. The set C' must include the extreme point c_2 of C. This means that the plane $\{w, v_1, v_2\}$ separates c_2 from the origin, so that the simplex S has negative orientation also along the face $\{w, v_1, v_2\}$. This contradicts Lemma 3.13. □

4. Decomposition stars

This chapter constructs a topological space DS such that each point of DS encodes the geometrical data surrounding a vertex in the packing. The points in this topological space are called decomposition stars. A decomposition star encodes all of the local geometrical information that will be needed in the local analysis of a sphere packing. These geometrical data are sufficiently detailed that it is possible to recover the V-cell at $v \in \Lambda$ from the corresponding point in the topological space. It is also possible to recover the simplices in the Q-system that have a vertex at $v \in \Lambda$. Thus, a decomposition star has a dual nature that encompasses both the Voronoi-like V-cell and the Delaunay-like simplices in the Q-system. By encoding both structures, the decomposition star becomes our primary geometric object of analysis.

It can be helpful at times to visualize the decomposition star as a polyhedral object formed by the union of the simplices at v in the Q-system with the V-cell at $v \in \Lambda$. Although such descriptions can be helpful to the intuition, the formal definition of a decomposition star is rather more combinatorial, expressed as a series of indexing sets that hold the data that are needed to reconstruct the geometry. The formal description of the decomposition star is preferred because it encodes more information than the polyhedral object.

The term "decomposition star" is derived from the earlier term "Delaunay star" that was used in [Hal93] as the name for the union of Delaunay simplices that shared a common vertex. Delaunay stars are star-convex. It is perhaps unfortunate that the term "star" has been retained, because (the geometric realization of) a decomposition star need not be star convex. In fact, Remark 3.10 suggests that V-cells can be rather poorly behaved in this respect.

4.1. *Indexing sets.* We are ready for the formal description of decomposition stars.

Let $\omega = \{0, 1, 2 \dots\}$. Pick a bijection $b : \omega \to \Lambda$ and use this bijection to index the vertices $b(i) = v_i \in \Lambda$, $i = 0, 1, 2 \dots$. Define the following indexing sets.

- Let $I_1 = \omega$.
- Let I_2 be the set of unordered pairs of indices $\{i, j\}$ such that $|v_i - v_j| \leq 2t_0 = 2.51$.
- Let I_3 be the set of unordered tuples of indices $\{i, j, k, \ell\}$ such that the corresponding simplex is a strict quarter.
- Let I_4 be the set of unordered tuples $\{i, j, k, \ell\}$ of indices such that the simplex $\{v_i, v_j, v_k, v_\ell\}$ is in the Q-system.
- Let I_5 be the set of unordered triples $\{i, j, k\}$ of indices such that v_i is an anchor of a diagonal $\{v_j, v_k\}$ of a strict quarter in the Q-system.
- Let I_6 be the set of unordered pairs $\{i, j\}$ of indices such that the edge $\{v_i, v_j\}$ has length in the open interval $(2t_0, \sqrt{8})$. (This set includes all such pairs, whether or not they are attached to the diagonal of a strict quarter.)
- Let I_7 be the set of unordered triples $\{i, j, k\}$ of indices such that the triangle $\{v_i, v_j, v_k\}$ is a face of a simplex in the Q-system and such that the circumradius is less than $\sqrt{2}$.

- Let I_8 be the set of unordered quadruples $\{i, j, k, \ell\}$ of indices such that the corresponding simplex $\{v_i, v_j, v_k, v_\ell\}$ is a quasi-regular tetrahedron with circumradius less than 1.41.

The data are highly redundant, because some of the indexing sets can be derived from others. But there is no need to strive for a minimal description of the data.

Set $d_0 = 2\sqrt{2} + 4\sqrt{3}$. We recall that $\Lambda(v, d_0) = \{w \in \Lambda : |w - v| \le d_0\}$. Let

$$T' = \{i : v_i \in \Lambda(v, d_0)\}.$$

It is the indexing set for a neighborhood of v.

Fix a vertex $v = v_a \in \Lambda$. Let $I'_0 = \{\{a\}\}$. Let

$$I'_j = \{x \in I_j : x \subset T'\}, \text{ for } 1 \le j \le 8.$$

Each I'_j is a finite set of finite subsets of ω. Hence $I'_j \in P(P(\omega))$, where $P(X)$ is the powerset of any set X.

Associate with each $v \in \Lambda$ the function $f : T' \to B(0, d_0)$ given by $f(i) = v_i - v$, and the tuple

$$t = (I'_0, \ldots, I'_8) \in P(P(\omega))^9.$$

There is a natural action of the permutation group of ω on the set of pairs (f, t), where a permutation acts on the domain of f and on $P(P(\omega))$ through its action on ω. Let $[f, t]$ be the orbit of the pair (f, t) under this action. The orbit $[f, t]$ is independent of the bijection $b : \omega \to \Lambda$. Thus, it is canonically attached to (v, Λ).

Definition 4.1. Let DS$^\circ$ be the set of all pairs $[f, t]$ that come from some v in a saturated packing Λ.

Put a topology on all pairs (f, t) (as we range over all saturated packings Λ, all choices of indexing $b : \omega \to \Lambda$, and all $v \in \Lambda$) by declaring (f, t) to be close to (f', t') if and only if $t = t'$, domain(f) = domain(f'), and for all $i \in$ domain(f), $f(i)$ is close to $f'(i)$. That is, we take the topology to be that inherited from the standard topology on $B(0, d_0)$ and the discrete topology on the finite indexing sets.

The topology on pairs (f, t) descends to the orbit space and gives a topology on DS$^\circ$.

There is a natural compactification of DS$^\circ$ obtained by replacing all open conditions by closed conditions. That is, for instance if $\{i, j\}$ is a pair in I_6, we allow $|f(i) - f(j)|$ to lie in the closed interval $[2t_0, \sqrt{8}]$. The conditions on each of the other indexing sets I_j are similarly relaxed so that they are closed conditions.

Compactness comes from the compactness of the closed ball $B(0, d_0)$, the closed conditions on indexing sets, and the finiteness of T'.

Definition 4.2. Let DS be the compactification given above of DS°. Call it the space of *decomposition stars*.

Definition 4.3. Let v be a vertex in a saturated packing Λ. We let $D(v, \Lambda)$ denote the decomposition star attached to (v, Λ).

Because of the discrete indexing sets, the space of decomposition stars breaks into a large number of connected components. On each connected component, the combinatorial data are constant. Motion within a fixed connected component corresponds to a motion of a finite set of sphere centers of the packing (in a direction that preserves all of the combinatorial structures).

In a decomposition star, it is no longer possible to distinguish some quasi-regular tetrahedra from quarters solely on the basis of metric relations. For instance, the simplex with edge lengths 2, 2, 2, 2, 2, $2t_0$ is a quasi-regular tetrahedron and is also in the closure of the set of strict quarters. The indexing set I'_2, which is part of the data of a decomposition star, determines whether the simplex is treated as a quasi-regular tetrahedron or a quarter.

Roughly speaking, two decomposition stars $D(v, \Lambda)$ and $D(v', \Lambda')$ are close if the translations $\Lambda(v, d_0) - v$ and $\Lambda'(v', d_0) - v'$ have the same cardinality, and there is a bijection between them that respects all of the indexing sets I'_j and proximity of vertices.

4.2. *Cells attached to decomposition stars.* To each decomposition star, we can associate a V-cell centered at 0 by a direct adaptation of Definition 3.6.

LEMMA 4.4. *The V-cell at v depends on Λ only through $\Lambda(v, d_0)$ and the indexing sets I'_j.*

Proof. We wish to decide whether a given x belongs to the V-cell at v or to another contender $w \in \Lambda$. We assume that $x \in I_v$, for otherwise x cannot belong to the V-cell at v. Similarly, we assume $x \in I_w$. We must determine whether v or w is obstructed at x. For this we must know whether barriers lie on the path between x and v (or w). Since $|x - w| \le 2\sqrt{3}$ and $|x - v| \le 2\sqrt{3}$, the point p of intersection of the barrier and the segment $\{x, v\}$ (or $\{x, w\}$) satisfies $|x - p| \le 2\sqrt{3}$. All the vertices of the barrier then have distance at most $\sqrt{8} + 2\sqrt{3}$ from x, and hence distance at most $d_0 = \sqrt{8} + 4\sqrt{3}$ from v. The decomposition star $D(v, \Lambda)$ includes all vertices in $\Lambda(v, d_0)$ and the indexing sets of the decomposition star label all the barriers in $\Lambda(v, d_0)$. Thus, the decomposition star at v gives all the data that are needed to determine whether $x \in I_v$ belongs to the V-cell at v. $\square$

COROLLARY 4.5. *There is a V-cell* $\mathrm{VC}(D)$ *attached to each decomposition star D such that if $D = D(v, \Lambda)$, then $\mathrm{VC}(D)+v$ is the V-cell attached to (v, Λ) in Definition* 3.6.

Proof. By the lemma, the map from (v, Λ) maps through the data determining the decomposition star $D(v, \Lambda)$. The definition of V-cell extends: the V-cell at 0 attached to $[f, t]$ is the set of points in $B(0, C_0)$ for which the origin is the unique closest unobstructed vertex of range(f). The barriers for the obstruction are to be reconstructed from the indexing data sets I'_j of t. □

LEMMA 4.6. $\mathrm{VC}(D)$ *is a finite union of nonoverlapping convex polyhedra. Moreover*, $D \mapsto \mathrm{vol}(\mathrm{VC}(D))$ *is continuous.*

Proof. For the proof, we ignore sets of measure zero, such as finite unions of planes. We may restrict our attention to a single connected component of the space of decomposition stars. On each connected component, the indexing set for each barrier (near the origin) is fixed. The indexing set for the set of vertices near the origin is fixed. For each D the VC-cell breaks into a finite union of convex polyhedra by Lemma 3.9.

As the proof of that lemma shows, some faces of the polyhedra are perpendicular bisecting planes between two vertices near the origin. Such planes vary continuously on (a connected component) of DS. The other faces of polyhedra are formed by planes through three vertices of the packing near the origin. Such planes also vary continuously on DS. It follows that the volume of each convex polyhedron is a continuous function on DS. The sum of these volumes, giving the volume of $\mathrm{VC}(D)$ is also continuous. □

LEMMA 4.7. *Let Λ be a saturated packing. The Voronoi cell $\Omega(v)$ at v depends on Λ only through $\Lambda(v, d_0)$.*

Proof. Let x be an extreme point of the Voronoi cell $\Omega(v)$. The vertex v is one of the vertices closest to x. If the distance from x to v is at least 2, then there is room to place another ball centered at x into the packing without overlap. Then Λ is not saturated.

Thus, the distance from x to v is less than 2. The Voronoi cell lies in the ball $B(v, 2)$. The Voronoi cell is bounded by the perpendicular bisectors of segments $\{v, w\}$ for $w \in \Lambda$. If w has distance 4 or more from v, then the bisector cannot meet the ball $B(v, 2)$ and cannot bound the cell. Since $4 < d_0$, the proof is complete. □

COROLLARY 4.8. *The vertex v and the decomposition star $D(v, \Lambda)$ determine the Voronoi cell at v. In fact, the Voronoi cell is determined by v and the first indexing set I'_1 of $D(v, \Lambda)$.*

Definition 4.9. The Voronoi cell $\Omega(D)$ of $D \in \mathrm{DS}$ is the set containing the origin bounded by the perpendicular bisectors of $\{0, v_i\}$ for $i \in I_1'$.

Remark 4.10. It follows from Corollary 4.8 that

$$\Omega(D(v, \Lambda)) = v + \Omega(v).$$

In particular, they have the same volume.

Remark 4.11. From a decomposition star D, we can recover the set of vertices $U(D)$ of distance at most $2t_0$ from the origin, the set of barriers at the origin, the simplices of the Q-system having a vertex at the origin, the V-cell $VC(D)$ at the origin, the Voronoi cell $\Omega(D)$ at the origin, and so forth. In fact, the indexing sets in the definition of the decomposition star were chosen specifically to encode these structures.

4.3. *Colored spaces.* In Section 1, we introduced a function σ that will be formally defined in Definition 5.8. The details of the definition of σ are not needed for the discussion that follows. The function σ on the space DS of decomposition stars is continuous. This section gives an alternate description of the sense in which this function is continuous.

We begin with an example that illustrates the basic issues. Suppose that we have a discontinuous piecewise linear function on the unit interval $[-1, 1]$, as in Figure 4.1. It is continuous, except at $x = 0$.

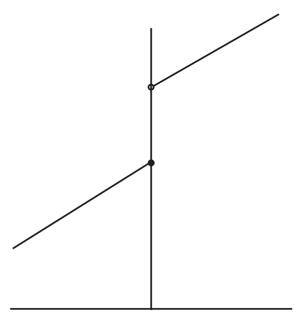

Figure 4.1: A piecewise linear function

We break the interval in two at $x = 0$, forming two compact intervals $[-1, 0]$ and $[0, 1]$. We have continuous functions $f_- : [-1, 0] \to \mathbb{R}$ and $f_+ : [0, 1]$, such that

$$f(x) = \begin{cases} f_-(x) & x \in [-1, 0], \\ f_+(x) & \text{otherwise.} \end{cases}$$

We have replaced the discontinuous function by a pair of continuous functions on smaller intervals, at the expense of duplicating the point of discontinuity

$x = 0$. We view this pair of functions as a single function F on the compact topological space with two components

$$[-1, 0] \times \{-\} \text{ and } [0, 1] \times \{+\},$$

where $F(x, a) = f_a(x)$, and $a \in \{-, +\}$.

This is the approach that we follow in general with the Kepler conjecture. The function σ is defined by a series of case statements, and the function does not extend continuously across the boundary of the cases. However, in the degenerate cases that land precisely between two or more cases, we form multiple copies of the decomposition star for each case, and place each case into a separate compact domain on which the function σ is continuous.

This can be formalized as a *colored space*. A colored space is a topological space X together with an equivalence relation on X with the property that no point x is equivalent to any other point in the same connected component as x. We refer to the connected components as colors, and call the points of X *colored points*. We call the set of equivalence classes of X the underlying uncolored space of X. Two colored points are equal as uncolored points if they are equivalent under the equivalence relation.

In our example, there are two colors "$-$" and "$+$." The equivalence class of (x, a) is the set of pairs (x, b) with the same first coordinate. Thus, if $x \neq 0$, the equivalence class contains one element $(x, \text{sign}(x))$, and in the boundary case $x = 0$ there are two equivalent elements $(0, -)$ and $(0, +)$.

In our treatment of decomposition stars, there are various cases: whether an edge has length less than or greater than $2t_0$, less than or greater than $\sqrt{8}$, whether a face has circumradius less than or greater than $\sqrt{2}$, and so forth. By duplicating the degenerate cases (say an edge of exact length $2t_0$), creating a separate connected component for each case, and expressing the optimization problem on a colored space, we obtain a continuous function σ on a compact domain X.

The colorings have in general been suppressed in places from the notation. To obtain consistent results, a statement about $x \in [2, 2t_0]$ should be interpreted as having an implicit condition saying that x has the coloring induced from the coloring on the component containing $[2, 2t_0]$. A later statement about $y \in [2t_0, \sqrt{8}]$ deals with y of a different color, and no relation between x and y of different colors is assumed at the endpoint $2t_0$.

5. Scoring (Ferguson, Hales)

This chapter is coauthored by Samuel P. Ferguson and Thomas C. Hales.

In earlier chapters, we describe each packing of unit balls by its set $\Lambda \subset \mathbb{R}^3$ of centers of the packing. We showed that we may assume that our packings are saturated in the sense that there is no room for additional balls to be inserted into the packing without overlap. Lemma 1.3 shows that the Kepler conjecture follows if for each saturated packing Λ we can find a function $A : \Lambda \to \mathbb{R}$ with two properties: the function is fcc-compatible and it is saturated in the sense of Definition 1.2.

The purpose of the first part of this chapter is to define a function $A : \Lambda \to \mathbb{R}$ for every saturated packing Λ and to show that it is negligible. The formula defining A consists of a term that is a correction between the volume of the Voronoi cell $\Omega(v)$ and that of the V-cell $\mathrm{VC}(v)$ and a further term coming from simplices of the Q-system that have a vertex at v.

A major theorem in this paper will be that this negligible function is fcc-compatible. The proof of fcc-compatibility can be expressed as a difficult nonlinear optimization problem over the compact topological space DS that was introduced in Chapter 4. In fact, we construct a continuous function A_0 on the space DS such that for each saturated packing Λ and each $v \in \Lambda$, the value of the function A at v is a value in the range of the function A_0 on DS. In this way, we are able to translate the fcc-compatibility of A into an extremal property of the function A_0 on the space DS.

The proof of fcc-compatibility is more conveniently couched as an optimization problem over a function that is related to the function A_0 by an affine rescaling. This new function is called the score and is denoted σ. (The exact relationship between A_0 and σ appears in Definition 5.12.) The function σ is a continuous function on the space DS. This function is defined in the final paragraphs of this chapter.

5.1. *Definitions.* For every saturated packing Λ, and $v \in \Lambda$, there is a canonically associated decomposition star $D(v, \Lambda)$. The negligible function $A : \Lambda \to \mathbb{R}$ that we define is a composite

$$A = A_0 \circ D(\cdot, \Lambda) : \Lambda \to DS \to \mathbb{R}, \quad v \mapsto D(v, \Lambda) \mapsto A_0(D(v, \Lambda)), \tag{5.1}$$

where $A_0 : \mathrm{DS} \to \mathbb{R}$ is as defined by Equations 5.2 and 5.5 below. Each simplex in the Q-system with a vertex at v defines by translation to the origin a simplex in the Q-system with a vertex at 0 attached to $D(v, \Lambda)$. Let $\mathcal{Q}_0(D)$ be this set of translated simplices at the origin. This set is determined by D.

Definition 5.1. Let Q be a quarter in $\mathcal{Q}_0(D)$. We say that the *context* of Q is (p, q) if there are p anchors and $p - q$ quarters along the diagonal of Q. Write $c(Q, D)$ for the context of $Q \in \mathcal{Q}_0(D)$.

Note that q is the number of "gaps" between anchors around the diagonal. For example, the context of a quarter in a quartered octahedron is $(4, 0)$. The context of a single quarter is $(2, 1)$.

The function A_0 will be defined to be a continuous function on DS of the form

$$A_0(D) = -\mathrm{vol}\,(\Omega(D)) + \mathrm{vol}\,(\mathrm{VC}(D)) + \sum_{Q \in \mathcal{Q}_0(D)} A_1(Q, c(Q, D), 0). \tag{5.2}$$

Thus, the function A_0 measures the difference in volume between the Voronoi cell and the V-cell, as well as certain contributions A_1 from the Q-system. The function $A_1(Q, c, v)$ depends on Q, its context c, and a vertex v of Q. The function $A_1(Q, c, v)$ will not depend on the second argument when Q is a quasi-regular tetrahedron. (The context is not defined for such simplices.)

Definition 5.2. An *orthosimplex* consists of the convex hull of $\{0, v_1, v_1 + v_2, v_1 + v_2 + v_3\}$, where v_2 is a vector orthogonal to v_1, and v_3 is orthogonal to both v_1 and v_2. We can specify an orthosimplex up to congruence by the parameters $a = |v_1|$, $b = |v_1 + v_2|$, and $c = |v_1 + v_2 + v_3|$, where $a \le b \le c$. This parametrization of the orthosimplex departs from the usual parametrization by the lengths $|v_1|$, $|v_2|$, $|v_3|$. For $a \le b \le c$, the *Rogers simplex* $R(a, b, c)$ is an orthosimplex of the form

$$R(a, b, c) = S(a, b, c, \sqrt{c^2 - b^2}, \sqrt{c^2 - a^2}, \sqrt{b^2 - a^2}).$$

See Figure 5.1.

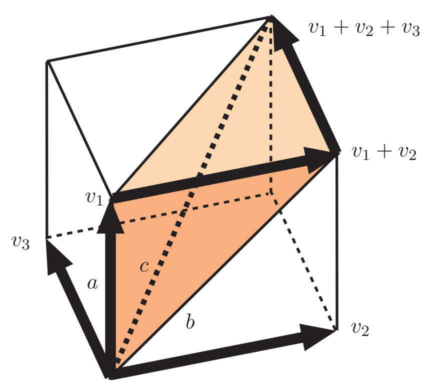

Figure 5.1: The Rogers simplex is an orthosimplex.

Definition 5.3. Let R be a Rogers simplex. We define the *quoin* of R to be the wedge-like solid (a quoin) situated above R. It is defined as the solid bounded by the four planes through the faces of R and a sphere of radius c at the origin. (See Figure 5.2.) We let $\mathrm{quo}(R)$ be the volume of the quoin over R. An explicit formula appears in [Hal06a].

Let S be a simplex and let v be a vertex of that simplex. Let $\mathrm{VC}(S, v)$ be the subset of $|S|$ consisting of points closer to v than to any other vertex of S.

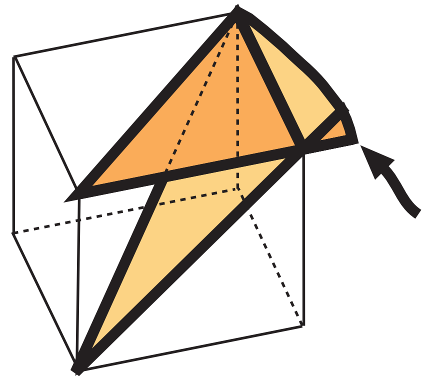

Figure 5.2: The quoin above a Rogers simplex is the part of the shaded solid outside the illustrated box. It is bounded by the shaded planes, the plane through the front face of the box, and a sphere centered at the origin passing through the opposite corner of the box.

By Lemma 3.28, if $S \in \mathcal{Q}_0(D)$, then

$$\mathrm{VC}(S,0) = \mathrm{VC}(D) \cap |S|.$$

Under the assumption that S contains its circumcenter and that every one of its faces contains its circumcenter, an explicit formula for the volume $\mathrm{vol}(\mathrm{VC}(S,v))$ has been calculated in [Hal97a, §8.6.3]. This volume formula is an algebraic function of the edge lengths of S, and may be analytically continued to give a function of S with chosen vertex v:

$$\mathrm{vol}\,\mathrm{VC}^{\mathrm{an}}(S,v).$$

Lemma 5.4. *Let $B(0,t)$ be a ball of radius t centered at the origin. Let v_1 and v_2 be vertices. Assume that $|v_1| < 2t$ and $|v_2| < 2t$. Truncate the ball by cutting away the caps*

$$\mathrm{cap}_i = \{x \in B(0,t) : |x - v_i| < |x|\}.$$

Assume that the circumradius of the triangle $\{0, v_1, v_2\}$ is less than t. Then the intersection of the caps, $\mathrm{cap}_1 \cap \mathrm{cap}_2$, is the union of four quoins.

Proof. This is true by inspection. See Figure 5.3. Slice the intersection $\mathrm{cap}_1 \cap \mathrm{cap}_2$ into four pieces by two perpendicular planes: the plane through $\{0, v_1, v_2\}$, and the plane perpendicular to the first and passing through 0 and the circumcenter of $\{0, v_1, v_2\}$. Each of the four pieces is a quoin. □

Definition 5.5. Let $v \in \mathbb{R}^3$ and let X be a measurable subset of $\mathbb{R}^3$. Let $\mathrm{sol}(X,v)$ be the area of the radial projection of $X \setminus \{0\}$ to the unit sphere

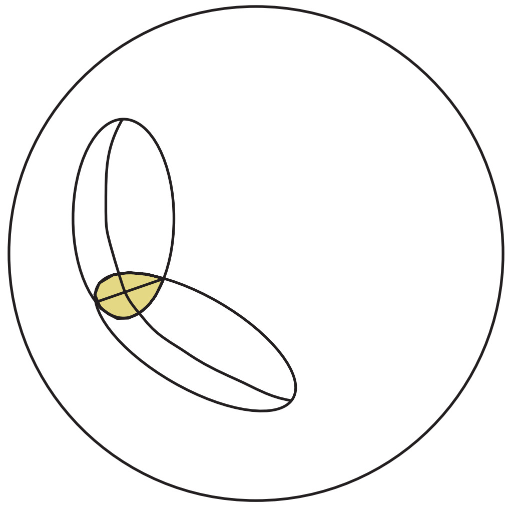

Figure 5.3: The intersection of two caps on the unit ball can be partitioned into four quoins (shaded).

centered at the origin. We call this area the *solid angle* of X (at v). When $v = 0$, we write the function as $\mathrm{sol}(X)$.

