A Proof of the Kepler Conjecture (unabridged)

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To the memory of László Fejes Tóth

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Contents

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 Section 2.5.

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Abstract: Historical Overview of the Kepler Conjecture This paper is the first in a series of six papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing. After some preliminary comments about the face-centered cubic and hexagonal close packings, the history of the Kepler problem is described, including a discussion of various published bounds on the density of sphere packings. There is also a general historical discussion of various proof strategies that have been tried with this problem.

Abstract: A Formulation of the Kepler Conjecture This paper is the second in a series of six papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing. The top level structure of the proof is described. A compact topological space is described. Each point of this space can be described as a finite cluster of balls with additional combinatorial markings. A continuous function on this compact space is defined. It is proved that the Kepler conjecture will follow if the value of this function is never greater than a given explicit constant.

Abstract: Sphere Packings III. Extremal Cases This paper is the third in a series of six papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing. In the previous paper in this series, a continuous function f on a compact space is defined, certain points in the domain are conjectured to give the global maxima, and the relation between this conjecture and the Kepler conjecture is established. This paper shows that those points are indeed local maxima. Various approximations to f are developed, that will be used in subsequent papers to bound the value of the function f. The function f can be expressed as a sum of terms, indexed by regions on a unit sphere. Detailed estimates of the terms corresponding to triangular and quadrilateral regions are developed.

Abstract: Sphere Packings IV. Detailed Bounds This paper is the fourth in a series of six papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing. In a previous paper in this series, a continuous function f on a compact space is defined, certain points in the domain are conjectured to give the global maxima, and the relation between this conjecture and the Kepler conjecture is established. The function f can be expressed as a sum of terms, indexed by regions on a unit sphere. In this paper, detailed estimates of the terms corresponding general regions are developed. These results form the technical heart of the proof of the Kepler conjecture, by giving detailed bounds on the function f. The results rely on long computer calculations.

Abstract: Sphere Packings V. Pentahedral Prisms This paper is the fifth in a series of papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing.

In this paper, we prove that decomposition stars associated with the plane graph of arrangements we term pentahedral prisms do not contravene. Recall that a contravening decomposition star is a potential counterexample to the Kepler conjecture. We use interval arithmetic methods to prove particular linear relations on components of any such contravening decomposition star. These relations are then combined to prove that no such contravening stars exist.

Abstract: Sphere Packings VI. Tame Graphs and Linear Programs This paper is the sixth and final part in a series of papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing. In a previous paper in this series, a continuous function f on a compact space is defined, certain points in the domain are conjectured to give the global maxima, and the relation between this conjecture and the Kepler conjecture is established. In this paper, we consider the set of all points in the domain for which the value of f is at least the conjectured maximum. To each such point, we attach a planar graph. It is proved that each such graph must be isomorphic to a *tame* graph, of which there are only finitely many up to isomorphism. Linear programming methods are then used to eliminate all possibilities, except for three special cases treated in earlier papers: pentahedral prisms, the face-centered cubic packing, and the hexagonal-close packing. The results of this paper rely on long computer calculations.

Paper I

Historical Overview of the Kepler Conjecture

Section 1

Introduction

The series of papers in this volume gives a proof of the Kepler conjecture, which asserts that the density of a packing of congruent spheres in three dimensions is never greater than $\pi/\sqrt{18} \approx 0.74048\ldots$. This is the oldest problem in discrete geometry and is an important part of Hilbert's 18th problem. An example of a packing achieving this density is the face-centered cubic packing.

1.1 The face-centered cubic packing

A packing of spheres is an arrangement of nonoverlapping spheres of radius 1 in Euclidean space. Each sphere is determined by its center, so equivalently it is a collection of points in Euclidean space separated by distances of at least 2. The density of a packing is defined as the lim sup of the densities of the partial packings formed by spheres inside a ball with fixed center of radius R. (By taking the lim sup, rather than lim inf as the density, we prove the Kepler conjecture in the strongest possible sense.) Defined as a limit, the density is insensitive to changes in the packing in any bounded region. For example, a finite number of spheres can be removed from the face-centered cubic packing without affecting its density.

Consequently, it is not possible to hope for any strong uniqueness results for packings of optimal density. The uniqueness established by this work is as strong as can be hoped for. It shows that certain local structures (decomposition stars) attached to the face-centered cubic (fcc) and hexagonal-close packings (hcp) are the only structures that maximize a local density function.

Although we do not pursue this point, Conway and Sloane develop a theory of tight packings that is more restrictive than having the greatest possible density [CS95]. An open problem is to prove that their list of tight packings in three dimensions is complete.

The face-centered cubic packing appears in Diagram 1.1.

The following facts about packings are well-known. However, there is a popular and persistent misconception in the popular press that the face-centered cubic packing is the only packing with density $\pi/\sqrt{18}$. The comments that follow correct

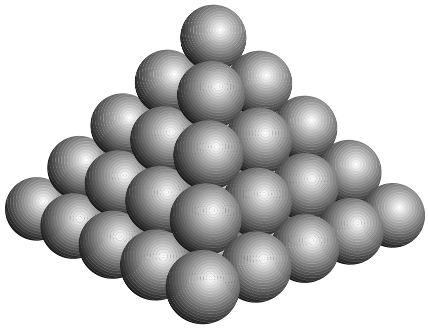

Figure 1.1. *The face-centered-cubic packing.*

that misconception.

In the face-centered cubic packing, each ball is tangent to twelve others. For each ball in the packing, this arrangement of twelve tangent balls is the same. We call it the fcc pattern. In the hexagonal-close packing, each ball is tangent to twelve others. For each ball in the packing, the arrangement of twelve tangent balls is again the same. We call it the hcp pattern. The fcc pattern is different from the hcp pattern. In the fcc pattern, there are four different planes through the center of the central ball that contain the centers of six other balls at the vertices of a regular hexagon. In the hcp pattern, there is only one such plane. We call the arrangement of balls tangent to a given ball the *local tangent arrangement* of the ball.

There are uncountably many packings of density $\pi/\sqrt{18}$ that have the property that every ball is tangent to twelve others and such that the tangent arrangement around each ball is either the fcc pattern or the hcp pattern.

By *hexagonal layer*, we mean a translate of the two-dimensional lattice of points M in the A_2 arrangement. That is, M is a translate of the planar lattice generated by two vectors of length 2 and angle $2\pi/3$. The face-centered cubic packing is an example of a packing built from hexagonal layers.

If M is a hexagonal layer, a second hexagonal layer M' can be placed parallel to the first so that each lattice point of M' has distance 2 from three different vertices of M. When the second layer is placed in the manner, it is as close to the first layer as possible. Fix M and a unit normal to the plane of M. The normal allows us to speak of the second layer M' as being "above" or "below" the layer M. There are two different positions in which M' can be placed closely above M and two different positions in which M' can be placed closely below M. As we build a packing, layer by layer, (M, M', M'', and so forth), there are two choices at each stage of the close placement of the layer above the previous layer. Running through different sequences of choices gives uncountably many packings. In each of these packings the tangent arrangement around each ball is that of the twelve spheres in the face-centered cubic or the twelve spheres in the hexagonal-close packing.

Let Λ be a packing built as a sequence of close-packed hexagonal layers in this fashion. If P is any plane parallel to the hexagonal layers, then there are at most three different orthogonal projections of the layers M to P. Call these projections A,

B, C. Each hexagonal layer has a different projection than the layers immediately above and below it. In the fcc packing, the successive layers are $A, B, C, A, B, C, \ldots$. In the hcp packing, the successive layers are $A, B, A, B, \ldots$. If we represent A, B, and C as the vertices of a triangle, then the succession of hexagonal layers can be described by a walk along the vertices of the triangle. Different walks through the triangle describe different packings.

In fact, the different walks through a triangle give all packings of infinitely many equal balls in which the tangent arrangement around every ball is either the fcc pattern of twelve balls or the hcp pattern of twelve balls.

> We justify the fact that different walks through a triangle give all such packings. Assume first that a packing Λ contains a ball (centered at v_0) in the hcp pattern. The hcp pattern contains a uniquely determined plane of symmetry. This plane contains v_0 and the centers of six others arranged in a regular hexagonal. If v is the center of one of the six others in the plane of symmetry, its local tangent arrangement of twelve balls must include v_0 and an additional four of the twelve balls around v_0. These five centers around v are not a subset of the fcc pattern. They can be uniquely extended to twelve centers arranged in the hcp pattern. This hcp pattern has the same plane of symmetry as the hcp pattern around v_0. In this way, as soon as there is a single center with the hcp pattern, the pattern propagates along the plane of symmetry to create a hexagonal layer M.
>
> Once a packing Λ contains a single hexagonal layer, the condition that each ball be tangent to twelve others forces a hexagonal layer M' above M and another hexagonal layer below M. Thus, a single hexagonal layer forces a sequence of close-packed hexagonal layers in both directions.
>
> We have justified the claim under the hypothesis that Λ contains at least one ball with the hcp pattern.
>
> Assume that Λ does not contain any balls whose local tangent arrangement is the hcp pattern. Then every local tangent arrangement is the fcc pattern, and Λ itself is then the face-centered cubic packing. This completes the proof.

1.2 Early History, Hariot, and Kepler

The study of the mathematical properties of the face-centered cubic packing can be traced back to a Sanskrit work composed around 499 CE. I quote an extensive passage from the commentary that K. Plofker has made about the formula for the number of balls in triangular piles[Plo00]:

> The excerpt below is taken from a Sanskrit work composed around 499 CE, the Āryabhaṭīya of Āryabhaṭa, and the commentary on it written in 629 CE by Bhāskara (I). The work is a compendium of various rules in mathematics and mathematical astronomy, and the results are probably not due the Āryabhaṭa himself but derived from an earlier source: however, this is the oldest source extant for them. (My translation's from the edition by K. S. Shukla,

The Āryabhaṭīya of Āryabhaṭa with the Commentary of Bhāskara I and Someśvara, New Delhi: Indian National Science Academy 1976; my inclusions are in square brackets. There is a corresponding English translation by Shukla and K. V. Sarma, *The Āryabhaṭīya of Āryabhaṭa*, New Delhi: Indian National Science Academy 1976. It might be easier to get hold of the earlier English translation by W. E. Clark, *The Āryabhaṭīya of Āryabhaṭa*, Chicago: University of Chicago Press, 1930.)

Basically, the rule considers the series in arithmetic progression $S_i = 1 + 2 + 3 + \ldots + i$ (for whose sum the formula is known) as the number of objects in the ith layer of a pile with a total of n layers, and specifies the following two equivalent formulas for the "accumulation of the pile" or $\sum_{i=1}^{n} S_i$:

$$\sum_{i=1}^{n} S_i = \frac{n(n+1)(n+2)}{6},$$

$$\sum_{i=1}^{n} S_i = \frac{(n+1)^3 - (n+1)}{6}.$$

What he says is this:

Āryabhaṭīya, Gaṇitapāda 21:

For a series [lit. "heap"] with a common difference and first term of 1, the product of three [terms successively] increased by 1 from the total, or else the cube of [the total] plus 1 diminished by [its] root, divided by 6, is the total of the pile [lit. "solid heap"].

Bhāskara's commentary on this verse:

[This] heap [or] series is specified as having one for its common difference and initial term. This same series with one for its common difference and initial term is said [to be] "heaped up." "The product of three [terms successively] increased by one from the total" of this so-called heaped-up "series with one for its common difference and initial term": i.e., the product of three terms, starting from the total and increasing by one. Namely, the total, that plus one, and [that] plus one again. That [can] be stated [as follows]: the total, that plus one, and that total plus two. The product of those three divided by 6 is the "solid heap," the accumulation of the series. Now another method: The cube of the root equal to that [total] plus one is diminished by its root, and divided by 6: thus it follows. "Or else": [i.e.], the cube of that root plus one, diminished by its own root, divided by 6, is the "solid heap." Example: Series with 5, 8, and 14 respectively for their total layers: tell me [their] triangular-shaped piles. In order, the totals are 5, 8, 14. Procedure: Total 5. This plus one: 6. This plus one again: 7. Product of those three: 210. This divided by 6 is the accumulation of the series: 35. [He goes on to give the answers for the second two cases, but you doubtless get the picture.] – K. Plofker

The modern mathematical study of spheres and their close packings can be traced to T. Hariot. Hariot's work – unpublished, unedited, and largely undated – shows a preoccupation with sphere packings. He seems to have first taken an interest in packings at the prompting of Sir Walter Raleigh. At the time, Hariot was Raleigh's mathematical assistant, and Raleigh gave him the problem of determining formulas for the number of cannonballs in regularly stacked piles. In 1591 he prepared a chart of triangular numbers for Raleigh. Shirley, Hariot's biographer, writes,

> Obviously, this is a quick reference chart prepared for Ralegh to give information on the ground space required for the storage of cannon balls in connection with the stacking of armaments for his marauding vessels. The chart is ingeniously arranged so that it is possible to read directly the number of cannon balls on the ground or in a pyramid pile with triangular, square, or oblong base. All of this Harriot had worked out by the laws of mathematical progression (not as Miss Rukeyser suggests by experiment), as the rough calculations accompanying the chart make clear. It is interesting to note that on adjacent sheets, Harriot moved, as a mathematician naturally would, into the theory of the sums of the squares, and attempted to determine graphically all the possible configurations that discrete particles could assume – a study which led him inevitably to the corpuscular or atomic theory of matter originally deriving from Lucretius and Epicurus. [Shi83, p.242]

Hariot connected sphere packings to Pascal's triangle long before Pascal introduced the triangle. See Diagram 1.2.

Hariot was the first to distinguish between the face-centered cubic and hexagonal close packings [Mas66, p.52].

Kepler became involved in sphere packings through his correspondence with Hariot in the early years of the 17th century. Kargon writes, in his history of atomism in England,

> Hariot's theory of matter appears to have been virtually that of Democritus, Hero of Alexandria, and, in a large measure, that of Epicurus and Lucretius. According to Hariot the universe is composed of atoms with void space interposed. The atoms themselves are eternal and continuous. Physical properties result from the magnitude, shape, and motion of these atoms, or corpuscles compounded from them. . ..
>
> Probably the most interesting application of Hariot's atomic theory was in the field of optics. In a letter to Kepler on 2 December 1606 Hariot outlined his views. Why, he asked, when a light ray falls upon the surface of a transparent medium, is it partially reflected and partially refracted? Since by the principle of uniformity, a single point cannot both reflect and transmit light, the answer must lie in the supposition that the ray is resisted by some points and not others.
>
> "A dense diaphanous body, therefore, which to the sense appears to be continuous in all parts, is not actually continuous. But it has corporeal parts which resist the rays, and incorporeal parts vacua which the rays penetrate. . ."
>
> It was here that Hariot advised Kepler to abstract himself mathematically into an atom in order to enter 'Nature's house'. In his reply of 2 August 1607, Kepler declined to follow Harriot, ad atomos et vacua. Kepler preferred to think of the reflection-refraction problem in terms of the union of two op-

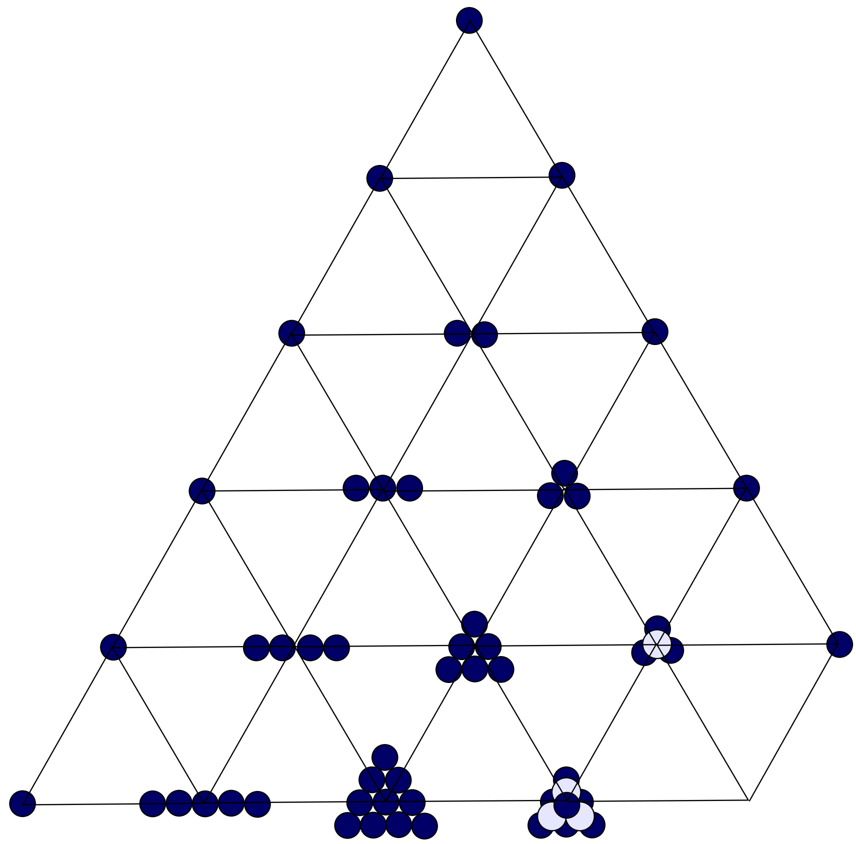

Figure 1.2. *Hariot's view of Pascal's triangle.*

> posing qualities – transparence and opacity. Hariot was surprised. "If those assumptions and reasons satisfy you, I am amazed." [Kar66, p.26]

Despite Kepler's initial reluctance to adopt an atomic theory, he was eventually swayed, and in 1611 he published an essay that explores the consequences of a theory of matter composed of small spherical particles. Kepler's essay was the "first recorded step towards a mathematical theory of the genesis of inorganic or organic form" [Why66, p.v].

Kepler's essay describes the face-centered cubic packing and asserts that "the packing will be the tightest possible, so that in no other arrangement could more pellets be stuffed into the same container." This assertion has come to be known as the Kepler conjecture. The purpose of this collection of papers is to give a proof of this conjecture.

1.3 History

The next episode in the history of this problem is a debate between Isaac Newton and David Gregory. Newton and Gregory discussed the question of how many spheres of equal radius can be arranged to touch a given sphere. This is the three-dimensional analogue of the simple fact that in two dimensions six pennies, but no more, can be arranged to touch a central penny. This is the kissing-number problem in n-dimensions. In three dimensions, Newton said that the maximum was twelve spheres, but Gregory claimed that thirteen might be possible.

Newton was correct. In the 19th century, the first papers claiming a proof of the kissing-number problem appeared in [Ben74], [Gun75], [Hop74]. Although some writers cite these papers as a proof, they are hardly rigorous by today's standards. Another incorrect proof appears in [Boe52]. The first proper proof was obtained by B. L. van der Waerden and Schütte in 1953 [SW53]. An elementary proof appears in Leech [Lee56]. The influence of van der Waerden, Schütte, and Leech upon the papers in this collection is readily apparent. Although the connection between the Newton-Gregory problem and Kepler's problem is not obvious, L. Fejes Tóth in 1953, in the first work describing a strategy to prove the Kepler conjecture, made a quantitative version of the Gregory-Newton problem the first step [Fej53].

The two-dimensional analogue of the Kepler conjecture is to show that the honeycomb packing in two dimensions gives the highest density. This result was established in 1892 by Thue, with a second proof appearing in 1910 ([Thu92], [Thu10]). G. Szpiro's book on the Kepler conjecture calls Thue's proofs into question ([Szp02]). C. Siegel said that Thue's original proof is "reasonable, but full of holes" ([Szp02]). A number of other proofs have appeared since then. Three are particularly notable. Rogers's proof generalizes to give a bound on the density of packings in any dimension [Rog58]. A proof by L. Fejes Tóth extends to give bounds on the density of packings of convex disks [Fej50]. A third proof, also by L. Fejes Tóth, extends to non-Euclidean geometries [Fej53]. Another early proof appears in [SM44].

In 1900, Hilbert made the Kepler conjecture part of his 18th problem [Hil01]. Milnor, in his review of Hilbert's 18th problem, breaks the problem into three parts [Mil76].

> 1. Is there in n-dimensional Euclidean Space ... only a finite number of essentially different kinds of groups of motions with a [compact] fundamental region?
>
> 2. Whether polyhedra also exist which do not appear as fundamental regions of groups of motions, by means of which nevertheless by a suitable juxtaposition of congruent copies a complete filling up of all [Euclidean] space is possible?

> 3. How can one arrange most densely in space an infinite number of equal solids of given form, e.g. spheres with given radii . . ., that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as great as possible?

Writing of the third part, Milnor states,

> For 2-dimensional disks this problem has been solved by Thue and Fejes Tóth, who showed that the expected hexagonal (or honeycomb) packing of circular disks in the plane is the densest possible. However, the corresponding problem in 3 dimensions remains unsolved. This is a scandalous situation since the (presumably) correct answer has been known since the time of Gauss. (Compare Hilbert and Cohn-Vossen.) All that is missing is a proof.

1.4 The Literature

Past progress toward the Kepler conjecture can be arranged into four categories:

- bounds on the density,
- descriptions of classes of packings for which the bound of $\pi/\sqrt{18}$ is known,
- convex bodies other than spheres for which the packing density can be determined precisely,
- strategies of proof.

1.4.1 Bounds

Various upper bounds have been established on the density of packings.

0.884 (Blichfeldt) [Bli19],
0.835 (Blichfeldt) [Bli29],
0.828 (Rankin) [Ran47],
0.7797 (Rogers) [Rog58],
0.77844 (Lindsey) [Lin86],
0.77836 (Muder)[Mud88],
0.7731 (Muder) [Mud93].