Let $S = \{v_0, v_1, v_2, v_3\}$ be a simplex. Fix t in the range $t_0 \le t \le \sqrt{2}$. Assume that t is at most the circumradius of S. Assume that it is at least the circumradius of each of the faces of S. Let $\mathrm{VC}_t(S, v_0)$ be the intersection of $\mathrm{VC}(S, v_0)$ with the ball $B(v_0, t)$. Under the assumption that S contains its circumcenter and that every one of its faces contains it circumcenter, an explicit formula for the volume

$$\mathrm{vol}(\mathrm{VC}_t(S, v_0))$$

is calculated by means of Lemma 5.4 through a process of inclusion and exclusion. In detail, start with $|S| \cap B(v_0, t)$. Truncate this solid by caps: cap_1, cap_2, and cap_3 bounded by the sphere of radius t centered at v_0 and the perpendicular bisectors (respectively) of $\{v_0, v_1\}$, $\{v_0, v_1\}$, $\{v_0, v_2\}$. If we subtract the volume of each cap, cap_i, then we must add back the volume of the doubly counted intersections of the caps. The intersections of caps are given as quoins (Lemma 5.4). This leads to the following formula. Let $h_i = |v_i|/2$ and $\eta_{ij} = \eta(0, v_i, v_j)$, and let S_3 be the group of permutations of $\{1, 2, 3\}$ in

(5.3)

$$\mathrm{vol}\,\mathrm{VC}_t(S, v_0) = \mathrm{sol}(S)/3 - \sum_{i=1}^{3} \frac{\mathrm{dih}(S, v_i)}{2\pi} \mathrm{vol}\,\mathrm{cap_i} + \sum_{(i,j,k)\in S_3} \mathrm{quo}(R(h_i, \eta_{ij}, t)).$$

We extend Formula 5.3 by setting

$$\mathrm{quo}(R(a, b, c)) = 0,$$

if the constraint $a < b < c$ fails to hold. Similarly, set $\mathrm{vol}\,\mathrm{cap}_i = 0$ if $|v_i| \ge 2t$. With these conventions, Formula 5.3 extends to all simplices. We write the extension of $\mathrm{vol}\,\mathrm{VC}_t(S, v)$ as

$$\mathrm{vol}\,\mathrm{VC}_t^+(S, v).$$

Definition 5.6. Let[2]

$$\begin{aligned}\text{s-vor}(S, v) &= 4(-\delta_{\mathrm{oct}}\mathrm{vol}\,\mathrm{VC}^{\mathrm{an}}(S, v) + \mathrm{sol}(S, v)/3),\\ \text{s-vor}(S, v, t) &= 4(-\delta_{\mathrm{oct}}\mathrm{vol}\,\mathrm{VC}_t^+(S, v) + \mathrm{sol}(S, v)/3),\end{aligned}$$

and

$$\text{s-vor}_0(S, v) = \text{s-vor}(S, v, t_0).$$

When it is clear from the context that the vertex v is fixed at the origin, we drop v from the notation of these functions. If $S = \{v_1, v_2, v_3, v_4\}$, we define $\Gamma(S)$ as the average

$$\Gamma(S) = \frac{1}{4}\sum_{i=1}^{4} \text{s-vor}(S, v_i). \tag{5.4}$$

The average $\Gamma(S)$ is called the *compression* of S.

Definition 5.7. Let Q be a quarter. Let $\eta^+(Q)$ be the maximum of the circumradii of the two faces of Q along the diagonal of Q.

Let Q be a simplex in the Q-system. We define an involution $v \to \hat{v}$ on the vertices of Q as follows. If Q is a quarter and v is an endpoint of the diagonal, then let $\hat{v}$ be the opposite endpoint of the diagonal. In all other cases, set $\hat{v} = v$.

We are ready to complete the definition of the function $A : \Lambda \to \mathbb{R}$. The definition of A was reduced to that of A_0 in Equation 5.1. The function A_0 was reduced in turn to that of A_1 in Equation 5.2. To complete the definition, we define A_1.

Definition 5.8. Set

$$A_1(S, c, v) = -\mathrm{vol}\,\mathrm{VC}(S, v) + \frac{\mathrm{sol}(S, v)}{3\delta_{\mathrm{oct}}} - \frac{\sigma(S, c, v)}{4\delta_{\mathrm{oct}}}, \tag{5.5}$$

where σ is given as follows:

[2] In the paper [Hal92], the volumes in this definition were volumes of Voronoi cells, and hence the notation vor for the function was adopted. We retain vor in the notation, although this direct connection with Voronoi cells has been lost.

1. When S is a quasi-regular tetrahedron:

   (a) If the circumradius of S is less than 1.41, set
   $$\sigma(S,-,v) = \Gamma(S).$$

   (b) If the circumradius of S is at least 1.41, set
   $$\sigma(S,-,v) = \text{s-vor}(S,v).$$

2. When S is a strict quarter:

   (a) If $\eta^+(S) < \sqrt{2}$:

      i. If the context c is $(2,1)$ or $(4,0)$, set
      $$\sigma(S,c,v) = \Gamma(S).$$

      ii. If the context of S is anything else, set
      $$\sigma(S,c,v) = \Gamma(S) + \frac{\text{s-vor}_0(S,v) - \text{s-vor}_0(S,\hat{v})}{2}.$$

   (b) If $\eta^+(S) \geq \sqrt{2}$:

      i. If the context of S is $(2,1)$, set
      $$\sigma(S,c,v) = \text{s-vor}(S,v).$$

      ii. If the context of S is $(4,0)$, set
      $$\sigma(S,c,v) = \frac{\text{s-vor}(S,v) + \text{s-vor}(S,\hat{v})}{2}.$$

      iii. If the context of S is anything else, set
      $$\sigma(S,c,v) = \frac{\text{s-vor}(S,v) + \text{s-vor}(S,\hat{v})}{2} + \frac{\text{s-vor}_0(S,v) - \text{s-vor}_0(S,\hat{v})}{2}.$$

When the context and vertex v are given, we often write $\sigma(S)$ or $\sigma(S,v)$ for $\sigma(S,c,v)$.

When $\eta^+ < \sqrt{2}$, we say that the quarter has compression type. Otherwise, we say it has Voronoi type. To say that a quarter has compression type means that $\Gamma(S)$ is one term of the function $\sigma(S,v)$. It does not mean that $\Gamma(S)$ is equal to $\sigma(S,v)$.

LEMMA 5.9. *$A_0 : \mathrm{DS} \to \mathbb{R}$ is continuous.*

Proof. The continuity of $D \mapsto \operatorname{vol} \mathrm{VC}(D)$ is proved in Lemma 4.6. The continuity of $D \mapsto \operatorname{vol} \Omega(D)$ is similarly proved. The terms $\operatorname{vol} \mathrm{VC}(S,v)$ and $\mathrm{sol}(S,v)$ are continuous. To complete the proof we check that the function $\sigma(S,c,v)$ is continuous. It is not continuous when viewed as a function of the set of quarters, because of the various cases breaking at circumradius 1.41 and

$\eta^+(S) = \sqrt{2}$. However, these cutoffs have been inserted into the data defining a decomposition star (in the indexing sets I_8 and I_9). Thus, the different cases in the definition of $\sigma(S, c, v)$ land in different connected components of the space DS and continuity is obtained. □

We conclude this section with a result that will be of use in the next section.

LEMMA 5.10. *Let $S = \{v_1, v_2, v_3, v_4\}$ be a simplex in the S-system, and c its context. Then*

$$\sum_{i=1}^{4} A_1(S, c, v_i) = 0.$$

Proof. By Formula 5.5, this is equivalent to

$$\sum_{i=1}^{4} \sigma(S, c, v_i) = \sum_{i=1}^{4} \text{s-vor}(S, c, v_i). \tag{5.6}$$

Equation 5.6 is evident from Definition 5.8 for σ. In fact, the terms of the form s-vor$_0$ have opposing signs and cancel when we sum. The other terms are weighted averages of the terms s-vor(S, c, v_i). Equation 5.6 is thus established because a sum is unaffected by taking weighted averages of its terms. □

5.2. *Negligibility.* Let $B(x, r)$ be the closed ball of radius $r \in \mathbb{R}$ centered at x. Let $\Lambda(x, r) = \Lambda \cap B(x, r)$.

Recall from Definition 1.2 that a function $A : \Lambda \to \mathbb{R}$ is said to be *negligible* if there is a constant C_1 such that for all $r \geq 1$,

$$\sum_{v \in \Lambda(x,r)} A(v) \leq C_1 r^2.$$

Recall the function $A : \Lambda \to \mathbb{R}$ given by Equation 5.1. Explicitly, let

$$A(v) = A_0(D(v, \Lambda)),$$

where A_0 in turn depends on functions A_1 and σ, as determined by Equations 5.2 and 5.5, and Definition 5.8.

THEOREM 5.11. *The function A of Equation* 5.1 *is negligible.*

Proof. First we consider a simplification, where we replace A with A' defined by

$$A'(v, \Lambda) = -\text{vol}(\Omega(D(v, \Lambda))) + \text{vol}(\text{VC}(D(v, \Lambda))).$$

(That is, at first we ignore the function A_1.) The Voronoi cells partition $\mathbb{R}^3$, as do the V-cells. We have $\Omega(v, \Lambda) \subset B(v, 2)$ (by saturation) and $\text{VC}(v, \Lambda) \subset$

$B(v, 2\sqrt{3})$ (by Definition 3.5). Hence the Voronoi cells with $v \in \Lambda(x, r)$ cover $B(x, r-2)$. Moreover, the V-cells with $v \in \Lambda(x, r)$ are contained in $B(x, r+2\sqrt{3})$. Hence

$$\sum_{v \in \Lambda(x,r)} A'(v) \leq -\mathrm{vol}\, B(x, r-2) + \mathrm{vol}\, B(x, r+2\sqrt{3}) \leq C_1' r^2$$

for some constant C_1'.

If we do not make the simplification, we must include the sum

$$\sum_{v \in \Lambda(x,r)} \sum_{Q \in \mathcal{Q}_v(D(v,\Lambda))} A_1(Q, c, v).$$

Each quarter $Q = \{v_1, v_2, v_3, v_4\}$ in the Q-system occurs in four sets $\mathcal{Q}_{v_i}(D(v_i, \Lambda))$. By Lemma 5.10 the sum cancels, except when some vertex of Q lies inside $\Lambda(x, r)$ and another lies outside. Each such simplex lies inside a shell of width $2\sqrt{8}$ around the boundary. The contribution of such boundary terms is again bounded by a constant times r^2. This completes the proof. □

5.3. Fcc-*compatibility.* We have constructed a negligible function A. The rest of this paper will prove that this function is fcc-compatible. This section translates fcc-compatibility into a property that will be easier to prove. To begin with, we introduce a rescaled version of the function A.

Definition 5.12. Let $\sigma : \mathrm{DS} \to \mathbb{R}$ be given by

$$\sigma(D) = -4\delta_{\mathrm{oct}}(\mathrm{vol}\, \Omega(D) + A_0(D)) + 16\pi/3.$$

It is called the *score* of the decomposition star.

Recall from Definition 1.6 the constant $\mathrm{pt} \approx 0.05537$. This constant is called a point.

LEMMA 5.13. *Let* A_0, A, *and* σ *be the functions defined by Equations* 5.1, 5.2, 5.5, *and Definition* 5.8. *The following are equivalent.*

1. *The minimum of the function on* DS *given by*

$$D \mapsto \mathrm{vol}\, \Omega(D) + A_0(D)$$

is $\sqrt{32}$.

2. *The maximum of* σ *on* DS *is* $8\,\mathrm{pt}$.

Moreover, these statements imply

- *For every saturated packing* Λ, *the function* A *is* fcc-*compatible.*

(Eventually, we prove fcc-compatibility by proving $\sigma(D) \leq 8\,\mathrm{pt}$ for all $D \in \mathrm{DS}$.)

Proof. To see the equivalence of the first and second statements, use Definition 5.12, and the identity

$$8\,\mathrm{pt} = -4\delta_{\mathrm{oct}}(\sqrt{32}) + 16\pi/3.$$

(Note that this identity is parallel in form to Definition 5.12 for σ.)

For a given saturated packing Λ, the function A has the form $A(v) = A_0(D(v,\Lambda))$. Also, $\Omega(D(v,\Lambda))$ is a translate of $\Omega(v)$, the Voronoi cell at v. In particular, they have the same volume. Thus, $\mathrm{vol}\,\Omega(v) + A(v)$ lies in the range of the function

$$\mathrm{vol}\,\Omega(D) + A_0(D)$$

on DS. The minimum of this function is $\sqrt{32}$ by the first of the equivalent statements. It now follows from the definition of fcc-compatibility, that $A : \Lambda \to \mathbb{R}$ is indeed fcc-compatible. $\square$

THEOREM 5.14. *If the maximum of the function σ on* DS *is* $8\,\mathrm{pt}$, *then for every saturated packing Λ there exists a negligible* fcc-*compatible function A.*

Proof. This follows immediately from Theorem 5.11 and Lemma 5.13. $\square$

5.4. *Scores of standard clusters.* The last section introduced a function σ called the score. We show that the function σ can be expressed as a sum over terms attached to each of the standard regions.

Definition 5.15. A *standard cluster* is a pair (R, D) where D is a decomposition star and R is one of its standard regions. A *quad cluster* is the standard cluster obtained when the standard region is a quadrilateral.

We break σ into a sum

$$\sigma(D) = \sum_R \sigma_R(D), \tag{5.7}$$

indexed by the standard clusters (R, D). Let

$$\mathrm{VC}_R(D) = \mathrm{VC}(D) \cap \mathrm{cone}(R),$$

whenever R is a measurable subset of the unit sphere. Let

$$\mathcal{Q}_0(R, D) = \{Q \in \mathcal{Q}_0(D) : Q \subset \mathrm{cone}(R)\}.$$

By Lemma 3.26, each Q is entirely contained in the cone over a single standard region.

Definition 5.16. Let R be a measurable subset of the unit sphere. Set

$$\mathrm{vor}_R(D) = 4\left(-\delta_{\mathrm{oct}}\mathrm{vol}\,\mathrm{VC}_R(D) + \mathrm{sol}(R)/3\right).$$

Let R be a standard region. Set

$$\sigma_R(D) = \mathrm{vor}_R(D) - 4\delta_{\mathrm{oct}} \sum_{Q\in\mathcal{Q}_0(R,D)} A_1(Q, c(Q,D), 0).$$

LEMMA 5.17. $\sigma(D) = \sum_R \sigma_R(D)$, *where the sum runs over all standard regions* R.

Proof.

$$\begin{aligned}
\sigma(D) &= -4\delta_{\mathrm{oct}}(\mathrm{vol}\,\Omega(D) + A_0(D)) + 16\pi/3\\
&= -4\delta_{\mathrm{oct}}(\mathrm{vol}\,\mathrm{VC}(D) + \textstyle\sum_{Q\in\mathcal{Q}_0(D)} A_1(Q, c(Q,D), 0)) + (4)(4\pi/3)\\
&= \textstyle\sum_R 4\Big(- \delta_{\mathrm{oct}}\mathrm{vol}\,\mathrm{VC}_R(D)\\
&\qquad\qquad - \delta_{\mathrm{oct}} \textstyle\sum_{Q\in\mathcal{Q}_0(R,D)} A_1(Q, c(Q,D), 0) + \mathrm{sol}(R)/3\Big).
\end{aligned}$$ □

LEMMA 5.18. *Let* $R' \subset R$ *be the part of a standard region that does not lie in any cone over any* $Q \in Q_0(R, D)$. *Then*

$$\sigma_R(D) = \mathrm{vor}_{R'}(D) + \sum_{Q\in\mathcal{Q}_0(R,D)} \sigma(Q, c(Q,D), 0).$$

Proof. Substitute the definition of A_1 (Equation 5.5) into the definition of $\sigma_R(D)$, noting that $\mathrm{VC}(Q, 0) = \mathrm{VC}_{R''}(D)$, where R'' is the intersection of Q with the unit sphere. □

Remark 5.19. Lemma 5.18 explains why we have chosen the same symbol σ for the functions $\sigma_R(D)$ and $\sigma(Q, c, v)$. We can view Lemma 5.18 as asserting a linear relation in the functions σ:

$$\sigma_R(D) = \sigma_{R'}(D) + \sum \sigma(Q, c, 0).$$

The sum runs over $Q \in \mathcal{Q}_0$ that lie in the cone over R.

6. Local optimality

The first several chapters have established the fundamental definitions and constructions of this paper. This chapter establishes the local optimality of the function $\sigma : \mathrm{DS} \to \mathbb{R}$ in a neighborhood of the decomposition stars of the face-centered cubic and hexagonal close packings.

6.1. *Results.* Here is a sketch of the proof of local optimality. The face-centered cubic and hexagonal close packings score precisely 8 pt. They also contain precisely eight tetrahedra around each vertex. In fact, the decomposition stars have eight quasi-regular tetrahedra and six other quad clusters. The proof shows that each of the eight quasi-regular tetrahedra scores at most 1 pt. Equality is obtained only when the tetrahedron is regular of side 2. Furthermore, the proof shows that each of six quad clusters have a nonpositive score. It will follows from these facts that any decomposition star with eight quasi-regular tetrahedra, six quad clusters, and no other standard clusters scores at most 8 pt. The case of equality is analyzed as well. The purpose of this chapter is to give a proof of the following theorem.

THEOREM 6.1 (Local optimality). *Let D be a contravening decomposition star. Let $U(D)$ be the set of sphere packing vectors at distance at most $2t_0$ from the origin. Assume that*

1. *The set $U(D)$ has twelve elements.*
2. *There is a bijection ψ between $U(D)$ and the kissing arrangement $U_{\rm fcc}$ of twelve tangent unit balls in the face-centered cubic configuration, or a bijection with $U_{\rm hcp}$ the twelve tangent unit balls in the hexagonal-close packing configuration; such that for all $v, w \in U(D)$, $|w - v| \le 2t_0$ if and only if $|\psi(w) - \psi(v)| = 2$. That is, the proximity graph of $U(D)$ is the same as the contact graph of $U_{\rm fcc}$ or $U_{\rm hcp}$.*

Then $\sigma(D) \le 8\,\mathrm{pt}$. Equality holds if and only if U coincides with $U_{\rm fcc}$ or $U_{\rm hcp}$ up to a Euclidean motion. Decomposition stars D exist with $U(D) = U_{\rm fcc}$ and others exist with $U(D) = U_{\rm hcp}$.

Remark 6.2. This theorem is one of the key claims of Section 1.3. This theorem is phrased slightly differently from the Claim 1.15 in Section 1.3. The reason for this is that we have not formally introduced the plane graph $G(D)$ of a decomposition star. (This happens in Section 9.2.) Once $G(D)$ has been formally introduced, then Theorem 6.1 can be expressed more directly, as follows. We let $G_{\rm fcc}$ and $G_{\rm hcp}$ be the plane graphs attached to the decomposition stars of vertices in the face-centered cubic and hexagonal-close packings, respectively. (These graphs are independent of the vertices selected.)

COROLLARY 6.3 (Local optimality - second version). *Contravening decomposition stars exist. If D is a contravening decomposition star, and if the plane graph of D is isomorphic to $G_{\rm fcc}$ or $G_{\rm hcp}$, then $\sigma(D) = 8\,\mathrm{pt}$. Moreover, up to Euclidean motion, $U(D)$ is the kissing arrangement of the twelve balls around a central ball in the face-centered cubic packing or the kissing arrangement of twelve balls in the hexagonal-close packing.*

The following theorem is also one of the main results of this chapter. It is a key part of the proof of local optimality.

THEOREM 6.4. *A quad cluster scores at most* 0, *and that only for a quad cluster whose corners have height* 2, *forming a square of side* 2. *That is*, $\sigma_R(D) \le 0$. *Other standard clusters have strictly negative scores*: $\sigma_R(D) < 0$.

The argument that the score of a quad cluster is nonpositive is general and can be used to prove that the score of any cluster attached to a non-triangular standard region (Definition 3.24) has nonpositive score.

6.2. *Rogers simplices.* To prove Theorem 6.4, we chop the cluster (R, D) into small pieces and show that the "density" of each piece is at most δ_{oct}. To prepare for this proof, this section describes various small geometric solids that have a density at most δ_{oct}. The first of these is the Rogers simplex.

LEMMA 6.5. *Let* $R(a, b, c)$ *be a Rogers simplex, with* $1 \le a < b < c$. *It has a distinguished vertex* (*the terminal point of the edges of lengths* a, b, *and* c), *which we assume to be the origin. Let* $A(a, b, c)$ *be the volume of the intersection of* $R(a, b, c)$ *with a ball of radius* 1 *at the origin. Then the ratio*

$$A(a, b, c)/\text{vol}(R(a, b, c))$$

is monotonically decreasing in each variable.

Proof. This is Rogers's lemma, as formulated in [Hal97a, Lemma 8.6]. □

LEMMA 6.6. *Consider the Rogers simplex* $R(a, b, \sqrt{2})$ *with vertex at the origin. Assume* $1 \le a \le b$ *and* $\eta(2, 2, 2) \le b \le \sqrt{2}$. *Let* A *be the volume of the intersection of the simplex with a closed ball of radius* 1 *at the origin. Then*

$$A \le \delta_{\text{oct}} \, \text{vol}(R(a, b, \sqrt{2})).$$

Equality is attained if and only if $a = 1$ *and* $b = \eta(2, 2, 2)$ *or for a degenerate simplex of zero volume.*

Proof. This is a special case of Lemma 6.5. See the third frame of Figure 6.1. □

LEMMA 6.7. *Consider the wedge of a cone*

$$W = W(\alpha, z_0) = \{t\, x : 0 \le t \le 1, x \in P(\alpha, z_0)\} \subset \mathbb{R}^3,$$

where $P(\alpha, z_0)$ *has the form*

$$P = \{(x_1, x_2, x_3) : x_3 = z_0,\ x_1^2 + x_2^2 + x_3^2 \le 2,\ 0 \le x_2 \le \alpha x_1\},$$

with $z_0 \ge 1$. *Let* A *be the volume of the intersection of the wedge with* $B(0, 1)$. *Then*

$$A \le \delta_{\text{oct}} \, \text{vol}(W).$$

Equality is attained if and only if W *has zero volume.*

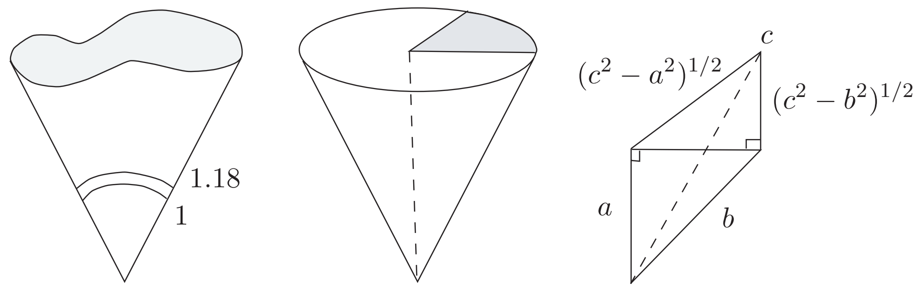

Figure 6.1: Some sets of low density.

Proof. This is calculated in [Hal97b, §4]. See the second frame of Figure 6.1. □

LEMMA 6.8. *Let C be the cone at the origin over a set P, where P is measurable and every point of P has distance at least* 1.18 *from the origin. Let A be the volume of the intersection of C with $B(0,1)$. Then*

$$A \leq \delta_{\text{oct}} \operatorname{vol}(C).$$

Equality is attained if and only if C has zero volume.

Proof. The ratio $A/\operatorname{vol}(C)$ is at most $1/1.18^3 < \delta_{\text{oct}}$. See the first frame of Figure 6.1. □

6.3. *Bounds on simplices.* In this and future chapters, we rely on some inequalities that are not proved in this paper. There is an archive of hundreds of inequalities that have been proved by computer. This full archive appears in [Hal05]. The justification for these inequalities appears in the same archive. (The proofs of these inequalities were executed by computer.) An explanation of how computers are able to prove inequalities can be found in [Hal03] and [Hal97a]. Each inequality carries a nine-digit identifying number. To invoke an inequality, we state it precisely, and give its identifying number, e.g. CALC-123456789. The first of these appears in Lemma 6.10. Some results rely on a simple combination of inequalities, rather than a single inequality. To make it easier to reference a group of inequalities, the archive at [Hal05] gives a separate nine-digit identifier to certain groups of inequalities. This permits us to reference such a group by a single number.

Definition 6.9. Recall that the constant pt, a *point*, is equal to $\sigma(S)$, where S is a regular tetrahedron with edges of length 2. We have $\mathrm{pt} = 4\arctan(\sqrt{2}/5) - \pi/3 \approx 0.05537$.

LEMMA 6.10. *A quasi-regular tetrahedron S satisfies $\sigma(S) \leq 1\,\mathrm{pt}$. Equality occurs if and only if the quasi-regular tetrahedron is regular of edge length* 2.

Proof. This is CALC-586468779. □

Remark 6.11. The reader who wishes to dig more deeply into this particular proof may do so. An early published proof of this lemma was not fully automated (see [Hal97a, Lemma 9.1.1]). This early proof show by conventional means that $\sigma(S) \le 1\,\mathrm{pt}$ in an explicit neighborhood of $(2,2,2,2,2,2)$.

LEMMA 6.12. *A quarter in the Q-system scores at most* 0. *That is,* $\sigma(Q) \le 0$. *Equality is attained if and only if five edges have length* 2 *and the diagonal has length* $\sqrt{8}$.

Proof. Throughout the proof of this lemma, we will refer to quarters with five edges of length 2 and one of length $\sqrt{8}$ as *extremal* quarters. We make use of the definition of σ on quarters from Definition 5.8. The general context (that is, contexts other than $(2,1)$ and $(4,0)$) of upright quarters is established by the inequalities[3] that hold for all upright quarters Q with distinguished vertex v:

$$\begin{aligned}&2\Gamma(Q) + \text{s-vor}_0(Q,v) - \text{s-vor}_0(Q,\hat{v}) \le 0\\&\text{s-vor}(Q,v) + \text{s-vor}(Q,\hat{v}) + \text{s-vor}_0(Q,v) - \text{s-vor}_0(Q,\hat{v}) \le 0.\end{aligned}$$

Equality is attained if and only if the quarter is extremal. For the remaining quarters (that is, contexts $(2,1)$ and $(4,0)$), it is enough to show that $\Gamma(Q) \le 0$, if $\eta^+ \le \sqrt{2}$ and $\text{s-vor}(Q,v) \le 0$, if $\eta^+ \ge \sqrt{2}$.