Rogers's is a particularly natural bound. As the dates indicate, it remained the best available bound for many years. His monotonicity lemma and his decomposition of Voronoi cells into simplices have become important elements in the proof of the Kepler conjecture. We give a new proof of Rogers's bound in "Sphere Packings III." A function τ, used throughout this collection, measures the departure of various objects from Rogers's bound.

Muder's bounds, although they appear to be rather small improvements of Rogers's bound, are the first to make use of the full Voronoi cell in the determination of densities. As such, they mark a transition to a greater level of sophistication and difficulty. Muder's influence on the work in this collection is also apparent.

A sphere packing admits a Voronoi decomposition: around every sphere take the convex region consisting of points closer to that sphere center than to any other sphere center. L. Fejes Tóth's dodecahedral conjecture asserts that the Voronoi cell of smallest volume is a regular dodecahedron with inradius 1 [Fej42]. The dodecahedral conjecture implies a bound of 0.755 on sphere packings. L. Fejes Tóth actually gave a complete proof except for one estimate. A footnote in his paper documents the gap, "In the proof, we have relied to some extent solely on intuitive observation [Anschauung]." As L. Fejes Tóth pointed out, that estimate is extraordinarily difficult, and the dodecahedral conjecture has resisted all efforts until now [McL98].

The missing estimate in L. Fejes Tóth's paper is an explicit form of the Newton-Gregory problem. What is needed is an explicit bound on how close the 13th sphere can come to touching the central sphere. Or more generally, minimize the sum of the distances of the 13 spheres from the central sphere. No satisfactory bounds are known. Boerdijk has a conjecture for the arrangement that minimizes the average distance of the 13 spheres from the central sphere. Van der Waerden has a conjecture for the closest arrangement of 13 spheres in which all spheres have the same distance from the central sphere. Bezdek has shown that the dodecahedral conjecture would follow from weaker bounds than those originally proposed by L. Fejes Tóth [Bez97].

A proof of the dodecahedral conjecture has traditionally been viewed as the first step toward a proof of the Kepler conjecture, and if little progress has been made until now toward a complete solution of the Kepler conjecture, the difficulty of the dodecahedral conjecture is certainly responsible to a large degree.

1.4.2 Classes of packings

If the infinite dimensional space of all packings is too unwieldy, we can ask if it is possible to establish the bound $\pi/\sqrt{18}$ for packings with special structures.

If we restrict the problem to packings whose sphere centers are the points of a lattice, the packings are described by a finite number of parameters, and the problem becomes much more accessible. Lagrange proved that the densest lattice packing in two dimensions is the familiar honeycomb arrangement [Lag73]. Gauss proved that the densest lattice packing in three dimensions is the face-centered cubic [Gau31]. In dimensions 4–8, the optimal lattices are described by their root systems, A_2, A_3, D_4, D_5, E_6, E_7, and E_8. A. Korkine and G. Zolotareff showed that D_4 and D_5 are the densest lattice packings in dimensions 4 and 5 ([KZ73], [KZ77]). Blichfeldt determined the densest lattice packings in dimensions 6–8 [Bli35]. Cohn and Kumar solved the problem in dimension 24 [CK04]. With the exception of dimension 24, beyond dimension 8, there are no proofs of optimality, and yet there are many excellent candidates for the densest lattice packings. For a proof of the existence of optimal lattices, see [Oes90].

Although lattice packings are of particular interest because they relate to so many different branches of mathematics, Rogers has conjectured that in sufficiently high dimensions, the densest packings are not lattice packings [Rog64]. In fact, the densest known packings in various dimensions are not lattice packings. The third edition of [CS93] gives several examples of nonlattice packings that are denser than any known lattice packings (dimensions 10, 11, 13, 18, 20, 22). The densest packings of typical convex sets in the plane, in the sense of Baire categories, are not lattice packings [Fej95].

Gauss's theorem on lattice densities has been generalized by A. Bezdek, W. Kuperberg, and E. Makai, Jr. [BKM91]. They showed that packings of parallel strings of spheres never have density greater than $\pi/\sqrt{18}$.

1.4.3 Other convex bodies

If the optimal sphere packings are too difficult to determine, we might ask whether the problem can be solved for other convex bodies. To avoid trivialities, we restrict our attention to convex bodies whose packing density is strictly less than 1.

The first convex body in Euclidean 3-space that does not tile for which the packing density was explicitly determined is an infinite cylinder [Bez90]. Here A. Bezdek and W. Kuperberg prove that the optimal density is obtained by arranging the cylinders in parallel columns in the honeycomb arrangement.

In 1993, J. Pach exposed the humbling depth of our ignorance when he issued the challenge to determine the packing density for some bounded convex body that does not tile space [MP93]. (Pach's question is more revealing than anything I can write on the subject of discrete geometry.) This question was answered by A. Bezdek [Bez94], who determined the packing density of a rhombic dodecahedron that has one corner clipped so that it no longer tiles. The packing density equals the ratio of the volume of the clipped rhombic dodecahedron to the volume of the unclipped rhombic dodecahedron.

1.4.4 Strategies of proof

In 1953, L. Fejes Tóth proposed a program to prove the Kepler conjecture [Fej53]. A single Voronoi cell cannot lead to a bound better than the dodecahedral conjecture. L. Fejes Tóth considered weighted averages of the volumes of collections of Voronoi cells. These weighted averages involve up to 13 Voronoi cells. He showed that if a particular weighted average of volumes is greater than the volume of the rhombic dodecahedron, then the Kepler conjecture follows. The Kepler conjecture is an optimization problem in an infinite number of variables. L. Fejes Tóth's weighted-average argument was the first indication that it might be possible to reduce the Kepler conjecture to a problem in a finite number of variables. Needless to say, calculations involving the weighted averages of the volumes of several Voronoi cells will be significantly more difficult than those involved in establishing the dodecahedral conjecture.

To justify his approach, which limits the number of Voronoi cells to 13, Fejes Tóth needs a preliminary estimate of how close a 13th sphere can come to a central sphere. It is at this point in his formulation of the Kepler conjecture that an explicit version of the Newton-Gregory problem is required. How close can 13 spheres come to a central sphere, as measured by the sum of their distances from the central sphere?

L. Fejes Tóth made another significant suggestion in [Fej64]. He was the first to suggest the use of computers in the Kepler conjecture. After describing his program, he writes,

> Thus it seems that the problem can be reduced to the determination of the minimum of a function of a finite number of variables, providing a programme realizable in principle. In view of the intricacy of this function we are far from attempting to determine the exact minimum. But, mindful of the rapid development of our computers, it is imaginable that the minimum may be approximated with great exactitude.

The most widely publicized attempt to prove the Kepler conjecture was that of Wu-Yi Hsiang [Hsi93a]. (See also [Hsi93b], [Hsi93c], [Hsi02].) Hsiang's approach can be viewed as a continuation and extension of L. Fejes Tóth's program. Hsiang's paper contains major gaps and errors [CHMS94]. The mathematical arguments against his argument appear in my debate with him in the *Mathematical Intelligencer* ([Hal94], [Hsi95]). There are now many published sources that agree with the central claims of [Hal94] against Hsiang. Conway and Sloane report that the paper "contains serious flaws." G. Fejes Tóth feels that "the greater part of the work has yet to be done" [Fej95]. K. Bezdek concluded, after an extensive study of Hsiang's work, "his work is far from being complete and correct in all details" [Bez97]. D. Muder writes, "the community has reached a consensus on it: no one buys it" [Mud97].

Section 2

Overview of the proof

2.1 Experiments with other Decompositions

The following two sections (added Jan 2003) describe some of the motivation behind the partitions of space that have been used in the proof of the Kepler conjecture. This discussion includes various ideas that were tried, found wanting, and discarded. However, this discussion provides motivation for some of the choices that appear in the proof of the Kepler conjecture.

Let S be a regular tetrahedron of side length 2. If we place a unit ball at each of the four vertices, the fraction of the tetrahedral solid occupied by the part of the four balls within the tetrahedron is $\delta_{tet} \approx 0.7797$. Let O be a regular octahedron of side length 2. If we place a unit ball at each of the four vertices, the fraction of the octahedral solid occupied by the four balls is $\delta_{oct} \approx 0.72$. The face-centered cubic packing can be obtained by packing eight regular tetrahedra and six regular octahedra around each vertex. The density $\pi/\sqrt{18}$ of this packing is a weighted average of δ_{tet} and δ_{oct}:

$$\frac{\pi}{\sqrt{18}} = \frac{1}{3}\delta_{tet} + \frac{2}{3}\delta_{oct}.$$

My early conception (around 1989) was that for every packing of congruent balls, there should be a corresponding partition of space into regions of high density and regions of low density. Regions of high density should be defined as regions having density between δ_{oct} and δ_{tet}, and regions of low density should be defined as those regions of density at most δ_{oct}. It was my intention to prove that all regions of high density had to be confined to a set of nonoverlapping tetrahedra whose vertices are centers of the balls in the packing.

Thus, the question naturally arises of how much a regular tetrahedron of edge length 2 can be deformed before its density drops below that of a regular octahedron δ_{oct}. The following graph (Figure 2.1) shows the density of a tetrahedron with five edges of length 2 and a sixth edge of length x. Numerically, we see that the density drops below δ_{oct}, when $x = x_0 \approx 2.504$. To achieve the design goal of confining regions of high density to tetrahedra, we want a tetrahedron of edge lengths $2, 2, 2, 2, 2, x$, for $x \leq x_0$, to be counted as a region of high density. Rounding upward, this example led to the cutoff parameter of 2.51 that distinguishes the tetrahedra (in the high density region) from the rest of space. This is the origin of the constant 2.51 that appears in the proof.

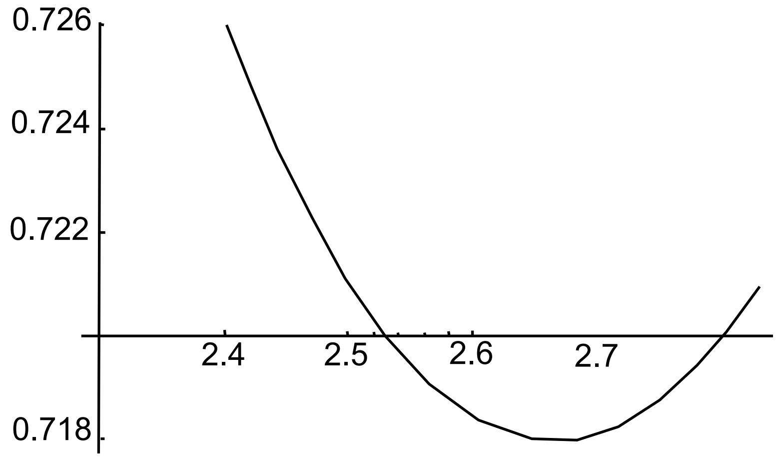

Figure 2.1. *The origin of the constant* 2.51.

Since the tetrahedra are chosen to have vertices at the centers of the balls in the packing, it was quite natural to base the decomposition of space on the Delaunay decomposition. According to this early conception, space was to be partitioned into Delaunay simplices. A Delaunay simplex whose edge lengths are at most 2.51 is called a quasi-regular tetrahedron. These were the regions of presumably high density. According to the strategy in those early days, all other Delaunay simplices were to be shown to belong to regions of density at most δ_{oct}.

The following problem occupied my attention for a long period.

Problem Fix a saturated packing. Let $X(oct)$ be the part of space of a saturated packing that is occupied by the Delaunay simplices having at least one edge of length at least 2.51. Let $X(tet)$ be the union of the complementary set of Delaunay simplices. Is it always true that the density of $X(oct)$ is at most δ_{oct}?

Early on, I viewed the positive resolution of this problem as crucial to the solution of the Kepler conjecture. Eventually, when I divided the proof of the Kepler conjecture into a five step program, a variant of this problem became the second step of the program. See [Hal97b].

To give an indication of the complexity of this problem, consider the simplex with edge lengths $(2, 2, 2, 2, \ell, \ell)$, where $\ell = \sqrt{2(3+\sqrt{6})} \approx 3.301$. Assume that the two longer edges meet at a vertex. This simplex can appear as the Delaunay simplex in a saturated packing. Its density is about 0.78469. This constant is not only greater than δ_{oct}; it is even greater than δ_{tet}, so that the problem is completely misguided at the level of individual Delaunay simplices in $X(oct)$. It is only in when the union of Delaunay simplices is considered that we can hope for an affirmative answer to the problem.

By the summer of 1994, I had lost hope of finding a partition of the set $X(oct)$ into small clusters of Delaunay simplices with the property that each cluster had density at most δ_{oct}. Progress had ground to a halt. The key insight came in the fall of 1994 (on Nov 12, 1994 to be precise). On that day, I introduced a hybrid decomposition that relied on the Delaunay simplices in the regions $X(tet)$ formed by quasi-regular tetrahedra, but that switched to the Voronoi decomposition in certain regions of $X(oct)$. By April 1995, I had reformulated the problem, worked out a proof of the problem [Hal97b] in its new form, and submitted it for publication. I submitted a revised version of [Hal97a] that same month. The revision mentions the new strategy: "The rough idea is to let the score of a simplex in a cluster be the compression $\Gamma(S)$ [a function based on the Delaunay decomposition] if the circumradius of every face of S small, and otherwise to let the score be defined by Voronoi cells (in a way that generalizes the definition for quasi-regular tetrahedra)." See [Hal97a, p.6].

The situation is somewhat more complicated than the previous paragraph suggests. Consider a Delaunay simplex S with edge lengths $(2, 2, 2, 2, 2, 2.52)$. Such a simplex belongs to the region $X(oct)$. However, if we break it into four pieces according to the Voronoi decomposition, the density of the two of the pieces is about $0.696 < \delta_{oct}$ and the density of the other two is about $0.7368 > \delta_{oct}$. It is desirable not to have any separate regions in $X(oct)$ of density greater than δ_{oct}. Hence it is preferable to keep the four Voronoi regions in S together as a single Delaunay simplex. A second reason to keep S together is that the proof of the local optimality of the face-centered cubic packing and hexagonal close packing seems to require it. A third reason was to treat pentahedral prisms. (This is a thorny class of counterexamples to a pure Delaunay simplex approach to the proof of the Kepler conjecture. See [Hal92], [Hal93], and [Fer97].) For these reasons, we identify a class of Delaunay simplices in $X(oct)$ (such as S) that are to be treated according to a special set of rules. They are called *quarters*. As the name suggests, they often occur as the four simplices comprising an octahedron that has been "quartered."

One of the great advantages of a hybrid approach is that there is a tremendous amount of flexibility in the choice of the details of the decomposition. The details of the decomposition continued to evolve during 1995 and 1996. Finally, during a stay in Budapest following the Second European Congress in 1996, I abandoned all vestiges of the Delaunay decomposition, and adopted definitions of quasi-regular tetrahedra and quarters that rely only on the metric properties of the simplices (as opposed to the Delaunay criterion based on the position of other sphere centers in relation to the circumscribing sphere of the simplex). This decomposition of space is essentially what is used in the final proof.

The hybrid construction depends on certain choices of functions (satisfying a rather mild set of constraints). To solve the Kepler conjecture appropriate functions had to be selected, and an optimization problem based on those functions had to be solved. This function is called *the score*. Samuel Ferguson and I realized that every time we encountered difficulties in solving the minimization problem, we could adjust the scoring function σ to skirt the difficulty. The function σ became more complicated, but with each change we cut months – or even years – from our work. This incessant fiddling was unpopular with my colleagues. Every time I presented my work in progress at a conference, I was minimizing a different function. Even worse, the function was mildly incompatible with what I did in earlier papers [Hal97a] [Hal97b], and this required going back and patching the earlier papers.

The definition of the scoring function σ did not become fixed until it came time for Ferguson to defend his thesis, and we finally felt obligated to stop tampering with it. The final version of the scoring function σ is rather complicated. The reasons for the precise form of σ cannot be described without a long and detailed description of dozens of sphere clusters that were studied in great detail during the design of this function. However, a few general design principles can be mentioned. These comments assume a certain familiarity with the design of the proof.

(1) Simplices (with vertices at the centers of the balls in the packing) should be used whenever careful estimates of the density are required. Voronoi cells should be used whenever crude estimates suffice. For Voronoi cells, it is clear what the scoring function should be $\mathrm{vor}(R)$ (and its truncated versions $\mathrm{vor}_0(R)$, and so forth).

(2) The definition of the scoring function for quasi-regular tetrahedra was fixed by [Hal97a] and this definition had to remain fixed to avoid rewriting that long paper.

Because of these first two points, most of the design effort for the function σ was focused on quarters.

(3) The decision to make the scoring for a quarter change when the circumradius of a face reaches $\sqrt{2}$ is to make the proof of the local optimality of the fcc and hcp packings run smoothly. From [Hal97b], we see that the cutoff value $\sqrt{2}$ is important for the success of that proof. The cutoff $\sqrt{2}$ is also important for the proof that standard regions (other than quasi-regular tetrahedra) score at most $0\,pt$.

(4) The purpose of adding terms to the scoring function σ that depend on the truncated Voronoi function vor_0 is to make interval arithmetic comparisons between σ and vor_0 easier to carry out. This is useful in arguments about "erasing upright quarters."

2.2 Contents of the Papers

In [Hal97a], a five-step program was described to prove the Kepler conjecture. It was planned that there would be five papers, each proving one step in the program. The papers [Hal97a] and [Hal97b] carry out the first two steps in the program. Because of the changes in the scoring function, it was necessary to issue a short paper [FH98] mid-stream whose purpose was to give some adjustments to the five-step program. This paper adjusts the definitions from [Hal97a] and checks that none of the results from [Hal97a] and [Hal97b] are affected in an essential way by these changes. Following this, the papers [Hal98b] and [Fer97] appeared in preprint form, completing the third and fifth steps of the program. The fourth step turned out to be particularly difficult. It occupies two separate papers [Hal98c] and [Hal98d].

The original series of papers suffers from the defect of being written over a span of several years. Some shifts in the conceptual framework of the research are evident. Based on comments from referees, a revision of these papers was prepared in 2002. The revisions were small, except for the paper [Hal98d], which was completely rewritten. The structure of the proof remains the same, but it adds a substantial amount of introductory material that lessens the dependence on [Hal97a] and [Hal97b].

The papers were reorganized again in 2003. The series of papers is no longer organized along the original five steps with a mid-stream correction. Instead, the proof is now arranged according to the logical development of the subject matter. Only minor modifications have been made to the original proof. (The earlier versions are still available from [arXiv].) In the 2003 revision, the exposition of the proof is entirely independent of the earlier papers [Hal97a] and [Hal97b].

An introduction to the ideas of the proof can be found in [Hal00]. An introduction to the algorithms can be found at [Hal03]. Speculation on a second-generation design of a proof can be found in [Hal03] and [Hal01].

2.3 Complexity

Why is this a difficult problem? There are many ways to answer this question.

This is an optimization problem in an infinite number of variables. In many respects, the central problem has been to formulate a good finite dimensional approximation to the density of a packing. Beyond this, there remains an extremely difficult problem in global optimization, involving nearly 150 variables. We recall that even very simple classes of nonlinear optimization problems, such as quadratic optimization problems, are NP-hard [HPT95]. A general highly nonlinear program of this size is regarded by most researchers as hopeless (at least as far as rigorous methods are concerned).

There is a considerable literature on many closely related nonlinear optimization problems (the Tammes problem, circle packings, covering problems, the Lennard-Jones potential, Coulombic energy minimization of point particles, and so forth). Many of our expectations about nonlattice packings are formed by the extensive experimental data that have been published on these problems. The literature leads one to expect a rich abundance of critical points, and yet it leaves one with a certain skepticism about the possibility of establishing general results rigorously.

The extensive survey of circle packings in [Mel97] gives a broad overview of the progress and limits of the subject. Problems involving a few circles can be trivial to solve. Problems involving several circles in the plane can be solved with sufficient ingenuity. With the aid of computers, various problems involving a few more circles can be treated by rigorous methods. Beyond that, numerical methods give approximations but no rigorous solutions. Melissen's account of the 20-year quest for the best separated arrangement of 10 points in a unit square is particularly revealing of the complexities of the subject.

Kepler's problem has a particularly rich collection of (numerical) local maxima that come uncomfortably close to the global maximum [Hal92]. These local maxima explain in part why a large number (around 5000) of planar maps are generated as part of the proof of the conjecture. Each planar map leads to a separate nonlinear optimization problem.

2.4 Computers

As this project has progressed, the computer has replaced conventional mathematical arguments more and more, until now nearly every aspect of the proof relies on computer verifications. Many assertions in these papers are results of computer calculations. To make the proof of Kepler's conjecture more accessible, I have posted extensive resources [arXiv].

Computers are used in various significant ways. They will be mentioned briefly here, and then developed more thoroughly elsewhere in the collection, especially in the final paper.

1. *Proof of inequalities by interval arithmetic.* "Sphere Packings I" describes a method of proving various inequalities in a small number of variables by computer by interval arithmetic.

2. *Combinatorics.* A computer program classifies all of the planar maps that are relevant to the Kepler conjecture.

3. *Linear programming bounds.* Many of the nonlinear optimization problems for the scores of decomposition stars are replaced by linear problems that dominate the original score. They are solved by linear programming methods by computer. A typical problem has between 100 and 200 variables and 1000 and 2000 constraints. Nearly 100000 such problems enter into the proof.

4. *Branch and bound methods.* When linear programming methods do not give sufficiently good bounds, they have been combined with branch and bound methods from global optimization.

5. *Numerical optimization.* The exploration of the problem has been substantially aided by nonlinear optimization and symbolic math packages.

6. *Organization of output.* The organization of the few gigabytes of code and data that enter into the proof is in itself a nontrivial undertaking.

2.5 Acknowledgments

I am indebted to G. Fejes Tóth's survey of sphere packings in the preparation of this overview [Fej97]. For a much more comprehensive introduction to the literature on sphere packings, I refer the reader to that survey and to standard references on sphere packings such as [CS93], [PA95], [Goo97], [Rog64], [Fej64], and [Fej72].

A detailed strategy of the proof was explained in lectures I gave at Mount Holyoke and Budapest during the summer of 1996 [Hal96]. See also the 1996 preprint, "Recent Progress on the Kepler Conjecture," [Hal96].

I owe the success of this project to a significant degree to S. Ferguson. His thesis solves a major step of the program. He has been highly involved in various other steps of the solution as well. He returned to Ann Arbor during the final three months of the project to verify many of the interval-based inequalities appearing in the appendices of "Sphere Packings IV" and "The Kepler Conjecture." It is a pleasure to express my debt to him.

Sean McLaughlin has been involved in this project through his fundamental work on the dodecahedral conjecture. By detecting many of my mistakes, by clarifying my arguments, and in many other ways, he has made an important contribution.

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Finally, I wish to give my special thanks to Kerri Smith, who has been my greatest source of support and encouragement through it all.

[1] www.isr.umd.edu/Labs/CACSE/FSQP/fsqp.html

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Paper II

A Formulation of the Kepler Conjecture

The following papers give a proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensional Euclidean space has density exceeding that of the face-centered cubic packing.

A historical overview of the Kepler conjecture is found in the first paper in this series. Since the history of this problem is treated there, this paper does not go into the details of the extensive literature on this problem. We mention that Hilbert included the Kepler conjecture as part of his eighteenth problem [Hil01]. L. Fejes Tóth was the first to formulate a plausible strategy for a proof [Fej72]. He also suggested that computers might play a role in the solution of this problem. The historical account also discusses the development of some of the key concepts of this paper.

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 [Hal05b].

The first section of this paper gives the top level structure of the proof of the Kepler conjecture. The next two sections describe the fundamental decompositions of space that are needed in the proof. The first decomposition, which is called the Q-system, is a collection of simplices that do not overlap. This decomposition was originally inspired by the Delaunay decomposition of space. The other decomposition, which is called the V-cell decomposition, is closely related to the Voronoi decomposition of space. In the following section, these two decompositions of space are combined into geometrical objects called *decomposition stars*. The decomposition star is the fundamental geometrical object in the proof of the Kepler conjecture.

The final section of this paper, which was coauthored with Samuel P. Ferguson, describes a particular nonlinear function on the set of all decomposition stars, called the scoring function. The Kepler conjecture reduces to an optimization problem involving this nonlinear function on the set of all decomposition stars. This is an optimization problem in a finite number of variables. The subsequent papers (Papers III – VI) solve that optimization problem.

The choice of the particular scoring function to use was arrived at jointly with Samuel P. Ferguson. He has contributed to this project in many important ways, including the results in Section 7.

Some history of the proof and this paper is as follows. The original proof, as envisioned in 1994 and accomplished in 1998, was divided into a five-step program. As a result, the original papers were called “Sphere Packings I,” “Sphere Packings II,” and so forth. The first two papers in the series were published in an earlier volume of DCG. As it turned out, the fourth step “Sphere Packings IV” is considerably more difficult than the other steps in the program. It became clear that a single paper would not suffice, and the fourth step of the proof was divided into two parts “Sphere Packings IV” and “Kepler Conjecture (Sphere Packings VI).” Samuel Ferguson’s thesis “Sphere Packings V” solved one of the five major steps in the proof. (Although “Sphere Packings IV” and “Sphere Packings VI” belonged together, because of the numbering scheme, Ferguson's theses "Sphere Packings V" was inserted between these two papers.)

The proof that is contained in this volume is a rewritten version of the proof. For historical reasons, the papers in this volume have retained the original titles, but because of extensive revisions over the past several years, the proof is no longer arranged according to the five steps of the 1994 program.

In addition to the $5 + 1$ papers corresponding to the five steps of the original program, there is the current paper. It has the following origin. In 1996, it became clear that progress on the problem required some adjustments in the main non-linear optimization problem of "Sphere Packings I" and "II." As the original 1996 manuscript put it, "There are infinitely many scoring schemes that should lead to a proof of the Kepler conjecture. The problem is to formulate the scheme that makes the Kepler conjecture as accessible as possible" [Hal96]. The original purpose of this paper was to make some useful improvements in the scoring function from "Sphere Packings I" and "II" and to make the changes in such a way that the main results of those papers would still hold true.

Over the past years, this paper has grown considerably in scope to the point that it is now lays the foundation for all of the papers in the series. In fact, all of the foundational material from "Sphere Packings I," and "II," and the 1998 preprint series has been collected together in this article. The scoring function is no longer the same as the one presented in "Sphere Packings I," and "II." This paper adapts the relevant material from these earlier papers to the current scoring function. This paper has expanded to the point that it is now possible to understand the entire proof of the Kepler conjecture without reading "I" and "II."

Section 3

The Top-Level Structure of the Proof

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

3.1 Statement of Theorems

Theorem 3.1 (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 $\pi/\sqrt{18} \approx 0.74$.

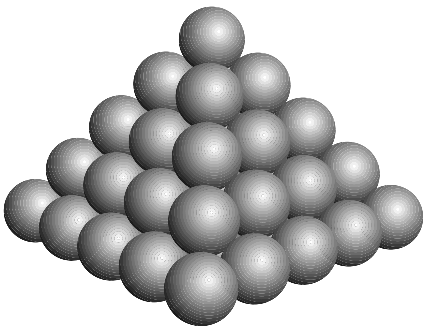

Figure 3.1. *The face-centered cubic packing*

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.

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 3.2. *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 3.3. *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

$$\mathrm{vol}\,B(x,r,\Lambda)\leq |\Lambda(x,r+1)|4\pi/3. \tag{3.1}$$

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

$$\begin{aligned}\sqrt{32}|\Lambda(x,r+1)| &\le \sum_{v\in\Lambda(x,r+1)} (A(v)+\mathrm{vol}(\Omega(v)))\\ &\le C_1(r+1)^2+\mathrm{vol}\,B(x,r+3)\\ &\le C_1(r+1)^2+(1+3/r)^3\mathrm{vol}\,B(x,r)\end{aligned}\quad . \tag{3.2}$$

Recall that $\delta(x,r,\Lambda)=\mathrm{vol}\,B(x,r,\Lambda)/\mathrm{vol}\,B(x,r)$. Divide Inequality 3.1 through by $\mathrm{vol}\,B(x,r)$. Use Inequality 3.2 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 3.3. 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 3.4. *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 3.3 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.*

Section 6 defines a compact topological space DS (the space of decomposition stars 6.2) 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 6.2 shows that the data in a decomposition star are sufficient to determine a Voronoi cell $\Omega(D)$ for each $D\in$ 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

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

Section 7 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 3.5. *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 7.11. 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)

$$\sqrt{32} \leq \operatorname{vol}\Omega(D) + A_0(D), \tag{3.3}$$

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 $\delta_{tet} = \sqrt{8}\arctan(\sqrt{2}/5)$.

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

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

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

In terms of these quantities,

$$\sigma(D) = -4\delta_{oct}(\operatorname{vol}(\Omega(D)) + A_0(D)) + \frac{16\pi}{3}. \tag{3.4}$$

Definition 3.6. *We define the constant*

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

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

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

In terms of the scoring function σ, the optimization problem in a finite number of variables (Inequality 3.3) takes the following form. The proof of this inequality is a central concern in this paper.

Theorem 3.7 (Finite dimensional reduction). *The maximum of σ on the topological space DS of all decomposition stars is the constant $8\,pt \approx 0.442989$.*

Remark 3.8. *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 3.7 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 3.9. *Let D be a decomposition star at which the function $\sigma : \mathrm{DS} \to \mathbb{R}$ attains its maximum. Then the set $U(D)$ of vectors at distance at most $2t_0$ from the center has cardinality twelve. Up to Euclidean motion, $U(D)$ is one of two arrangements: 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.*

There is a complete description of all packings in which every sphere center is surrounded by twelve 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 Paper I.

3.2 Basic Concepts in the Proof

To prove Theorems 3.1, 3.7, and 3.9, we wish to show that there is no counterexample. In particular, we wish to show that there is no decomposition star D with value $\sigma(D) > 8\,pt$. We reason by contradiction, assuming the existence of such a decomposition star. With this in mind, we call D a *contravening decomposition star*, if

$$\sigma(D) \geq 8\,pt.$$

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 18.3. 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 [Hal05b]. 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}.

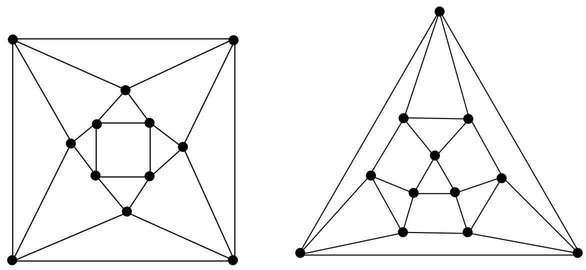

Figure 3.2. *The plane graphs G_{fcc} and G_{hcp}*

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 3.3). (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 Paper V.

Theorem 3.10 (Ferguson). *There are no contravening decomposition stars D whose associated plane graph is isomorphic to G_{pent}.*

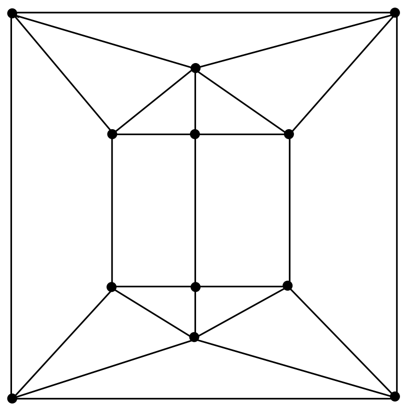

Figure 3.3. *The plane graph G_{pent}*
of the pentahedral prism.

3.3 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 3.1, 3.7, and 3.9) all follow from these claims.

Claim 3.11. *If the maximum of the function σ on* DS *is $8\,pt$, then for every saturated packing Λ there exists a negligible fcc-compatible function A.*

Claim 3.12. *Let D be a contravening decomposition star. Then its plane graph $G(D)$ is tame.*

Claim 3.13. *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 3.14. *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 3.15. *There do not exist any contravening decomposition stars D whose associated graph is isomorphic to G_{pent}.*

Claim 3.16. *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 $\sigma(D) = 8\,pt$. 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.*

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

Lemma 3.17. *Assume Claims 3.12, 3.13, 3.14, and 3.15. 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 3.15. $\square$

Lemma 3.18. *Assume Claims 3.12, 3.13, 3.14, 3.15, and 3.16. Then Theorem 3.7 holds.*

Proof. By Claim 3.16 and Lemma 3.17, the value $8\,pt$ lies in the range of the function σ on DS. Assume for a contradiction that there exists a decomposition star $D \in$ DS that has $\sigma(D) > 8\,pt$. By definition, this is a contravening star. By Lemma 3.17, its plane graph is isomorphic to G_{hcp} or G_{fcc}. By Claim 3.16, $\sigma(D) = 8\,pt$, in contradiction with $\sigma(D) > 8\,pt$. $\square$

Lemma 3.19. *Assume Claims 3.12, 3.13, 3.14, 3.15, and 3.16. Then Theorem 3.9* *holds.*

Proof. By Theorem 3.7, 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 3.17 implies that the plane graph is isomorphic to G_{hcp} or G_{fcc}. The hypotheses of Claim 3.16 are satisfied. The conclusion of Claim 3.16 is the conclusion of Theorem 3.9. □

Lemma 3.20. *Assume Claims 3.11–3.16. Then the Kepler conjecture (Theorem 3.1) holds.*

Proof. As pointed out in Remark 3.4, 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 3.11 (and Lemma 3.18). By Lemma 3.3, 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 3.21. *One other theorem (Theorem 3.5) was stated without proof in Section 3.1. This result was placed there to motivate the other results. However, it is not an immediate consequence of Claims 3.11–3.16. Its proof appears in Theorem 7.11.*

3.4 Proofs of the Central Claims

The previous section showed that the main results in the introduction (Theorems 3.1, 3.7, and 3.9) follow from six claims. This section indicates where each of these claims is proved, and mentions a few facts about the proofs.

Claim 3.11 is proved in Theorem 7.14. Claim 3.12 is proved in Theorem 20.20. Claim 3.13, the classification of tame graphs, is proved in Theorem 19.1. 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 3.14 in a moment. Claim 3.15 is Ferguson's thesis, cited as Theorem 3.10.

Claim 3.16 is the local optimality of the face-centered cubic and hexagonal close packings. In Section 8, the necessary local analysis is carried out to prove Claim 3.16 as Corollary 8.3.

Now we return to Claim 3.14. This claim is proved as Theorem 23.1. 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 volume is organized in the following way. Sections 4 through 7 introduce the basic definitions. Section 7 gives a proof of Claim 3.11. Section 8 proves Claim 3.16. Sections 9 through 14 present the fundamental estimates. Sections 18 through 19 give a proof of Claim 3.13. Sections 20 through 22 give a proof of Claim 3.12. Sections 23 through 25 give a proof of Claim 3.14. Claim 3.15 (Ferguson's thesis) appears in Paper V.

Section 4

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 section, 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 section 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 section, we give the proof that the simplices in the Q-system do not overlap.

4.1 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 4.1. *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 Paper I.*

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 4.2. *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 4.3. *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 4.4. *Two manifolds with boundary overlap if their interiors intersect.*

Definition 4.5. *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 4.6. *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 4.7. *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 4.8. *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 section.

Theorem 4.9. *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 sections that follow.

Lemma 4.10. *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. □

4.2 Geometric Considerations

Remark 4.11. *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 4.1.) $S(y_1, y_2, \ldots, y_6)$ 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 4.12. *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 4.13. *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 4.14. *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 4.1).

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

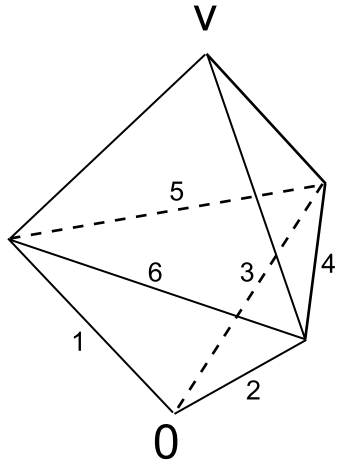

Figure 4.1. *$\mathcal{E}$ measures the distance between the vertices at* 0 *and* v. *The standard indexing of the edges of a simplex is marked on the lower simplex.*

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, Sec. 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 $y_i \geq 2$ and $y_4, y_5, y_6 \leq 2t_0$ and $S' = S(y'_1, y'_2, y'_3, y_4, y_5, y_6)$ satisfies $y'_i \geq 2$, 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

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

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[2] 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 $|v| > 2.75$.

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.

4.3 Incidence Relations

Lemma 4.15. *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 4.16. *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 4.17. *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. □

[2] Compare Lemma 4.21.

Definition 4.18. *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 4.19. *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

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

□

Definition 4.20. *Let $\eta(x, y, z)$ denote the circumradius of a triangle with edge-lengths x, y, and z.*

Lemma 4.21. *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

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

□

Lemma 4.22. *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 4.2).*

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

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

□

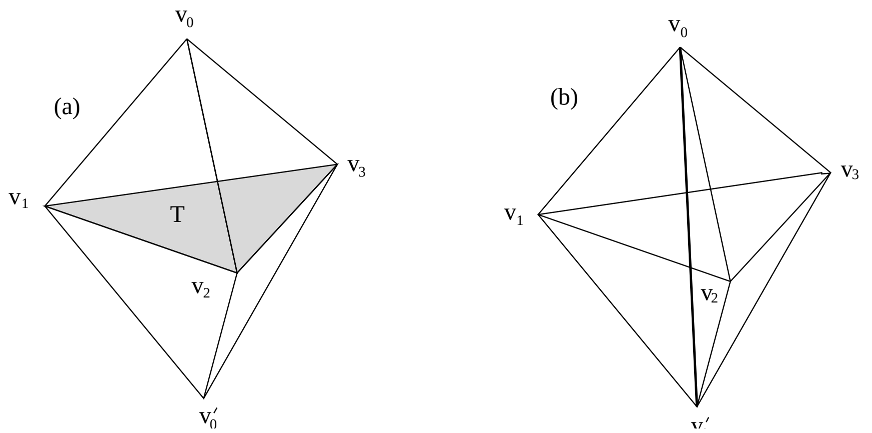

Figure 4.2. *Frame (a) depicts two quasi-regular tetrahedra that share a face. The same convex body may also be viewed as three quarters that share a diagonal, as in Frame (b).*

Lemma 4.23. *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 Lemma 4.22, 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 4.21. This implies that no other quarter overlaps these quasi-regular tetrahedra. $\square$

Lemma 4.24. *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 4.25. *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 4.26. *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 4.27. *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 4.28. *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 4.29. *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 4.30. *Suppose that there exist four nonzero vertices $v_1, \ldots, v_4$ of height at most $2t_0$ (that is, $|v_i| \leq 2t_0$) 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

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

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 4.31. *If, under the same hypotheses as Lemma 4.30, 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 $|w - v_1|, |w - v_3| \leq 2t_0$ (Lemma 4.24), where $\{v_1, v_3\}$ is a diagonal. Similarly, the distance from w to the other two corners is at most $2t_0$. □

Lemma 4.32. *Let v_1 and v_2 be anchors of $\{0, w\}$ with $2t_0 \leq |w| \leq \sqrt{8}$. 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 $|v_3 - v_4| \leq \sqrt{8}$. 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

$$\mathrm{dih}(S(\sqrt{8}, 2, y_3, 2, y_5, 2)) > 1.075, \quad y_3, y_5 \in [2, 2t_0], \tag{4.1}$$

$$\mathrm{dih}(S(\sqrt{8}, y_2, y_3, 2, y_5, y_6)) > 1, \quad y_2, y_3, y_5, y_6 \in [2, 2t_0]. \tag{4.2}$$

Then

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

Therefore, the figure does not exist. □

Lemma 4.33. *Two vertices w, w' of height at most $\sqrt{8}$ cannot be enclosed over a triangle $\{v_1, v_2, v_3\}$ satisfying $|v_1 - v_2| \leq \sqrt{8}$, $|v_1 - v_3| \leq 2t_0$, and $|v_2 - v_3| \leq 2t_0$.*

Proof. For a contradiction, assume the figure exists. The long edge $\{v_1, v_2\}$ must have length at least $2t_0$ by Lemma 4.22. 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 4.32 gives the contradiction $|w'| > \sqrt{8}$. □

Lemma 4.34. *Let v_1, v_2, v_3 be anchors of $\{0, w\}$, where $2t_0 \leq |w| \leq \sqrt{8}$, $|v_1 - v_3| \leq \sqrt{8}$, and the edge $\{v_1, v_3\}$ passes through the face $\{0, w, v_2\}$. Then $\min(|v_1 - v_2|, |v_2 - v_3|) \leq 2t_0$. Furthermore, if the minimum is $2t_0$, then $|v_1 - v_2| = |v_2 - v_3| = 2t_0$.*

Proof. Assume $\min \geq 2t_0$. As in the proof of Lemma 4.32, 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. □

4.4 Overlap of Simplices

This section gives a proof of Theorem 4.9 (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 4.35. *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 4.19). If a diagonal of a strict quarter passes through the face of a quasi-regular tetrahedron, then Lemma 4.23 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 4.36. *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 4.19). A diagonal of a strict quarter cannot pass through an external face either, because of Lemma 4.22. □

Lemma 4.37. *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 4.27.)

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 4.33 and 4.32, 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 4.32 and it cannot end inside the simplex by Corollary 4.17. 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 4.24 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 three 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 4.19, 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. $\square$

Remark 4.38. *We have seen in the proof of Lemma 4.37 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 4.39. *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 4.38, assume that neither is adjacent to another quarter. 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 4.24, 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 4.34). 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 4.19. 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 4.19. 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 4.32). Either $\{u, w'\}$ or $\{w', 0\}$ has length at most $2t_0$ by Lemma 4.34, 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 4.3). It follows that the two quarters form an isolated pair. $\square$

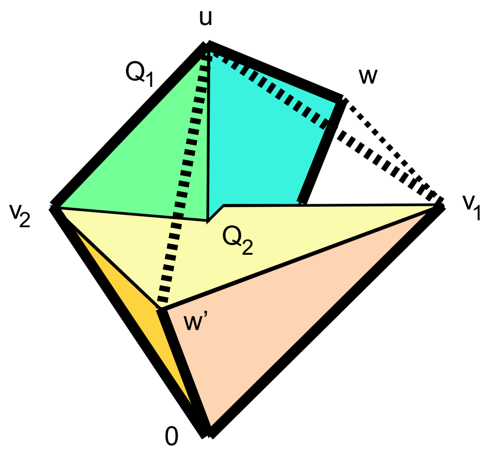

Figure 4.3. *An isolated pair. The isolated pair consists of two simplices* $Q_1 = \{0, u, w, v_2\}$ *and* $Q_2 = \{0, w', v_1, v_2\}$*. The six extremal vertices form an octahedron. This is not a quartered octahedron because the edges* $\{u, w'\}$ *and* $\{w, v_1\}$ *have length greater than* $2t_0$*.*

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 section.