Consider the case $\eta^+ \le \sqrt{2}$. If Q is a quarter such that every face has circumradius at most $\sqrt{2}$, then[4] $\Gamma(Q) \le 0$. Equality is attained if and only if the quarter is extremal. Because of this, we may assume that the circumradius of Q is greater than $\sqrt{2}$. The inequality $\eta^+(Q) \le \sqrt{2}$ implies that the faces of Q along the diagonal have nonnegative orientation. The other two faces have positive orientation, by Lemma 3.17. Since (Definition 5.6)

$$4\Gamma(Q) = \sum_{i=1}^{4} \text{s-vor}(Q, v_i),$$

it is enough to show that $\text{s-vor}(Q) < 0$. Since the orientation of every face is nonnegative and the circumradius is greater than $\sqrt{2}$, $\text{s-vor}(Q,\sqrt{2})$ is a strict truncation of the V-cell in Q, so that

$$\text{s-vor}(Q) < \text{s-vor}(Q,\sqrt{2}).$$

We show the right-hand side is nonpositive. Let v be the distinguished vertex of Q. Let A be $1/3$ the solid angle of Q at v . By the definition of $\text{s-vor}(Q,\sqrt{2})$,

[3] CALC-522528841 and CALC-892806084
[4] CALC-346093004

it is nonpositive if and only if

$$A \leq \delta_{\text{oct}} \operatorname{vol}(\mathrm{VC}(Q, v) \cap B(v, \sqrt{2})). \tag{6.1}$$

($\mathrm{VC}(Q,0)$ is defined in Section 5.1.) The intersection $\mathrm{VC}(Q,v) \cap B(v,\sqrt{2})$ consists of six Rogers simplices $R(a,b,\sqrt{2})$, three conic wedges (extending out to $\sqrt{2}$), and the intersection of $B(v,\sqrt{2})$ with a cone over v. By Lemmas 6.6, 6.7, and 6.8, these three types of solids give inequalities like that of Equation 6.1. Summing the inequalities from these lemmas, we get Equation 6.1.

Consider the case $\eta^+ \geq \sqrt{2}$ and $\sigma = \text{s-vor}$. If the quarter is upright, then[5] $\text{s-vor}(Q) \leq 0$. The quarters achieving equality are extremal. Thus, we may assume the quarter is flat. If the orientation of a flat quarter is negative along the face containing the origin and the diagonal, then[6] $\text{s-vor}(Q) \leq 0$. The quarters achieving equality are extremal. In the remaining case, the only possible face along which the orientation is negative is the top face. This means that the analytic continuation defining $\text{s-vor}(Q)$ is the same as

$$4(-\delta_{\text{oct}} \operatorname{vol}(X) + \operatorname{sol}(X)/3),$$

where X is the subset of the cone at v over Q consisting of points in that cone closer to v than to any other vertex of Q. The extreme point of X has distance at least $\sqrt{2}$ from v (since η^+ and hence the circumradius of Q are at least $\sqrt{2}$). Thus,

$$\text{s-vor}(Q) \leq \text{s-vor}(Q, \sqrt{2}).$$

We have $\text{s-vor}(Q,\sqrt{2}) \leq 0$ as in the previous paragraph, by Lemma 6.6, 6.7, and 6.8. If equality is attained, the wedges and cones must have zero volume, and each Rogers simplex must have the form $R(1, \eta(2,2,2), \sqrt{2})$ (or zero volume). This happens exactly when the flat quarter has five edges of length 2 and a diagonal of length $\sqrt{8}$. This completes the proof. □

LEMMA 6.13. *Let S be a simplex all of whose faces have circumradius at most $\sqrt{2}$. Assume that S is not a quasi-regular tetrahedron or quarter. Then* $\text{s-vor}(S) < 0$.

Proof. The assumptions imply that the orientation is positive along each face. Let v be the distinguished vertex of S.

Assume first that there are at least two edges of length at least $2t_0$ at the origin or that there are two opposite edges of length at least $2t_0$. Then the circumradius b of each of the three faces at v is at least $\eta(2, 2t_0, 2) > 1.207$. By the monotonicity properties of the circumradius of S, the simplex S has circumradius at least that of the simplex $S(2,2,2,2,2,2t_0)$, which a calculation

[5] CALC-40003553
[6] CALC-5901405

shows is greater than 1.3045. By definition, s-vor$(S) < 0$ if and only if

$$\mathrm{sol}(|S| \cap B(v,1))/3 < \delta_{\mathrm{oct}} \mathrm{vol}(\mathrm{VC}(S,0)).$$

This inequality breaks into six separate inequalities corresponding to the six Rogers's simplices $R(a,b,c)$ constituting $\mathrm{VC}(S,0)$. Rogers's Lemma 6.5 shows each of the six Rogers's simplices has density at most that of $R(1, 1.207, 1.3045)$, which is less than δ_{oct}. The result follows in this case.

Now assume that there is at most one edge of length at least $2t_0$ at the origin, and that there is not a pair of opposite edges of length at most $2t_0$. There are four cases up to symmetry, depending on which edges have length at least $2t_0$, and which have shorter length. Let S be a simplex such that every face has circumradius at most $\sqrt{2}$. We have[7] s-vor$(S(y_1, y_2, \ldots, y_6)) < 0$ for $(y_1, \ldots, y_6)$ in any of the following four domains:

$$[2t_0, \sqrt{8}][2, 2t_0]^3[2t_0, \sqrt{8}][2, 2t_0], \quad [2t_0, \sqrt{8}][2, 2t_0]^3[2t_0, \sqrt{8}]^2,$$
$$[2, 2t_0]^3[2t_0, \sqrt{8}]^2[2, 2t_0], \quad [2, 2t_0]^3[2t_0, \sqrt{8}]^3.$$

□

6.4. *Breaking clusters into pieces.* As we stated above, the strategy in the proof of local optimality will be to break quad clusters into smaller pieces and then to show that each piece has density at most δ_{oct}. There are several preliminary lemmas that will be used to prove that this decomposition into smaller pieces is well-defined. These lemmas are presented in this section.

LEMMA 6.14. *Let T be a triangle whose circumradius is less than $\sqrt{2}$. Assume that none of its edges passes through a barrier in $\mathcal{B}$. Then T does not overlap any barrier in $\mathcal{B}$.*

Proof. By hypothesis no edge of T passes through an edge in the barrier. By Lemma 2.21, no edge of a barrier passes through T. Hence they do not overlap. □

LEMMA 6.15. *Let $T = \{u, v, w\}$ be a set of three vertices whose circumradius is less than $\sqrt{2}$. Assume that one of its edges $\{v, w\}$ passes through a barrier $b = \{v_1, v_2, v_3\}$ in $\mathcal{B}$. Then*

- *The edge $\{v, w\}$ has length between $2t_0$ and $\sqrt{8}$.*
- *The vertex u is a vertex of b.*
- *One of the endpoints $y \in \{v, w\}$ is such that $\{y, v_1, v_2, v_3\}$ is a simplex in $\mathcal{Q}$.*

[7] CALC-629256313, CALC-917032944, CALC-738318844, and CALC-587618947

Proof. The edge $\{v, w\}$ must have length at least $2t_0$ by Lemma 2.19. If the edge $\{u, v\}$ has length at least $2t_0$, it cannot pass through b because of Lemma 2.33. If it has length at most $2t_0$, it cannot pass through b because of Lemma 2.19. Hence $\{u, v\}$ and similarly $\{u, w\}$ do not pass through b. The edges of b do not pass through T. The only remaining possibility is for u to be a vertex of b.

If b is a quasi-regular triangle, Lemma 2.22 gives the result. If b is a face of a quarter in the Q-system, then Lemma 2.34 gives the result. □

Definition 6.16 (Law of Cosines). Consider a triangle with sides a, b, and c. The angle opposite the edge of length c is given as

$$\begin{aligned}\operatorname{arc}(a,b,c) &= \arccos((a^2+b^2-c^2)/(2ab)) = \tfrac{\pi}{2} + \arctan \tfrac{c^2-a^2-b^2}{\sqrt{u(a^2,b^2,c^2)}}\\ &\quad \text{with } u(x,y,z) = -x^2-y^2-z^2+2xy+2yz+2zx.\end{aligned}$$

LEMMA 6.17 (First separation lemma). *Let v be a vertex of height at most $\sqrt{8}$. Let v_2 and v_3 be such that*

- 0, v, v_2, *and* v_3 *are distinct vertices,*
- $\eta(0, v_2, v_3) < \sqrt{2}$.

Then the open cone at the origin over the set $B(0, \sqrt{2}) \cap B(v, \sqrt{2})$ does not meet the closed cone C at the origin over the convex hull of $\{v_2, v_3\}$.

Proof. Let D be the open disk spanning the circle of intersection of $B(0, \sqrt{2})$ and $B(v, \sqrt{2})$. It is enough to show that this disk does not meet C. This disk is contained in $B(v, \sqrt{2})$, and so we bound this ball away from the given cone.

Assume for a contradiction that these two sets meet. Let v' be the reflection of v through the plane $P = \{0, v_2, v_3\}$.

If the closest point p in P to v lies outside C, then the edge constraints $|v| \le \sqrt{8}$ forces the closest point in C to lie along the edge $\{0, v_2\}$ or $\{0, v_3\}$. Since $|v_2|, |v_3| \le \sqrt{8}$, this closest point has distance at least $\sqrt{2}$ from v. Thus, we may assume that the closest point in P to v lies in C.

Assume next that the closest point in P to v lies in the convex hull of 0, v_2, and v_3. We obtain an edge $\{v, v'\}$ of length at most $\sqrt{8}$ that passes through a triangle of circumradius less than $\sqrt{2}$. This contradicts Lemma 2.21.

Assume finally that the closest point lies in the cone over $\{v_2, v_3\}$ but not in the convex hull of 0, v_2, v_3. By moving v toward C (preserving $|v|$), we may assume that $|v - v_2| = |v - v_3| = 2$. Stretching the edge $\{v_2, v_3\}$, we may assume that the circumradius of $\{0, v_2, v_3\}$ is precisely $\sqrt{2}$. Since the closest point in P is not in the convex hull of $\{0, v_2, v_3\}$, we may move v_2 and v_3 away from v while preserving the circumradius and increasing the lengths $|v - v_2|$ and $|v - v_3|$. By moving v again toward C, we may assume without loss of generality that $|v_2| = |v_3| = 2$ and $|v_2 - v_3| = \sqrt{8}$. We have reduced to a one-parameter family of arrangements, parametrized by $|v|$. We observe that the disk in the statement of the lemma is tangent to the segment $\{v_2, v_3\}$ at its midpoint, no matter what the value of $|v|$ is. Thus, in the extremal case, the open disk does not intersect the segment $\{v_2, v_3\}$ or the cone C that it generates. This completes the proof. $\square$

Lemma 6.18 (Second separation lemma). *Let v_1 be a vertex of height at most $2t_0$. Let v_2 and v_3 be such that*

- *0, v_1, v_2, and v_3 are distinct vertices,*
- *$\{0, v_1, v_2, v_3\} \notin \mathcal{Q}_0$, and*
- *$\{0, v_2, v_3\}$ is a barrier.*

Then the open cone at the origin over the set $B(0, \sqrt{2}) \cap B(v_1, \sqrt{2})$ does not meet the closed cone C at the origin over $\{v_2, v_3\}$.

Proof. Since v_1 has height at most $2t_0$, and $\{0, v_2, v_3\}$ is a barrier, it follows from Lemma 2.10 that $\{0, v_1, v_2, v_3\}$ is in the Q-system if $|v_1 - v_2| \le 2t_0$ and $|v_1 - v_3| \le 2t_0$. This is contrary to hypothesis. Thus, we may assume without loss of generality that $|v_1 - v_2| > 2t_0$.

By arguing as in the proof of Lemma 6.17, we may assume that the orthogonal projection of v_1 to the plane P is a point in the cone C. Let v_1' be the reflection of v_1 through C. We have that either $\{v_2, v_3\}$ passes through $\{0, v_1, v_1'\}$ or $\{v_1, v_1'\}$ passes through $\{0, v_2, v_3\}$. We may assume for a contradiction that $|v_1 - v_1'| < \sqrt{8}$.

If $\{v_2, v_3\}$ passes through $\{0, v_1, v_1'\}$, then v_2 and v_3 are anchors of the diagonal $\{v_1, v_1'\}$ by Lemma 2.24. This gives the contradiction $|v_1 - v_2| \le 2t_0$.

If $\{v_1, v_1'\}$ passes through $\{0, v_2, v_3\}$, then by Lemma 2.22 $\{0, v_2, v_3\}$ is a face of a quarter. Moreover, v_1 and v_1' are anchors of the diagonal of that quarter by Lemma 2.24. Since $|v_1 - v_2| > 2t_0$, the diagonal must not have v_2 as an endpoint, so that the diagonal is $\{0, v_3\}$. Lemma 2.34 forces one of $|v_1 - v_2|$ or $|v_1' - v_2|$ to be at most $2t_0$. But these are both equal to $|v_1 - v_2| > 2t_0$, a contradiction. $\square$

Definition 6.19. We define an enlarged set of simplices $\mathcal{Q}_0'$. Let $\mathcal{Q}_0'$ be the set of simplices S with a vertex at the origin such that either $S \in \mathcal{Q}_0$, or S is a simplex with a vertex at the origin and with circumradius less than $\sqrt{2}$ such that none of its edges passes through a barrier.

Lemma 6.20. *The simplices in $\mathcal{Q}_0'$ do not overlap one another.*

Proof. The simplices in $\mathcal{Q}_0$ are in the Q-system and do not overlap. No edge of length less than $\sqrt{8}$ passes through any edge of a simplex in $\mathcal{Q}_0' \setminus \mathcal{Q}_0$, by Lemma 2.21. By construction, none of the edges of a simplex in $\mathcal{Q}_0' \setminus \mathcal{Q}_0$ can pass through a barrier, and this includes all the faces of $\mathcal{Q}_0$. Thus, there is no overlap. $\square$

Definition 6.21. Let v be a vertex of height at most $2.36 = 2(1.18)$. Let $C(v)$ be the cone at the origin generated by the intersection $B(v, \sqrt{2}) \cap B(0, \sqrt{2})$. Define a subset $C'(v)$ of $C(v)$ by the conditions:

1. $x \in C(v)$.
2. x is closer to 0 than to v.
3. $x \in B(0, \sqrt{2})$.
4. x does not lie in the cone over any simplex in $\mathcal{Q}_0$.
5. For every vertex $u \neq 0, v$ such that the face $\{0, u, v\}$ is a barrier or has circumradius less than $\sqrt{2}$ and such that none of the edges of this face pass through a barrier, we have that x and v lie in the same half-space bounded by the plane perpendicular to $\{0, u, v\}$ and passing through 0 and the circumcenter of $\{0, u, v\}$.
6. For every simplex $\{0, v_1, v_2, v\} \in \mathcal{Q}_0$, the segment $\{x, v\}$ does not cross through the cone $C(\{0, v_1, v_2\})$.

LEMMA 6.22. *For every vertex v of height at most* 2.36, *we have* $C'(v) \subset \mathrm{VC}(0)$.

Proof. Assume for a contradiction that $x \in C'(v) \cap \mathrm{VC}(u)$, with $u \neq 0$. Lemma 3.20 implies that x is unobstructed at 0. Thus $|x - u| < |x| \leq \sqrt{2}$.

Assume that the hypotheses of Condition 5 in Definition 6.21 are satisfied. This, together with $x \in C(v)$ implies that $\eta(\{0, u, v\}) < \sqrt{2}$. An element x that is closer to 0 than to v and in the same half-space as v (in the half-space bounded by the perpendicular plane to $\{0, u, v\}$ through 0 and the circumcenter of $\{0, u, v\}$) is closer to 0 than to u, which is contrary to $x \in \mathrm{VC}(u)$. This completes the proof, except in the case that an edge of the triangle $\{0, u, v\}$ passes through a barrier b. Assume that this is so.

The edge $\{0, v\}$ cannot pass through a barrier because it is too short (length less than $2t_0$).

Suppose that the edge $\{u, v\}$ passes through a barrier b. By Lemma 6.15 applied to $T = \{0, u, v\}$, the origin is a vertex of b. There are three possibilities:

1. x is obstructed from u by b.
2. x is obstructed from v by b.
3. x is not obstructed from either u or v by b.

The first possibility runs contrary to the hypothesis $x \in \mathrm{VC}(u)$. The second possibility, together with Lemma 6.18, implies that $\{v, b\}$ is a simplex in the Q-system. This is contrary to Condition 6 defining $C'(v)$.

The third possibility is eliminated as follows. Every point in the half-space containing v and bounded by the plane of b

- is obstructed at u by b, or
- has distance at least $\sqrt{2}$ from u (because each edge of b has this property).

Since x has neither of these properties, we find that x must lie in the same half space bounded by the plane of b as u. Let S be the simplex formed by b and v. If $S \notin \mathcal{Q}_0$, then Lemma 6.18 shows that no part of the cone $C(v)$ lies in the same half space as u. So $S \in \mathcal{Q}_0$. By Condition 6 on $C'(v)$, the line from x to v does not intersect the cone at the origin over b. But then the arc-length of the geodesic on the unit sphere running from the projection of x to the projection of v is at least $\mathrm{arc}(|v|, \sqrt{8}, 2) \geq \mathrm{arc}(|v|, \sqrt{2}, \sqrt{2})$. This measurement shows that x lies outside the cone $C(v)$, which is contrary to assumption.

Suppose that the edge $\{0, u\}$ passes through the barrier b. By Lemma 6.15 applied to $T = \{0, u, v\}$, we get that v is a vertex of b. There are again three possibilities

1. x is obstructed from u by b.
2. x is not obstructed from either u or 0 by b.
3. x is obstructed from 0 by b.

The first possibility runs contrary to the hypothesis $x \in \mathrm{VC}(u)$. The second places x outside the convex hull of 0, b, u and gives $|x - u| + |x| > \sqrt{8}$, which is contrary to $|x - u| \leq |x| \leq \sqrt{2}$. The third possibility cannot occur by the observation made at the beginning of the proof that x is unobstructed at 0. $\square$

It follows from the definition that $C'(v)$ is star convex at the origin. We make this more explicit in the following lemma.

LEMMA 6.23. *Assume* $|v| \leq 2.36$. *Let* $F(v)$ *be the intersection of* $\Omega(0) \cap \Omega(v)$; *that is, the face of the Voronoi cell of* $\Omega(0)$ *associated with the vertex* v. *Let* $F'(v)$ *be the part of* $F(v) \cap B(0, 1.18)$ *that is not in the cone over any simplex in* $\mathcal{Q}_0$. *Let* $H(v)$ *be the closure of the union of segments from the origin to points of* $F'(v)$. *Let* $C''(v)$ *be the cone at the origin spanned by* $B(0, 1.18) \cap B(v, 1.18)$. *Then the closure of* $C'(v) \cap C''(v)$ *is equal to* $H(v)$.

Proof. We have $F'(v) \subset C''(v)$. First we show that $F'(v)$ lies in the closure of $C'(v)$. For this, we check that points of $F'(v)$ satisfy the (closed counterparts of) Conditions 1–6 defining $C'(v)$ (see Definition 6.21). Conditions 1–4 are immediate from the definitions. If u is a vertex as in Condition 5, then the half-space it determines is that containing the origin and the edge of the Voronoi cell determined by u and v. Condition 5 now follows. Consider Condition 6. Suppose that $\{x,v\}$ crosses the cone $\{0,v_1,v_2\}$ and that $x\in F'(v)$. (The point of intersection has height at most $\sqrt{2}$ and hence lies in the convex hull of $\{0,v_1,v_2\}$.) This implies that x is obstructed at v. By Lemma 3.22, this implies that $|x-v|\ge t_0$. Since x is equidistant from v and the origin, we find that $|x|\ge t_0$, which is contrary to $x\in B(0,1.18)$.

To finish the proof, we show that $C'(v)\cap C''(v)\subset H(v)$. For a contradiction, consider a point $x\in C'(v)\cap C''(v)$ that is not in $H(v)$. It must lie in the cone over some other face of the Voronoi cell; say that of u. The constraints force the circumradius of $T=\{0,v,u\}$ to be at most 1.18. The edges of T are too short to pass through a barrier. Thus, Condition 5 defining $C'(v)$ places a bounding plane that is perpendicular to T and that runs through the origin and the circumcenter of T. This prevents x from lying in the cone over the face of the Voronoi cell attached to u. $\square$

Remark 6.24. In the lemma, it is enough to consider simplices along $\{0,w\}$, because

$$\operatorname{arc}(|v|,\sqrt{8},2)>\operatorname{arc}(|v|,1.18,1.18).$$

COROLLARY 6.25. *If $x\in \mathrm{VC}(0)$, with $0<|x|\le 1.18$, if the point at distance 1.18 from 0 along the ray $(0,x)$ does not lie in $\mathrm{VC}(0)$, and if x is not in the cone over any simplex of $\mathcal{Q}_0$, then there is some v such that $x\in C'(v)$, and $|v|\le 2.36$.*

Proof. If $x\in \mathrm{VC}(0)\cap B(0,1.18)$, then $x\in\Omega(0)\cap B(0,1.18)$ by Lemma 3.23. Also x lies in the cone over some face $F(v)$ of the Voronoi cell $\Omega(0)$. The hypotheses imply that x lies in the cone over $F'(v)$. Lemma 6.23 implies that $x\in C'(v)$. $\square$

LEMMA 6.26. *Assume that $|u|\le 2.36$ and that $|v|\le 2.36$. The sets $C'(u)$, $C'(v)$ do not overlap for $u\ne v$.*

Proof. If there is some x in the overlap, then the circumradius of $\{0,u,v\}$ is less than $\sqrt{2}$. If no edge of $\{0,u,v\}$ passes through a barrier, then the defining conditions of $C'(u)$ and $C'(v)$ separate them along the plane perpendicular to $\{0,u,v\}$ and passing through the origin and the circumcenter of $\{0,u,v\}$.

If some edge of $\{0,u,v\}$ passes through a barrier, then an argument like that in the proof of Lemma 6.22 shows they do not overlap. $\square$

LEMMA 6.27. *Let S be a simplex whose circumradius is less than $\sqrt{2}$. If five of the six edges of the simplex do not pass through a barrier, then the sixth* *edge e does not pass through a barrier either, unless both endpoints of the edge opposite e in S are vertices of the barrier.*

Proof. We leave this as an exercise. The point is that it is impossible to draw the barrier without having one of its edges pass through a face of S, which is ruled out by Lemma 2.21. □

6.5. *Proofs.* We are finally prepared to give a proof of Theorem 6.4. We break the proof into two lemmas.

Lemma 6.28. *If R is a standard region that is not a triangle, then $\sigma_R(D) \le 0$.*

Proof. This proof is an adaptation of the main result in [Hal97b, Th. 4.1]. We consider the V-cell at a vertex, which we take to be the origin. We will partition the V-cell into pieces. On each piece it will be shown that σ is nonpositive.

Throughout the proof we make use of the correspondence between $\sigma_R(D$ ≤ 0 and the bound of δ_{oct} on densities, on standard regions R (away from simplices in the Q-system). This correspondence is evident from Lemma 5.18, which gives the formula

$$\sigma_R(D) = 4\left(-\delta_{\text{oct}} \mathrm{vol}\,\mathrm{VC}_{R'}(D) + \mathrm{sol}(R')/3\right) + \sum_{Q\in\mathcal{Q}_0(R,D)} \sigma(Q, c(Q,D), 0).$$

If $\sigma(Q, c(Q,D), 0) \le 0$, and $\mathrm{vol}\,\mathrm{VC}_{R'}(D) \ne 0$ then $\sigma_R(D) \le 0$ follows from the inequality

$$(\mathrm{sol}(R')/3)/\mathrm{vol}\,\mathrm{VC}_{R'}(D) \le \delta_{\text{oct}}.$$

This is an assertion about the ratio of two volumes, that is, a bound δ_{oct} on the density of $\mathrm{VC}_{R'}(D)$.

The parts of $\mathrm{VC}(D)$ that lie in the cone over some simplex in $\mathcal{Q}_0$ are easily treated. If S is in $\mathcal{Q}_0$, then it is either a quasi-regular tetrahedron or a quarter. If it is a quasi-regular tetrahedron, it is excluded by the hypothesis of the lemma. If it is a quarter, $\sigma(S) \le 0$ by Lemma 6.12. The parts of $\mathrm{VC}(D)$ that lie in the cone over some simplex in $\mathcal{Q}_0' \setminus \mathcal{Q}_0$ are also easily treated. The simplex $S = \{0, v, w, w'\}$ has circumradius less than $\sqrt{2}$. Use s-vor(S) on the simplex. Lemma 6.13 shows that s-vor$(S) < 0$ as desired.

Next we consider the parts of $\mathrm{VC}(D)$ that are not in any $C'(v)$ (with $|v| \le 2.36$) and that are not in any cone over a simplex in $\mathcal{Q}_0'$. (Note that by Lemmas 6.17 and 6.18, if a cone over some simplex in $\mathcal{Q}_0'$ meets $C'(v)$, then v must be a vertex of that simplex.) By Corollary 6.25, if x belongs to this set, then all the points out to radius 1.18 in the same direction belong to this set. By Lemma 6.8, the density of such parts is less than δ_{oct}.