Proof. **(Theorem 4.9)** 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 4.35 shows that quasi-regular tetrahedra do not overlap other simplices in the Q-system. Lemma 4.36 shows that the quarters in quartered octahedra are well-behaved. Lemma 4.37 shows that other quarters in adjacent pairs do not overlap other simplices in the Q-system. Finally, we treat isolated quarters in Lemma 4.39. 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. $\square$

Section 5

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 section. 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 section, 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 5.28). A second compatibility result between these two structures is proved in Lemma 5.29.

The purpose of this section 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 Section 6, 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.

5.1 V-Cells

Definition 5.1. *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 5.2. *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 5.3. *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 4.21 and that the length $|w_1 - w_2|$ is greater than $2t_0$ by Lemma 4.19. 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 4.22 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 5.4. *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 5.5. *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 5.6. *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 5.7. *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 5.8. *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 5.9. □

Lemma 5.9. *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 5.10. *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 5.1, 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.*

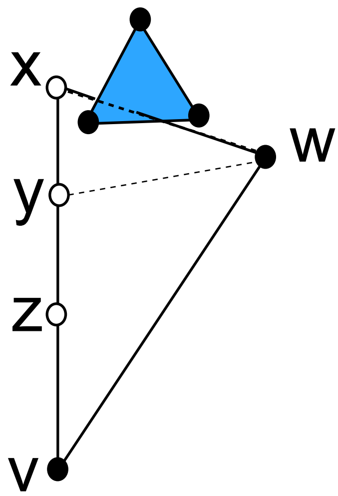

Figure 5.1. *A hypothetical arrangement that leads to a nonconvex V-cell at v.*

Remark 5.11. *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 5.23 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 (to be defined later).

Truncation will be justified later in Lemma 7.18, 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.*

5.2 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 5.12. *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 5.13. *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 5.14. *Define the polynomial χ by*

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

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 5.15. *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, Sec. 8.1]). Thus, t and χ have the same sign. The result follows. □

Lemma 5.16. *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 5.15). 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 5.17. *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 5.16. 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 5.18. *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
$$\chi(y_1^2, \ldots, y_6^2) \geq \chi(4, 4, 4, y_4^2, y_5^2, y_6^2) = 2y_4^2 y_5^2 y_6^2 (2/\eta(y_4, y_5, y_6)^2 - 1) > 0.$$
(Here y_i are the edge-lengths of the simplex.) □

5.3 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 5.19. *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 5.16.) We consider the implications of negative orientation for each kind of barrier. If the barrier is a quasi-regular triangle, then Lemma 5.17 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 5.16 gives that Q is a flat-quarter in the Q-system as well. Hence $Q \in \mathcal{Q}_0$.

The rest is clear. $\square$

Lemma 5.20. *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 4.22 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 4.34, 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 4.10. This contradicts the hypothesis of the lemma. $\square$

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

Corollary 5.21. *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 5.20 and invoke Lemma 4.19.) $\square$

Lemma 5.22. *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 5.20, 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 4.19, 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. $\square$

Lemma 5.23. *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 5.22, the origin is unobstructed at x. Thus, $|x - v| \leq |x| \leq t_0$. By Lemma 5.22 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 $x \in \mathrm{VC}(0)$. $\square$

Definition 5.24. *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 5.25. *Let v_1, v_2, v_3, and v_4 be distinct vertices such that $|v_i| \leq 2t_0$ for*

$i = 1, 2, 3, 4$ and $|v_1 - v_3|, |v_2 - v_4| \leq 2t_0$. Then the edges $\{v_1, v_3\}$ and $\{v_2, v_4\}$ do not cross. In particular, the arcs of Definition 5.24 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

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

□

Lemma 5.26. *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 5.3. □

Remark 5.27. *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 5.28 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 5.29 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 5.28. *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. □

Let $\mathcal{B}'_0$ be the set of triangles T such that at least 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 5.29 (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 5.30. *The Decoupling Lemma is a crucial result. It permits estimates of the scoring function in Section 7 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 Section 23.*

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 5.2. 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. 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 5.16 and 5.17, 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 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

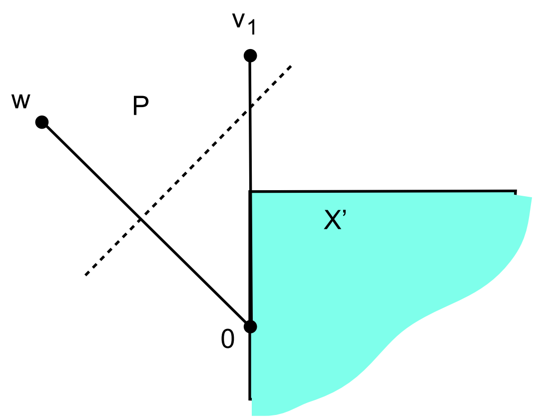

Figure 5.2. *The perpendicular bisector to* $\{0, w\}$ *(dashed line) cannot meet the quadrant* X' *(shaded).*

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 5.13. □

We draw out a simple consequence of the proof. Let $F = \{0, v_1, v_2\}$ with edges of length between 2 and $\sqrt{8}$. Let $S = \{0, w, v_1, v_2\}$, and assume that S has negative orientation along F. 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 both v_1 and v_2. Let x lie in this convex hull C.

Lemma 5.31. *In this context, w is obstructed at x.*

Proof. This is what the final paragraph of the previous proof proves by contradiction. □

Section 6

Decomposition Stars

This section 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 5.10 suggests that V-cells can be rather poorly behaved in this respect.

6.1 Indexing Sets

We are ready for the formal description of decomposition stars.

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

- Let $I_1 = \omega$.
- Let I_2 be the set of unordered pairs of indices $\{i, j\}$ such that $|v_i - v_j| \le 2t_0 = 2.51$.
- 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 6.1. *Let* DS° *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 $t = t'$, $\mathrm{domain}(f) = \mathrm{domain}(f')$, and for all $i \in \mathrm{domain}(f)$, $f(i)$ 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°.

There is a natural compactification of DS° obtained by replacing 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 6.2. *Let* DS *be the compactification given above of* DS°. *Call it the space of decomposition stars.*

Definition 6.3. *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.

6.2 Cells attached to Decomposition Stars

To each decomposition star, we can associate a V-cell centered at 0 by a direct adaptation of Definition 5.6.

Lemma 6.4. *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. □

Corollary 6.5. *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 5.6.*

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 6.6. $\mathrm{VC}(D)$ *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 5.9.

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 VC(D) is also continuous. ∎

Lemma 6.7. *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 6.8. *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 6.9. *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 6.10. *It follows from Corollary 6.8 that*

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

In particular, they have the same volume.

Remark 6.11. *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 $\mathrm{VC}(D)$ 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.*

6.3 Colored Spaces

In Section 3, we introduced a function σ that will be formally defined in Definition 7.8. 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 6.1. It is continuous, except at $x=0$.

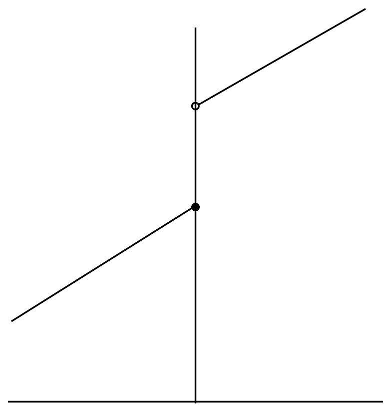

Figure 6.1. *A piecewise linear function*

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 $(x, \mathrm{sign}(x))$, 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 $2t_0$.

Section 7

Scoring (Ferguson, Hales)

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

In earlier sections, 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 3.3 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 3.2.

The purpose of the first part of this section 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 volume 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 Section 6. 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 7.12.) The function σ is a continuous function on the space DS. This function is defined in the final paragraphs of this section.

7.1 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

$$A = A_0 \circ D(\cdot, \Lambda) : \Lambda \to \mathrm{DS} \to \mathbb{R}, \quad v \mapsto D(v, \Lambda) \mapsto A_0(D(v, \Lambda)), \tag{7.1}$$

where $A_0 : \mathrm{DS} \to \mathbb{R}$ is as defined by Equations 7.2 and 7.6 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 7.1. *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

$$A_0(D) = -\mathrm{vol}\,(\Omega(D)) + \mathrm{vol}\,(\mathrm{VC}(D)) + \sum_{Q \in \mathcal{Q}_0(D)} A_1(Q, c(Q, D), 0). \tag{7.2}$$

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 7.2. *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 7.1.

Definition 7.3. *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 7.2.) We let $\mathrm{quo}(R)$ be the volume of the quoin over R. If $R = R(a, b, c)$ is*

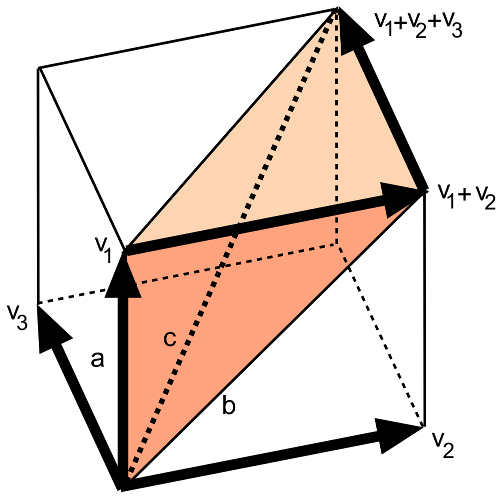

Figure 7.1. *The Rogers simplex is an orthosimplex.*

a Rogers simplex, the volume $\mathrm{quo}(R)$ *is given explicitly as follows*

$$\begin{aligned} 6\,\mathrm{quo}(R) &= (a+2c)(c-a)^2 \arctan(e) + a(b^2-a^2)e \\ &\quad -4c^3 \arctan(e(b-a)/(b+c)), \end{aligned} \tag{7.3}$$

where $e \geq 0$ *is given by* $e^2(b^2-a^2) = (c^2-b^2)$.

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. By Lemma 5.28, 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, Section 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 7.4. *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.*

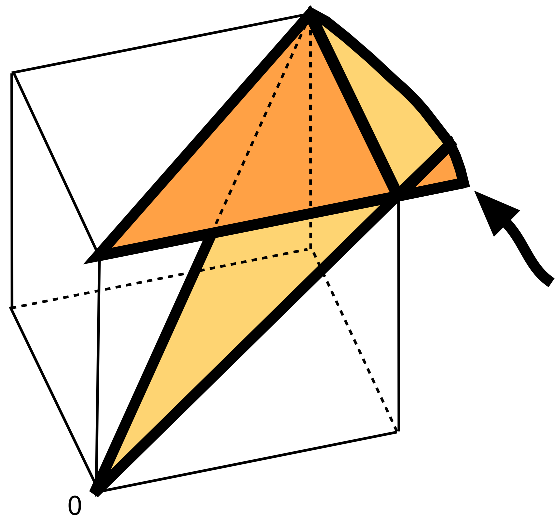

Figure 7.2. *The quoin above a Rogers simplex is the part of the shaded solid outside the illustrated box. It is bounded by the shaded planes, the plane through the front face of the box, and a sphere centered at the origin passing through the opposite corner of the box.*

Proof. This is true by inspection. See Figure 7.3. 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 7.5. *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 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 7.4 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

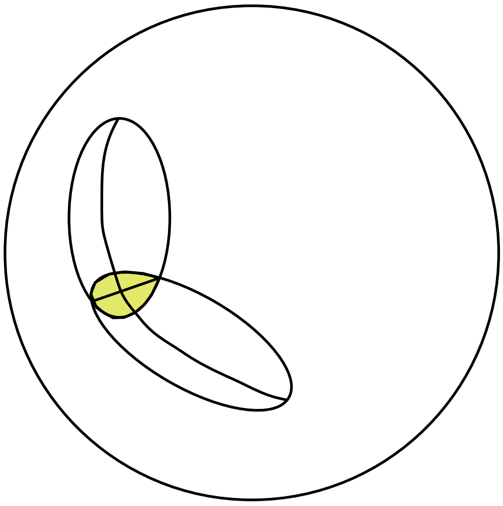

Figure 7.3. *The intersection of two caps on the unit ball can be partitioned into four quoins (shaded).*

caps. The intersections of caps are given as quoins (Lemma 7.4). 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

$$\operatorname{vol}\mathrm{VC}_t(S, v_0) = \operatorname{sol}(S)/3 - \sum_{i=1}^{3} \frac{\operatorname{dih}(S, v_i)}{2\pi} \operatorname{vol}\mathrm{cap_i} + \sum_{(i,j,k)\in S_3} \operatorname{quo}(R(h_i, \eta_{ij}, t)). \quad (7.4)$$

We extend Formula 7.4 by setting

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

if the constraint $a < b < c$ fails to hold. Similarly, set $\operatorname{vol}\mathrm{cap}_i = 0$ if $|v_i| \geq 2t$. With these conventions, Formula 7.4 extends to all simplices. We write the extension of $\operatorname{vol}\mathrm{VC}_t(S, v)$ as

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

Definition 7.6. *Let*[3]

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

and

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

[3]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.

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

$$\Gamma(S) = \frac{1}{4}\sum_{i=1}^{4} \text{s-vor}(S, v_i). \tag{7.5}$$

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

Definition 7.7. *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 7.1. The function A_0 was reduced in turn to that of A_1 in Equation 7.2. To complete the definition, we define A_1.

Definition 7.8. *Set*

$$A_1(S, c, v) = -\mathrm{vol}\,\mathrm{VC}(S, v) + \frac{\mathrm{sol}(S, v)}{3\delta_{oct}} - \frac{\sigma(S, c, v)}{4\delta_{oct}}. \tag{7.6}$$

where σ is given as follows:

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* $\sigma(S,v)$*.*

The definition of σ on quarters can be expressed a second way in terms of a function μ. If S is a quarter, set

$$\mu(S,v) = \begin{cases} \Gamma(S), & \text{if } \eta^+(S) < \sqrt{2}, \\ \text{s-vor}(S,v), & \text{otherwise.} \end{cases} \tag{7.7}$$

If S is a flat quarter, we have $\sigma(S,c,v) = \mu(S,v)$, for all contexts c.

Suppose S is an upright quarter. Definition 7.8 can be expressed as follows.

- context $(2,1)$: Set $\sigma(S,c,v) = \mu(S,v)$.
- context $(4,0)$: Set $\sigma(S,c,v) = (\mu(S,v) + \mu(S,\hat{v}))/2$.
- other contexts: Set $\sigma(S,c,v) = (\mu(S,v)+\mu(S,\hat{v})+\text{s-vor}_0(S,v)-\text{s-vor}_0(S,\hat{v}))/2$.

Lemma 7.9. $A_0 : \mathrm{DS} \to \mathbb{R}$ *is continuous.*

Proof. The continuity of $D \mapsto \operatorname{vol}\mathrm{VC}(D)$ is proved in Lemma 6.6. 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 7.10. *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 7.6, this is equivalent to

$$\sum_{i=1}^{4} \sigma(S, c, v_i) = \sum_{i=1}^{4} \text{s-vor}(S, c, v_i). \tag{7.8}$$

Equation 7.8 is evident from Definition 7.8 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 $\text{s-vor}(S, c, v_i)$. Equation 7.8 is thus established because a sum is unaffected by taking weighted averages of its terms. □

7.2 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 3.2 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 7.1. 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 7.2 and 7.6, and Definition 7.8.

Theorem 7.11. *The function A of Equation 7.1 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 5.5). 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

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

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 7.10 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. $\square$

7.3 Fcc-compatibility

We have constructed a negligible function A. The rest of this volume 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 7.12. *Let $\sigma : \mathrm{DS} \to \mathbb{R}$ be given by*

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

It is called the score of the decomposition star.

Recall from Definition 3.6 the constant $pt \approx 0.05537$. This constant is called a point.

Lemma 7.13. *Let A_0, A, and σ be the functions defined by Equations 7.1, 7.2 7.6, and Definition 7.8. 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 $8\,pt$.*

Moreover, these statements imply

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

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

Proof. To see the equivalence of the first and second statements, use Definition 7.12, and the identity

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

(Note that this identity is parallel in form to Definition 7.12 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. □

Theorem 7.14. *If the maximum of the function σ on* DS *is $8\,pt$, then for every saturated packing Λ there exists a negligible fcc-compatible function A.*

Proof. This follows immediately from Theorem 7.11 and Lemma 7.13. □

7.4 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 7.15. *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

$$\sigma(D) = \sum_R \sigma_R(D), \tag{7.9}$$

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 5.26, each Q is entirely contained in the cone over a single standard region.

Definition 7.16. *Let R be a measurable subset of the unit sphere. Set*

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

Let R be a standard region. Set

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

Lemma 7.17. *$\sigma(D) = \sum_R \sigma_R(D)$, where the sum runs over all standard regions R.*

Proof.

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

∎

Also, we have

$$\mathrm{vor}(D) = \sum_{R\in\mathcal{R}(D)} \mathrm{vor}_R(D). \tag{7.10}$$

Lemma 7.18. *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 7.6) 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 7.19. *Lemma 7.18 explains why we have chosen the same symbol σ for the functions $\sigma_R(D)$ and $\sigma(Q,c,v)$. We can view Lemma 7.18 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.

7.5 Scores of Simplices and Cones

Many of the functions in this paper are defined by terms involving volumes of simple solids. To give estimates on the functions, it is often convenient to partition the solids into smaller pieces and then define corresponding functions on each of the pieces. For this reason, we define some variants of the functions vor and σ.

Remark 7.20. *We now define a few more variants of the function* vor. *The function* s-vor *and its truncated version* s-vor$(\cdot, t)$ *have been defined already. The function* $\mathrm{vor}_R(D)$ *will also be given a truncated version* $\mathrm{vor}_R(D, t)$*, for a real truncation parameter* $t \geq 0$*. The special case,* $\mathrm{vor}_R(D, t_0)$ *will be abbreviated* $\mathrm{vor}_{0,R}(D)$*. There will be another variant* r-vor *for Rogers simplices, and another* c-vor *for general sets. The general form of these functions is*

$$\text{c-vor}(X) = 4(-\delta_{oct}\mathrm{vol}(X) + \mathrm{sol}(X)/3),$$

for any subset $X \subset \mathbb{R}^3$*. The differences between the different versions of* vor *come from the different choices of the set* X *and the way they are parametrized.*

Definition 7.21. *Let* $R = R(a, b, c)$ *be a Rogers simplex. Assume that the vertex terminating the edges of lengths* a*,* b*, and* c *is situated at the origin. Let*

$$\text{r-vor}(R) = 4(-\delta_{oct}\mathrm{vol}(R) + \mathrm{sol}(R)/3).$$

Definition 7.22. *Let* $C(h, t)$ *denote the compact cone of height* h *and circular base. Set*

$$\phi(h, t) = 2(2 - \delta_{oct} th(h + t))/3.$$

Then

$$\text{c-vor}(C(h, t)) = 2\pi(1 - h/t)\phi(h, t). \tag{7.11}$$

Remark 7.23. *Below, we introduce variants of the function* σ*. We have already encountered* σ *in Definitions 7.8, 7.12, and 7.16. Informally, we call* σ *(and various functions that are closely related to it) the score. Equation 7.11 represents the score of* $C(h, t)$*. The solid angle of* $C(h, t)$ *is* $2\pi(1 - h/t)$*, so* $\phi(h, t)$ *is the score per unit area. Also,* $\phi(t, t)$ *is the score per unit area of a ball of radius* t*. That is,* $\phi(t, t) = 4(-\delta_{oct}\mathrm{vol}/\mathrm{sol} + 1/3)$*.*

We set

$$\begin{aligned} \text{s-vor}(S, t) &= \mathrm{sol}(S)\phi(t, t) + \textstyle\sum_{i=1,\ h_i \leq t}^{3} d_i(1 - h_i/t)(\phi(h_i, t) - \phi(t, t)) \\ &\quad - \textstyle\sum_{(i,j,k)\in S_3} 4\delta_{oct}\,\mathrm{quo}(R(h_i, \eta(y_i, y_j, y_{k+3}), t)). \end{aligned} \tag{7.12}$$

In the definition, we adopt the convention that $\mathrm{quo}(R) = 0$, if $R = R(a, b, c)$ does not exist (that is, if the condition $0 < a \leq b \leq c$ is violated). In the second sum, S_3 is the set of permutations on three letters. This definition is compatible with Definition 7.6.

Similarly, we define $\mathrm{vor}_P(D,t)$ for arbitrary standard clusters (P,D). (We shift notation from R to P for a standard region to avoid conflict with Rogers simplices R in the following definition.) Extending the notation in an obvious way, we have

$$\begin{aligned}\mathrm{vor}_P(D,t) &= \mathrm{sol}(P)\phi(t,t) + \textstyle\sum_{|v_i|\le 2t} d_i(1-|v_i|/(2t))(\phi(|v_i|/2,t)-\phi(t,t)) \\ &\quad - \textstyle\sum_R 4\delta_{oct}\,\mathrm{quo}(R).\end{aligned} \tag{7.13}$$

The first sum runs over vertices in P of height at most $2t$. The second sum runs over Rogers simplices $R(|v_i|/2,\eta(F),t)$ in P, where $F=\{0,v_1,v_2\}$ is a face of circumradius $\eta(F)$ at most t, formed by vertices in P. The constant d_i is the total dihedral angle along $\{0,v_i\}$ of the standard cluster. The truncations $t=t_0=1.255$ and $t=\sqrt{2}$ will be of particular importance. Set $A(h)=(1-h/t_0)(\phi(h,t_0)-\phi(t_0,t_0))$.

Remark 7.24. *We have introduced both untruncated and truncated versions of functions* vor *and* σ. *The truncated versions are used to give upper bounds on the untruncated versions. For example, in the function* $\sigma(D)$, *the* V*-cell contributes through its volume, as in Remark 7.20. The volume appears with a negative coefficient* $-4\delta_{oct}$. *Thus, we obtain an upper bound on* $\sigma(D)$ *by discarding bits of volume from the* V*-cell. This suggests that we might try to give upper bounds on the score* $\sigma(D)$ *by truncating the* V*-cell in various ways. This is the reason for the truncated versions of these functions.*

7.6 The Example of a Dodecahedron

Example 7.25. *The following example illustrates why better bounds on the density of packings can be obtained with* $\sigma(D)$ *than with a naive approach based on the volume of Voronoi cells. By scoring quasi-regular tetrahedra with the compression function* $\Gamma(S)$ *rather than* s-vor(S), *we will find that the score is lowered below* $8\,pt$ *for configurations with many quasi-regular tetrahedra. To work one example, let us assume that the decomposition star consists of twelve vertices located at distance* 2 *from the origin, at the vertices of a regular icosahedron. The score is approximately*

$$20\,\Gamma(S(2,2,2,2.10292,2.10292,2.10292)\approx 1.8\,pt < 8\,pt.$$

If s-vor(S) *had been used, the score would violate Theorem 1.7:*

$$20\,\text{s-vor}(S)\approx 13.5493\,pt > 8\,pt.$$

(This is tied to the fact that the regular dodecahedron of inradius 1 *has smaller volume than the rhombic dodecahedron of inradius* 1.*)*

Paper III

Sphere Packings III. Extremal Cases

This paper is the third in a series of six papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing. In the previous paper in this series, a continuous function f on a compact space is defined, certain points in the domain are conjectured to give the global maxima, and the relation between this conjecture and the Kepler conjecture is established. This paper shows that those points are indeed local maxima. Various approximations to f are developed, that will be used in subsequent papers to bound the value of the function f. The function f can be expressed as a sum of terms, indexed by regions on a unit sphere. Detailed estimates of the terms corresponding to triangular and quadrilateral regions are developed.

This paper has three objectives. The first is dealing with the two types of decomposition stars that attain the optimal Kepler conjecture bound. The second is obtaining general upper bounds on the score of decomposition star by truncation. The third is obtaining various upper bounds on the score associated to individual triangular and quadrilateral regions of a general decomposition star.

The first section contains a proof that the decomposition stars attached to the face-centered cubic and hexagonal-close packings give local maxima to the scoring function on the space of all decomposition stars. The proof describes precisely determined neighborhoods of these critical points. These special decomposition stars are shown to yield the global maximum of the scoring function on these restricted neighborhoods.

The second section gives an approximation to a decomposition star that provides an upper bound approximation to the scoring function σ. In the simplest cases, the approximation to the decomposition star is obtained by truncating the decomposition star at distance $t_0 = 1.255$ from the origin. More generally, we define a collection of simplices (that do not overlap any simplices in the Q-system), and define a somewhat different truncation for each type of simplex in the collection. For want of a more suggestive term, these simplices are said to form the $\mathcal{S}$-system.

When truncation at t_0 cuts too deeply, we reclaim a scrap of volume that lies outside the ball of radius t_0 but still inside the V-cell. This scrap is called a *crown*. These scraps are studied in that same section.

In a final section, we develop a series of bounds on the score function in triangular and quadrilateral regions, for use in later papers.

Section 8

Local Optimality

The first several sections have established the fundamental definitions and constructions of this volume. This section 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.

8.1 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 section is to give a proof of the following theorem.

Theorem 8.1 (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_{fcc} of twelve tangent unit balls in the face-centered cubic configuration, or a bijection with U_{hcp} the twelve tangent unit balls in the hexagonal-close packing configuration; such that for all $v, w \in U(D)$, $|w - v| \leq 2t_0$ 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_{fcc} or U_{hcp}.*

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

Remark 8.2. *This theorem is one of the key claims of Section 3.3. This theorem is phrased slightly differently from the Claim 3.15 in Section 3.3. The reason for this is that we have not formally introduced the plane graph $G(D)$ of a decomposition star. (This happens in Section 20.2.) Once $G(D)$ has been formally introduced, then Theorem 8.1 can be expressed more directly, as follows. We let G_{fcc} and G_{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 8.3 (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_{fcc} or G_{hcp}, then $\sigma(D) = 8\,pt$. 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 section. It is a key part of the proof of local optimality.

Theorem 8.4. *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, $\sigma_R(D) \leq 0$. 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 5.24) has nonpositive score.

8.2 Rogers Simplices

To prove Theorem 8.4, 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 8.5. *Let $R(a, b, c)$ be a Rogers simplex, with $1 \leq a < b < c$. 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*

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

is monotonically decreasing in each variable.

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

Lemma 8.6. *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*

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

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 8.5. See the third frame of Figure 8.1. □

Lemma 8.7. *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

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

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

Proof. This is calculated in [Hal97b, Sec. 4]. See the second frame of Figure 8.1.
□

Lemma 8.8. *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*

$$A \le \delta_{oct}\,\mathrm{vol}(C).$$

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

Proof. The ratio $A/\mathrm{vol}(C)$ is at most $1/1.18^3 < \delta_{oct}$. See the first frame of Figure 8.1. □

8.3 Bounds on Simplices

In this and future sections, 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

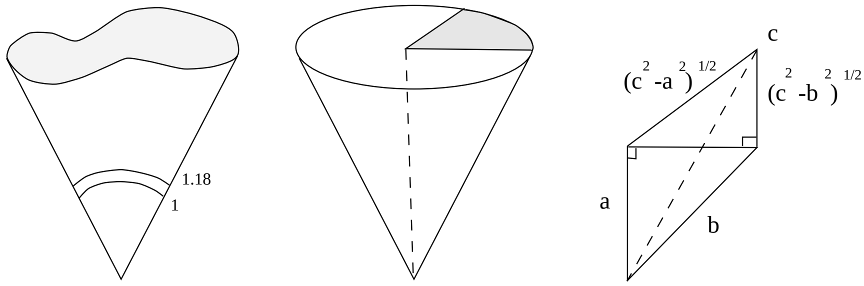

Figure 8.1. *Some sets of low density.*

computer. This full archive appears in [Hal05b]. The justification of 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 8.10. 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 [Hal05b] gives a separate nine-digit identifier to certain groups of inequalities. This permits us to reference such a group by a single number.

Definition 8.9. *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* $pt = 4\arctan(\sqrt{2}/5) - \pi/3 \approx 0.05537$.

Lemma 8.10. *A quasi-regular tetrahedron S satisfies $\sigma(S) \le 1\,pt$. Equality occurs if and only if the quasi-regular tetrahedron is regular of edge length* 2*.*

Proof. This is CALC-586468779. □

Remark 8.11. *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 $\sigma(S) \le 1\,pt$ in an explicit neighborhood of* $(2,2,2,2,2,2)$*.*

Lemma 8.12. *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 7.8. The general context (that is, contexts other than $(2,1)$ and $(4,0)$) of upright quarters is established by the inequalities[4] 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[5] $\Gamma(Q) \le 0$. 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 5.17. Since (Definition 7.6)

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

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 $\text{s-vor}(Q,\sqrt{2})$, it is nonpositive if and only if

$$A \le \delta_{oct}\,\text{vol}(\text{VC}(Q,v) \cap B(v,\sqrt{2})). \tag{8.1}$$

($\text{VC}(Q,0)$ is defined in Section 7.1.) The intersection $\text{VC}(Q,v) \cap B(v,\sqrt{2})$ 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 8.6, 8.7, and 8.8, these three types of solids give inequalities like that of Equation 8.1. Summing the inequalities from these lemmas, we get Equation 8.1.

Consider the case $\eta^+ \ge \sqrt{2}$ and $\sigma = \text{s-vor}$. If the quarter is upright, then[6] $\text{s-vor}(Q) \le 0$. 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[7] $\text{s-vor}(Q) \le 0$. The quarters achieving equality are extremal. In the remaining case, the only possible face along which the

[4] CALC-522528841 and CALC-892806084
[5] CALC-346093004
[6] CALC-40003553
[7] CALC-5901405

orientation is negative is the top face. This means that the analytic continuation defining s-vor(Q) is the same as

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

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,

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

We have s-vor$(Q, \sqrt{2}) \le 0$ as in the previous paragraph, by Lemma 8.6, 8.7, and 8.8. 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 8.13. *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* 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 shows is greater than 1.3045. By definition, s-vor$(S) < 0$ if and only if

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

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 8.5 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[8] s-vor$(S(y_1, y_2, \ldots, y_6)) < 0$ for $(y_1, \ldots, y_6)$ in any of the following four domains:

$$\begin{array}{ll} [2t_0, \sqrt{8}][2, 2t_0]^3[2t_0, \sqrt{8}][2, 2t_0], & [2t_0, \sqrt{8}][2, 2t_0]^3[2t_0, \sqrt{8}]^2, \\ [2, 2t_0]^3[2t_0, \sqrt{8}]^2[2, 2t_0], & [2, 2t_0]^3[2t_0, \sqrt{8}]^3 \end{array}$$

□

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

8.4 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 8.14. *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 4.21, no edge of a barrier passes through T. Hence they do not overlap. □

Lemma 8.15. *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 $\mathcal{Q}$.*

Proof. The edge $\{v, w\}$ must have length at least $2t_0$ by Lemma 4.19. If the edge $\{u, v\}$ has length at least $2t_0$, it cannot pass through b because of Lemma 4.33. If it has length at most $2t_0$, it cannot pass through b because of Lemma 4.19. 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 4.22 gives the result. If b is a face of a quarter in the Q-system, then Lemma 4.34 gives the result. □

Definition 8.16 (Law of Cosines). *Consider a triangle with sides a, b, and c. The angle opposite the edge of length c is given as*

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

Lemma 8.17 (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 4.21.

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. □

Lemma 8.18 (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 4.10 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 8.17, 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 4.24. 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 4.22 $\{0, v_2, v_3\}$ is a face of a quarter. Moreover, v_1 and v_1' are anchors of the diagonal of that quarter by Lemma 4.24. 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 4.34 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. □

Definition 8.19. *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 8.20. *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 4.21. 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. □

Definition 8.21. *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 $u \ne 0, v$ 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 8.22. *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 5.20 implies that x is unobstructed at 0. Thus $|x - u| < |x| \leq \sqrt{2}$.

Assume that the hypotheses of Condition 5 in Definition 8.21 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 8.15 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 8.18, 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 8.18 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 8.15 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 $|x-u| \le |x| \le \sqrt{2}$. 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 8.23. *Assume $|v| \le 2.36$. 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 8.21). 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 5.22, 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 8.24. *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 8.25. *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 5.23. 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 8.23 implies that $x \in C'(v)$. $\square$

Lemma 8.26. *Assume that $|u| \leq 2.36$ and that $|v| \leq 2.36$. The sets $C'(u)$, $C'(v)$ do not overlap for $u \neq v$.*

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 8.22 shows they do not overlap. In fact, the edges $\{0, u\}$ and $\{0, v\}$ are too short to pass through a barrier Suppose the edge $\{u, v\}$ passes through a barrier b. By Lemma 8.15 applied to $T = \{0, u, v\}$, the origin is a vertex of b. If neither of the simplices $\{u, b\}$ and $\{v, b\}$ are in $\mathcal{Q}_0$, then the plane through b separates $C'(u)$ from $C'(v)$. Assume without loss of generality that $S = \{v, b\} \in \mathcal{Q}_0$. By Condition 6 of the definition of C' (Definition 8.21), the segment from x to v does not intersect the cone at the origin formed by b. As in the proof of Lemma 8.22, x lies outside the cone $C(v)$; unless x and v lie in the same half space formed by the plane of b. The cone $C(u)$ intersects this half space at x. By Lemma 8.18, we have $\{u, b\} \in \mathcal{Q}_0$. Condition 6 in the definition of C' now keeps x at distance at least $\sqrt{2}$ from u. This completes the proof. □

Lemma 8.27. *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 4.21. □

8.5 Proofs

We are finally prepared to give a proof of Theorem 8.4. We break the proof into two lemmas.

Lemma 8.28. *If R is a standard region that is not a triangle, then $\sigma_R(D) \leq 0$.*

Proof. This proof is an adaptation of the main result in [Hal97b, Theorem 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 $\sigma_R(D) \leq 0$ 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 7.18, which gives the formula

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

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

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

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 8.12. 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 8.13 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 8.17 and 8.18, if a cone over some simplex in $\mathcal{Q}'_0$ meets $C'(v)$, then v must be a vertex of that simplex.) By Corollary 8.25, 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 8.8, 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 8.2. 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'.

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.

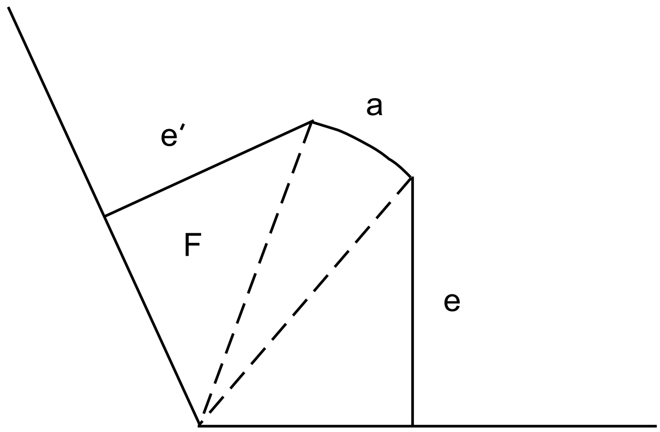

Figure 8.2. *A planar region.*

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 8.27.

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 5.18, 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 5.16 and 5.17). This is contrary to our assumption above that $\{0, v, w, w'\}$ is not in $\mathcal{Q}_0$.

These comments show that Figure 8.2 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 8.6 and 8.7, 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 8.29. *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 8.8 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 8.7, 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:

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

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

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

Proof. **Theorem 8.1 (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 8.10, 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 8.4, 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. □

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Section 9

The $\mathcal{S}$-system

9.1 Overview

In this section, we define a decomposition of a V-cell. Let VC be the V-cell at the origin. For any $t > 0$, let $V(t)$ be the intersection of VC with the ball $B(0,t)$ at the origin of radius t. We write VC as the disjoint union of $V(t_0)$ and its complement δ.

Assume that there is an upright quarter in the Q-system with diagonal $\{0, v\}$. As usual, we call $\{0, v\}$ an *upright diagonal*. We will define $\delta(v) \subset \delta$. It will be a subset of a set of the form $C(D_v) \cap \delta$ for some subset D_v of the unit sphere. The sets D_v will be defined so as not to overlap one another for distinct v. Then the sets $\delta(v)$ do not overlap one another either. We will give an explicit formula for the volume of $\delta(v)$.

We will define a set $\mathcal{S}$ of simplices, each having a vertex at the origin. (The letter '$\mathcal{S}$' is for simplex.) The vertices of the simplices will be vertices of the packing, and their edges will have length at most $2\sqrt{2}$. The sets $C(S)$, for distinct $S \in \mathcal{S}$, will not overlap. Over a simplex $S \in \mathcal{S}$, the V-cell will be truncated at a radius $t_S \geq t_0$. After defining the constants t_S, we will set

$$V_S(t_S) = C(S) \cap V(t_S) = C(S) \cap B(t_S) \cap \mathrm{VC}(0).$$

That is, $V_S(t_S)$ is the part of the V-cell at the origin, contained in the cone over S and in the ball of radius t_S. If $\mathrm{VC}(0) \cap C(S) \subset B(t_S) \subset B(t'_S)$, then $V_S(t_S) = V_S(t'_S)$.

Since $t_S \geq t_0$, the sets $V_S(t_S)$ and δ may overlap. Nevertheless, we will show that $V_S(t_S)$ does not overlap any $\delta(v)$. Let $V^{\mathcal{S}}(t_0)$ be the set of points in $V(t_0)$ that do not lie in $C(S)$, $S \in \mathcal{S}$. We will derive an explicit formula for the volume of $V^{\mathcal{S}}(t_0)$.

In VC(0), there are nonoverlapping sets

$$\delta(v), \quad V_S(t_S), \quad V^{\mathcal{S}}(t_0).$$

Let δ' be the complement in VC(0) of the union of these sets. These sets give a decomposition of VC(0). Corresponding to this decomposition is a formula for $\sigma(D)$ of the form

$$\sigma(D) = \text{c-vor}(V^{\mathcal{S}}(t_0)) + \sum_{\mathcal{S}} \text{c-vor}(V_S(t_S)) - \sum_v 4\delta_{oct}\text{vol}(\delta(v)) - 4\delta_{oct}\text{vol}(\delta').$$

Since $\text{vol}(\delta') \geq 0$, we obtain an upper bound on $\sigma(D)$ by dropping the rightmost term.

9.2 The set $\delta(v)$

Let $\{0, v\}$ be the diagonal of an upright quarter in $\mathcal{Q}_0$. We define $\delta(v) \subset C(D_v) \cap \delta$ for an appropriate subset D_v of the unit sphere.

Definition 9.1. *Set* $\eta_0(h) = \eta(2h, 2, 2t_0)$.

If $h \leq \sqrt{2}$, then $\eta_0(h) \leq \eta_0(\sqrt{2}) < 1.453$.

Let D_0 be the spherical cap on the unit sphere, centered along $\{0, v\}$ and having arcradius θ, where $\cos\theta = |v|/(2\eta_0(|v|/2))$.

The area of D_0 is $2\pi(1 - \cos\theta)$. Let $v_1, \ldots, v_k$ be the anchors around $\{0, v\}$ indexed cyclically. The radial projections of the edges $\{v, v_i\}$ (extended as necessary) slice the spherical cap into k wedges W_i, between $\{v, v_i\}$ and $\{v, v_j\}$, where $j \equiv i + 1 \mod k$, so that $D_0 = \cup W_i$.

Definition 9.2. *Let* $\mathcal{W}$ *be the set of wedges* $W = W_i$ *such that either*

1. W *occupies more than half the spherical cap (so that its area is at least* $\pi(1 - \cos\theta)$*), or*
2. $|v_i - v_j| \geq 2.77$, $\text{rad}(0, v, v_i, v_j) \geq \eta_0(|v|/2)$, *and the circumradius of* $\{0, v_i, v_j\}$ *or* $\{v, v_i, v_j\}$ *is* $\geq \sqrt{2}$.

Fix i, j, with $j \equiv i + 1 \mod k$. If $W = W_i$ is a wedge in $\mathcal{W}$, let $\{0, v_i, v\}^\perp$ be the plane through the origin and the circumcenter of $\{0, v_i, v\}$, perpendicular to $\{0, v_i, v\}$. Skip the following step if the circumradius of $\{0, v_i, v\}$ is greater than $\eta_0(|v|/2)$, but if the circumradius is at most this bound, let c_i be the intersection of $\{0, v_i, v\}^\perp$ with the circular boundary of W. Extend W by adding to W the spherical triangle with vertices the radial projections of v, v_i, and c_i. Similarly, extend W with the triangle from $\{v, v_j, c_j\}$, if the circumradius of $\{0, v_j, v\}$ permits. (An example of this is illustrated in Fig. 9.1.) Let W^e be extension of the wedge obtained by adding these two spherical triangles.

We will define $\delta(v, W^e) \subset C(W^e) \cap \delta$. Then $\delta(v)$ is defined as the union of $\delta(v, W^e)$, for $W \in \mathcal{W}$. Let

$$E_w = \{x : 2x \cdot w \leq w \cdot w\},$$

for $w = v, v_i, v_j$. These are half-spaces bounding the Voronoi cell. Set $E_\ell = E_{v_\ell}$.

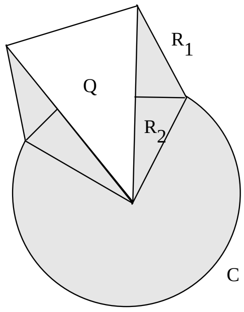

Figure 9.1. *An example of a set W^e (shaded region).*

If (2) holds, we let c be the radial projection of the circumradius of $\{0, v_i, v_j, v\}$ to the unit sphere. The arclength from c to the radial projection of v is θ', where

$$\cos\theta' = |v|/(2\,\mathrm{rad}) < |v|/(2\eta_0) = \cos\theta.$$

We conclude that $\theta' > \theta$ and c does not lie in D_0.

Definition 9.3. *In both cases (1) and (2), set*

$$\begin{aligned} \Delta(v, W^e) &= (E_v \cap E_i \cap E_j \cap C(W^e)) \\ \delta(v, W^e) &= \Delta(v, W^e) \setminus B(t_0). \end{aligned}$$

Remark 9.4. *There are some degenerate cases in this construction depending on the number of anchors. If there is no anchor, then $\Delta(v, W^e)$ is to be defined simply as $(E_v \cap C(W^e))$. If there is one anchor v_i, then*

$$\Delta(v, W^e) = (E_v \cap E_i \cap C(W^e)).$$

Remark 9.5. *The following remark applies when the points c_i and c_j have been constructed, and is irrelevant when that step was skipped in the construction described above. Observe that*

$$E_v \cap E_i \cap E_j \cap C(W^e)$$

is the union of four Rogers simplices

$$R(|w|/2, \eta(0, v, v_\ell), \eta_0(|v|/2)), \quad w = v, v_\ell, \quad \ell = i, j$$

and a conic wedge over W between c_i and c_j. (The inequality $\theta' > \theta$ implies that the Rogers simplices do not overlap.)