Finally, we treat the parts of $\mathrm{VC}(D)$ that are in some $C'(v)$ but that lie outside all cones over simplices in $\mathcal{Q}_0'$.

Fix v of height at most 2.36. Let $w_1, w_2, \ldots, w_k$ be the vertices w near $\{0, v\}$ such that either $\{0, v, w\}$ is a barrier or it has circumradius less than $\sqrt{2}$, and such that none of its edges passes through a barrier. We view the triangles $\{0, v, w_i\}$ as a fan of triangles around the edge $\{0, v\}$. We assume that the vertices are indexed so that consecutive triangles in this fan have consecutive indices (modulo k). We will analyze the densities separately within each wedge, where a wedge is the intersection along the line $\{0, v\}$ of half spaces bounded by the half planes $\{0, v, w_i\}$ and $\{0, v, w_{i+1}\}$. Space is partitioned by these k different wedges. Fix i and write $w = w_i$, $w' = w_{i+1}$. Let $S = \{0, v, w, w'\}$.

Let F be the convex planar region in the perpendicular bisector of $\{0, v\}$ defined by the points inside the closure of $C'(v)$, inside the wedge between $\{0, v, w\}$ and $\{0, v, w'\}$, closer to v than to w, and closer to v than to w'. This planar region is illustrated in Figure 6.2. The edge e lies in the line perpendicular to $\{0, v, w\}$ and through the circumcenter of $\{0, v, w\}$. It extends from the circumcenter out to distance $\sqrt{2}$ from the vertices 0, v, w. If the circumradius of $\{0, v, w\}$ is greater than $\sqrt{2}$, the edge e reduces to a point, and only the arc a at distance $\sqrt{2}$ from 0 and v appears. Similar comments apply to e'.

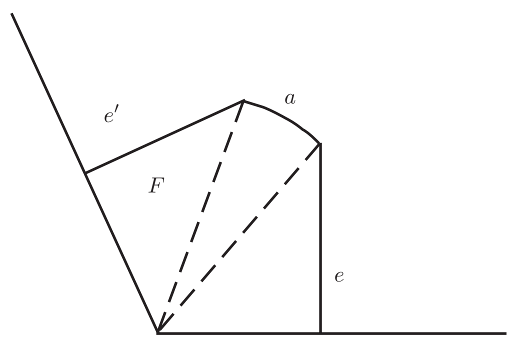

Figure 6.2: A planar region.

Case 1. *Circumradius of S is less than $\sqrt{2}$.* We show that this case does not occur. If none of the edges of this simplex pass through a barrier, then this simplex belongs to $\mathcal{Q}_0'$, a case already considered. By definition of the wedges, the edges $\{0, v\}$, $\{0, w\}$, $\{0, w'\}$, $\{v, w\}$, and $\{v, w'\}$ do not pass through a barrier. Since five of the six edges do not pass through a barrier, and since S is formed by consecutive triangles in the fan around $\{0, v\}$, the sixth does not pass through a barrier either, by Lemma 6.27.

Case 2. *Circumradius of S is at least $\sqrt{2}$.* Let $r \geq \sqrt{2}$ be the circumradius. We claim that the edge e cannot extend beyond the wedge through the half plane through $\{0, v, w'\}$. In fact, the circumcenter of $\{0, v, w, w'\}$ lies on the extension (in one direction or the other) of the segment e to a point at distance r from the origin. If this circumcenter does not lie in the wedge, then the orientation is negative along one of the faces $\{0, v, w\}$ or $\{0, v, w'\}$. This face must have circumradius at least $\sqrt{2}$, by Lemma 3.18, and this forces the face to be a barrier. If the orientation is negative along a barrier, then the simplex $\{0, v, w, w'\}$ is a simplex in $\mathcal{Q}_0$ (Lemmas 3.16 and 3.17). This is contrary to our assumption above that $\{0, v, w, w'\}$ is not in $\mathcal{Q}_0$.

These comments show that Figure 6.2 correctly represents the basic shape of F, with the understanding that the edges e and e' may degenerate to a point. By construction, every point x in the open convex hull $\{F, 0\}$ of F and 0 lies in $C'(v) \subset \mathrm{VC}(0)$. The convex hull $\{F, 0\}$ is the union of three solids, two Rogers simplices along the triangles $\{0, v, w\}$ and $\{0, v, w'\}$ respectively, and the conic solid given by the convex hull of the arc a, $v/2$ and 0. By Lemmas 6.6 and 6.7, these solids have density at most δ_{oct}.

This completes the proof that $\sigma_R(D)$ is never positive on non-triangular standard regions R. Note that the decomposition into the parts of cones $C'(v)$ inside a wedge is compatible with the partition of the unit sphere into standard regions, so that the estimate holds over each standard region, and not just over the union of the standard regions. □

LEMMA 6.29. *If R is a standard region that is not a triangle, and if $\sigma_R(D) = 0$, then (R, D) is a quad cluster. Moreover, the four corners of R in the quad cluster have height* 2, *forming a square of side* 2.

Proof. To analyze the case of equality, first we note that any truncation at 1.18 produces a strict inequality (Lemma 6.8 is strict if the volume is nonzero), so that every point must lie over a simplex in $\mathcal{Q}'_0$ or over some $C'(v)$. We have $\text{s-vor}(S) < 0$ for simplices with circumradius less than $\sqrt{2}$. The only simplices in $\mathcal{Q}_0$ that produce equality are those with five edges of length 2 and a diagonal of length $\sqrt{8}$. Any nontrivial arc a produces strict inequality (see Lemma 6.7, so we must have that e and e' meet at exactly distance $\sqrt{2}$ from 0 and v. Moreover, if e does not degenerate to a point, the corresponding Rogers simplex gives strict inequality, unless $\{0, v, w\}$ is an equilateral triangle with side length 2. We conclude that the entire part of the V-cell over the standard region must be assembled from Rogers simplices $R(1, \eta(2, 2, 2), \sqrt{2})$, and quarters with lengths $(2, 2, 2, 2, 2, \sqrt{8})$. This forces each vertex v of height at most $2t_0$ to have height 2. It forces each pair of triangles $\{0, v_1, v_2\}$ $\{0, v_2, v_3\}$, that determine consecutive edges along the boundary of the standard region to meet at right angles:

$$\mathrm{dih}(0, v_2, v_1, v_3) = 0.$$

This forces the object to be a quad cluster of the indicated form. □

We conclude the chapter with a proof of the main theorem. With all our preparations in place, the proof is short.

Proof of Theorem 6.1 (*Local optimality*). The hypothesis implies that there are six quad clusters and eight quasi-regular tetrahedra at the origin of the decomposition star. By Lemma 6.10, each quasi-regular tetrahedron scores at most 1 pt with equality if and only if the tetrahedron is regular with edge-length 2. By Theorem 6.4, each quad cluster scores at most 0, with equality if and only if the corners of the quad cluster form a square with edge-length 2 at distance 2 from the origin. Thus, $\sigma(D)$ is at most 8 pt. In the case of equality, there are twelve vertices at distance 2 from the origin, forming eight equilateral triangles and six squares (all of edge-length 2). These conditions are satisfied precisely when the arrangement is U_{fcc} or U_{hcp} up to a Euclidean motion. □

7. Tame graphs

This chapter defines a class of plane graphs. Graphs in this class are said to be *tame*. In the next chapter, we give a complete classification of all tame graphs. This classification of tame graphs was carried out by computer and is a major step of the proof of the Kepler conjecture.

7.1. *Basic definitions.*

Definition 7.1. An *n-cycle* is a finite set C of cardinality n, together with a cyclic permutation s of C. We write s in the form $v \mapsto s(v, C)$, for $v \in C$. The element $s(v, C)$ is called the *successor* of v (in C). A *cycle* is an n-cycle for some natural number n. By abuse of language, we often identify C with the cycle. The natural number n is the *length* of the cycle.

Definition 7.2. Let G be a nonempty finite set of cycles (called faces) of length at least 3. The elements of faces are called the *vertices* of G. An unordered pair of vertices $\{v, w\}$ such that one element is the successor of the other in some face is called an *edge*. The vertices v and w are then said to be *adjacent*. The set G is a *plane graph* if four conditions hold.

1. If an element v has successor w in some face F, then there is a unique face (call it $s'(F, v)$) in G for which v is the successor of w. (Thus, $v = s(w, s'(F, v))$, and each edge occurs twice with opposite orientation.)

2. For each vertex v, the function $F \mapsto s'(F, v)$ is a cyclic permutation of the set of faces containing v.

3. Euler's formula holds relating the number of vertices V, the number of edges E, and the number of faces F:
$$V - E + F = 2.$$

4. The set of vertices is connected. That is, the only nonempty set of vertices that is closed under $v \mapsto s(v, C)$ for all C is the full set of vertices.

Remark 7.3. The set of vertices and edges of a plane graph form a planar graph in the usual graph-theoretic sense of admitting an embedding into the plane. Every planar graph carries an orientation on its faces that is inherited from an orientation of the plane. (Use the right-hand rule on the face, to orient it with the given outward normal of the oriented plane.) For us, the orientation is built into the definition, so that properly speaking, we should call these objects *oriented plane graphs*. We follow the convention of distinguishing between planar graphs (which admit an embedding into the plane) and plane graphs (for which a choice of embedding has been made). Our definition is more restrictive than the standard definition of plane graph in the literature, because we require all faces to be simple polygons with at least 3 vertices. Thus, a graph with a single edge does not comply with our narrow definition of plane graph. Other graphs that are excluded by this definition are shown in Figure 7.1. Standard results about plane graphs can be found in any of a number of graph theory textbooks. However, this paper is written in such a way that it should not be necessary to consult outside graph theory references.

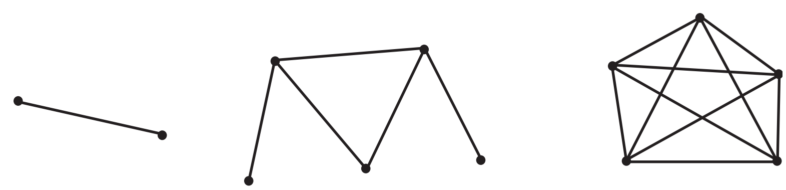

Figure 7.1: Some examples of graphs that are excluded from the narrow definition of plane graph, as defined in this section.

Definition 7.4. Let *len* be the length function on faces. Faces of length 3 are called *triangles*, those of length 4 are called *quadrilaterals*, and so forth. Let $\text{tri}(v)$ be the number of triangles containing a vertex v. A face of length at least 5 is called an *exceptional* face.

Two plane graphs are *properly* isomorphic if there is a bijection of vertices inducing a bijection of faces. For each plane graph, there is an opposite plane graph G^{op} obtained by reversing the cyclic order of vertices in each face. A plane graph G is isomorphic to another if G or G^{op} is properly isomorphic to the other.

Definition 7.5. The *degree* of a vertex is the number of faces it belongs to. An *n-circuit* in G is a cycle C in the vertex-set of G, such that for every $v \in C$, it forms an edge in G with its successor: that is, $(v, s(v, C))$ is an edge of G.

In a plane graph G we have a combinatorial form of the Jordan curve theorem: each n-circuit determines a partition of G into two sets of faces.

Definition 7.6. The *type* of a vertex is defined to be a triple of nonnegative integers (p, q, r), where p is the number of triangles containing the vertex, q is the number of quadrilaterals containing it, and r is the number of exceptional faces. When $r = 0$, we abbreviate the type to the ordered pair (p, q).

7.2. *Weight assignments.* We call the constant $\mathrm{tgt} = 14.8$, which arises repeatedly in this section, the *target*. (This constant arises as an approximation to $4\pi\zeta - 8 \approx 14.7947$, where $\zeta = 1/(2\arctan(\sqrt{2}/5))$.)

Define $a : \mathbb{N} \to \mathbb{R}$ by

$$a(n) = \begin{cases} 14.8 & n = 0, 1, 2, \\ 1.4 & n = 3, \\ 1.5 & n = 4, \\ 0 & \text{otherwise.} \end{cases}$$

Define $b : \mathbb{N} \times \mathbb{N} \to \mathbb{R}$ by $b(p, q) = 14.8$, except for the values in the following table (with $\mathrm{tgt} = 14.8$):

	$q = 0$	1	2	3	4
$p = 0$	tgt	tgt	tgt	7.135	10.649
1	tgt	tgt	6.95	7.135	tgt
2	tgt	8.5	4.756	12.981	tgt
3	tgt	3.642	8.334	tgt	tgt
4	4.139	3.781	tgt	tgt	tgt
5	0.55	11.22	tgt	tgt	tgt
6	6.339	tgt	tgt	tgt	tgt.

Define $c : \mathbb{N} \to \mathbb{R}$ by

$$c(n) = \begin{cases} 1 & n = 3, \\ 0 & n = 4, \\ -1.03 & n = 5, \\ -2.06 & n = 6, \\ -3.03 & \text{otherwise.} \end{cases}$$

Define $d : \mathbb{N} \to \mathbb{R}$ by

$$d(n) = \begin{cases} 0 & n = 3, \\ 2.378 & n = 4, \\ 4.896 & n = 5, \\ 7.414 & n = 6, \\ 9.932 & n = 7, \\ 10.916 & n = 8, \\ \mathrm{tgt} = 14.8 & \text{otherwise.} \end{cases}$$

A set V of vertices is called a *separated* set of vertices if the following four conditions hold.

1. For every vertex in V there is an exceptional face containing it.
2. No two vertices in V are adjacent.
3. No two vertices in V lie on a common quadrilateral.
4. Each vertex in V has degree 5.

A *weight assignment* of a plane graph G is a function $w : G \to \mathbb{R}$ taking values in the set of nonnegative real numbers. A weight assignment is *admissible* if the following properties hold:

1. If the face F has length n, then $w(F) \geq d(n)$.
2. If v has type (p, q), then
$$\sum_{F:\, v\in F} w(F) \geq b(p, q).$$
3. Let V be any set of vertices of type $(5, 0)$. If the cardinality of V is $k \leq 4$, then
$$\sum_{F:\, V\cap F\neq\emptyset} w(F) \geq 0.55k.$$
4. Let V be any separated set of vertices. Then
$$\sum_{F:\, V\cap F\neq\emptyset} (w(F) - d(\mathrm{len}(F))) \geq \sum_{v\in V} a(\mathrm{tri}(v)).$$

The sum $\sum_F w(F)$ is called the *total weight* of w.

7.3. *Plane graph properties.* We say that a plane graph is *tame* if it satisfies the following conditions.

1. The length of each face is at least 3 and at most 8.
2. Every 3-circuit is a face or the opposite of a face.
3. Every 4-circuit surrounds one of the cases illustrated in Figure 7.2.
4. The degree of every vertex is at least 2 and at most 6.
5. If a vertex is contained in an exceptional face, then the degree of the vertex is at most 5.

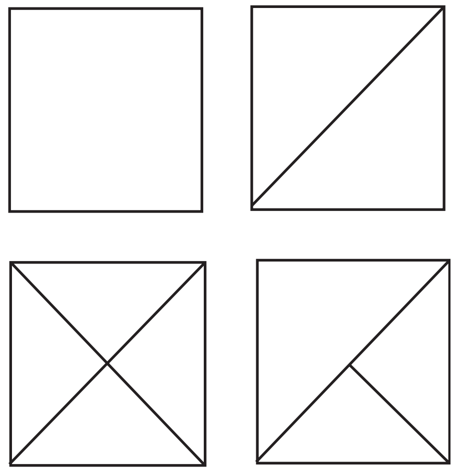

Figure 7.2: Tame 4-circuits

6. $$\sum_F c(\mathrm{len}(F)) \geq 8,$$

7. There exists an admissible weight assignment of total weight less than the target, $\mathrm{tgt} = 14.8$.

8. There are never two vertices of type $(4, 0)$ that are adjacent to each other.

It follows from the definitions that the abstract vertex-edge graph of G has no loops or multiple joins. Also, by construction, every vertex lies in at least two faces. Property 6 implies that the graph has at least eight triangles.

Remark 7.7. We pause to review the strategy of the proof of the Kepler conjecture as described in Section 1.2. The decomposition stars that violate the main inequality $\sigma(D) \geq 8\,\mathrm{pt}$ are said to contravene. A plane graph is associated with each contravening decomposition star. These are the contravening plane graphs. The main object of this paper is to prove that the only two contravening graphs are G_{fcc} and G_{hcp}, the graphs associated with the face-centered cubic and hexagonal close packings.

We have defined a set of plane graphs, called *tame graphs*. The next chapter will give a classification of tame plane graphs. (There are several thousand.) Chapter 9 gives a proof that all contravening plane graphs are tame. By the classification result, this reduces the possible contravening graphs to an explicit finite list. Case-by-case linear programming arguments will show that none of these tame plane graphs is a contravening graph (except G_{fcc} and G_{hcp}). Having eliminated all possible graphs, we arrive at the resolution of the Kepler conjecture.

8. Classification of tame plane graphs

8.1. *Statement of the theorem.* A list of several thousand plane graphs appears at [Hal05]. The following theorem is listed as one of the central claims in the proof in Section 1.3.

THEOREM 8.1. *Every tame plane graph is isomorphic to a plane graph in this list.*

The results of this section are not needed except in the proof of Theorem 8.1.

Computers are used to generate a list of all tame plane graphs and to check them against the archive of tame plane graphs. We will describe a finite state machine that produces all tame plane graphs. This machine is not particularly efficient, and so we also include a description of pruning strategies that prevent a combinatorial explosion of possibilities.

8.2. *Basic definitions.* In order to describe how all tame plane graphs are generated, we need to introduce *partial plane graphs* that encode an incompletely generated tame graph. A partial plane graph is itself a graph, but marked in such a way as to indicate that it is in a transitional state that will be used to generate further plane graphs.

Definition 8.2. A *partial plane graph* is a plane graph with additional data: every face is marked as "complete" or "incomplete." We call a face *complete* or *incomplete* according to the markings. We require the following condition.

- *No two incomplete faces share an edge.*

Each unmarked plane graph is identified with the marked plane graph in which every face is complete. We represent a partial plane graph graphically by deleting one face (the face at infinity) and drawing the others and shading those that are complete.

A *patch* is a partial plane graph P with two distinguished faces F_1 and F_2, such that the following hold.

- Every vertex of P lies in F_1 or F_2.
- The face F_2 is the only complete face.
- F_1 and F_2 share an edge.
- Every vertex of F_2 that is not in F_1 has degree 2.

F_1 and F_2 will be referred to as the distinguished incomplete and the distinguished complete faces, respectively.

Patches can be used to modify a partial plane graph as follows. Let F be an incomplete face of length n in a partial plane graph G. Let P be a patch whose incomplete distinguished face F_1 has length n. Replace P with a properly isomorphic patch P' in which the image of F_1 is equal to $F^{\rm op}$ and in which no other vertex of P' is a vertex of G. Then

$$G' = \{F' \in G \cup P' : F' \neq F^{\rm op}, F' \neq F\}$$

is a partial plane graph. Intuitively, we cut away the faces F and F_1 from their plane graphs, and glue the holes together along the boundary (Figure 8.1). (It is immediate that the Condition 8.2 in the definition of partial plane graphs is maintained by this process.) There are n distinct proper ways of identifying F_1 with $F^{\rm op}$ in this construction, and we let ϕ be this identification. The isomorphism class of G' is uniquely determined by the isomorphism class of G, the isomorphism class of P, and ϕ (ranging over proper bijections $\phi : F_1 \mapsto F^{\rm op}$).

8.3. *A finite state machine.* For a fixed N we define a finite state machine as follows. The states of the finite state machine are isomorphism classes of partial plane graphs G with at most N vertices. The transitions from one state G to another are isomorphism classes of pairs (P, ϕ) where P is a patch, and ϕ pairs an incomplete face of G with the distinguished incomplete face of P. However, we exclude a transition (P, ϕ) at a state if the resulting partial plane graphs contains more than N vertices. Figure 8.1 shows two states and a transition between them.

The initial states I_n of the finite state machine are defined to be the isomorphism classes of partial plane graphs with two faces:

$$\{(1, 2, \ldots, n), (n, n-1, \ldots, 1)\}$$

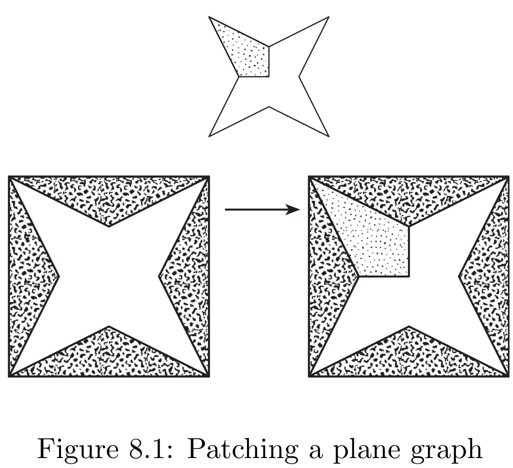

Figure 8.1: Patching a plane graph

where $n \leq N$, one face is complete, and the other is incomplete. In other words, they are patches with exactly two faces.

A terminal state of this finite state machine is one in which every face is complete. By construction, these are (isomorphism classes of) plane graphs with at most N vertices.

Lemma 8.3. *Let G be a plane graph with at most N vertices. Then its state in the machine is reachable from an initial state through a series of transitions.*

Proof. Pick a face in G of length n and identify it with the complete face in the initial state I_n. At any stage at state G', we have an identification of all of the vertices of the plane graph G' with some of the vertices of G, and an identification of all of the complete faces of G' with some of the faces of G (all faces of G are complete). Pick an incomplete face F of G' and an oriented edge along that face. We let F' be the complete face of G with that edge, with the same orientation on that edge as F. Create a patch with distinguished faces $F_1 = F^{\mathrm{op}}$ and $F_2 = F'$. (F_1 and F_2 determine the patch up to isomorphism.) It is immediate that the conditions defining a patch are fulfilled. Continue in this way until a graph isomorphic to G is reached. □

Remark 8.4. It is an elementary matter to generate all patches P such that the distinguished faces have given lengths n and m. Patching is also entirely algorithmic, and thus by following all paths through the finite state machine, we obtain all plane graphs with at most N vertices.

8.4. *Pruning strategies.* Although we reach all graphs in this manner, it is not computationally efficient. We introduce pruning strategies to increase the efficiency of the search. We can terminate our search along a path through the finite state machine, if we can determine:

1. Every terminal graph along that path violates one of the defining properties of tameness, or

2. An isomorphic terminal graph will be reached by some other path that will not be terminated early.

Here are some pruning strategies of the first type (1). They are immediate consequences of the conditions of the defining properties of tameness.

- If the current state contains an incomplete face of length 3, then eliminate all transitions, except for the transition that carries the partial plane graph to a partial plane graph that is the same in all respects, except that the face has become complete.

- If the current state contains an incomplete face of length 4, then eliminate all transitions except those that lead to the possibilities of Section 7.3, Property 3, where in Property 3 each depicted face is interpreted as being complete.

- Remove all transitions with patches whose complete face has length greater than 8.

- It is frequently possible to conclude from the examination of a partial plane graph that no matter what the terminal position, any admissible weight assignment will give total weight greater than the target (tgt = 14.8). In such cases, all transitions out of the partial plane graph can be pruned.

To take a simple example of the last item, we observe that weights are always nonnegative, and that the weight of a complete face of length n is at least $d(n)$. Thus, if there are complete faces $F_1, \ldots, F_k$ of lengths $n_1, \ldots, n_k$, then any admissible weight assignment has total weight at least $\sum_{i=1}^{k} d(n_i)$. If this number is at least the target, then no transitions out of that state need be considered.

More generally, we can apply all of the inequalities in the definition of admissible weight assignment to the complete portion of the partial plane graph to obtain lower bounds. However, we must be careful, in applying Property 4 of admissible weight assignments, because vertices that are not adjacent at an intermediate state may become adjacent in the complete graph. Also, vertices that do not lie together in a quadrilateral at an intermediate state may do so in the complete graph.

Here are some pruning strategies of the second type (2).

- At a given state it is enough to fix one incomplete face and one edge of that face and then to follow only the transitions that patch along that face and add a complete face along that edge. (This is seen from the proof of Lemma 8.3.)

- In leading out from the initial state I_n, it is enough to follow paths in which every added complete face has length at most n. (A graph with a face of length m, for $m > n$, will be also be found downstream from I_m.)

- Make a list of all type (p, q) with $b(p, q) < \text{tgt} = 14.8$. Remove the initial states I_3 and I_4, and create new initial states $I_{p,q}$ ($I'_{p,q}$, $I''_{p,q}$, etc.) in the finite state machine. Define the state $I_{p,q}$ to be one consisting of $p+q+1$ faces, with p complete triangles and q complete quadrilaterals all meeting at a vertex (and one other incomplete face away from v). (If there is more than one way to arrange p triangles and q quadrilaterals, create states

$I_{p,q}$, $I'_{p,q}$, $I''_{p,q}$, for each possibility. See Figure 8.2.) Put a linear order on states $I_{p,q}$. In state transitions downstream from $I_{p,q}$ disallow any transition that creates a vertex of type (p', q'), for any (p', q') preceding (p, q) in the imposed linear order.