In general, we break $\Delta(v, W^e)$ into an inner part $\Delta^-(v, W^e)$ (the part outside the Rogers simplices together with (as many as) two Rogers simplices along $(0, v)$), and the Rogers simplices R_w, for $w = v_i, v_j$. We take R_w to be the empty set, when there is no anchor w with $\eta(0, v, w) < \eta_0(|v|/2)$.

We present a series of lemmas that explore the geometry of the sets $\Delta(v, W^e)$. In the next few lemmas we make use of a function ϵ, which is defined as follows.

Definition 9.6. *If Λ is a set of vertices containing v, let $\epsilon_v(\Lambda, x) \in \Lambda$ be given as the vertex $w \in \Lambda\setminus\{v\}$ such that the ray from v through x intersects the perpendicular bisecting plane of $\{v, w\}$ before that of any other $w' \in \Lambda \setminus \{v\}$. If the ray from v through x does not intersect any of the planes, then we set ϵ to the default value v. In cases of ties, resolve the tie in any consistent manner. If $x \in \Omega(0)$ (the Voronoi cell at the origin), then x lies in the cone over the face attached to the vertex $\epsilon_0(\Lambda, x) \in \Lambda$.*

We define a function ϵ' in a similar fashion. Assume $\epsilon_v(\Lambda, x) = w$, where the ray from v to x intersects the perpendicular bisector to $\{v, w\}$ at x'. Set

$$\epsilon'_v(\Lambda, x) = \epsilon_{w/2}(\Lambda \setminus \{w\}, x').$$

That is, move along the face of the Voronoi cell from x until another face is encountered. Let the corresponding vertex be the value of ϵ'. If $x \in \Omega(0)$ in the cone over the face attached to the vertex w, and if $w/2$ lies on that face, then x' lies in the sector of the face formed by the cone at $w/2$ generated by the edge of the Voronoi cell between the faces associated to w and $\epsilon'_0(\Lambda, x)$.

Lemma 9.7. *Let $S = \{0, v, w, u\}$ be a simplex. Assume that $\{0, v\}$ is an upright diagonal of a quarter in the Q-system, that w and v are anchors of $\{0, v\}$, and that $\mathrm{rad}(S) < \eta_0(|v|/2)$. Assume there is a wedge W of $\mathcal{W}$ along the face $\{0, v, w\}$ (on the same side of the face as u). Let R_w be the Rogers simplex $R(|w|/2, \eta(0, v, w), \eta_0(|v|/2))$ along the face $\{0, w, v\}$ along the edge of $\{0, w\}$ on the same side of the face as u. Then*

1. *There exists an anchor w' between u and w with $|w-w'| \le 2t_0$, and $|w'-w| \ge 2.77$.*
2. *$\{0, v, u, w'\}$ is an upright quarter in the Q-system and its face $\{0, v, w'\}$ is a barrier.*
3. *The barrier $\{0, v, w'\}$ obstructs every point of R_w from u.*

Proof. Since $\mathrm{rad}(S) < \eta_0(|v|/2)$ is contrary to the conditions defining wedges, the wedge must run from the face $\{0, v, w\}$ to a face $\{0, v, w'\}$, where w' is an anchor between w and u. By the hypotheses defining wedges $W \in \mathcal{W}$, we have that the length of $\{u, w'\}$ is at least 2.77. For the same reason, the circumradius of $\{0, v, w, w'\}$ is at least $\eta_0(|v|/2)$.

We claim that R_w lies in the convex hull of $S = \{0, v, w, w'\}$. Since $|w - w'| \ge 2.77$, we see that the orientation of each face of $\{0, v, w, w'\}$ is positive. Since $\mathrm{rad}(S) \ge \eta_0$, we have

$$R_w \subset R(|w|/2, \eta(0, v, w), \mathrm{rad}(S)) \subset S.$$

Thus it is enough to show that each point of the convex hull of S is obstructed.

For this, it is enough to show that the extreme point w is obstructed from u by the barrier $\{0, v, w'\}$. In other words, we show that the edge $\{w, v\}$ passes through $\{0, v, w'\}$. For this we show that no other geometrical configuration of points is possible.

w' is not in the convex hull of $\{0, v, w, u\}$ by Lemma 4.15. The vertex w' is not enclosed over $\{0, v, w, u\}$ because

$$\mathcal{E}(S(2, 2, 2t_0, 2t_0, 2t_0, 2(1.453), 2, 2, 2) > 2t_0.$$

(The constant 1.453 is from Definition 9.1.) The edge $\{v, w'\}$ does not pass through $\{0, w, u\}$, for otherwise we would reach a contradiction

$$2\eta_0(|v|/2) > 2\,\mathrm{rad}(S) \geq |u-w| \geq \mathcal{E}(S(2, 2, 2, \sqrt{8}, 2, 2), 2, 2, 2.77) \geq 2(1.453) \geq 2\eta_0(|v|/2).$$

We conclude that $\{u, w\}$ passes through $\{0, v, w'\}$. $\square$

Lemma 9.8. *Let $F = \{0, u_1, u_2\}$ be a quasi-regular triangle. Let $\{0, v\}$ be the diagonal of an upright quarter in the Q-system. The set $\Delta(v, W^e)$ does not overlap the cone at 0 over the triangle F.*

Proof. We prove the lemma for the subsets $\Delta^-(v, W^e)$ and R_w in two separate cases, beginning with $\Delta^-(v, W^e)$. Let S be the simplex $\{0, u_1, u_2, v\}$.

Assume that the orientation of S along F is negative. The simplex S is an upright quarter, so that u_1 and u_2 are anchors of v. This is contrary to the construction of the wedges W in $\mathcal{W}$. Thus, the orientation of F must be positive.

Assume that $\mathrm{rad}(S) < \eta_0(|v|/2)$. Then again, u_1 and u_2 are anchors. It follows that S is an upright quarter. As in the previous paragraph, this is contrary to construction. Thus, $\mathrm{rad}(S) \geq \eta_0(|v|/2)$.

We now have that the orientation of F is positive and that $\mathrm{rad}(S) \geq \eta_0(|v|/2)$. These two facts allow us to separate $\Delta^-(v, W^e)$ from $\{0, u_1, u_2, v\}$ as follows. Each interior point x of $\Delta^-(v, W^e)$ has

$$\epsilon_0(\{0, u_1, u_2, v\}, x) = v.$$

Let F_0 be the set of points in the intersection of $\Omega(0)$ with the convex hull of F. Each point y in F_0 has

$$\epsilon_0(\{0, u_1, u_2, v\}, y) \in \{u_1, u_2\}.$$

Since ϵ_0 takes distinct values on these two sets, they are disjoint.

Next consider the subset R_w, in the case that $w \in \{u_1, u_2\}$. To be definite, assume that $w = u_1$. The same argument as above establishes that the orientation of F is positive and that $\mathrm{rad}(S) \geq \eta_0(|v|/2)$. Each interior point x of R_w has

$$\epsilon_0'(\{0, u_1, u_2, v\}, x) = v$$

But each point y in F_0 has

$$\epsilon_0'(\{0, u_1, u_2, v\}, y) \in \{u_1, u_2\}.$$

This proves this case.

Until the end of the proof, we may assume that $w \notin \{u_1, u_2\}$. If the value of $\epsilon_0(\{0, u_1, u_2, w\}, \cdot)$ is w on interior points of R_w and in $\{u_1, u_2\}$ on F_0, then we have separated the sets. Assume to the contrary, that ϵ takes value w at a point x of F_0. Let $S'' = \{0, u_1, u_2, w\}$. This assumption implies that the orientation of S'' is negative along F. This in turn implies that S'' is a quasi-regular tetrahedron. The vertex v is not enclosed over S'', because the simplices in the Q-system do not overlap. For similar reasons, the face $\{0, v, w\}$ does not overlap the simplex S''. By the previous case (when $w \in \{u_1, u_2\}$), the interior of R_w does not intersect the faces of the quasi-regular tetrahedron S'' along the edge $\{0, w\}$. These facts imply that The interior of R_w is disjoint from S''. In particular, it does not meet the cone at 0 over the triangle F.

Assume finally that ϵ takes value u_1 or u_2 at an interior point y of R_w. (Say u_1.) Let $S' = \{0, v, w, u_1\}$. Assume that R_w lies on the same side of $\{0, v, w\}$ as u_1. If $\mathrm{rad}(S') < \eta_0(|v|/2)$, then each point of R_w is obstructed from u_1 (by Lemma 9.7). But no point of F_0 is obstructed from u_1. Thus, R_w and F_0 are disjoint in this case. Assume that $\mathrm{rad}(S') \geq \eta_0(|v|/2)$. If the orientation of $\{0, v, w\}$ in S' is negative, then S' is a quarter and the result follows. Assume that the orientation is positive. Now $\epsilon_0(S', x) = w$ for $x \in R_w$, contrary to assumption.

We may now assume that R_w lies outside the simplex S' on the opposite side of the face $\{0, v, w\}$. This case is dismissed by Lemma 5.31, which guarantees that the interior of R_w with $\epsilon = u_1$ are obstructed from u_1 by $\{0, v, w\}$. However, none of the points of F_0 with $\epsilon = u_1$ are obstructed from u_1. □

Corollary 9.9. *Each $\Delta(v, W^e)$ lies entirely in the cone over the standard region that contains $\{0, v\}$.*

Proof. The cone over a standard region is bounded by the cones over the quasi-regular triangles. □

Lemma 9.10. *Let $F = \{0, u_1, u_2\}$ be a triangle. Assume that $|u_1| \leq 2t_0$, $|u_2| \leq 2t_0$, and $2t_0 \leq |u_1 - u_2| \leq \sqrt{8}$. Let $\{0, v\}$ be the diagonal of an upright quarter in the Q-system. Assume that if u_1 and u_2 are both anchors of v, then they are consecutive anchors around v. Under these conditions, the set $\Delta(v, W^e)$ does not overlap the cone at 0 over the triangle F.*

Proof. The proof is similar to that of Lemma 9.8. We prove the lemma for the subsets $\Delta^-(v, W^e)$ and R_w in two separate cases, beginning with $\Delta^-(v, W^e)$. Let S be the simplex $\{0, u_1, u_2, v\}$. The orientation of S along F is positive.

Assume that $\mathrm{rad}(S) < \eta_0(|v|/2)$. Then u_1 and u_2 are anchors. By the hypotheses of the lemma, they are consecutive anchors. By the rules defining $\Delta^-(v, W^e)$, there is no wedge W^e between u_1 and u_2. Thus, the result follows in this case.

We now have that the orientation of F is positive and that $\mathrm{rad}(S) \geq \eta_0(|v|/2)$. These two facts allow us to separate $\Delta^-(v, W^e)$ from the cone over $\{0, u_1, u_2, v\}$ as follows. Each interior point x of $\Delta^-(v, W^e)$ has

$$\epsilon_0(\{0, u_1, u_2, v\}, x) = v.$$

Let F_0 be the intersection of $\Omega(0)$ with the convex hull of F. Each point y in F_0 has

$$\epsilon_0(\{0, u_1, u_2, v\}, y) \in \{u_1, u_2\}.$$

Next consider the subset R_w, in the case that $w \in \{u_1, u_2\}$. To be definite, assume that $w = u_1$. The same argument as above establishes that the orientation of F is positive and that $\mathrm{rad}(S) \geq \eta_0(|v|/2)$. Each interior point x of R_w has

$$\epsilon_0'(\{0, u_1, u_2, v\}, x) = v$$

But each point y in F_0 has

$$\epsilon_0'(\{0, u_1, u_2, v\}, y) \in \{u_1, u_2\}.$$

This proves this case.

Consider the subset R_w, in the case that $w \notin \{u_1, u_2\}$. As in the previous proof, if the value of $\epsilon_0(\{0, u_1, u_2, w\}, \cdot)$ is w on interior points of R_w and in $\{u_1, u_2\}$ on F_0, then we have separated the sets. Assume first to the contrary, that ϵ_0 takes value w at a point x of F_0. Let $S'' = \{0, u_1, u_2, w\}$. Our assumption on ϵ_0 implies that the orientation of S'' is negative along F, so that S'' is a flat quarter. The vertex v cannot be enclosed over S'', for otherwise w, u_1, and u_2 would all be anchors of v, which would mean that there is no region $W \in \mathcal{W}$. Similarly, the triangle $\{0, v, w\}$ cannot overlap the triangle $\{0, u_1, u_2\}$, for otherwise w, u_1, and u_2 would again be anchors, contrary to the hypothesis that u_1 and u_2 are consecutive anchors. Now we invoke Lemma 9.8, to establish that R_w does not intersect S'' and is therefore disjoint from F_0.

Assume finally, that ϵ_0 takes value u_1 or u_2 at an interior point y of R_w. (Say u_1.) This case is identical to the parallel case in the proof of Lemma 9.8. □

Lemma 9.11. *Let $F = \{0, u_1, u_2\}$ be a triangle. Assume that $2t_0 \leq |u_1| \leq \sqrt{8}$, $2 \leq |u_2| \leq 2t_0$, and $2 \leq |u_1 - u_2| \leq 2t_0$. Let $\{0, v\}$ be the diagonal of an upright quarter in the Q-system. Under these conditions, the set $\Delta(v, W^e)$ does not overlap the cone at 0 over the triangle F.*

Proof. Let $S = \{0, u_1, u_2, v\}$. The orientation of S along $\{0, u_1, u_2\}$ is positive. The circumradius $\mathrm{rad}(S)$ is at least $\eta_0(0, v, u_1) \geq \eta_0(|v|/2)$.

We now have that the orientation of F is positive and that $\mathrm{rad}(S) \geq \eta_0(|v|/2)$. We can then argue as in the proof of Lemmas 9.8 and 9.10, to get the result for $\Delta^-(v, W^e)$ and R_w (with $w = u_2$).

Consider the case R_w, with $w \neq u_2$. As in these earlier proofs, we may assume that ϵ_0 takes value w at a point x of F_0 (or that ϵ_0 takes value in $\{u_1, u_2\}$ at a point y of R_w).

In the case $\epsilon_0 = w$ at $x \in F_0$, let $S'' = \{0, u_1, w, u_2\}$. We have that $\epsilon_0 = w$ implies that the orientation of S'' along $\{0, u_1, u_2\}$ is negative. This in turn implies that S'' is an upright quarter. It is checked without difficulty that v is not enclosed over S'' and that the face $\{0, w, v\}$ does not cross the face $\{0, u_1, u_2\}$. It follows from Lemma 9.8 and the already treated cases of this lemma that R_w cannot intersect S''. Thus, it does not intersect the face $\{0, u_1, u_2\}$ of S''.

Finally, assume that ϵ_0 takes value in $\{u_1, u_2\}$ at a point y of R_w. The orientation of the face $\{0, v, w\}$ is positive in the simplex $\{0, v, w, u_1\}$ and the circumradius of $\{0, v, w, u_1\}$ is greater than $\eta_0(|v|/2)$. This implies that ϵ_0 does not take the value u_1. Assume that $\epsilon_0 = u_2$. This case is excluded in the same manner as the parallel case in the earlier Lemmas 9.8 and 9.10. ◻

Lemma 9.12. *Let $\{0, v\}$ be an upright diagonal of a quarter in the Q-system. If x lies in the interior of $\Delta(v, W^e)$, then x is unobstructed at* 0.

Proof. For a contradiction, assume that x is obstructed at 0 by barrier $T = \{u_1, u_2, u_3\}$.

The convex hull of T can be partitioned into three sets $T(i)$ depending on which vertex of T is closest to a given point in the convex hull. (Ties can be resolved in any consistent manner.) Let $y \in \Delta(v, W^e)$ be the point in the convex hull of T on the segment from 0 to x. Fix i so that $y \in T(i)$. If $v = u_i$, then each point y of $T(i)$ is closer to v than to 0. But each point of $\Delta(v, W^e)$ is closer to 0 than to v. So x is not obstructed by T at 0.

We may now assume that $v \neq u_i$.

Partition $\mathbb{R}^3$ geometrically into three sets $V(u_i)$, $V(0)$, $V(v)$ according to which of $\{u_i, 0, v\}$ a point $z \in \mathbb{R}^3$ is closest to. (Again resolve ties in any consistent manner.)

Assume further that $\max_j u_j \geq 2t_0$. This implies that $y \in T(i) \subset V(v) \cup V(u_i)$. On the other hand, we have by construction that $y \in \Delta(v, W^e) \subset V(0)$. (There are two cases involved in this conclusion, depending on whether u_i is an anchor of $\{0, v\}$.) However, the sets $V(\cdot)$ are disjoint; and we reach a contradiction. Thus, under these assumptions, x is unobstructed at 0.

Next assume that $\max_j u_j < 2t_0$. Let $S = \{0, u_1, u_2, u_3\}$. Since T is a barrier, $S \in \mathcal{Q}_0$. By assumption, $\{0, v\}$ is a diagonal of an upright quarter in $\mathcal{Q}_0$. By the nonoverlap of quarters in $\mathcal{Q}_0$, we see that v is not enclosed over S. The wedge W^e on the unit sphere is spherically star convex with respect to the center $v/|v|$. Thus, if $\Delta(v, W^e)$ intersects the convex hull of T at y, then $\Delta(v, W^e)$ intersects the cone over a face $\{0, u_1, u_2\}$ of S at y'. (We can take $y'/|y'|$ to lie on the cone generated by the arc running from $v/|v|$ to $y/|y|$. This is impossible by Lemmas 9.8 and 9.10. ◻

Lemma 9.13. *Let $\{0, v\}$ be the upright diagonal of a quarter in the $\mathcal{Q}_0$-system. Then the interior of $\Delta(v, W^e)$ is a subset of* VC(0).

Proof. We begin by showing that $\Delta^-(v, W^e) \subset \mathrm{VC}(0)$. Suppose to the contrary, that a point x in the interior of Δ^- lies in VC(w), with $w \neq 0$. Then x is closer to w than to 0. Thus, $\eta(0, v, w) < \eta_0(|v|/2)$, and w is an anchor of $\{0, v\}$. The face E_w in the construction $\Delta^-(v, W^e)$ prevents this from happening.

Now consider a point x of R_w, which we assume to lie in VC(u), with $u \neq 0$. To avoid a trivial case, we may assume that $w \neq u$.

Assume that the orientation of $S = \{0, v, w, u\}$ is negative along the face $\{0, v, w\}$. Then S must be an upright quarter. By the construction of wedges $W \in \mathcal{W}$, we have that R_w must lie on the opposite side of the plane $\{0, v, w\}$ from u (for there is no wedge between the anchors of an upright quarter). The result now follows from Lemma 5.31.

If $\mathrm{rad}(S) < \eta_0(|v|/2)$, then u and w are anchors. In this case, the result follows from Lemma 9.7.

Finally if the orientation is positive and if $\mathrm{rad}(S) \geq \eta(|v|/2)$, then a point of R_w cannot be closer to u than to 0. ∎

9.3 Overlap

Lemma 9.14. *The sets $\Delta(v, W^e)$ do not overlap one another.*

Proof. This is clear for two sets around the same vertex v. Consider the sets $\Delta(u, W^e)$ and $\Delta(v, W^e)$ at u and v.

To treat the points in $\Delta^-(u, W^e)$ and $\Delta^-(v, W^e)$, we may contract $\{u, v\}$ until $|u - v| = 2$. By the constraints on the edges of $\{0, u, v\}$, the circumcenter c of this triangle lies in the convex hull of the triangle. We have $\eta(0, u, v) \geq \eta_0(|v|/2)$ and $\eta(0, u, v) \geq \eta_0(|u|/2)$. So the plane through $\{0, c\}$ perpendicular to the plane $\{0, u, v\}$ separates $\Delta^-(u, W^e)$ from $\Delta^-(v, W^e)$.

Next we separate points in $\Delta^-(u, W^e)$ from points of $R_w^{(v)}$, where w is an anchor of v and $u \neq v$. Let $S = \{0, u, v, w\}$. The orientation of S along $\{0, v, w\}$ is positive. The circumradius of S satisfies

$$\mathrm{rad}(S) \geq \eta(0, u, v) > \eta_0(|v|/2).$$

Thus, $\epsilon_0(S, \cdot)$ takes different values on $\Delta^-(u, W^e)$ and $R_w^{(v)}$, so that the sets are disjoint.

Next we separate points of $R_w^{(v)}$ from $R_w^{(u)}$. (Notice that we assume that the anchor is the same for the two Rogers simplices.) Let $S = \{0, u, v, w\}$. As above, we have

$$\mathrm{rad}(S) \geq \eta_0(|v|/2), \quad \eta_0(|w|/2).$$

The simplex S has positive orientation along the faces $\{0, u, w\}$ and $\{0, v, w\}$. Let c_u be the circumcenter of $\{0, u, w\}$, let c_v be the circumcenter of $\{0, v, w\}$, and let

c be the circumcenter of S. Then $R_w^{(v)}$ lies in the convex hull of $\{0, w, c_v, c\}$, but $R_w^{(u)}$ lies in the convex hull of $\{0, w, c_u, c\}$. Thus, the sets are disjoint.

Finally, we separate points of $R_w^{(u)}$ from points of $R_{w'}^{(v)}$, where $w \neq w'$ and $u \neq v$. If the function $\epsilon_0(\{0, w, w'\}, \cdot)$ separates the sets, we are done. Otherwise, we may assume say that $\epsilon_0(\{0, w, w'\}, x) = w'$ from some $x \in R_w^{(u)}$. Let $S = \{0, u, w, w'\}$.

If w' is not an anchor of u, then $\mathrm{rad}(S) \geq \eta_0(|u|/2)$ and the orientation of S along $\{0, w, u\}$ is positive. In this case, we have $\epsilon_0 = w$ on $R_w^{(u)}$, which is contrary to assumption. Thus, we may assume that w' is an anchor of u.

If the orientation of $\{0, u, w, w'\}$ is negative along $\{0, w, u\}$, then $\{0, u, w, w'\}$ is a quarter, contrary to the existence of $W \in \mathcal{W}$. So the orientation is positive. If $\mathrm{rad}(\{0, u, w, w'\}) < \eta_0(|u|/2)$, then Lemma 9.7 implies that each point of R_w is obstructed from w'. But no point of $R_{w'}^{(v)}$ is obstructed from w. (In fact, a barrier that crosses $\Delta(v, W^e)$ is inconsistent with Lemmas 9.8, 9.10, 9.11.) So $\mathrm{rad}(\{0, u, w, w'\}) \geq \eta_0(|u|/2)$. This is contrary to $\epsilon_0(\{0, w, w'\}, x) = w'$ from some $x \in R_w^{(u)}$. □

9.4 The $\mathcal{S}$-system defined

We consider three types of simplices A, B, C. Each type has its vertices at vertices of the packing. The edge lengths of these simplices are at most $2\sqrt{2}$.

A. This family consists of simplices $S(y_1, \ldots, y_6)$ whose edge lengths satisfy

$$y_1, y_2, y_3 \in [2, 2t_0], \quad y_4, y_5 \in [2t_0, 2.77], \quad y_6 \in [2, 2t_0], \quad \text{and } \eta(y_4, y_5, y_6) < \sqrt{2}.$$

(These conditions imply $y_4, y_5 < 2.697$, because $\eta(2.697, 2t_0, 2) > \sqrt{2}$.)

B. This family consists of certain flat quarters that are part of an isolated pair of flat quarters. It consists of those satisfying $y_2, y_3 \leq 2.23$, $y_4 \in [2t_0, 2\sqrt{2}]$.

C. This family consists of certain simplices $S(y_1, \ldots, y_6)$ with edge lengths satisfying $y_1, y_4 \in [2t_0, 2\sqrt{2}]$, $y_2, y_3, y_5, y_6 \in [2, 2t_0]$. We impose the condition that the first edge is the diagonal of some upright quarter in the Q-system, and that the upper endpoints of the second and third edges (that is, the second and third vertices of the simplex) are consecutive anchors of this diagonal. We also assume that $y_4 < 2.77$, or that both face circumradii of S along the fourth edge are less than $\sqrt{2}$.

Lemma 9.15. *If a vertex w is enclosed over a simplex S of type A, B, or C, then its height is greater than 2.77. Also, $\{0, w\}$ is not the diagonal of an upright quarter in the Q-system.*

Proof. In case A, $\eta(y_4, y_5, y_6) < \sqrt{2}$, so an enclosed vertex must have height greater than $2\sqrt{2}$. It is too long to be the diagonal of a quarter.

In case B, we use the fact that the isolated quarter does not overlap any quarter in the Q-system. We recall that a function $\mathcal{E}$, defined in Section 4.2, measures the distance between opposing vertices in a pair of simplices sharing a face. An enclosed vertex has length at least

$$\mathcal{E}(S(2,2,2,2\sqrt{2},2t_0,2t_0),2t_0,2,2) > 2.77.$$

By the symmetry of isolated quarters, this means that the diagonal of a flat quarter must also be at least 2.77.

In case C, the same calculation gives that the enclosed vertex w has height at least 2.77. Let the simplex S be given by $\{0,v,v_1,v_2\}$, where $\{0,v\}$ is the upright diagonal. By Lemma 4.24, v_1 and v_2 are anchors of $\{0,w\}$. The edge between w and its anchor cannot cross $\{v,v_i\}$ by Lemma 4.19. (Recall that two sets are said to *cross* if their radial projections overlap.) The distance between w and v is at most $2t_0$ by Lemma 4.32. If $\{0,w\}$ is the diagonal of an upright quarter, the quarter takes the form $\{0,w,v_1,v_3\}$, or $\{0,w,v_2,v_3\}$ for some v_3, by Lemma 4.32. If both of these are quarters, then the diagonal $\{v_1,v_2\}$ has four anchors v, w, 0, and v_3. The selection rules for the Q-system place the quarters around this diagonal in the Q-system. So neither $\{0,w,v_1,v_3\}$ nor $\{0,w,v_2,v_3\}$ is in the Q-system. Suppose that $\{0,w,v_1,v_3\}$ is a quarter, but that $\{0,w,v_2,v_3\}$ is not. Then $\{0,w,v_1,v_3\}$ forms an isolated pair with $\{v_1,v_2,v,w\}$. In either case, the quarters along $\{0,w\}$ are not in the Q-system. □

Remark 9.16. *The proof of this lemma does not make use of all the hypotheses on C. The conclusion holds for any simplex $S(y_1,\ldots,y_6)$, with $y_1,y_4 \in [2t_0,2\sqrt{2}]$, $y_2,y_3,y_5,y_6 \in [2,2t_0]$.*

9.5 Disjointness

Let $S = \{0,v_1,v_2,v_3\}$ be a simplex of type A, B, or C. An edge $\{v_4,v_5\}$ of length at most $2\sqrt{2}$ such that $|v_4|,|v_5| \le 2t_0$ cannot cross two of the edges $\{v_i,v_j\}$ of S. In fact, it cannot cross any edge $\{v_i,v_j\}$ with $|v_i|,|v_j| \le 2t_0$ by Lemma 4.30. The only possibility is that the edge $\{v_4,v_5\}$ crosses the two edges with endpoint v_1, with $|v_1| \ge 2t_0$ in case C. But this too is impossible by Lemma 4.32.

Similar arguments show that the same conclusion holds for an edge $\{v_4,v_5\}$ of length at most $2t_0$ such that $|v_4| \le 2t_0$, $v_5 \le 2\sqrt{2}$. The only additional fact that is needed is that $\{v_4,v_5\}$ cannot cross the edge between the vertex v of an upright diagonal $\{0,v\}$ and an anchor (Lemma 4.19).

Lemma 9.17. *Consider two simplices S, S', each of type A, B, C, or a quarter in the Q-system. Assume that S and S' do not lie in the cone over a quadrilateral region. Then S and S' do not overlap.*

Proof. By hypothesis, the standard region is not a quadrilateral, and we thus exclude the case of conflicting diagonals in a quad cluster. We claim that no vertex w of S is enclosed over S'. Otherwise, w must have height at least $2t_0$, so that $\{0,w\}$ is the diagonal of an upright in the Q-system, and this is contrary to Lemma 9.15. Similarly, no vertex of S' is enclosed over S.

Let $\{v_1, v_2\}$ be an edge of S crossing an edge $\{v_3, v_4\}$ of S'. By the preceding remarks, neither of these edges can cross two edges of the other simplex. The endpoints of the edges are not enclosed over the other simplex. This means that one endpoint of each edge $\{v_1, v_2\}$ and $\{v_3, v_4\}$ is a vertex of the other simplex. This forces S and S' to have three vertices in common, say 0, v_2, and v_3. We have $S = \{0, v_1, v_3, v_2\}$ and $S' = \{0, v_3, v_2, v_4\}$. If $|v_2| \in [2t_0, 2\sqrt{2}]$, then we see that the anchors v_3, v_4 of $\{0, v_2\}$ are not consecutive. This is impossible for simplices of type C and upright quarters. Thus, v_2 and v_3 have height at most $2t_0$. We conclude, without loss of generality, that $|v_4| \in [2t_0, 2\sqrt{2}]$ and $|v_1 - v_2| \geq 2t_0$.

The heights of the vertices of S are at most $2t_0$, so it has type A or B, or it is a flat quarter in the Q-system. If S' is an upright quarter in the Q-system, then it does not overlap an isolated quarter or a flat quarter in the Q-system, so S has type A. This imposes the contradictory constraints on A

$$2.77 \geq |v_1 - v_2| \geq \mathcal{E}(S(2t_0, 2, 2, 2\sqrt{2}, 2t_0, 2t_0), 2, 2, 2) > 2.77.$$

Thus S' has type C. This forces S to have type A. We reach the same contradiction $2.77 \geq \mathcal{E} > 2.77$. □

9.6 Separation of simplices of type A

Let $V_S = \mathrm{VC}(0) \cap C(S)$, for a simplex S of type A, B, or C. We truncate V_S to $V_S(t_S)$ by intersecting V_S with a ball of radius t_S. The parameters t_S depend on S.

If S has type A, we use $t_S = +\infty$ (no truncation). If v is enclosed over $S = \{0, v_1, v_2, v_3\}$, then since $\eta(v_1, v_2, v_3) < \sqrt{2}$, the face $\{v_1, v_2, v_3\}$ has positive orientation for S and $\{v, v_1, v_2, v_3\}$. This implies that the V-cells at v and 0 do not intersect, and there is no need to truncate. If a simplex adjacent to S has negative orientation along a face shared with A, then it must be a quarter $Q = \{0, v_4, v_1, v_2\}$ (Lemma 5.13) or quasi-regular tetrahedron. It cannot be an isolated quarter because of the edge length constraint 2.77 on simplices of type A. If it is in the Q-system, the face between S and the adjacent simplex is a barrier, and it does not interfere with the V-cell over S. Assume that it is not in the Q-system. There must be a conflicting diagonal $\{0, w\}$, where w is enclosed over Q. (w cannot be enclosed over S by results of Lemma 9.17.) This shields the V-cell at v_4 from $C(S)$ by the two barriers $\{0, w, v_1\}$ and $\{0, w, v_2\}$ of quarters in the Q-system.

This shows that nothing external to a simplex of type A affects the shape of $V_S(t_S)$ (that is, $\mathrm{VC}(0) \cap C(S)$ consists of points of S that are closer to 0 than to the other vertices of S). Thus, $V_S(t_S)$ can be computed from S alone. Similarly, $V_S(t_S)$ does not influence the external geometry, since all faces have positive orientation.

We also remark that $V_S(t_S)$ does not overlap any of the sets $\Delta(v, W^e)$. This is evident from Lemmas 9.8 and 9.10.

Our justification that $V_S(t_S)$ can be treated as an independently scored entity is now complete.

9.7 Separation of simplices of type B

If $S(y_1, \ldots, y_6)$ has type B, we label vertices so that the diagonal is the fourth edge, with length y_4. We set $t_S = 1.385$. The calculation of $\mathcal{E}$ in Lemma 9.15 shows that any enclosed vertex over S has height at least $2.77 = 2t_S$.

Vertices outside $C(S)$ cannot affect the shape of $V_S(t_S)$. In fact, such a vertex v' would have to form a quarter or quasi-regular tetrahedron with a face of S. The V-cell at v' cannot meet $C(S)$ unless it is a quarter that is not in the Q-system. But by definition, an isolated quarter is not adjacent (along a face along the diagonal) to any other quarters.

To separate the scoring of $V_S(t_S)$ from the rest of the standard cluster, we also show that the terms of Formula 7.12 for $V_S(t_S)$ are represented geometrically by solids that lie in the cone $C(S)$. This is more than a formality because S can have negative orientation along the face F formed by the origin and the diagonal (the fourth edge).

Definition 9.18. *Let $\beta_\psi(\theta) \in [0, \pi/2]$ be defined by the equations*

$$\cos^2 \beta_\psi = (\cos^2 \psi - \cos^2 \theta)/(1 - \cos^2 \theta), \text{ for } \psi \leq \theta,$$

Let p and q be points on the unit sphere separated by arclength θ. If we place a spherical cap of arcradius ψ on the unit sphere centered at p, then $\beta_\psi(theta)$ is the angle at q between the arc (q, p) and the tangent to the cap which passes through q.

Let $S = \{0, v_1, v_2, v_3\}$, where v_i is the endpoint of the ith edge. We establish that the solids representing the conic and Rogers terms of Formula 7.12 lie over $C(S)$ by showing[9] that $\beta_\psi(\text{arc}(y_1, y_3, y_5)) < \text{dih}_3(S(y_1, \ldots, y_6))$, where dih_3 is the dihedral angle along the third edge. We use $\cos \psi = y_1/2.77$ and assume $y_2, y_3 \in [2, 2.23]$.

The reasons given in Section 9.6 for the disjointness of $\delta(v)$ and $V_S(t_S)$ apply to simplices of type B as well. This completes the justification that $V_S(t_S)$ is an object that can be treated in separation from the rest of the local V-cell.

9.8 Separation of simplices of type C

If $S(y_1, \ldots, y_6)$ is of type C, we label vertices so that the upright diagonal is the first edge. We use $t_S = +\infty$ (no truncation). Each face of S has positive orientation by Lemma 5.13. So $V_S(t_S) \subset S$.

Vertices outside S cannot affect the shape of $V_S(t_S)$. Any vertex v' would have to form a quarter along a face of S. If the shared face lies along the first edge, it is a quarter Q in the Q-system, because one and hence all quarters along this edge are in the Q-system. The faces of this quarter are then barriers. If the shared face lies along the fourth edge, then its length is at most 2.77, so that the quarter cannot be part of an isolated pair. If it is not in the Q-system, there must be a conflicting diagonal. The two faces along this conflicting diagonal of the adjacent

[9] CALC-193836552

pair in the Q-system (that is, the pair taking precedence over Q in the Q-system) are barriers that shield the V-cell at v' from S.

The reasons given in Section 9.6 for the disjointness of $\delta(v)$ and $V_S(t_S)$ apply to simplices of type C as well. This completes the justification that $V_S(t_S)$ is an object that can be treated in separation from the rest of the local V-cell.

9.9 Simplices of type C'

We introduce a small variation on simplices of type C, called type C'. We define a simplex $\{0, v, v_1, v_2\}$ of type C' to be one satisfying the following conditions.

1. The edge $\{0, v\}$ is an upright diagonal of an upright quarter in the Q-system.
2. $|v_2| \in [2.45, 2t_0]$.
3. v_1 and v_2 are anchors of v.
4. $|v - v_2| \in [2.45, 2t_0]$.
5. The edge $\{v_1, v_2\}$ is a diagonal of a flat quarter with face $\{0, v_1, v_2\}$.

It follows that v_1 and v_2 are consecutive anchors of $\{0, v\}$.

On simplices S of type C', we label vertices so that the upright diagonal is the first edge. We use $t_S = +\infty$ (no truncation). Each face of S has positive orientation by Lemma 5.13. So $V_S(t_S) \subset S$.

Simplices of type C' are separated from quarters in the Q-system and simplices of types A and B by procedures similar to those described for type C. The following lemma is helpful in this regard.

Lemma 9.19. *The flat quarter along the face $\{0, v_1, v_2\}$ is in the Q-system.*

Proof.

$$\mathcal{E}(S(2, 2, 2.45, 2\sqrt{2}, 2t_0, 2t_0), 2, 2, 2) > 2\sqrt{2},$$

so nothing is enclosed over the flat quarter.

$$\mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2t_0, 2t_0), 2t_0, 2.45, 2) > 2\sqrt{2},$$

so no edge between vertices of the packing can cross inside the anchored simplex. This implies that the flat quarter does not have a conflicting diagonal and is not part of an isolated pair. $\square$

Similar arguments show that there is not a simplex with negative orientation along the top face of S.

Unlike the other cases, there can in fact be overlap between $\Delta(v, W^e)$ and simplex of type C', when the upright diagonal of the simplex is $\{0, v\}$. This is because the conditions defining a wedge $W \in \mathcal{W}$ are not incompatible with the conditions defining type C'. Nevertheless, except in the obvious case where the simplex of type C' and the wedge are both constructed between the same consecutive anchors of $\{0, v\}$, there can be no overlap of a $\Delta(v, W^e)$ with a simplex of type C'.

9.10 Scoring

The construction of the decomposition of the V-cell VC(0) is now complete. It consists of the pieces

- $\delta(v)$, for each diagonal $\{0, v\}$ of an upright quarter in the Q-system,
- truncations of Voronoi pieces $V_S(t_S)$ for simplices of type A, B, or C (and on rare occasion C'),
- $V^{\mathcal{S}}(t_0)$, the truncation at t_0 of all parts of VC(0) that do not lie in any of the cones $C(S)$ over simplices of type A, B or C,
- δ', the part not lying in any of the preceding.

By the results of Sections 9.6, 9.7, 9.8, $\sigma(D)$ can be broken into a corresponding sum,

$$\begin{aligned} \sigma_R(D) &= \textstyle\sum_Q \sigma(Q) + \sigma(V_P), \text{ for quarters } Q \text{ in the } Q\text{-system, where} \\ \sigma(V_P) &= \text{c-vor}(V_P^{\mathcal{S}}(t_0)) + \textstyle\sum_{A,B,C} \text{c-vor}(V_S(t_S)) - \sum_v 4\delta_{oct}\text{vol}(\delta_P(v)) - 4\delta_{oct}\text{vol}(\delta'_P). \end{aligned}$$

By dropping the final term, $4\delta_{oct}\text{vol}(\delta'_P)$, we obtain an upper bound on $\sigma(V_P)$. Because of the separation results of Sections 9.6–9.7, we may score $V_P^{\mathcal{S}}(t_0)$ by Formula 7.13. Bounds on the score of simplices of type B appear in CALC-193836552.

Lemma 9.20. *Let R be a standard region that is not a triangle in a decomposition start D. $\tau_{0,R}(D) \geq 0$.*

Proof. Everything truncated at t_0 can be broken into three types of pieces: Rogers simplices $R(a, b, t_0)$, wedges of t_0-cones, and spherical regions. (See Figure 8.1.) The wedges of t_0-cones and spherical regions can be considered as the degenerate cases $b = t_0$ and $a = b = t_0$ of Rogers simplices, so it is enough to show that $\tau(R(a, b, t_0)) \geq 0$. We have $t_0 > \sqrt{3/2}$, so by Rogers's lemma [Hal97a, Lemma 8.6.2],

$$\tau(R(a, b, t_0)) > \tau(R(1, \eta(2, 2, 2), \sqrt{3/2})).$$

The right-hand side is zero. (In fact, the vanishing of the right-hand side is essentially Rogers's bound. When Rogers's bound is met, $\tau = 0$.) ∎

Section 10

Bounds on the Score in Triangular and Quadrilateral Regions

10.1 The function τ

We consider the functions $\sigma_R(D) - \lambda\zeta \operatorname{sol}(R)\, pt$, for $\lambda = 0$, 1, or 3.2, where R is a standard cluster. We write

$$\tau_R(D) = \operatorname{sol}(R)\zeta\, pt - \sigma_R(D).$$

We will see that $\tau_R(D)$ has a simple interpretation. If D is a decomposition star with standard clusters $\{R\}$, set $\tau(D) = \sum_R \tau_R(D)$.

Lemma 10.1. *$\tau_R(D) \geq 0$, for all standard clusters R.*

Proof. If R is not a quasi-regular tetrahedron, then $\sigma_R(D) \leq 0$ by Theorem 8.4 and $\operatorname{sol}(R) > 0$, so that the result is immediate. If R is a quasi-regular tetrahedron, the result appears in the archive of inequalities CALC-53415898. □

Lemma 10.2.

$$\sigma(D) = 4\pi\zeta\, pt - \tau(D).$$

Proof. Let $\{R\}$ be the standard clusters in D. Then

$$\sigma(D) = \sum_R \sigma_{R_i}(D) + (4\pi - \sum_R \operatorname{sol}(R_i))\zeta\, pt = 4\pi\zeta\, pt - \sum_R \tau_{R_i}(D).$$

□

Since $22.8 > 4\pi\zeta$ and $14.8\, pt > 4\pi\zeta\, pt - 8\, pt$, we find as an immediate corollary that if there are standard clusters satisfying $\tau_{R_1}(D) + \cdots + \tau_{R_k}(D) \geq 14.8\, pt$, then D does not contravene.

The function $\tau_R(D)$ gives the amount *squandered* by a particular standard cluster R. If nothing is squandered, then $\tau_{R_i}(D) = 0$ for every standard cluster, and the upper bound is $4\pi\zeta\, pt \approx 22.8\, pt$. To say that a decomposition star does not contravene is to say that at least $(4\pi\zeta - 8)pt \approx 14.8\, pt$ are squandered.

Remark 10.3. *(This remark is not used elsewhere.) The bound $\sigma(D) \leq 4\pi\zeta\, pt$ implies Rogers's bound on density. It is the unattainable bound that would be obtained by packing regular tetrahedra around a common vertex with no distortion and no gaps. (More precisely, in the terminology of [Hal92], the score $s_0 = 4\pi\zeta\, pt$ corresponds to the effective density $16\pi\delta_{oct}/(16\pi - 3s_0) = \sqrt{2}/\zeta \approx 0.7796$, which is Rogers's bound.) Every positive lower bound on some $\tau_R(D)$ translates into an improvement on Rogers's bound.*

Lemma 10.4. *A triangular standard region does not contain any enclosed vertices.*

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

10.2 Types

Let v be a vertex of height at most $2t_0$. We say that v has *type* (p, q) if every standard region with a vertex at $\bar{v}$ (the radial projection of v) is a triangle or a quadrilateral, and if there are exactly p triangular faces and q quadrilateral faces that meet at $\bar{v}$. We write (p_v, q_v) for the type of v.

This section derives the bounds on the scores of the clusters around a given vertex as a function of the type of the vertex. Define constants $\tau_{\mathrm{LP}}(p, q)/pt$ by Table 10.1. The entries marked with an asterisk will not be needed.