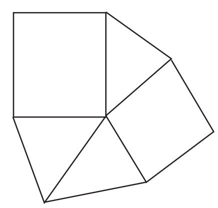

Figure 8.2: States $I_{3,2}$ and $I'_{3,2}$

This last pruning strategy is justified by the following lemma, which classifies vertices of type (p, q).

LEMMA 8.5. *Let A and B be triangular or quadrilateral faces that have at least 2 vertices in common in a tame graph. Then the faces have exactly two vertices in common, and an edge is shared by the two faces.*

Proof. Exercise. Some of the configurations that must be ruled out are shown in Figure 8.3. Some properties that are particularly useful for the exercise are Properties 2 and 3 of tameness, and Property 2 of admissibility. □

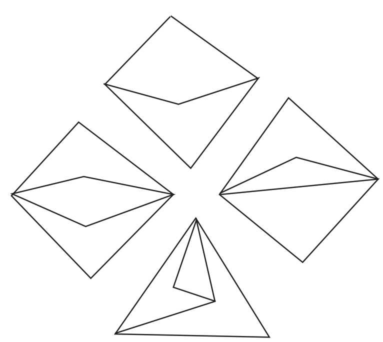

Figure 8.3: Some impossibilities

Once a terminal position is reached it is checked to see whether it satisfies all the properties of tameness.

Duplication is removed among isomorphic terminal plane graphs. It is not an entirely trivial procedure for the computer to determine whether there exists an isomorphism between two plane graphs. This is accomplished by computing a numerical invariant of a vertex that depends only on the local structure of the vertex. If two plane graphs are properly isomorphic then the numerical invariant is the same at vertices that correspond under the proper isomorphism. If two graphs have the same number of vertices with the same numerical invariants, they become candidates for an isomorphism. All possible numerical-invariant preserving bijections are attempted until a proper isomorphism is found, or until it is found that none exist. If there is no proper isomorphism, the same procedure is applied to the opposite plane graph to find any possible orientation-reversing isomorphism.

This same isomorphism-producing algorithm is used to match each terminal graph with a graph in the archive. It is found that each terminal graph matches with one in the archive. (The archive was originally obtained by running the finite state machine and making a list of all the terminal states up to isomorphism that satisfy the given conditions.)

In this way Theorem 8.1 is proved.

9. Contravening graphs

We have seen that a system of points and arcs on the unit sphere can be associated with a decomposition star D. The points are the radial projections of the vertices of $U(D)$ (those at distance at most $2t_0 = 2.51$ from the origin). The arcs are the radial projections of edges between $v, w \in U(D)$, where $|v - w| \leq 2t_0$. If we consider this collection of arcs combinatorially as a graph, then it is not always true that these arcs form a plane graph in the restrictive sense of Chapter 7.

The purpose of this chapter is to show that if the original decomposition star contravenes, then minor modifications can be made to the system of arcs of the graph so that the resulting combinatorial graph has the structure of a plane graph in the sense of Chapter 7. These plane graphs are called contravening plane graphs, or simply contravening graphs.

9.1. *A review of earlier results.* In this chapter, we will make use of several results that appear in the unabridged version of this paper. Full proofs appear in Section 20 of the unabridged version. In this section, we collect together the most important of these results.

Let $\zeta = 1/(2\arctan(\sqrt{2}/5))$. Let $\mathrm{sol}(R)$ denote the solid angle of a standard region R. We write τ_R for the following modification of σ_R:

$$\tau_R(D) = \mathrm{sol}(R)\zeta\mathrm{pt} - \sigma_R(D) \tag{9.1}$$

and

$$\tau(D) = \sum \tau_R(D) = 4\pi\zeta\mathrm{pt} - \sigma(D). \tag{9.2}$$

Since $4\pi\zeta\mathrm{pt}$ is a constant, τ and σ contain the same information, but τ is often more convenient to work with. A contravening decomposition star satisfies

$$\tau(D) \le 4\pi\zeta\mathrm{pt} - 8\,\mathrm{pt} = (4\pi\zeta - 8)\mathrm{pt}. \tag{9.3}$$

The constant $(4\pi\zeta - 8)\,\mathrm{pt}$ (and its upper bound $\mathrm{tgt}\,\mathrm{pt}$ where $\mathrm{tgt} = 14.8$) will occur repeatedly in the discussion that follows.

Recall that a standard cluster is a pair (R, D) consisting of a decomposition star D and one of its standard regions R. If F is a finite set (or finite union) of standard regions, let

$$\sigma_F(D) = \sum_R \sigma_R(D), \quad \tau_F(D) = \sum_R \tau_R(D), \tag{9.4}$$

where the sum runs over all the standard regions in F. When the sum runs over all standard regions,

$$\sigma(D) = \sum \sigma_R(D), \quad \tau(D) = \sum \tau_R(D). \tag{9.5}$$

A natural number $n(R)$ is associated with each standard region. If the boundary of that region is a simple polygon, then $n(R)$ is the number of sides. If the boundary consists of k disjoint simple polygons, with $n_1, \ldots, n_k$ sides then

$$n(R) = n_1 + \cdots + n_k + 2(k - 1).$$

LEMMA 9.1. *Let R be a standard region in a contravening decomposition star D. The boundary of R is a simple polygon with at most eight edges, or one of the configurations of Figure* 9.1.

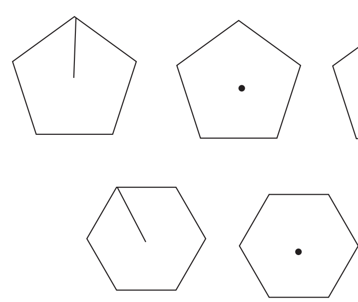

Figure 9.1: Nonpolygonal standard regions ($n(R) = 7, 7, 8, 8, 8$)

Proof. See [Hal06a]. □

LEMMA 9.2. *Let R be a standard region. We have $\tau_R(D) \ge t_n$, where $n = n(R)$, and*

$$\begin{array}{lll} t_3 = 0, & t_4 = 0.1317, & t_5 = 0.27113, \\ t_6 = 0.41056 & t_7 = 0.54999, & t_8 = 0.6045. \end{array}$$

Furthermore, $\sigma_R(D) \le s_n$, *for* $5 \le n \le 8$, *where*

$$s_3 = 1\,\mathrm{pt}, \qquad s_4 = 0, \qquad s_5 = -0.05704,$$
$$s_6 = -0.11408, \qquad s_7 = -0.17112, \qquad s_8 = -0.22816.$$

Proof. [Hal06a]. □

LEMMA 9.3. *Let F be a set of standard regions bounded by a simple polygon with at most nine edges. Assume that*

$$\sigma_F(D) \le s_9 \quad \textit{and } \tau_F(D) \ge t_9,$$

where $s_9 = -0.1972$ *and* $t_9 = 0.6978$. *Then D does not contravene.*

Proof. [Hal06a]. □

LEMMA 9.4. *Let (R, D) be a standard cluster. If R is a triangular region, then*

$$\sigma_R(D) \le 1\,\mathrm{pt}.$$

If R is not a triangular region, then

$$\sigma_R(D) \le 0.$$

Proof. See Lemma 6.10 and Theorem 6.4. □

LEMMA 9.5. $\tau_R(D) \ge 0$, *for all standard clusters R.*

Proof. [Hal06a]. □

Recall that v has *type* (p, q) if every standard region with a vertex at v is a triangle or quadrilateral, and if there are exactly p triangular faces and q quadrilateral faces that meet at v (see Definition 7.6). We write (p_v, q_v) for the type of v. Define constants $\tau_{\mathrm{LP}}(p, q)/\mathrm{pt}$ by Table 9.6. The entries marked with an asterisk will not be needed.

(9.6)

$\tau_{\mathrm{LP}}(p,q)/\mathrm{pt}$	$q = 0$	1	2	3	4	5
$p = 0$	*	*	15.18	7.135	10.6497	22.27
1	*	*	6.95	7.135	17.62	32.3
2	*	8.5	4.756	12.9814	*	*
3	*	3.6426	8.334	20.9	*	*
4	4.1396	3.7812	16.11	*	*	*
5	0.55	11.22	*	*	*	*
6	6.339	*	*	*	*	*
7	14.76	*	*	*	*	*

LEMMA 9.6. *Let $S_1, \dots, S_p$ and $R_1, \dots, R_q$ be the tetrahedra and quad clusters around a vertex of type (p,q). Consider the constants of Table* 9.6. *Now,*

$$\sum^p \tau(S_i) + \sum^q \tau(R_i) \geq \tau_{\mathrm{LP}}(p,q).$$

Proof. [Hal06a]. □

LEMMA 9.7. *Let $v_1, \dots, v_k$, for some $k \leq 4$, be distinct vertices of type $(5,0)$. Let $S_1, \dots, S_r$ be quasi-regular tetrahedra around the edges $(0, v_i)$, for $i \leq k$. Then*

$$\sum_{i=1}^{r} \tau(S_i) > 0.55k\,\mathrm{pt},$$

and

$$\sum_{i=1}^{r} \sigma(S_i) < r\,\mathrm{pt} - 0.48k\,\mathrm{pt}.$$

Proof. [Hal06a]. □

LEMMA 9.8. *Let D be a contravening decomposition star. If the type of the vertex is (p,q,r) with $r = 0$, then (p,q) must be one of the following*:

$$\{(6,0),(5,0),(4,0),(5,1),(4,1),(3,1),(2,1),$$
$$(3,2),(2,2),(1,2),(2,3),(1,3),(0,3),(0,4)\}.$$

Proof. [Hal06a]. □

LEMMA 9.9. *A triangular standard region does not contain any enclosed vertices.*

Proof. This fact is proved in [Hal97a, Lemma 3.7]. □

LEMMA 9.10. *A quadrilateral region does not enclose any vertices of height at most $2t_0$.*

Proof. [Hal06a]. □

LEMMA 9.11. *Let F be a union of standard regions. Suppose that the boundary of F consists of four edges. Suppose that the area of F is at most 2π. Then there is at most one enclosed vertex over F.*

Proof. This is [Hal97a, Prop. 4.2]. □

LEMMA 9.12. *Let F be the union of two standard regions, a triangular region and a pentagonal region that meet at a vertex of type $(1,0,1)$ as shown in Figure* 9.2. *Then*

$$\tau_F(D) \geq 11.16\,\mathrm{pt}.$$

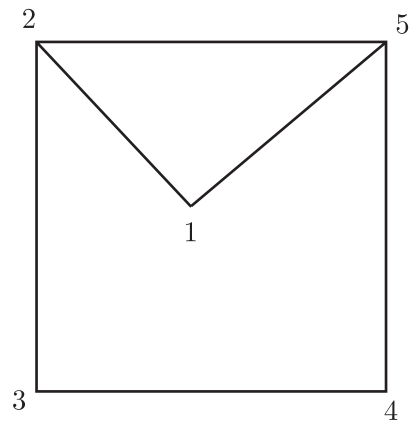

Figure 9.2: A 4-circuit

Proof. [Hal06a]. □

LEMMA 9.13. *Let R be an exceptional standard region. Suppose that R has r different interior angles that are pairwise nonadjacent and such that each is at most* 1.32. *Then*

$$\tau_R(D) \geq t_n + r(1.47)\,\mathrm{pt}.$$

Proof. [Hal06a]. □

LEMMA 9.14. *Every interior angle of every standard region is at least* 0.8638. *Every interior angle of every standard region that is not a triangle is at least* 1.153.

Proof. CALC-208809199 and CALC-853728973-1. □

Definition 9.15. The *central vertex* of a flat quarter is defined to be the one that does not lie on the triangle formed by the origin and the diagonal.

LEMMA 9.16. *If the interior angle at a corner v of a non-triangular standard region is at most* 1.32, *then there is a flat quarter over R whose central vertex is v.*

Proof. [Hal06a]. □

9.2. *Contravening plane graphs defined.* A plane graph G is attached to every contravening decomposition star as follows. From the decomposition star D, it is possible to determine the coordinates of the set $U(D)$ of vertices at distance at most $2t_0$ from the origin.

If we draw a geodesic arc on the unit sphere at the origin with endpoints at the radial projections of v_1 and v_2 for every pair of vertices v_1, $v_2 \in U(D)$

such that $|v_1|, |v_2|, |v_1 - v_2| \le 2t_0$, we obtain a plane graph that breaks the unit sphere into standard regions. (The arcs do not meet except at endpoints by Lemma 2.19.)

For a given standard region, we consider the arcs forming its boundary together with the arcs that are internal to the standard region. We consider the points on the unit sphere formed by the endpoints of the arcs, together with the radial projections to the unit sphere of vertices in U whose radial projection lies in the interior of the region.

Remark 9.17. The system of arcs and vertices associated with a standard region in a contravening example must be a polygon, or one of the configurations of Figure 9.1 (see Lemma 9.1).

Remark 9.18. Observe that one case of Figure 9.1 is bounded by a triangle and a pentagon, and that the others are bounded by a polygon. Replacing the triangle-pentagon arrangement with the bounding pentagon and replacing the others with the bounding polygon, we obtain a partition of the sphere into simple polygons. Each of these polygons is a single standard region, except in the triangle-pentagon case (Figure 9.3), which is a union of two standard regions (a triangle and an eight-sided region).

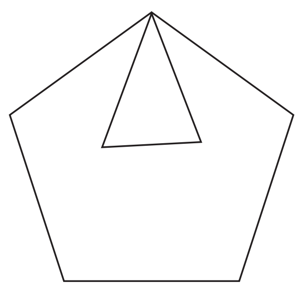

Figure 9.3: An aggregate forming a pentagon

Remark 9.19. To simplify further, if we have an arrangement of six standard regions around a vertex formed from five triangles and one pentagon, we replace it with the bounding octagon (or hexagon). See Figure 9.4. (It will be shown in Lemma 10.11 that there is at most one such configuration in the standard decomposition of a contravening decomposition star, so we will not worry here about how to treat the case of two overlapping configurations of this sort.)

In summary, we have a plane graph that is approximately that given by the standard regions of the decomposition star, but simplified to a bounding polygon when one of the configurations of Remarks 9.18 and 9.19 occur. We

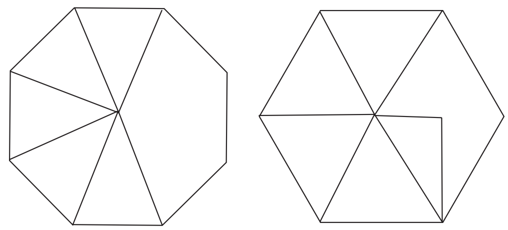

Figure 9.4: Degree 6 aggregates

refer to the combination of standard regions into a single face of the graph as *aggregation*. We call it the plane graph $G = G(D)$ attached to a contravening decomposition star D.

Proposition 10.1 will show the vertex set U is nonempty and that the graph $G(D)$ is nonempty.

When we refer to the plane graph in this manner, we mean the combinatorial plane graph as opposed to the embedded metric graph on the unit sphere formed from the system of geodesic arcs. Given a vertex v in $G(D)$, there is a uniquely determined vertex $v(D)$ of $U(D)$ whose radial projection to the unit sphere determines v. We call $v(D)$ the *corner* in $U(D)$ over v.

By construction, the plane graphs associated with a decomposition star do not have loops or multiple joins. In fact, the edges of $G(D)$ are defined by triangles whose sides vary between lengths 2 and $2t_0$. The angles of such a triangle are strictly less than π. This implies that the edges of the metric graph on the unit sphere always have arc-length strictly less than π. In particular, the endpoints are never antipodal. A loop on the combinatorial graph corresponds to an edge on the metric graph that is a closed geodesic. A multiple join on the combinatorial graph corresponds on the metric graph to a pair of points joined by multiple minimal geodesics, that is, a pair of antipodal points on the sphere. By the arc-length constraints on edges in the metric graph, there are no loops or multiple joins in the combinatorial graph $G(D)$.

In Definition 7.3, a plane graph satisfying a certain restrictive set of properties is said to be *tame*. If a plane graph $G(D)$ is associated with a contravening decomposition star D, we call $G(D)$ a *contravening plane graph*.

Theorem 9.20. *Let D be a contravening decomposition star. Then its plane graph $G(D)$ is tame.*

This theorem is one of the main steps in the proof of the Kepler conjecture. It is advanced as one of the central claims in Section 1.3. Its proof occupies Chapters 10 and 11. In Theorem 8.1, the tame graphs are classified up to isomorphism. As a corollary, we have an explicit list of graphs that contains all contravening plane graphs.

10. Contravention is tame

This section begins the proof of Theorem 9.20 (contravening graphs are tame). To prove Theorem 9.20, it is enough to show that each defining property of tameness is satisfied for every contravening graph. This is the substance of results in the following sections. The proof continues through the end of Chapter 11. This chapter verifies all the properties of tameness, except for the last one (weight assignments).

10.1. *First properties.* This section verifies Properties 1, 2, 4, and 8 of tameness. First, we prove the promised nondegeneracy result.

Proposition 10.1. *The construction of Section* 9.2 *associates a* (*non-empty*) *plane graph with at least two faces to every decomposition star* D *with* $\sigma(D) > 0$.

Proof. First we show that decomposition stars with $\sigma(D) > 0$ have nonempty vertex sets U. (Recall that U is the set of vertices of distance at most $2t_0$ from the center.) The vertices of U are used in Chapters 2 and 3 to create all of the structural features of the decomposition star: quasi-regular tetrahedra, quarters, and so forth. If U is empty, the V-cell is a solid containing the ball $B(t_0)$ of radius t_0, and $\sigma(D)$ satisfies

$$\begin{aligned}\sigma(D) &= \mathrm{vor}(D)\\ &= -4\delta_{\mathrm{oct}}\mathrm{vol}(\mathrm{VC}(D)) + 4\pi/3\\ &< -4\delta_{\mathrm{oct}}\mathrm{vol}(B(t_0)) + 4\pi/3 \quad < 0.\end{aligned}$$

By hypothesis, $\sigma(D) > 0$. So U is not empty.

Equation 9.5 shows that the function σ can be expressed as a sum of terms σ_R indexed by the standard regions R. It is proved in Theorem 6.4 that $\sigma_R \le 0$, unless R is a triangle. Thus, a decomposition star with positive $\sigma(D)$ must have at least one triangle. Its complement contains a second standard region. Even after we form aggregates of distinct standard regions to form the simplified plane graph (Remarks 9.18 and 9.19), there certainly remain at least two faces. □

Proposition 10.2. *The plane graph of a contravening decomposition star satisfies Property* 1 *of tameness*: *The length of each face is at least* 3 *and at most* 8.

Proof. By the construction of the graph, each face has at least three edges. The upper bound of 8 edges is Lemma 9.1. Note that the aggregates of Remarks 9.19 and 9.18 have between 5 and 8 edges. □

Proposition 10.3. *The plane graph of a contravening decomposition star satisfies Property* 2 *of tameness*: *Every* 3*-circuit is a face or the opposite of a face.*

Proof. The simplifications of the plane graph in Remarks 9.18 and 9.19 do not produce any new 3-circuits. (See the accompanying figures.) The result is Lemma 9.9. □

Proposition 10.4. *Contravening graphs satisfy Property* 4 *of tameness*: *The degree of every vertex is at least* 2 *and at most* 6*.*

Proof. The statement that degrees are at least 2 trivially follows because each vertex lies on at least one polygon, with two edges at that vertex.

If the type is (p, q), then the impossibility of a vertex of degree 7 or more is found in Lemma 9.8. If the type is (p, q, r), with $r \geq 1$, then Lemma 9.14 shows that the interior angles of the standard regions cannot sum to 2π:

$$6(0.8638) + 1.153 > 2\pi. \qquad \square$$

Proposition 10.5. *Contravening graphs satisfy Property* 8 *of tameness*: *There are never two vertices of type* $(4, 0)$ *that are adjacent to each other*.

Proof. This is proved in [Hal97a, 4.2]. □

10.2. *Computer calculations and their consequences.* This section continues in the proof that all contravening plane graphs are tame. The next few sections verify Properties 6, 5, and then 3 of tameness.

In this chapter, we rely on some inequalities that are not proved in this paper. Recall from Section 6.3 that there is an archive of hundreds of inequalities that have been proved by computer. This full archive appears in [Hal05]. The justification of these inequalities appears in the same archive. (The proofs of these inequalities were executed by computer.) Each inequality carries a nine digit identifying number. To invoke an inequality, we state it precisely, and give its identifying number, e.g. calc-123456789.

To use these inequalities systematically, we combine inequalities into linear programs and solve the linear programs on computer. At first, our use of linear programs will be light, but our reliance will become progressively strong as the argument develops.

To start out, we will make use of several calculations[8] that give lower bounds on $\tau_R(D)$ when R is a triangle or a quadrilateral. To obtain lower

[8]The sequence of five inequalities starting with calc-927432550, Lemma 9.5, and for quads calc-310151857, calc-655029773, calc-73283761, calc-15141595, calc-574391221, calc-396281725

bounds through linear programming, we take a linear relaxation. Specifically, we introduce a linear variable for each function τ_R and a linear variable for each interior angle α_R. We substitute these linear variables for the nonlinear functions $\tau_R(D)$ and nonlinear interior angle function into the given inequalities. Under these substitutions, the inequalities become linear. Given p triangles and q quadrilaterals at a vertex, we have the linear program to minimize the sum of the (linear variables associated with) $\tau_R(D)$ subject to the constraint that the (linear variables associated with the) angles at the vertex sum to at most d. Linear programming yields[9] a lower bound $\tau_{\rm LP}(p, q, d)$ to this minimization problem. This gives a lower bound to the corresponding constrained sum of nonlinear functions τ_R.

Similarly, another group of inequalities[10] yields upper bounds $\sigma_{\rm LP}(p, q, d)$ on the sum of $p+q$ functions σ_R, with p standard regions R that are triangular, and another q that are quadrilateral. These linear programs find their first application in the proof of the following proposition.

10.3. *Linear programs.* To continue with the proof that contravening plane graphs are tame, we need to introduce more notation and methods.

If F is a face of $G(D)$, let

$$\sigma_F(D) = \sum \sigma_R(D),$$

where the sum runs over the set of standard regions associated with F. This sum reduces to a single term unless F is an aggregate in the sense of Remarks 9.19 and 9.18.

LEMMA 10.6. *The plane graph of a contravening decomposition star satisfies Property* 6 *of tameness*:

$$\sum_F c(\mathrm{len}(F)) \ge 8.$$

Proof. We will show that

$$c(\mathrm{len}(F))\,\mathrm{pt} \ge \sigma_F(D). \tag{10.1}$$

Assuming this, the result follows for contravening stars D:

$$\begin{aligned} \textstyle\sum_F c(\mathrm{len}(F))\,\mathrm{pt} &\ge \textstyle\sum_F \sigma_F(D) \\ &= \sigma(D) \ge 8\,\mathrm{pt}. \end{aligned}$$

We consider three cases for Inequality 10.1. In the first case, assume that the face F corresponds to exactly one standard region in the decompo-

[9] Although they are closely related, the function $\tau_{\rm LP}$ of three arguments introduced here is distinct from the function of two variables of the same name that is introduced in Section 9.1.

[10] CALC-539256862, CALC-864218323, CALC-776305271, and for quads CALC-310151857, CALC-655029773, CALC-73283761, CALC-15141595, CALC-574391221, CALC-396281725

sition star. In this case, Inequality 10.1 follows directly from the bounds of Lemma 9.2:

$$\sigma_F(D) \le s_n \le c(n)\,\mathrm{pt}.$$

In the second case, assume the context of a pentagon F formed in Remark 9.18. Then, again by Theorem 9.2, we have

$$\sigma_F(D) \le s_3 + s_8 \le (c(3)+c(8))\,\mathrm{pt} \le c(5)\,\mathrm{pt}.$$

(Just examine the constants $c(k)$.)

In the third case, we consider the situation of Remark 9.19. The six standard regions give

$$\sigma_F(D) \le s_5 + \sigma_{\mathrm{LP}}(5,0,2\pi - 1.153) < c(8)\,\mathrm{pt}.$$

The constant 1.153 comes from Lemma 9.14. □

PROPOSITION 10.7. *Let F be a face of a contravening plane graph $G(D)$. Then*

$$\tau_F(D) \ge d(\mathrm{len}(F))\mathrm{pt}.$$

Proof. Similar. □

LEMMA 10.8. *If v is a vertex of an exceptional standard region, and if there are six standard regions meeting at v, then the exceptional region is a pentagonal region and the other five standard regions are triangular.*

Proof. There are several cases according to the number k of triangular regions at the vertex.

$(k \le 2)$ If there are at least four non-triangular regions at the vertex, then the sum of interior angles around the vertex is at least $4(1.153) + 2(0.8638) > 2\pi$, which is impossible. (See Lemma 9.14.)

$(k = 3)$ If there are three non-triangular regions at the vertex, then $\tau(D)$ is at least $2t_4 + t_5 + \tau_{\mathrm{LP}}(3,0,2\pi - 3(1.153)) > (4\pi\zeta - 8)\,\mathrm{pt}$.

$(k = 4)$ If there are two exceptional regions at the vertex, then $\tau(D)$ is at least $2t_5 + \tau_{\mathrm{LP}}(4,0,2\pi - 2(1.153)) > (4\pi\zeta - 8)\,\mathrm{pt}$.

If there are two non-triangular regions at the vertex, then $\tau(D)$ is at least $t_5 + \tau_{\mathrm{LP}}(4,1,2\pi - 1.153) > (4\pi\zeta - 8)\,\mathrm{pt}$.

$(k = 5)$ We are left with the case of five triangular regions and one exceptional region.

When there is an exceptional standard region at a vertex of degree six, we claim that the exceptional region must be a pentagon. If the region is a heptagon or more, then $\tau(D)$ is at least $t_7 + \tau_{\mathrm{LP}}(5,0,2\pi - 1.153) > (4\pi\zeta - 8)\,\mathrm{pt}$.

If the standard region is a hexagon, then $\tau(D)$ is at least $t_6+\tau_{\text{LP}}(5,0,2\pi-1.153) > t_9$. Also, $s_6+\sigma_{\text{LP}}(5,0,2\pi-1.153) < s_9$. The aggregate of the six standard regions is 9-sided. Lemma 9.3 gives the bound of 8 pt. $\square$

LEMMA 10.9. *Consider the standard regions of a contravening star D.*

1. *If a vertex of a pentagonal standard region has degree six, then the aggregate F of the six faces satisfies*

$$\sigma_F(D) < s_8,$$
$$\tau_F(D) > t_8.$$

2. *An exceptional standard region has at most two vertices of degree six. If there are two, then they are nonadjacent vertices on a pentagon, as shown in Figure* 10.1.

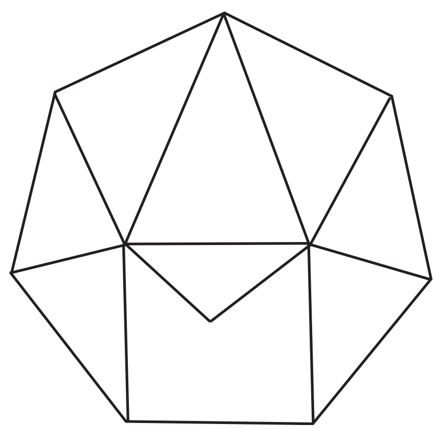

Figure 10.1: Nonadjacent vertices of degree six on a pentagon

Proof. We begin with the first part of the lemma. The sum $\tau_F(D)$ over these six standard regions is at least

$$t_5+\tau_{\text{LP}}(5,0,2\pi-1.153) > t_8.$$

Similarly,

$$s_5+\sigma_{\text{LP}}(5,0,2\pi-1.153) < s_8.$$

We note that there can be at most one exceptional region with a vertex of degree six. Indeed, if there are two, then they must both be vertices of the same pentagon:

$$t_8+t_5 > (4\pi\zeta-8)\,\text{pt}.$$

Such a second vertex on the octagonal aggregate leads to one of the following constants greater than $(4\pi\zeta - 8)\,\mathrm{pt}$. These same constants show that such a second vertex on a hexagonal aggregate must share two triangular faces with the first vertex of degree six.

$$\begin{array}{ll} t_8 & +\tau_{\mathrm{LP}}(4, 0, 2\pi - 1.32 - 0.8638), \quad \text{or} \\ t_8 & +1.47\,\mathrm{pt} + \tau_{\mathrm{LP}}(4, 0, 2\pi - 1.153 - 0.8638), \quad \text{or} \\ t_8 & +\tau_{\mathrm{LP}}(5, 0, 2\pi - 1.153). \end{array}$$

(The relevant constants are found at Lemma 9.13 and Lemma 9.14.) □

10.4. *A non-contravening 4-circuit.* This subsection rules out the existence of a particular 4-circuit on a contravening plane graph. The interior of the circuit consists of two faces: a triangle and a pentagon. The circuit and its enclosed vertex are show in Figure 9.2 with vertices marked $p_1, \ldots, p_5$. The vertex p_1 is the enclosed vertex, the triangle is (p_1, p_2, p_5) and the pentagon is $(p_1, \ldots, p_5)$. Let $v_1, \ldots, v_4, v_5$ be the corresponding vertices of $U(D)$.

The diagonals $\{v_5, v_3\}$ and $\{v_2, v_4\}$ have length at least $2\sqrt{2}$ by Lemma 2.19. If an interior angle of the quadrilateral is less than 1.32, then by Lemma 9.16, $|v_1 - v_3| \le \sqrt{8}$. Thus, we assume in the following lemma, that all interior angles of the quadrilateral aggregate are at least 1.32.

LEMMA 10.10. *A decomposition star that contains this configuration does not contravene.*

Proof. Let P denote the quadrilateral aggregate of these two standard regions. By Lemma 9.12, we have $\tau_P(D) \ge 11.16\,\mathrm{pt}$. There are no other exceptional faces, because $11.16\,\mathrm{pt} + t_5 > (4\pi\zeta - 8)\,\mathrm{pt}$. Every vertex not on P has type $(5, 0)$, by Lemma 9.6. In particular, there are no quadrilateral regions. The interior angles of P are at least 1.32. There are at most four triangles at every vertex of P, because

$$11.16\,\mathrm{pt} + \tau_{\mathrm{LP}}(5, 0, 2\pi - 1.32) > (4\pi\zeta - 8)\,\mathrm{pt}.$$

There are at least three triangles at every vertex of P, otherwise we contradict Lemma 9.9 or Lemma 9.11.

The only triangulation with these properties is obtained by removing one edge from the icosahedron (Exercise). This implies that there are two opposite corners of P each having four quasi-regular tetrahedra. Since the diagonals of P have lengths greater than $2\sqrt{2}$, the results of CALC-325738864 show that the union F of these eight quasi-regular tetrahedra satisfies

$$\tau_F(D) \ge 2(1.5)\,\mathrm{pt}.$$

There are two additional vertices of type $(5, 0)$ whose tetrahedra are distinct from these eight quasi-regular tetrahedra. They give an additional $2(0.55)\,\mathrm{pt}$.

Now $(11.16 + 2(1.5) + 2(0.55))\,\mathrm{pt} > (4\pi\zeta - 8)\,\mathrm{pt}$ by Lemma 9.7. The result follows. □

LEMMA 10.11. *A contravening plane graph satisfies Property* 5 *of tameness*: *If a vertex is contained in an exceptional face*, *then the degree of the vertex is at most* 5.

Proof. An exceptional standard region with a vertex of degree six must be pentagonal by Lemma 10.9. If that pentagonal region has two or more such vertices, then by the same lemma, it must be the arrangement shown in Figure 10.1. This arrangement does not appear on a contravening graph by Lemma 10.10. □

Remark 10.12. We have now fully justified the claim made in Remark 9.19: there is at most one vertex on six standard regions, and it is part of an aggregate in such a way that it does not appear as the vertex of $G(D)$.

10.5. *Possible* 4-*circuits.* Every 4-circuit divides a plane graph into two aggregates of faces that we may call the interior and exterior. We call vertices of the faces in the aggregate that do not lie on the 4-cycle *enclosed vertices*. Thus, every vertex lies in the 4-cycle, is enclosed over the interior, or is enclosed over the exterior.

Lemma 9.11 asserts that either the interior or the exterior has at most 1 enclosed vertex. When choosing which aggregate is to be called the interior, we may make our choice so that the interior has area at most 2π, and hence contains at most 1 vertex. With this choice, we have the following proposition.

PROPOSITION 10.13. *Let D be a contravening plane graph. A* 4-*circuit surrounds one of the aggregates of faces shown in Property* 3 *of tameness.*

Proof. If there are no enclosed vertices, then the only possibilities are for it to be a single quadrilateral face or a pair of adjacent triangles.

Assume there is one enclosed vertex v. If v is connected to three or four vertices of the quadrilateral, then that possibility is listed as part of the conclusion.

If v is connected to two opposite vertices in the 4-cycle, then the vertex v has type $(0, 2)$ and the bounds of Lemma 9.6 show that the graph cannot be contravening.

If v is connected to two adjacent vertices in the 4-cycle, then we appeal to Lemma 10.10 to conclude that the graph does not contravene.

If v is connected to 0 or 1 vertices, then we appeal to Lemma 9.10. This completes the proof. □

11. Weight assignments

The purpose of this section is to prove the existence of a good admissible weight assignment for contravening plane graphs. This will complete the proof that all contravening graphs are tame.

Theorem 11.1. *Every contravening plane graph has an admissible weight assignment of total weight less than* $\mathrm{tgt} = 14.8$.

Given a contravening decomposition star D, we define a weight assignment w by

$$F \mapsto w(F) = \tau_F(D)/\mathrm{pt}.$$

Since D contravenes,

$$\begin{aligned} \textstyle\sum_F w(F) &= \textstyle\sum_F \tau_F(D)/\mathrm{pt} \\ &= \tau(D)/\mathrm{pt} \ \leq\ (4\pi\zeta - 8)\,\mathrm{pt}/\mathrm{pt} \\ &< \mathrm{tgt} = 14.8. \end{aligned}$$

The challenge of the theorem will be to prove that w, when defined by this formula, is admissible.

11.1. *Admissibility.* The next three lemmas establish that this definition of $w(F)$ for contravening plane graphs satisfies the first three defining properties of an admissible weight assignment.

Lemma 11.2. *Let F be a face of length n in a contravening plane graph. Define $w(F)$ as above. Then $w(F) \geq d(n)$.*

Proof. This is Proposition 10.7. □

Lemma 11.3. *Let v be a vertex of type (p, q) in a contravening plane graph. Define $w(F)$ as above. Then*

$$\sum_{v \in F} w(F) \geq b(p, q).$$

Proof. This is Lemma 9.6. □

Lemma 11.4. *Let V be any set of vertices of type $(5, 0)$ in a contravening plane graph. Define $w(F)$ as above. If the cardinality of V is $k \leq 4$, then*

$$\sum_{V \cap F \neq \emptyset} w(F) \geq 0.55k.$$

Proof. This is Lemma 9.7. □

The following proposition establishes the final property that $w(F)$ must satisfy to make it admissible. *Separated sets* are defined in Section 7.2.

PROPOSITION 11.5. *Let V be any separated set of vertices in a contravening plane graph. Define $w(F)$ as above. Then*

$$\sum_{V\cap F\neq\emptyset}(w(F)-d(\mathrm{len}(F)))\geq\sum_{v\in V}a(\mathrm{tri}(v)),$$

where $\mathrm{tri}(v)$ *denotes the number of triangles containing the vertex v.*

The proof will occupy the rest of this chapter. Since the degree of each vertex is five, and there is at least one face that is not a triangle at the vertex, the only constants $\mathrm{tri}(v)$ that arise are

$$\mathrm{tri}(v)\in\{0,\ldots,4\}.$$

We will prove that in a contravening plane graph the Properties (1) and (4) of a separated set are incompatible with the condition $\mathrm{tri}(v)\leq 2$, for some $v\in V$. This will allows us to assume that

$$\mathrm{tri}(v)\in\{3,4\},$$

for all $v\in V$. These cases will be treated in Section 11.3.

First we prove the inequality when there are no aggregates involved. Afterwards, we show that the conclusions can be extended to aggregate faces as well.

11.2. *Proof that* $\mathrm{tri}(v)>2$. In this subsection D is a contravening decomposition star with associated graph $G(D)$. Let V be a separated set of vertices in $G(D)$. Let v be a vertex in V such that none of its faces is an aggregate in the sense of Remarks 9.18 and 9.19.

LEMMA 11.6. *Under these conditions, for every $v\in V$,* $\mathrm{tri}(v)>1$.

Proof. If there are p triangles, q quadrilaterals, and r other faces, then

$$\begin{aligned}\tau(D)&\geq\textstyle\sum_{v\in R}\tau_R(D)\\&\geq r\,t_5+\tau_{\mathrm{LP}}(p,q,2\pi-r(1.153)).\end{aligned}$$

If there is a vertex w that is not on any of the faces containing v, then the sum of $\tau_F(D)$ over the faces containing w yield an additional 0.55 pt by Lemma 9.7. We calculate these constants for each (p,q,r) and find that the bound is always greater than $(4\pi\zeta-8)$ pt. This implies that D cannot be contravening.

(p,q,r)	lower bound	justification
$(0,5,0)$	22.27 pt	Lemma 9.6
$(0,q,r\geq 1)$	$t_5+4t_4\approx 14.41$ pt	
$(1,4,0)$	17.62 pt	Lemma 9.6
$(1,3,1)$	$t_5+12.58$ pt	(τ_{LP})
$(1,2,2)$	$2t_5+7.53$ pt	(τ_{LP})
$(1,q,r\geq 3)$	$3t_5+t_4$.	

∎

Lemma 11.7. *Under these same conditions, for every* $v \in V$, $\mathrm{tri}(v) > 2$.

Proof. Assume that $\mathrm{tri}(v) = 2$. We will show that this implies that D does not contravene. Let e be the number of exceptional faces at v. We have $e + \mathrm{tri}(v) \le 5$.

The constants $0.55\,\mathrm{pt}$ and $0.48\,\mathrm{pt}$ used throughout the proof come from Lemma 9.7. The constants t_n comes from Lemma 9.2.

($e = 3$): First, assume that there are three exceptional faces around vertex v. They must all be pentagons ($2t_5 + t_6 > (4\pi\zeta - 8)\,\mathrm{pt}$). The aggregate of the five faces is an m-gon (some $m \le 11$). If there is a vertex not on this aggregate, use $3t_5 + 0.55\,\mathrm{pt} > (4\pi\zeta - 8)\,\mathrm{pt}$. So there are at most nine triangles away from the aggregate, and

$$\sigma(D) \le 9\,\mathrm{pt} + (3s_5 + 2\,\mathrm{pt}) < 8\,\mathrm{pt}.$$

The argument if there is a quad, a pentagon, or a hexagon is the same ($t_4 + t_6 = 2t_5, s_4 + s_6 = 2s_5$).

($e = 2$): Assume next that there are two pentagons and a quadrilateral around the vertex. The aggregate of the two pentagons, quadrilateral, and two triangles is an m-gon (some $m \le 10$). There must be a vertex not on the aggregate of five faces, for otherwise we have

$$\sigma(D) \le 8\,\mathrm{pt} + (2s_5 + 2\,\mathrm{pt}) < 8\,\mathrm{pt}.$$

The interior angle of one of the pentagons is at most 1.32. For otherwise, $\tau_{\mathrm{LP}}(2, 1, 2\pi - 2(1.32)) + 2t_5 + 0.55\,\mathrm{pt} > (4\pi\zeta - 8)\,\mathrm{pt}$.

Lemma 9.13 shows that any pentagon R with an interior angle less than 1.32 yields $\tau_R(D) \ge t_5 + (1.47\,\mathrm{pt})$. If both pentagons have an interior angle < 1.32 the lemma follows easily from this calculation: $2(t_5 + 1.47\,\mathrm{pt})\,\mathrm{pt} + \tau_{\mathrm{LP}}(2, 1, 2\pi - 2(1.153)) + 0.55\,\mathrm{pt} > (4\pi\zeta - 8)\,\mathrm{pt}$. If there is one pentagon with angle > 1.32, we then have $t_5 + (1.47\,\mathrm{pt}) + \tau_{\mathrm{LP}}(2, 1, 2\pi - 1.153 - 1.32) + t_5 + 0.55\,\mathrm{pt} > (4\pi\zeta - 8)\,\mathrm{pt}$.

($e = 1$): Assume finally that there is one exceptional face at the vertex. If it is a hexagon (or more), we are done: $t_6 + \tau_{\mathrm{LP}}(2, 2, 2\pi - 1.153) > (4\pi\zeta - 8)\,\mathrm{pt}$. Assume it is a pentagon. The aggregate of the five faces at the vertex is bounded by an m-circuit (some $m \le 9$). If there are no more than nine quasi-regular tetrahedra outside the aggregate, then $\sigma(D)$ is at most $(9 - 2(0.48))\,\mathrm{pt} + s_5 + \sigma_{\mathrm{LP}}(2, 2, 2\pi - 1.153) < 8\,\mathrm{pt}$ (Lemma 9.7). So we may assume that there are at least three vertices not on the aggregate.

If the interior angle of the pentagon is greater than 1.32,

$$\tau_{\mathrm{LP}}(2, 2, 2\pi - 1.32) + 3(0.55)\,\mathrm{pt} + t_5 > (4\pi\zeta - 8)\,\mathrm{pt};$$

then, if it is less than 1.32, by Lemma 9.13

$$\tau_{\mathrm{LP}}(2, 2, 2\pi - 1.153) + 3(0.55)\mathrm{pt} + 1.47\,\mathrm{pt} + t_5 > (4\pi\zeta - 8)\,\mathrm{pt}. \qquad \square$$

Lemma 11.8. *The bound* $\mathrm{tri}(v) > 2$ *holds if* v *is a vertex of an aggregate face.*

Proof. The exceptional region enters into the preceding two proofs in a purely formal way. Pentagons enter through the bounds

$$t_5,\ s_5,\ 1.47\,\mathrm{pt}$$

and angles 1.153, 1.32. Hexagons enter through the bounds

$$t_6,\ s_6$$

and so forth. These bounds hold for the aggregate faces. Hence the proofs hold for aggregates as well. □

11.3. *Bounds when* $\mathrm{tri}(v) \in \{3, 4\}$. In this subsection D is a contravening decomposition star with associated graph $G(D)$. Let V be a separated set of vertices. For every vertex v in V, we assume that none of its faces is an aggregate in the sense of Remarks 9.18 and 9.19. We assume that there are three or four triangles containing v, for every $v \in V$.

To prove the Inequality 4 in the definition of admissible weight assignments, we will rely on the following reductions. Define an equivalence relation on exceptional faces by $F \sim F'$ if there is a sequence $F_0 = F, \ldots, F_r = F'$ of exceptional faces such that consecutive faces share a vertex of type $(3, 0, 2)$. (That is, $\mathrm{tri}(v) = 3$.) Let $\mathcal{F}$ be an equivalence class of faces.

Lemma 11.9. *Let* V *be a separated set of vertices. For every equivalence class of exceptional faces* $\mathcal{F}$, *let* $V(\mathcal{F})$ *be the subset of* V *whose vertices lie in the union of faces of* $\mathcal{F}$. *Suppose that for every equivalence class* $\mathcal{F}$, *the Inequality* 4 (*in the definition of admissible weight assignments*) *holds for* $V(\mathcal{F})$. *Then Inequality* 4 *holds for* V.

Proof. By construction, each vertex in V lies in some F, for an exceptional face. Moreover, the separating property of V insures that the triangles and quadrilaterals in the inequality are associated with a well-defined $\mathcal{F}$. Thus, the inequality for V is a sum of the inequalities for each $V(\mathcal{F})$. □

Lemma 11.10. *Let* v *be a vertex in a separated set* V *at which there are* p *triangles*, q *quadrilaterals*, *and* r *other faces. Suppose that for some* $p' \le p$ *and* $q' \le q$, *we have*

$$\tau_{\mathrm{LP}}(p', q', \alpha) > (p' d(3) + q' d(4) + a(p))\,\mathrm{pt}$$

for some upper bound α *on the angle occupied by* p' *triangles and* q' *quadrilaterals at* v. *Suppose further that Inequality* 4 (*in the definition of admissible weight assignments*) *holds for the separated set* $V' = V \setminus \{v\}$. *Then the inequality holds for* V.

Proof. Let $F_1, \ldots, F_m$, $m = p' + q'$, be faces corresponding to the triangles and quadrilaterals in the lemma. The hypotheses of the lemma imply that

$$\sum_1^m (w(F_i) - d(\mathrm{len}(F_i))) > a(p).$$

Clearly, the inequality for V is the sum of this inequality, the inequality for V', and $d(n) \geq 0$. □

Recall that the central vertex of a flat quarter is defined to be the one that does not lie on the triangle formed by the origin and the diagonal.

LEMMA 11.11. *Let R be an exceptional standard region. Let V be a set of vertices of R. If $v \in V$, let p_v be the number of triangular regions at v and let q_v be the number of quadrilateral regions at v. Assume that V has the following properties:*

1. *The set V is separated.*
2. *If $v \in V$, then there are five standard regions at v.*
3. *If $v \in V$, then the corner over v is a central vertex of a flat quarter in the cone over R.*
4. *If $v \in V$, then $p_v \geq 3$. That is, at least three of the five standard regions at v are triangular.*
5. *If $R' \neq R$ is an exceptional region at v, and if R has interior angle at least 1.32 at v, then R' also has interior angle at least 1.32 at v.*

Let F be the union of $\{R\}$ with the set of triangular and quadrilateral regions that have a vertex at some $v \in V$. Then

$$\tau_F(D) > \sum_{v \in V} (p_v d(3) + q_v d(4) + a(p_v))\,\mathrm{pt}.$$

Proof. If $(p_v, q_v) = (3, 1)$ and the internal angle of R at v is at least 1.32, then we use

$$\tau_{\mathrm{LP}}(3, 1, 2\pi - 1.32) > 1.4\,\mathrm{pt} + t_4.$$

In this case, the inequality of the lemma is a consequence of this inequality and the inequality for $V \setminus \{v\}$. Thus, we may assume without loss of generality that if $(p_v, q_v) = (3, 1)$, then the internal angle of R at v is at most 1.32. The conclusion is now found in [Hal06a]. □

LEMMA 11.12. *Property 4 of admissibility holds. That is, let V be any separated set of vertices. Then*

$$\sum_{F:\, V \cap F \neq \emptyset} (w(F) - d(\mathrm{len}(F))) \geq \sum_{v \in V} a(\mathrm{tri}(v)).$$

Proof. Let V be a separated set of vertices. The results of Section 11.2 reduce the lemma to the case where $\mathrm{tri}(v) \in \{3, 4\}$ for every vertex $v \in V$.

We will say that there is a flat quarter centered at v, if the corner v' over v is the central vertex of a flat quarter and that flat quarter lies in the cone over an exceptional region.

One case is easy to deal with. Assume that there are three triangles, a quadrilateral, and an exceptional face at the vertex. Assume the interior angle on the exceptional region is least 1.32; then

$$\tau_{\mathrm{LP}}(3, 1, 2\pi - 1.32) > 1.4\,\mathrm{pt} + t_4. \tag{11.1}$$

This gives the bound in the sense of Lemma 11.10 at such a vertex. For the rest of the proof, assume that the interior angle on the exceptional region is less than 1.32 at vertices of type $(p, q, r) = (3, 1, 1)$. This implies in particular by Lemma 9.16 that there is a flat quarter centered at each vertex of this type.

Let v be vertex with no flat quarter centered at v. By Lemma 9.16, the interior angles of the exceptional regions at v are at least 1.32. It follows[11] that

$$\tau_{\mathrm{LP}}(p_v, q_v, \alpha) > (p_v d(3) + q_v d(4) + a(p_v))\,\mathrm{pt}. \tag{11.2}$$

Thus, by Lemma 11.10, we reduce to the case where for each $v \in V$, there is a flat quarter centered at v. Assume that V has this property.

Pick a function f from the set V to the set of exceptional standard regions as follows. If there is only one exceptional region at v, then let $f(v)$ be that exceptional region. If there are two exceptional regions at v, then let $f(v)$ be one of these two exceptional regions. Pick it to be an exceptional region with interior angle at most 1.32 if one of the two exceptional regions has this property. Pick it to have a flat quarter centered at v. Note that by Lemma 9.16, if the exceptional region has interior angle at most 1.32, then $f(v)$ will have a flat quarter centered at v.

For each exceptional region R, let

$$V_R = \{v \in V : f(v) = R\}.$$

By Lemma 11.11, the Property 4 of admissibility is satisfied for each V_R. Since this property is additive in V_R and since V is the disjoint union of the sets V_R, the proof is complete. □

11.4. *Weight assignments for aggregates.*

LEMMA 11.13. *Consider a separated set of vertices V on an aggregated face F as in Remark* 9.18. *Then Inequality* 4 *holds* (*in the definition of admis-*

[11] CALC-551665569, CALC-824762926, and CALC-325738864

sible weight assignments):

$$\sum_{V\cap F\neq\emptyset}(w(F)-d(\mathrm{len}(F)))\geq\sum_{v\in V}a(\mathrm{tri}(v)).$$

Proof. We may assume that $\mathrm{tri}(v)\in\{3,4\}$. First consider the aggregate of Remark 9.18 of a triangle and eight-sided region, with pentagonal hull F. There is no other exceptional region in a contravening decomposition star with this aggregate:

$$t_8+t_5>(4\pi\zeta-8)\,\mathrm{pt}.$$

A separated set of vertices V on F has cardinality at most 2. This gives the desired bound

$$t_8>t_5+2(1.5)\,\mathrm{pt}.$$

Next, consider the aggregate of a hexagonal hull with an enclosed vertex. Again, there is no other exceptional face. If there are at most $k\leq 2$ vertices in a separated set, then the result follows from

$$t_8>t_6+k(1.5)\,\mathrm{pt}.$$

There are at most three vertices in V on a hexagon, by the non-adjacency conditions defining V. A vertex v can be removed from V if it is not the central vertex of a flat quarter (Lemma 11.10 and Inequalities 11.1 and 11.2). If there is an enclosed vertex w, it is impossible for there to be three nonadjacent vertices, each the central vertex of a flat quarter:

$$\mathcal{E}(2,2,2,\sqrt{8},\sqrt{8},\sqrt{8},2t_0,2t_0,2)>2t_0.$$

($\mathcal{E}$ is as defined in Definition 2.14.)

Finally consider the aggregate of a pentagonal hull with an enclosed vertex. There are at most $k\leq 2$ vertices in a separated set in F. There is no other exceptional region:

$$t_7+t_5>(4\pi\zeta-8)\,\mathrm{pt}.$$

The result follows from

$$t_7>t_5+2(1.5)\,\mathrm{pt}.\qquad\square$$

LEMMA 11.14. *Consider a separated set of vertices V on an aggregate face of a contravening plane graph as in Remark* 9.19. *Inequality* 4 *holds in the definition of admissible weight assignments.*

Proof. There is at most one exceptional face in the plane graph:

$$t_8+t_5>(4\pi\zeta-8)\,\mathrm{pt}.$$

Assume first that an aggregate face is an octagon (Figure 9.4). At each of the vertices of the face that lies on a triangular standard region in the aggregate, we can remove the vertex from V using Lemma 11.10 and the estimate

$$\tau_{\mathrm{LP}}(4, 0, 2\pi - 2(0.8638)) > 1.5\,\mathrm{pt}.$$

This leaves at most one vertex in V, and it lies on a vertex of F which is "not aggregated," so that there are five standard regions of the associated decomposition star at that vertex, and one of those regions is pentagonal. The value $a(4) = 1.5\,\mathrm{pt}$ can be estimated at this vertex in the same way it is done for a non-aggregated case in Section 11.3.

Now consider the case of an aggregate face that is a hexagon (Figure 9.4). The argument is the same: we reduce to V containing a single vertex, and argue that this vertex can be treated as in Section 11.3. (Alternatively, use the fact that the pentagon-triangle combination in this aggregate has been eliminated by Lemma 10.10.) $\square$

The proof that contravening plane graphs are tame is complete.

12. Linear program estimates

We have completed the first half of the proof of the Kepler conjecture by proving that every contravening plane graph is tame.

The second half of the proof of the Kepler conjecture consists in showing that tame graphs are not contravening, except for the isomorphism class of graphs isomorphic to G_{fcc} and G_{hcp} associated with the face-centered cubic and hexagonal close packings.

This part of the proof treats all contravening tame graphs except for three cases G_{fcc}, G_{pent}, and G_{hcp}. The two cases G_{fcc} and G_{hcp} are treated in Theorem 6.1, and the case G_{pent} is treated in [Fer97].

The primary tool that will be used is linear programming. The linear programs are obtained as relaxations of the original nonlinear optimization problem of maximizing $\sigma(D)$ over all decomposition stars whose associated graph is a given tame graph G. The upper bounds obtained through relaxation are upper bounds to the nonlinear problem.

To eliminate a tame graph, we must show that it is not contravening. By definition, this means we must show that $\sigma(D) < 8\,\mathrm{pt}$. When a single linear program does not yield an upper bound under 8 pt, we branch into a sequence of linear programs that collectively imply the upper bound of 8 pt. This will call for a sequence of increasingly complex linear programs.

For each of the tame plane graphs produced in Theorem 8.1, we define a linear programming problem whose solution dominates the value of $\sigma(D)$ on the set of decomposition stars associated with the plane graph. A description of the linear programs is presented in this chapter.

THEOREM 12.1. *If the plane graph of a contravening decomposition star is isomorphic to one in the list* [Hal05], *then it is isomorphic to one of the following three plane graphs*: *the plane graph of the pentahedral prism*, *that of the hexagonal-close packing*, *or that of the face-centered cubic packing.*

This theorem is one of the central claims described in Section 1.3 that lead to the proof of the Kepler conjecture.

12.1. *Relaxation.*

(NLP): Let $f : P \to \mathbb{R}$ be a function on a nonempty set P. Consider the nonlinear maximization problem

$$\max_{p \in P} f(p).$$

(LP): Consider a linear programming problem

$$\max\ c \cdot x$$

such that $A\,x \leq b$, where A is a matrix, b, c are vectors of real constants and x is a vector of variables $x = (x_1, \ldots, x_n)$. We write the linear programming problem as

$$\max(c \cdot x : A\,x \leq b).$$

An *interpretation* I of a linear programming problem (LP) is a nonempty set $|I|$, together with an assignment $x_i \mapsto x_i^I$ of functions $x_i^I : |I| \to \mathbb{R}$ to variables x_i. We say the constraints $A\,x \leq b$ of the linear program are *satisfied* under the interpretation I if for all $p \in |I|$,

$$A\,x^I(p) \leq b.$$

The interpretation I is said to be a *relaxation* of the nonlinear program (NLP), if the following three conditions hold.

1. $P = |I|$.

2. The constraints are satisfied under the interpretation.

3. $f(p) \leq c \cdot x^I(p)$, for all $p \in |I|$.

LEMMA 12.2. *Let* (LP) *be a linear program with relaxation* I *to* (NLP). *Then* (LP) *has a feasible solution. Moreover, if* (LP) *is bounded above by a constant* M, *then* M *is an upper bound on the function* $f : |I| \to \mathbb{R}$.

Proof. A feasible solution is $x_i = x_i^I(p)$, for any $p \in |I|$. The rest is clear. $\square$

Remark 12.3. In general, it is to be expected that the interpretations $A\,x^I \le b$ will be nonlinear inequalities on the domain P. In our situation, satisfaction of the constraints will be proved by interval arithmetic. Thus, the construction of an upper bound to (NLP) breaks into two tasks: to solve the linear programs and to prove the nonlinear inequalities required to satisfy the constraints.

There are many nonlinear inequalities entering into our interpretation. These have been proved by interval arithmetic on computer and are listed at [Hal05].

Remark 12.4. There is a second method of establishing the satisfaction of inequalities under an interpretation. Suppose we wish to show that the inequality $e\cdot x \le b'$ is satisfied under the interpretation I. Suppose that we have already established that a system of inequalities $A\,x \le b$ is satisfied under the interpretation I. We solve the linear programming problem $\max(e\cdot x : A\,x \le b)$. If this maximum is at most b', then the inequality $e \cdot x \le b'$ is satisfied under the interpretation I. We will refer to $e \cdot x \le b'$ as an *LP-derived inequality* (with respect to the system $A\,x \le b$).

12.2. *The linear programs.* Let G be a tame plane graph. Let $\mathrm{DS}(G)$ be the space of all decomposition stars whose associated plane graph is isomorphic to G.

THEOREM 12.5. *For every tame plane graph G other than G_{fcc}, G_{hcp}, and G_{pent}, there exists a finite sequence of linear programs with the following properties.*

1. *Every linear program has an admissible solution and its solution is strictly less than* $8\,\mathrm{pt}$.
2. *For every linear program in this sequence, there is an interpretation I of the linear program that is a relaxation of the nonlinear optimization problem*
$$\sigma : |I| \to \mathbb{R},$$
where $|I|$ is a subset of $\mathrm{DS}(G)$.
3. *The union of the subsets $|I|$, as we run over the sequence of linear programs, is* $\mathrm{DS}(G)$.

The proof is constructive. For every tame plane graph G a sequence of linear programs is generated by computer and solved. The optimal solutions are all bounded above by $8\,\mathrm{pt}$. It will be clear from construction of the sequence that the union of the sets $|I|$ exhausts $\mathrm{DS}(G)$. We estimate that nearly

10^5 linear programs are involved in the construction. The rest of this paper outlines the construction of some of these linear programs. Details are found in [Hal06a].

Remark 12.6. The paper [Hal03, §3.1.1] shows how the linear programs that arise in connection with the Kepler conjecture can be formulated in such a way that they always have a feasible solution and so that the optimal solution is bounded. We assume that all our linear programs have been constructed in this way.

COROLLARY 12.7. *If a tame graph G is not isomorphic to $G_{\rm fcc}$, $G_{\rm hcp}$, or $G_{\rm pent}$, then it is not contravening.*

Proof. This follows immediately from Theorem 12.5 and Lemma 12.2. □

12.3. *Basic linear programs.* Let G be a tame plane graph. Specifically, G is one of the several thousands of graphs that appear in the explicit classification [Hal05].

To describe the basic linear program, we need the following indexing sets. Let `VERTEX` be the set of all vertices in G. Let `FACE` be the set of all faces in G. (Recall that by construction each face F of the graph carries an orientation.) Let `ANGLE` be the set of all angles in G, defined as the set of pairs (v, F), where the vertex v lies in the face F. Let `DIRECTED` be the set of directed edges. It consists of all ordered pairs $(v, s(v, F))$, where $s(v, F)$ denotes the successor of the vertex v in the oriented face F. Let `TRIANGLES` be the subset of `FACE` consisting of those faces of length 3. Let `UNDIRECTED` be the set of undirected edges. It consists of all unordered pairs $\{v, s(v, F)\}$, for $v \in F$.

We introduce variables indexed by these sets. Following AMPL notation, we write for instance $y\{\texttt{VERTEX}\}$ to declare a collection of variables $y[v]$ indexed by vertices v in `VERTEX`. With this in mind, we declare the variables

$$\begin{array}{lll} \alpha\{\texttt{ANGLE}\}, & y\{\texttt{VERTEX}\}, & e\{\texttt{UNDIRECTED}\}, \\ \sigma\{\texttt{FACE}\}, & \tau\{\texttt{FACE}\}, & \mathrm{sol}\{\texttt{FACE}\}. \end{array}$$

We obtain an interpretation I on the compact space $\mathrm{DS}(G)$. First, we define an interpretation at the level of indexing sets. A decomposition star determines the set $U(D)$ of vertices of height at most $2t_0$ from the origin of D. Each decomposition star $D \in \mathrm{DS}(G)$ determines a (metric) graph with geodesic edges on the surface of the unit sphere, which is isomorphic to G as a (combinatorial) plane graph. There is a map from the vertices of G to $U(D)$ given by $v \mapsto v^I$, if the radial projection of v^I to the unit sphere at the origin corresponds to v under this isomorphism. Similarly, each face F of G corresponds to a set F^I of standard regions. Each edge e of G corresponds to a geodesic edge e^I on the unit sphere.

Now we give an interpretation I to the linear programming variables at a decomposition star D. As usual, we add a superscript I to a variable to indicate its interpretation. Let $\alpha[v,F]^I$ be the sum of the interior angles at v^I of the metric graph in the standard regions F^I. Let $y[v]^I$ be the length $|v^I|$ of the vertex $v^I \in U(D)$ corresponding to v. Let $e[v,w]^I$ be the length $|v^I - w^I|$ of the edge between v^I and $w^I \in U(D)$. Let

$$\begin{aligned} \sigma[F]^I &= \sigma_F(D), \\ \mathrm{sol}[F]^I &= \mathrm{sol}(F^I), \\ \tau[F]^I &= \tau_F(D). \end{aligned}$$

The objective function for the optimization problems is

$$\max: \quad \sum_{F \in \mathtt{FACE}} \sigma[F].$$

Its interpretation under I is the score $\sigma(D)$.

We can write a number of linear inequalities that will be satisfied under our interpretation. For example, we have the bounds

$$\begin{array}{ll} 0 \le y[v] \le 2t_0, & v \in \mathtt{VERTEX}, \\ 0 \le e[v,w] \le 2t_0, & (v,w) \in \mathtt{EDGE}, \\ 0 \le \alpha[v,F] \le 2\pi, & (v,F) \in \mathtt{ANGLE}, \\ 0 \le \mathrm{sol}[F] \le 4\pi, & F \in \mathtt{FACE}. \end{array}$$

There are other linear relations that are suggested directly by the definitions or the geometry. Here, v belongs to VERTEX.

$$\begin{aligned} \tau[F] &= \mathrm{sol}[F]\zeta\mathrm{pt} - \sigma[F], \\ 2\pi &= \textstyle\sum_{F: v\in F} \alpha[v,F], \\ \mathrm{sol}[F] &= \textstyle\sum_{v\in F} \alpha[v,F] - (\mathrm{len}(F) - 2)\pi. \end{aligned}$$

There are long lists of additional inequalities that come from interval arithmetic verifications. Many are specifically designed to give relations between the variables.

$$\begin{array}{lll} \sigma[F], & \tau[F], & \alpha[v,F], \\ \mathrm{sol}[F], & y[v], & e[v,w] \end{array}$$

whenever F^I is a single standard region having three sides. Similarly, other computer calculations give inequalities for $\sigma[F]$ and related variables, when the length of F is four. A complete list of inequalities that are used for triangular and quadrilateral faces is found in [Hal05].

For exceptional faces, we have an admissible weight function $w(F)$. According to definitions $w(F) = \tau[F]/pt$, so that the inequalities for the weight function can be expressed in terms of the linear program variables.

When the exceptional face is not an aggregate, then it also satisfies the inequalities of Lemma 9.2.

12.4. *Error analysis.* The variables of the linear programming problem are the dihedral angles, the scores of each of the standard clusters, and their edge lengths.

We subject these variables to a system of linear inequalities. First of all, the dihedral angles around each vertex sum to 2π. The dihedral angles, solid angles, and score are related by various linear inequalities as described in Section 12.3. The solid-angle variables are linear functions of dihedral angles. We have

$$\sigma(D) = \sigma_{S_1}(D) + \cdots + \sigma_{S_p}(D) + \sigma_{R_1}(D) + \cdots + \sigma_{R_q}(D).$$

Forgetting the origin of the scores, solid angles, and dihedral angles as nonlinear functions of the standard clusters and treating them as formal variables subject only to the given linear inequalities, we obtain a linear programming bound on the score.

Floating-point arithmetic was used freely in obtaining these bounds. The linear programming package CPLEX was used (see *www.cplex.com*). However, the results, once obtained, could be checked rigorously as follows.[12]

We present an informal analysis of the floating-point errors. For each quasi-regular tetrahedron S_i we have a nonnegative variable $x_i = \mathrm{pt} - \sigma(S_i)$. For each quad cluster R_k, we have a nonnegative variable $x_k = -\sigma(R_k)$. A bound on $\sigma(D)$ is $p\,\mathrm{pt} - \sum_{i\in I} x_i$, where p is the number of triangular standard regions, and I indexes the faces of the plane graph. We give error bounds for a linear program involving scores and dihedral angles. Similar estimates can be made if there are edges representing edge lengths. Let the dihedral angles be x_j, for j in some indexing set J. Write the linear constraints as $Ax \le b$. We wish to maximize $c\cdot x$ subject to these constraints, where $c_i = -1$, for $i \in I$, and $c_j = 0$, for $j \in J$. Let z be an approximate solution to the inequalities $zA \ge c$ and $z \ge 0$ obtained by numerical methods. Replacing the negative entries of z by 0 we may assume that $z \ge 0$ and that $zA_i > c_i - \epsilon$, for $i \in I \cup J$, and some small error ϵ. If we obtain the numerical bound $p\,\mathrm{pt} + z\cdot b < 7.9999\,\mathrm{pt}$, and if $\epsilon < 10^{-8}$, then $\sigma(D)$ is less than $8\,\mathrm{pt}$. In fact, we note that

$$\left(\frac{z}{1+\epsilon}\right) A_i$$

is at least c_i for $i \in I$ (since $c_i = -1$), and that it is greater than $c_i - \epsilon/(1+\epsilon)$, for $i \in J$ (since $c_i = 0$). Thus, if $N \le 60$ is the number of vertices, and

[12] The output from each linear program that has no exceptional regions has been double checked with interval arithmetic. Predictably, the error bounds presented here were satisfactory. 1/2002

$p \le 2(N-2) \le 116$ is the number of triangular faces,

$$\begin{aligned}\sigma(D) &\le p\,\mathrm{pt} + c\cdot x \le p\,\mathrm{pt} + \left(\frac{z}{1+\epsilon}\right) Ax + \frac{\epsilon}{1+\epsilon}\sum_{j\in J} x_j \\ &\le p\,\mathrm{pt} + \frac{z\cdot b}{1+\epsilon} + \frac{\epsilon}{1+\epsilon} 2\pi N \\ &\le \left[p\,\mathrm{pt} + z\cdot b + \epsilon(p\,\mathrm{pt} + 2\pi N)\right]/(1+\epsilon) \\ &\le \left[7.9999\,\mathrm{pt} + 10^{-8}(116\,\mathrm{pt} + 500)\right]/(1+10^{-8}) < 8\,\mathrm{pt}.\end{aligned}$$

In practice, we used $0.4429 < 0.79984\,\mathrm{pt}$ as our cutoff, and $N \le 14$ in the interesting cases, so that much tighter error estimates are possible.

13. Elimination of aggregates

The proof of the following theorem occupies the entire chapter. It eliminates all the pathological cases that we have had to carry along until now.

THEOREM 13.1. *Let D be a contravening decomposition star, and let G be its tame graph. Every face of G corresponds to exactly one standard region of D. No standard region of D has any enclosed vertices from $U(D)$. (That is, a decomposition star with one of the aggregates shown in Figure* 9.1 *is not contravening.)*

13.1. *Triangle and quad branching.* Chapter 14 will discuss branch and bound strategies. Branch and bound strategies replace a single linear program with a series of linear program, when a single linear program does not suffice. There is one case of branch and bound that we need before Chapter 14. This is a branching on triangular and quadrilateral faces.

We divide triangular faces with corners v_1, v_2, v_3 into two cases:

$$e[v_1,v_2] + e[v_2,v_3] + e[v_3,v_1] \le 6.25,$$
$$e[v_1,v_2] + e[v_2,v_3] + e[v_3,v_1] \ge 6.25,$$

whenever sufficiently good bounds are not obtained as a single linear program. We also divide quadrilateral faces into four cases: two flat quarters, two flat quarters with diagonal running in the other direction, four upright quarters forming a quartered octahedron, and the mixed case. (A mixed cases by definition is any case that is not one of the other three.) In general, if there are r_1 triangles and r_2 quadrilaterals, we obtain as many as $2^{r_1+2r_2}$ cases by breaking the various triangles and quadrilaterals into subcases.

We break triangular faces and quadrilaterals into subcases, as needed in the linear programs that follow, without further comment.

13.2. *A pentagonal hull with* $n = 8$. The next few sections treat the nonpolygonal standard regions described in Remark 9.18. In this subsection, there is an aggregate of the octagonal region and a triangle has a pentagonal hull. Let P denote this aggregate.

LEMMA 13.2. *Let G be a contravening plane graph with the aggregate of Remark* 9.18*. Some vertex on the pentagonal face has type not equal to* $(3, 0, 1)$.

Proof. If every vertex on the pentagonal face has type $(3, 0, 1)$, then at the vertex of the pentagon meeting the aggregated triangle, the four triangles together with the octagon give

$$t_8 + \sum_{(4)} \tau_{\mathrm{LP}}(4, 0, 2\pi - 2(1.153)) > (4\pi\zeta - 8)\,\mathrm{pt},$$

so that the graph does not contravene. □

For a general contravening plane graph with this aggregate, we have bounds

$$\sigma_F(D) \le \mathrm{pt} + s_8,$$
$$\tau_F(D) \ge t_8.$$

We add the inequalities $\tau[F] > t_8$ and $\sigma[F] < \mathrm{pt} + s_8$ to the exceptional face. There is no other exceptional face, because $t_8 + t_5 > (4\pi\zeta - 8)\,\mathrm{pt}$. We run the linear programs for all tame graphs with the property asserted by Lemma 13.2. Every upper bound is less than $8\,\mathrm{pt}$, so that there are no contravening decomposition stars with this configuration.

13.3. $n = 8$, *hexagonal hull.* We treat the two cases from Remark 9.18 that have a hexagonal hull (Figure 9.1). One can be described as a hexagonal region with an enclosed vertex that has height at most $2t_0$ and distance at least $2t_0$ from each corner over the hexagon. The other is described as a hexagonal region with an enclosed vertex of height at most $2t_0$, but this time with distance less than $2t_0$ from one of the corners over the hexagon.

The argument for the case $n = 8$ with hexagonal hull is similar to the argument of Section 13.2. Add the inequalities $\tau[R] > t_8$ and $\sigma[R] < s_8$ for each hexagonal region. Run the linear programs for all tame graphs, and check that these additional inequalities yield linear programming bounds under $8\,\mathrm{pt}$.

13.4. $n = 7$, *pentagonal hull.* We treat the two cases illustrated in Figure 9.1 that have a pentagonal hull. These cases require more work. One can be described as a pentagon with an enclosed vertex that has height at most $2t_0$ and distance at least $2t_0$ from each corner of the pentagon. The other is described as a pentagon with an enclosed vertex of height at most $2t_0$, but this time with distance less than $2t_0$ from one of the corners of the pentagon.

In discussing various maps, we let v_i be the corners of the regions, and we set $y_i = |v_i|$ and $y_{ij} = |v_i - v_j|$. The subscript F is dropped, when there is no great danger of ambiguity.

Add the inequalities $\tau[F] > t_7$, $\sigma[F] < s_7$ for the pentagonal face. There is no other exceptional region, because $t_5 + t_7 > (4\pi\zeta - 8)\,\mathrm{pt}$. With these changes, of all the tame plane graphs with a pentagonal face and no other exceptional face, all but one of the linear programs give a bound under 8 pt.

The plane graph G_0 that remains is easy to describe. It is the plane graph with 11 vertices, obtained by removing from an icosahedron a vertex and all five edges that meet at that vertex.

We treat the case G_0. Let v_{12} be the vertex enclosed over the pentagon. We let $v_1, \ldots, v_5$ be the five corners of $U(D)$ over the pentagon. Break the pentagon into five simplices along $\{0, v_{12}\}$: $S_i = \{0, v_{12}, v_i, v_{i+1}\}$. We have LP-derived bounds (in the sense of Remark 12.4) $y[v_i] \le 2.168$, and $\alpha[v_i, F] \le 2.89$, for $i = 1, 2, 3, 4, 5$. In particular, the pentagonal region is convex, for every contravening star $D \in \mathrm{DS}(G_0)$.

Further LP-derived inequalities are

$$\sigma[F] > -0.2345 \text{ and } \tau[F] < 0.644.$$

By using branch and bound arguments on the triangular faces, as described in Section 13.1, we can improve the LP-derived inequality to

$$\tau[F] < 0.6079.$$

Another LP-derived inequality gives a bound on the perimeter:

$$\sum |v_i - v_{i+1}| \le 11.407.$$

Yet another LP-derived inequality states that if v_1, v_2, v_3 are consecutive corners over the pentagonal region, then

$$|v_1 - v_2| + |v_2 - v_3| < 4.804.$$

Lemma 13.3. *Assume that R is a pentagonal standard region with an enclosed vertex v of height at most $2t_0$. Assume further that*

- $|v_i| \le 2.168$ *for each of the five corners.*
- *Each interior angle of the pentagon is at most* 2.89.
- *If v_1, v_2, v_3 are consecutive corners over the pentagonal region, then* $|v_1 - v_2| + |v_2 - v_3| < 4.804$.
- $\sum_5 |v_i - v_{i+1}| \le 11.407$.

Then $\sigma_R(D) < -0.2345$ or $\tau_R(D) > 0.6079$.

Proof. This appears in [Hal06a]. □

Since the bound $\tau_R(D) > 0.6079$ contradicts the LP-derived inequality $\tau[F] < 0.6079$, this case does not occur in a contravening graph.

13.5. *Type* $(p, q, r) = (5, 0, 1)$. We return briefly to the case of six standard regions around a vertex discussed in Remark 9.19. In the plane graph they are aggregated into an octagon. We take each of the remaining cases with an octagon, and replace the octagon with a pentagon and six triangles around a new vertex. There are eight ways of doing this. All eight ways in each of the cases gives an LP bound under 8 pt. This completes this case.

The second aggregate shown in Figure 9.4 contains a pentagon-triangle combination that was ruled out by Lemma 10.10.

13.6. *Summary.*

Lemma 13.4. *None of the aggregates of Remark* 9.19 *and Remark* 9.18 *appear in a contravening star. In particular, all regions are bounded by simple polygons, and each face of the graph* $G(D)$ *corresponds to exactly one standard region.*

The proof is the main result of this chapter. □

14. Branch and bound strategies

When a single linear program does not give sufficiently good bounds, we apply branch and bound methods to improve the bound. By branching repeatedly, we are able to show in every case that a given tame graph is not contravening.

By relying to a greater degree on results from the unabridged version of the proof and on results that appear in unpublished (but publicly available) computer logs, this chapter is more technical than the others. The purpose of the chapter is to give a sketch of the various ways that the various decomposition stars are divided into cases according to a branch and bound strategy. This final chapter is intended as a brief introduction to the unabridged version.

The first branching strategy has already been described in Section 13.1. It divides the decomposition stars with a given graph into subcases according to the structural properties of triangular and quadrilateral standard regions.

We assume the results from the Section 13 that eliminate the most unpleasant types of configurations.

14.1. *Review of internal structures.* For the past several chapters, it has not been necessary to refer to the internal structure of the standard clusters.

This chapter is different. To describe the branching operations, it will be necessary to use details about the structure of standard clusters.

Recall that a *quarter* is a set of four vertices with five edges of length at least 2 and at most $2t_0$ and a sixth edge of length at least $2t_0$ and at most $2\sqrt{2}$. The long edge of the quarter is called its diagonal. A set of quarters with pairwise disjoint interiors has been selected. Quarters in this set are said to belong to the Q-system. The Q-system has been constructed in such a way that if one quarter along a diagonal lies in the Q-system, then all quarters along that diagonal lie in the Q-system. An anchor is a vertex of the packing that has distance at least 2 and at most $2t_0$ from both endpoints of a diagonal. Each diagonal has a context (n, k), with $n \geq k$, where n is the number of anchors around the diagonal and $n - k$ is the number of quarters that have that diagonal as an edge. If a diagonal has context (n, k), then k is the number of *gaps* that occur between anchors; that is, spaces that are not filled in by quarters. The context of a quarter is defined to be the context of its diagonal.

Recall that a quarter (or its diagonal) is said to be upright if one endpoint of its diagonal is the origin. A quarter is said to be flat if it is not upright and if some vertex of the quarter is the origin.

There is a process of simplification of the decomposition stars and their scoring functions that eliminates[13] many of the contexts (n, k). (The upright quarters are said to be *erased*.) We assume in the following discussion and lemmas that this procedure has been carried out.

An upright diagonal is said to be a *loop* when there is a reasonable scheme of inserting a simplex into each gap so that the diagonal is completely surrounded by quarters and the inserted simplices. The simplices that are inserted in the gaps are called *anchored simplices*. They are constructed in such a way that every edge of an anchored simplex has length at most 3.2. All simplices in a given loop lie over a single standard region. If the gaps cannot be filled with anchored simplices, the upright diagonal is not a loop. Details of this construction can be found in the unabridged proof [Hal06a].

In every case, the simplices around a given upright diagonal lie in the cone over a single standard region.

LEMMA 14.1. *Consider an upright diagonal that is a loop. Let R be the standard region that contains the upright diagonal and its surround simplices. Then the following contexts (n, k) are the only ones possible. Moreover, the constants that appear in the columns marked σ and τ are upper and lower bounds respectively for $\sigma_R(D)$ and $\tau_R(D)$ when R contains one loop of that context.*

[13]In detail, we assume that all of the contexts that do not carry a penalty have been erased. We leave loops, 3-crowded, 4-crowded, and 3-unconfined upright diagonals unerased at this point.

std. region	(n,k)	σ	τ
R quad:	$(4,0)$	-0.0536	0.1362
R pentagon:	$(4,1)$	s_5	0.27385
	$(5,0)$	-0.157	0.3665
R hexagon:	$(4,1)$	s_6	0.41328
	$(4,2)$	-0.1999	0.5309
	$(5,1)$	-0.37595	0.65995
R heptagon:	$(4,1)$	s_7	0.55271
	$(4,2)$	-0.25694	0.67033
R octagon:	$(4,1)$	s_8	0.60722
	$(4,2)$	-0.31398	$0.72484.$

Proof. See [Hal06a]. □

14.2. 3-*crowded and* 4-*crowded upright diagonals.*

Definition 14.2. Consider an upright diagonal that is not a loop. Let R be the standard region that contains the upright diagonal and its surrounding quarters. Then the contexts $(4,1)$ and $(5,1)$ are the only contexts possible. In the context $(4,1)$, if there does not exist a plane through the upright diagonal such that all three quarters lie in the same half-space bounded by the plane, then we say that the context is 3-*unconfined.* If such a plane exists, then we say that the context is 3-crowded. We call the context $(5,1)$ a 4-crowded upright diagonal. Thus, every upright diagonal is exactly one of the following: a loop, 3-unconfined, 3-crowded, or 4-crowded. A contravening decomposition star contains at most one upright diagonal that is 3-crowded or 4-crowded. See [Hal06a] for a proof of these facts and for further details.

Lemma 14.3. *Let R be a standard region that contains an upright diagonal that is* 4*-crowded. Then*

$$\sigma_R(D) < -0.25 \text{ and } \tau_R(D) > 0.4.$$

Let R be a standard region that contains an upright diagonal that is 3*-crowded. Then*

$$\sigma_R(D) < -0.4339 \text{ and } \tau_R(D) > 0.5606.$$

Proof. See [Hal06a]. □

LEMMA 14.4. *A contravening decomposition star does not contain any upright diagonals that are* 3*-crowded.*

Proof. If we have an upright diagonal that is 3-crowded, then there is only one exceptional region $(0.5606 + t_5 > (4\pi\zeta - 8)\,\mathrm{pt})$. We add the inequalities $\tau > 0.5606$ and $\sigma < -0.4339$ to the exceptional region. All linear programming bounds drop under 8 pt when these changes are made. □

Upright diagonals that are 4-crowded require more work. We begin with a lemma.

LEMMA 14.5. *Let α be the dihedral angle along the large gap along an upright diagonal that is* 4*-crowded. Let F be the union of the four upright quarters along the upright diagonal. Let v_1 and v_2 be the anchors of $U(D)$ lying along the large gap. If $|v_1| + |v_2| < 4.6$, then $\alpha > 1.78$ and $\sigma_F(D) < -0.31547$.*

Proof. The bound $\alpha > 1.78$ comes from the inequality archive.[14] The upper bound on the score is a linear programming calculation involving the inequality $\alpha > 1.78$ and the known inequalities on the score of an upright quarter. □

LEMMA 14.6. *A contravening decomposition star does not contain any upright diagonals that are* 4*-crowded.*

Proof. Add the inequalities $\sigma_R(D) < -0.25$ and $\tau_R(D) > 0.4$ at the exceptional regions. An upright diagonal that is 4-crowded does not appear in a pentagon for purely geometrical reasons. Run the linear programs for all tame plane graphs with an exceptional region that is not a pentagon. If this linear program fails to produce a bound of 8 pt, we use the lemma to branch into two cases: either $y[v_1] + y[v_2] \geq 4.6$ or $\sigma[R] < -0.31547$. In every case the bound drops below 8 pt. □

14.3. *Five anchors.* Now turn to the decomposition stars with an upright diagonal with five anchors. Five quarters around a common upright diagonal in a pentagonal region can certainly occur. We claim that any other upright diagonal with five anchors leads to a decomposition star that does not contravene. In fact, the only other possible context is $(n, k) = (5, 1)$ (see Lemma 14.1).

LEMMA 14.7. *Let D be a contravening decomposition star. Then there are no loops with context $(5, 1)$ in D.*

[14] CALC-161665083

Proof. By Lemma 14.1, the standard region R that contains the loop must be a hexagon. By the same lemma, we have

$$\tau_R(D) > 0.65995 \text{ and } \sigma_R(D) < -0.37595.$$

Add these constraints to the linear program of the tame graphs with a hexagonal face. The LP-bound on $\sigma(D)$ with these additional inequalities is less than 8 pt. □

14.4. *Penalties.* From now on, we assume that there are no loops with context $(5, 1)$, and no 3-crowded or 4-crowded upright diagonals. This leaves various loops and 3-unconfined upright diagonals.

At times, it is necessary to *erase*[15] certain loops and 3-unconfined upright diagonals. There is a *penalty* for doing so. Let D be a decomposition star with an upright diagonal $\{0, v\}$. Let D' be the decomposition star that is identical in all respects, except that v and all indices in the decomposition star that point to v (in the sense of Section 4.1) have been deleted. Let R be the standard region of D over which v is located, and let R' be the corresponding standard region of D'. We say that the upright diagonal can be *erased with penalty* π_R if

$$\sigma_R(D) \leq \sigma_{R'}(D') + \pi_R.$$

Definition 14.8. When we break a single region into smaller regions (by taking the part of the region that meets the cone over a quarter, anchored simplex, and so forth) the smaller regions will be called subregions. An anchored simplex that overlaps a flat quarter is said to *mask* the flat quarter. (Masked flat quarters are not in the Q-system.)

Remark 14.9. A function $\hat{\sigma}$ has been defined in [Hal06a]. The details of the definition of this function are not important here. It is proved there that $\hat{\sigma}$ is a good upper bound on the scoring function on flat quarters no matter what the origin of the flat quarter. It gives bounds for flat quarters in the Q-system, masked quarters, isolated quarters, and all the other types of flat quarters. The function $\hat{\tau}$ on the space of flat quarters is defined as

$$\hat{\tau}(Q) = \mathrm{sol}(Q)\zeta\mathrm{pt} - \hat{\sigma}(Q).$$

Remark 14.10. At times, we work with various upper bounds to $\sigma_R(D)$, say,

$$\sigma_R(D) \leq f_R(D).$$

[15] Penalties are a major topic in the unabridged version of this paper. In this paper, we give a short summary

When we have a specific upper bound $f_R(D)$ in view, then we will also say that the upright diagonal can be erased with penalty π_R if

$$f_R(D) \le f_{R'}(D') + \pi_R.$$

In more detail, let $R = \{R_1, \ldots, R_k\}$ be the set of subregions over the anchored simplices in a loop. Let $f_{R_i}(D)$ be the approximations of the score of each anchored simplex. Let $Q_1, \ldots, Q_\ell$ be the flat quarters masked by the anchored simplices in the loop. Let R' be the subregion of points in the union of R that are not in the cone over any Q_i. Then we erase with penalty π_R if

$$\sum_i f_{R_i}(D) \le \sum_\ell \hat\sigma(Q_j) = \mathrm{vor}_{R',0}(D) + \pi_R.$$

If the upright diagonal is not a loop, we include in the set R all regions along the "gaps" around the upright diagonal.

The unabridged proof makes various estimates of the penalties that are involved in erasing various loops and 3-unconfined upright diagonals. Most of the penalties are calculated as integer combinations of the constants $\xi_\Gamma = 0.01561$, $\xi_V = 0.003521$, and 0.008. It is proved[16] in [Hal06a] that ξ_Γ is the penalty for erasing a single upright quarter of compression type, and that ξ_V is the penalty for erasing a single upright quarter of Voronoi type.

Lemma 14.11. *Let* $\{0, v\}$ *be an upright diagonal.*

- *If the upright diagonal is* 3*-unconfined, then the upright diagonal can be erased with penalty* 0.008*.*
- *If the upright diagonal is* 3*-unconfined and it masks a flat quarter, then the upright diagonal can be erased with penalty* 0*.*
- *If a flat quarter is masked, then its diagonal has length at least* 2.6*. Also, if the diagonal of a masked flat quarter has length at most* 2.7*, then the height of its central vertex is at least* 2.2*.*

Proof. See [Hal06a]. □

14.5. Pent *and* hex *branching.* If a single linear program does not yield the bound $\sigma(D) < 8\,\mathrm{pt}$, then we divide the set of decomposition stars with graph G into several subsets, according to the arrangements of quarters inside each standard cluster. This section gives a rough classification of possible arrangements of quarters in the cone over pentagonal and hexagonal standard regions.

[16] CALC-751772680 and CALC-310679005

The possibilities are listed in the diagram only up to symmetry by the dihedral group action on the polygon. We do not prove the completeness of the list, but its completeness can be seen by inspection, in view of the comments that follow here and in Section 14.4. Details about the size of the penalties can be found in [Hal06a].

The conventions for generating the possibilities are different for the pentagons and hexagons than for the heptagons and octagons. We describe the pentagons and hexagons first. We erase all 3-unconfined upright diagonals. If there is one loop we leave the loop in the figure. If there are two loops (so that both necessarily have context $(n,k)=(4,1)$), we erase one and keep the other.

The figures are interpreted as follows. An internal vertex in the polygon represents an upright diagonal. Edges from that vertex are in one-to-one correspondence with the anchors around that upright diagonal. Edges between nonadjacent vertices of the polygon represent the diagonals of flat quarters. We draw all edges from an upright diagonal to its anchors, and all edges of length $[2t_0, 2\sqrt{2}]$ that are not masked by upright quarters. Since the only remaining upright quarters belong to loops, the four simplices around a loop are anchored simplices and the edge opposite the diagonal has length at most 3.2.

Various inequalities in the inequality archive have been designed for subregions of pentagons. Additional inequalities have been designed for subregions in hexagonal regions. Thus, we are able to obtain greatly improved linear programming bounds when we break each pentagonal region into various cases, according to the list of Figures 14.1 and 14.2.

14.6. *Hept and oct branching.* When the figure is a heptagon or octagon, we proceed differently. We erase all 3-unconfined upright diagonals and all loops (either context $(n,k)=(4,1)$ or $(4,2)$) and draw only the flat quarters. An undrawn diagonal of the polygon has length at least $2t_0$. Overall, in these cases much less internal structure is represented.

In the cases where 3-confined upright diagonals or loops have been erased, a number indicating a penalty accompanies the diagram (Figures 14.2 and 14.3). These penalties are derived in [Hal06a].

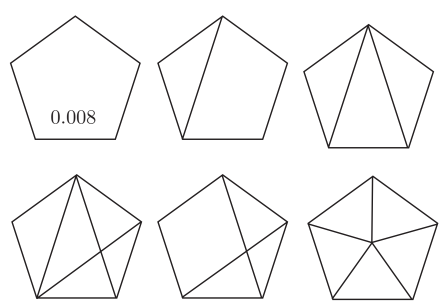

Figure 14.1: Pentagonal face refinements

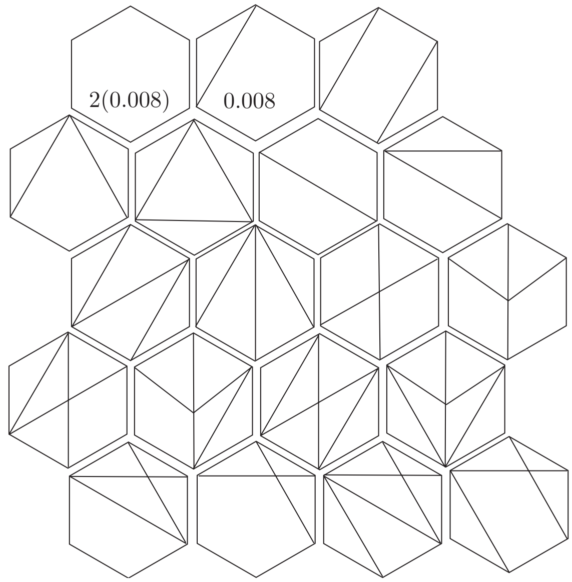

Figure 14.2: Hexagonal face refinements. The only figures with a penalty are the first two on the top row and those on the bottom row. The first two on the top row have penalties 2(0.008) and 0.008. Those on the bottom row have penalties $3\xi_\Gamma$, $3\xi_\Gamma$, $\xi_\Gamma + 2\xi_V$, and $\xi_\Gamma + 2\xi_V$.

Define values

$$Z(3,1) = 0.00005 \quad \text{and } D(3,1) = 0.06585.$$

Here are some special arguments that are used for heptagons and octagons.

14.6.1. *One flat quarter.* Suppose that the standard region breaks into two subregions: the triangular region of a flat quarter Q and one other. Let $n = n(R) \in \{7, 8\}$. We have the inequality:

$$\sigma_R(D) < (\hat\sigma(Q) - Z(3,1)) + s_n + \xi_\Gamma + 2\xi_V.$$

The penalty term $\xi_\Gamma + 2\xi_V$ comes from a possible anchored simplex masking a flat quarter. Let v be the central vertex of the flat quarter Q. Let $\{v_1, v_2\}$ be its diagonal. Masked flat quarters satisfy restrictive edge constraints. It follows from [Hal06a] that we have one of the following three possibilities:

1. $y[v] \geq 2.2$,
2. $e[v_1, v_2] \geq 2.7$,
3. $\sigma_R(D) < (\hat\sigma(Q) - Z(3,1)) + s_{n(R)}$.

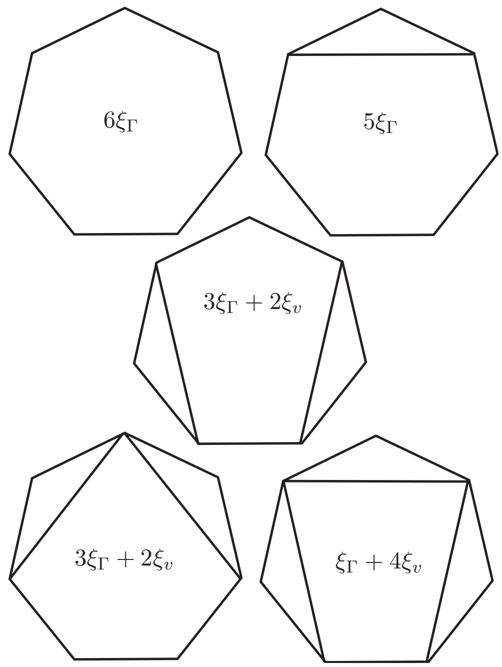

Figure 14.3: Hept face refinements

14.6.2. *Two flat quarters.* We proceed similarly if the standard region R breaks into three subregions: two regions R_1 and R_2 cut out by flat quarters Q_1, Q_2 and one other region made from what remains. Write $\hat{\sigma}_1$ for $\hat{\sigma}(Q_1)$, and so forth. It follows from [Hal06a] that we have one of the following three possibilities:

1. The height of a central vertex is at least 2.2.

2. The diagonal of a flat quarter is at least 2.7.

3. $$\begin{aligned} \sigma_R(D) &< (\hat{\sigma}_1 - Z(3,1)) + (\hat{\sigma}_2 - Z(3,1)) + s_{n(R)}, \\ \tau_R(D) &> (\hat{\tau}_1 - D(3,1)) + (\hat{\tau}_2 - D(3,1)) + t_{n(R)}. \end{aligned}$$

With heptagons, it is helpful on occasion to use an upper bound on the penalty of $3\xi_\Gamma = 0.04683$. This bound holds if neither flat quarter is masked by a loop. For this, it suffices to show that the first two of the given three cases do not hold.

If there is a loop of context $(n,k) = (4,2)$, we have the upper bounds of Lemma 14.1. If, on the other hand, there is no loop of context $(n,k) = (4,2)$, then we have the upper bound

$$\sigma_R(D) \leq (\hat{\sigma}(Q_1) - Z(3,1)) + (\hat{\sigma}(Q_2) - Z(3,1)) + s_{n(R)} + 2(\xi_\Gamma + 2\xi_V),$$

where $n(R) \in \{7,8\}$.

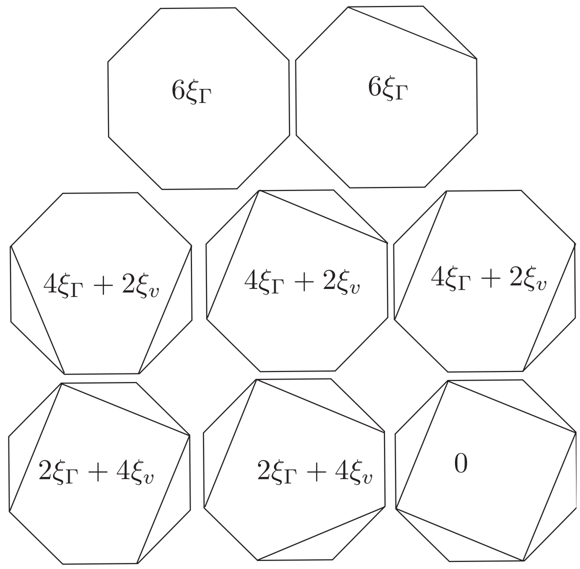

Figure 14.4: Oct face refinements

14.7. *Branching on upright diagonals.* We divide the upright simplices into two domains depending on the height of the upright diagonal, using $|v| = 2.696$ as the dividing point. We break the upright diagonals (of unerased quarters in the Q-system) into cases:

1. The upright diagonal has height at most 2.696.
2. The upright diagonal $\{0, v\}$ has height at least 2.696, and some anchor w along the flat quarter satisfies $|w| \geq 2.45$ or $|v - w| \geq 2.45$. (There is a separate case here for each anchor w.)
3. The upright diagonal $\{0, v\}$ has height at least 2.696, and every anchor w along the flat quarter satisfies $|w| \leq 2.45$ and $|v - w| \leq 2.45$.

Many inequalities have been specially designed to hold on these smaller domains. They are included into the linear programming problems as appropriate.

When all the upright quarters can be erased, then the case for upright quarters follows from some other case without the upright quarters. An upright quarter can be erased in the following situations. If the upright quarter Q has compression type (in the sense of Definition 5.8) and the diagonal has height at least 2.696, then[17]

$$\sigma(Q) < \text{s-vor}_0(Q).$$

[17] CALC-214637273.

(If there are masked flat quarters, they become scored by $\hat{\sigma}$.) If an upright quarter has Voronoi type and the anchors w satisfy $|w| \leq 2.45$ and $|v-w| \leq 2.45$, then the quarter can be erased[18]

$$\sigma(Q) < \text{s-vor}_0(Q).$$

In general, we only have the weaker inequality[19]

$$\sigma(Q) < \text{s-vor}_0(Q) + 0.003521.$$

In a pentagon or hexagon, consider an upright diagonal with three upright quarters, that is, context $(n,k) = (4,1)$. If the upright diagonal has height at most 2.696, and if an upright quarter shares both faces along the upright diagonal with other upright quarters, then we may assume that the upright quarter has compression type. For otherwise, there is a face of circumradius at least $\sqrt{2}$, and hence two upright quarters of Voronoi type. The inequality

$$\text{octavor} < \text{octavor}_0 - 0.008, \tag{14.1}$$

if $y_1 \in [2t_0, 2.696]$, and $\eta_{126} \geq \sqrt{2}$ shows that the upright quarters can be erased without penalty because

$$\xi_\Gamma - 0.008 - 0.008 < 0.$$

If erased, the case is treated as part of a different case.

This allows the inequalities[20] to be used that relate specifically to upright quarters of compression type. Furthermore, it can often be concluded that all three upright quarters have compression type. For this, we use various inequalities in the archive which can often be used to show that if the anchored simplex has a face of circumradius at least $\sqrt{2}$, then the linear programming bound on $\sigma(D)$ is less than 8 pt.

14.8. *Branching on flat quarters.* We make a few general remarks about flat quarters.

Remark 14.12. Information about the internal structure of an exceptional face gives improvements to the constants 1.4 pt and 1.5 pt of Property 4 in the definition of admissible weight assignments. (The bounds remain fixed at 1.4 pt and 1.5 pt, but these arguments allow us to specify more precisely which simplices contribute to these bounds.) These constants contribute to the bound on $\tau(D)$ through the admissible weight assignment. Assume that at the vertex v there are four quasi-regular tetrahedra and an exceptional face, and that the exceptional face has a flat quarter with central vertex v. The calculations of

[18] CALC-378432183.
[19] CALC-310679005.
[20] See, for example, CALC-867513567-*

Section 11.3 show that the union F of the four quasi-regular tetrahedra and exceptional region give $\tau_F(D) \geq 1.5\,\mathrm{pt}$. If there is no flat quarter with central vertex v, then the union F of four quasi-regular tetrahedra along $\{0, v\}$ give $\tau_F(D) \geq 1.5\,\mathrm{pt}$. We can make similar improvements when $\mathrm{tri}(v) = 3$.

Remark 14.13. There are a few other interval-based inequalities that are used in particular cases. The inequalities $y_1 \leq 2.2, y_4 \leq 2.7, \eta_{234}, \eta_{456} \leq \sqrt{2}$ imply that the flat quarter has compression type (see Section 5.1). The circumradius is not a linear-programming variable, so its upper bound must be deduced from edge-length information.

If all three corners of a flat quarter have height at most 2.14, and if the diagonal has length less than 2.77, then the circumradius of the face containing the origin and diagonal is at most $\eta(2.14, 2.14, 2.77) < \sqrt{2}$. This allows us to branch combine into three cases.

LEMMA 14.14. *Let Q be a flat quarter whose corners v_i have height at most* 2.14 *and whose diagonal is at most* 2.77*. Then one of the following is true.*

1. $\sigma(Q) = \Gamma(Q)$.

2. *The diagonal has length* ≤ 2.7, $\eta(y_4, y_5, y_6) \geq \sqrt{2}$, *and* $\sigma(Q) \leq \text{s-vor}_0(Q)$.

3. *The diagonal has length* ≥ 2.7 *and* $\sigma(Q) \leq \text{s-vor}_0(Q)$.

Proof. Case 1 holds when Q is a quarter of compression type in the Q-system. If Q is in the Q-system but is not of compression type, then $\eta(y_4, y_5, y_6) \geq \sqrt{2}$ and $\sigma(Q) \leq \text{s-vor}_0(Q)$. If Q is not in the Q-system, then $\text{s-vor}_0(Q)$ is an upper bound [Hal06a]. If Q is not in the Q-system, then its diagonal has length at least 2.7, or the central vertex has height at most 2.2 (see Lemma 14.11.) In this case, we use the upper bound $\text{s-vor}_0(Q)$. □

Various inequalities in the archive have been designed specifically for each of these three cases. Thus, whenever the hypotheses of the lemma are met, we are able to improve on the linear programming bounds by breaking into these three cases.

14.9. *Branching on simplices that are not quarters.*

LEMMA 14.15. *Suppose that a triangular subregion comes from a simplex S with one vertex at the origin and three other vertices of height at most $2t_0$. Suppose that the edge lengths of the fourth, fifth, and sixth edges satisfy $y_5, y_6 \in [2t_0, 2\sqrt{2}]$, $y_4 \in [2, 2t_0]$. Suppose that* $\min(y_5, y_6) \leq 2.77$*. Then one of the following is true.*

1. *The edges have lengths* $y_5, y_6 \in [2t_0, 2.77]$, $\eta_{456} \geq \sqrt{2}$, *and* $\sigma(S) \leq$ s-vor$_0(S)$.

2. $y_5, y_6 \in [2t_0, 2.77]$, *and* $\sigma(S) \leq$ s-vor(S) (*the analytic Voronoi function*).

3. *An edge* (*say* y_6) *has length* $y_6 \geq 2.77$ *and* $\sigma(S) \leq$ s-vor$_0(S)$.

Proof. If we ignore the statements about σ, then the conditions in the Lemma concerning edge-length are exhaustive. The bounds on σ in each case are given by [Hal06a]. □

There are linear programming inequalities that are tailored to each case.

14.10. *Conclusion.* By combinations of branching along the lines set forth in the preceding sections, a sequence of linear programs is obtained that establishes that $\sigma(D)$ is less than 8 pt. For details of particular cases, the interested reader can consult the log files in [Hal05], which record which branches are followed for any given tame graph. (For most tame graphs, a single linear program suffices.)

This completes the (abridged) proof of the Kepler conjecture.

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