$\tau_{\mathrm{LP}}(p,q)/pt$	$q=0$	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	*	*	*	*	*

(10.1)

Lemma 10.5. *Let $S_1, \ldots, S_p$ and $R_1, \ldots, R_q$ be the tetrahedra and quad clusters around a vertex of type (p, q). Consider the constants of Table 10.1. Now,*

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

Proof. Set

$$(d_i^0, t_i^0) = (\mathrm{dih}(S_i), \tau(S_i)), \qquad (d_i^1, t_i^1) = (\mathrm{dih}(R_i), \tau(R_i)).$$

The linear combination $\sum^p \tau(S_i) + \sum^q \tau_{R_i}(D)$ is at least the minimum of $\sum^p t_i^0 + \sum^q t_i^1$ subject to $\sum^p d_i^0 + \sum^q d_i^1 = 2\pi$ and to the system of linear inequalities CALC-830854305 and the system of linear inequalities CALC-940884472 (obtained by replacing τ and dihedral angles by t_i^j and d_i^j). The constant $\tau_{\mathrm{LP}}(p,q)$ was chosen to be slightly smaller than the actual minimum of this linear programming problem.

The entry $\tau_{\mathrm{LP}}(5,0)$ is based on Lemma 10.6, $k=1$. □

Lemma 10.6. *Let $v_1, \ldots, v_k$, for some $k \le 4$, be distinct vertices of a decomposition star of type $(5,0)$. Let $S_1, \ldots, S_r$ be quasi-regular tetrahedra around the edges $\{0, v_i\}$, for $i \le k$. Then*

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

and

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

Proof. We have $\tau(S) \ge 0$, for any quasi-regular tetrahedron S. We refer to the edges y_4, y_5, y_6 of a simplex $S(y_1, \ldots, y_6)$ as its top edges. Set $\xi = 2.1773$.

The proof of the first inequalities relies on seven calculations[10]. Throughout the proof, we will refer to these inequalities simply as Inequality i, for $i = 1, \ldots, 7$.

We claim (Claim 1) that if $S_1, \ldots, S_5$ are quasi-regular tetrahedra around an edge $\{0, v\}$ and if $S_1 = S(y_1, \ldots, y_6)$, where $y_5 \ge \xi$ is the length of a top edge e on S_1 shared with S_2, then $\sum_1^5 \tau(S_i) > 3(0.55)\,pt$. This claim follows from Inequalities 1 and 2 if some other top edge in this group of quasi-regular tetrahedra has length greater than ξ. Assuming all the top edges other than e have length at most ξ, the estimate follows from $\sum_1^5 \mathrm{dih}(S_i) = 2\pi$ and Inequalities 3, 4.

Now let $S_1, \ldots, S_8$ be the eight quasi-regular tetrahedra around two edges $\{0, v_1\}$, $\{0, v_2\}$ of type $(5,0)$. Let S_1 and S_2 be the simplices along the face $\{0, v_1, v_2\}$. Suppose that the top edge $\{v_1, v_2\}$ has length at least ξ. We claim (Claim 2) that $\sum_1^8 \tau(S_i) > 4(0.55)\,pt$. If there is a top edge of length at least ξ that does not lie on S_1 or S_2, then this claim reduces to Inequality 1 and Claim 1. If any of the top edges of S_1 or S_2 other than $\{v_1, v_2\}$ has length at least ξ, then the claim follows from Inequalities 1 and 2. We assume all top edges other than $\{v_1, v_2\}$ have length at most ξ. The claim now follows from Inequalities 3 and 5, since the dihedral angles around each vertex sum to 2π.

We prove the bounds for τ. The proof for σ is entirely similar, but uses the constant $\xi = 2.177303$ and seven new calculations[11] rather than the seven given

[10] CALC-636208429
[11] CALC-129662166

above. Claims analogous to Claims 1 and 2 hold for the σ bound by this new group of seven inequalities.

Consider τ for $k = 1$. If a top edge has length at least ξ, this is Inequality 1. If all top edges have length less than ξ, this is Inequality 3, since dihedral angles sum to 2π.

We say that a top edge lies around a vertex v if it is an edge of a quasi-regular tetrahedron with vertex v. We do not require v to be the endpoint of the edge.

Take $k = 2$. If there is an edge of length at least ξ that lies around only one of v_1 and v_2, then Inequality 1 reduces us to the case $k = 1$. Any other edge of length at least ξ is covered by Claim 1. So we may assume that all top edges have length less than ξ. And then the result follows easily from Inequalities 3 and 6.

Take $k = 3$. If there is an edge of length at least ξ lying around only one of the v_i, then Inequality 1 reduces us to the case $k = 2$. If an edge of length at least ξ lies around exactly two of the v_i, then it is an edge of two of the quasi-regular tetrahedra. These quasi-regular tetrahedra give $2(0.55)\,pt$, and the quasi-regular tetrahedra around the third vertex v_i give $0.55\,pt$ more. If a top edge of length at least ξ lies around all three vertices, then one of the endpoints of the edge lies in $\{v_1, v_2, v_3\}$, so the result follows from Claim 1. Finally, if all top edges have length at most ξ, we use Inequalities 3, 6, 7.

Take $k = 4$. Suppose there is a top edge e of length at least ξ. If e lies around only one of the v_i, we reduce to the case $k = 3$. If it lies around two of them, then the two quasi-regular tetrahedra along this edge give $2(0.55)\,pt$ and the quasi-regular tetrahedra around the other two vertices v_i give another $2(0.55)\,pt$. If both endpoints of e are among the vertices v_i, the result follows from Claim 2. This happens in particular if e lies around four vertices. If e lies around only three vertices, one of its endpoints is one of the vertices v_i, say v_1. Assume e is not around v_2. If v_2 is not adjacent to v_1, then Claim 1 gives the result. So taking v_1 adjacent to v_2, we adapt Claim 1, by using all seven Inequalities, to show that the eight quasi-regular tetrahedra around v_1 and v_2 give $4(0.55)\,pt$. Finally, if all top edges have length at most ξ, we use Inequalities 3, 6, 7. □

In a special case, the constant of Lemma 10.6 can be improved by a small amount. This small improvement will be used in Paper V.

Lemma 10.7. *Let v be a vertex of a decomposition star of type $(5, 0)$. Let $S_1, \ldots, S_5$ be quasi-regular tetrahedra around the edge $\{0, v\}$. Then*

$$\sum_{i=1}^{5} \sigma(S_i) < 4.52\,pt - 10^{-8}.$$

Proof. If any of the top edges has length greater than ξ, we use a slightly improved calculation[12] that yields this constant. Otherwise, the same calculation[13] that was

[12] CALC-241241504-1
[13] CALC-82950290

used in the previous lemma gives the desired estimate

$$\sum \sigma < 5(0.31023815) - 2\pi(0.207045) < 4.52\,pt - 10^{-8}$$

□

10.3 Limitations on Types

Recall that a vertex of a planar map has type (p, q) if it is the vertex of exactly p triangles and q quadrilaterals. This section restricts the possible types that appear in a decomposition star.

Let t_4 denote the constant $0.1317 \approx 2.37838774\,pt$.

Lemma 10.8. *If R is a quad cluster, then*

$$\tau_R(D) \geq t_4.$$

Proof. A calculation[14] asserts precisely this. □

Lemma 10.9. *The following eight types (p, q) are impossible: (1) $p \geq 8$, (2) $p \geq 6$ and $q \geq 1$, (3) $p \geq 5$ and $q \geq 2$, (4) $p \geq 4$ and $q \geq 3$, (5) $p \geq 2$ and $q \geq 4$, (6) $p \geq 0$ and $q \geq 6$, (7) $p \leq 3$ and $q = 0$, (8) $p \leq 1$ and $q = 1$.*

Proof. Calculations[15] give a lower bound on the dihedral angle of p simplices and q quadrilaterals at $0.8638p + 1.153q$ and an upper bound of $1.874445p + 3.247q$. If the type exists, these constants must straddle 2π. One readily verifies in Cases 1–8 that these constants do not straddle 2π. □

Lemma 10.10. *If the type of any vertex of a decomposition star is one of $(4, 2)$, $(3, 3)$, $(1, 4)$, $(1, 5)$, $(0, 5)$, $(0, 2)$, then the decomposition star does not contravene.*

Proof. According to Table 10.1, we have $\tau_{\mathrm{LP}}(p, q) > (4\pi\zeta - 8)\,pt$, for $(p, q) = (4, 2)$, $(3, 3)$, $(1, 4)$, $(1, 5)$, $(0, 5)$, or $(0, 2)$. By Lemma 10.2, the result follows in these cases. □

Remark 10.11. *In summary of the preceding two lemmas, we find that we may*

[14] CALC-996268658

[15] CALC-657406669, CALC-208809199, CALC-984463800, and CALC-277330628

restrict our attention to the following types of vertices.

$$\begin{array}{cccc}
(7,0) & & & \\
(6,0) & & & \\
(5,0) & (5,1) & & \\
(4,0) & (4,1) & & \\
 & (3,1) & (3,2) & \\
 & (2,1) & (2,2) & (2,3) \\
 & & (1,2) & (1,3) \\
 & & & (0,3) \quad (0,4)
\end{array}$$

It will be shown in Lemma 12.3, that the type $(7,0)$ *does not occur in a contravening decomposition star.*

10.4 Bounds on the Score in Quadrilateral Regions

If the quad cluster has a diagonal of length at most $\sqrt{8}$ between two corners, there are three possible decompositions. (1) The two quarters formed by the diagonal lie in the Q-system so that the scoring rules for the Q-system are used. (2) There is a second diagonal of length at most $\sqrt{8}$, and we use the two quarters from the second diagonal for the scoring. (3) There is an enclosed vertex that makes the quad cluster into a quartered octahedron and the four upright quarters are in the Q-system.

Now suppose that neither diagonal is less than $\sqrt{8}$ and the quad cluster is not a quartered octahedron. If there is no enclosed vertex of length at most $\sqrt{8}$, the quad cluster contains no quarters. An upper bound on the score of the quad cluster (P, D) is $\mathrm{vor}_P(D, \sqrt{2})$. The remaining cases are called *mixed* quad clusters. Mixed quad clusters enclose a vertex of height at most $\sqrt{8}$ and do not contain flat quarters.

Lemma 10.12. *Assume a figure exists with vertices* $v_1, \ldots, v_4$, v *subject to the constraints*

$$\begin{array}{rl}
2 \leq & |v_i| \leq 2t_0, \\
2 \leq & |v_i - v_{i+1}| \leq 2t_0, \\
2 \leq & |v_i - v_{i+2}|, \\
h_i \leq & |v - v_i|, \\
2 \leq & |v| \leq 2t_0, \ \textit{for } i = 1, \ldots, 4 \ (\textit{mod } 4)
\end{array}$$

where h_i *are fixed constants that satisfy* $h_i \in [2, 2\sqrt{2})$. *Let* L *be the quadrilateral on the unit sphere with vertices* $v_i/|v_i|$ *and edges running between consecutive vertices. Assume that* v *lies in the cone at the origin obtained by scaling* L. *Then another figure exists made of a (new) collection of vectors* $v_1, \ldots, v_4$ *and* v *subject to the constraints above together with the additional constraints*

$$\begin{array}{l}
|v_i - v_{i+1}| = 2t_0 \\
|v_i| = 2, \ \textit{for } i = 1, \ldots, 4, \\
|v| = 2t_0.
\end{array}$$

Moreover, the quadrilateral L may be assumed to be convex.

Proof. This lemma in pure geometry is a special case of [Hal97a, Lemma 4.3]. □

Lemma 10.13. *A quadrilateral region does not enclose any vertices of height at most $2t_0$.*

Proof. Let $v_1, \ldots, v_4$ be the corners of the quad cluster, and let v be an enclosed vertex of height at most $2t_0$. We cannot have $|v_i - v| \le 2t_0$ for two different vertices v_i, because two such inequalities would partition the region into two separate standard regions instead of a single quadrilateral region.

We apply Lemma 10.12 to assume

$$|v_i - v_{i+1}| = 2t_0, \quad |v_i| = 2, \quad |v| = 2t_0,$$

for $i = 1, \ldots, 4$. Reindexing and perturbing v as necessary, we may assume that $2 \le |v_1 - v| \le 2t_0$ and $|v_i - v| \ge 2t_0$, for $i = 2, 3, 4$. Moving v, we may assume it reaches the minimal distance to two adjacent corners (2 for v_1 or $2t_0$ for v_i, $i > 1$). Keeping v fixed at this minimal distance, perturb the quad cluster along its remaining degree of freedom until v attains its minimal distance to three of the corners. This is a rigid figure. There are four possibilities depending on which three corners are chosen. Pick coordinates to show that the distance from v to the remaining vertex violates its inequality. □

Lemma 10.14. *The score of a mixed quad cluster is less than $-1.04\,pt$.*

Proof. Any enclosed vertex in a quad cluster has length at least $2t_0$ by Lemma 10.13. In particular, the anchors of an enclosed vertex are corners of the quad cluster. There are no flat quarters.

We generally truncate the V-cell at $\sqrt{2}$ as in the proof of Theorem 8.4. By that lemma, it breaks the V-cell into pieces whose score is nonpositive. Thus, if we identify certain pieces that score less than $-1.04\,pt$, the result follows. Nevertheless, a few simplices will be left untruncated in the following argument. We will leave a simplex untruncated only if we are certain that each of its faces has positive orientation and that the simplices sharing a face F with S either lie in the Q-system or have positive orientation along F. If these conditions hold, we may use[16] the function s-vor on S rather than truncation s-vor$_0$.

In this proof, by enclosed vertex, we mean one of height at most $2\sqrt{2}$. Let v be an enclosed vertex with the fewest anchors. If there are no anchors, the right circular cone $C(h, \eta_0(h))$ (aligned along $\{0, v\}$; see Definition 7.22) belongs to VC(0), where $\eta_0(h) = \eta(2h, 2, 2t_0)$ as in Definition 9.1 and $|v| = 2h$. In fact, if such a point lies in VC(u), with $u \ne v$, then u must be a corner of the quad cluster or an enclosed vertex of height at least $2t_0$. In either case, the right circular cone belongs to VC(0). By

[16] CALC-185703487, CALC-69785808, and CALC-104677697

Formula 7.11, the score of this cone is $2\pi(1 - h/\eta_0(h))\phi(h, \eta_0(h))$. An optimization in one variable gives an upper bound of $-4.52\,pt$, for $t_0 \le h \le \sqrt{2}$. This gives the bound of $-1.04\,pt$ in this case.

If there is one anchor, we cut the cone in half along the plane through $\{0, v\}$ perpendicular to the plane containing the anchor and $\{0, v\}$. The half of the cone on the far side of the anchor lies under the face at v of the V-cell. We get a bound of $-4.52\,pt/2 < -1.04\,pt$.

To treat the remaining cases, we define a function $K(S)$ on certain simplices S with circumradius at least $\sqrt{2}$. Let $S = S(y_1, y_2, \ldots, y_6)$. Let $R(a, b, c)$ denote a Rogers simplex. Set

$$K(S) = K_0(y_1, y_2, y_6) + K_0(y_1, y_3, y_5) + \mathrm{dih}(S)(1 - y_1/\sqrt{8})\phi(y_1/2, \sqrt{2}), \quad (10.2)$$

where

$$\begin{aligned} K_0(y_1, y_2, y_6) \quad &= \text{r-vor}(R(y_1/2, \eta(y_1, y_2, y_6), \sqrt{2})) + \text{r-vor}(R(y_2/2, \eta(y_1, y_2, y_6), \sqrt{2})) \\ &- \mathrm{dih}(R(y_1/2, \eta(y_1, y_2, y_6), \sqrt{2}))(1 - y_1/\sqrt{8})\phi(y_1/2, \sqrt{2}). \end{aligned}$$

(If the given Rogers simplices do not exist because the condition $0 < a < b < c$ is violated, we set the corresponding terms in these expressions to 0.) The function $K(S)$ represents the part of the score coming from the four Rogers simplices along two of the faces of S, and the conic region extending out to $\sqrt{2}$ between the two Rogers simplices along the edge y_1 (Figure 10.1). This region is closely related to the solids $\Delta(v, W^e)$ of Section 9.3, with the difference that the solids Δ lie in a ball of radius $\eta_0(|v|/2)$, but the solids here are truncated at $\sqrt{2}$.

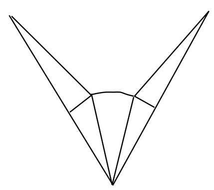

Figure 10.1. *The set measured by the function $K(S)$.*

In the remaining cases, each enclosed vertex has at least two anchors. Each anchor is a corner of the quad cluster. Fix an enclosed vertex v. Suppose that v_1, a corner, is an anchor of v. Assume that the face $\{0, v, v_1\}$ bounds at most one upright quarter. We sweep around the edge $\{0, v_1\}$, away from the upright quarter if there is one, until we come to another enclosed vertex v' such that $\{0, v_1, v'\}$ has circumradius less than $\sqrt{2}$ or such that v_1 is an anchor of $\{0, v'\}$. If such a vertex v' does not exist, we sweep all the way to v_2 a corner of the quad cluster adjacent to v_1.

If v' exists, then various calculations[17] give the bound $-1.04\,pt$, depending on the size of the circumradius of $\{0, v, v'\}$. This allows us to assume that we do not

[17] CALC-104677697, CALC-69785808, CALC-586706757, and CALC-87690094

encounter such an enclosed vertex v' whenever we sweep away, as above, from the face formed by an anchor.

Now consider the simplex $S = \{0, v_1, v_2, v\}$, where v_1 is an anchor of $\{0, v\}$. We assume that it is not an upright quarter. There are three alternatives. The first is that S decreases the score of the quarter by at least $0.52\,pt$. Calculations[18] show that this occurs if the circumradius of the face $\{0, v, v_2\}$ is less than $\sqrt{2}$, or if the circumradius of the face is greater than $\sqrt{2}$, provided that the length of $\{v, v_1\}$ is at most 2.2. The second alternative[19] is that the face $\{0, v, v_1\}$ of S is shared with a quarter Q and that S and Q taken together bring the score down by $0.52\,pt$. In fact, if there are two such simplices S and S' along Q, then the three simplices Q, S, and S' pull the score[20] below $-1.04\,pt$. The third alternative is that there is a simplex $S' = \{0, v, v, v_3\}$ sharing the face $\{0, v, v_1\}$, which, like S, scores less than $-0.31\,pt$. In each case, S and the adjacent simplex through $\{0, v, v_1\}$ score less than $-0.52\,pt$. Since v has at least two anchors, the quad cluster scores less than $2(-0.52)\,pt = -1.04\,pt$. $\square$

10.5 A Volume Formula

In Definition 9.3, we found a solid $\delta(v, W^e)$ that lies outside the ball of radius t_0 at 0 but inside VC(0). We now develop a formula for its volume.

Set $\phi_0 = \phi(t_0, t_0) \approx -0.5666$. We define

$$\mathrm{crown}(h) = 2\pi(1 - h/\eta_0(h))(\phi(h, \eta_0(h)) - \phi_0). \tag{10.3}$$

It is equal to $-4\delta_{oct}$ times the volume of the region outside the sphere of radius t_0 and inside the finite cone $C(h, \eta_0(h))$. If v is an enclosed vertex of height $2h \in [2t_0, \sqrt{8}]$, such that every other vertex v' of the standard cluster satisfies

$$\eta(|v|, |v'|, |v - v'|) \geq \eta_0(h),$$

then the solid represented by crown$(|v|/2)$ lies outside the truncated V-cell, but inside the V-cell, so that if P is a quad cluster,

$$\text{c-vor}(V_P) < \text{c-vor}_0(V_P) + \mathrm{crown}(|v|/2).$$

If a vertex v' satisfies $\eta(|v|, |v'|, |v - v'|) \leq \eta_0(h)$, then by the monotonicity of the circumradius of acute triangles, v' is an anchor of v. This anchor clips the crown just defined, and we add a correction term anc$(|v'|, |v|, |v - v'|)$ to account for this. Figure 10.2 illustrates the terms in the definition of anc().

Set

$$\begin{aligned}\mathrm{anc}(y_1, y_2, y_6) \quad &= -\,\mathrm{dih}(R_1)\,\mathrm{crown}(y_1/2)/(2\pi) - \mathrm{sol}(R_1)\phi_0 + \text{r-vor}(R_1)\\ &\quad - \mathrm{dih}(R_2)(1 - y_2/2t_0)(\phi(y_2/2, t_0) - \phi_0) - \mathrm{sol}(R_2)\phi_0 + \text{r-vor}(R_2),\end{aligned} \tag{10.4}$$

[18] CALC-185703487 and CALC-441195992
[19] CALC-848147403, CALC-969320489, and CALC-975496332.
[20] CALC-766771911

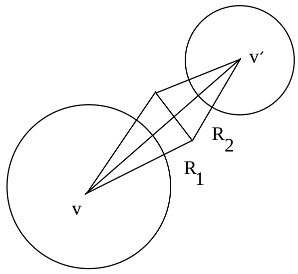

Figure 10.2. *An illustration of the terms* anc.

where $R_i = R(y_i/2, \eta(y_1, y_2, y_6), \eta_0(y_1/2))$, for $i = 1, 2$. In general, there are Rogers simplices on both sides of the face $\{0, v, v')$, and this gives a factor of 2. For example, if v has a single anchor v', then

$$\text{c-vor}(V_P) < \text{c-vor}_0(V_P) + \text{crown}(|v|/2) + 2\,\text{anc}(|v|, |v'|, |v - v'|).$$

However, if the anchor gives a face of an upright quarter, only one side of the face lies in the V-cell, so that the factor of 2 is not required. For example, v' has context $(2, 1)$ with upright quarter Q, and if there are no other enclosed vertices, and if v', v'' are the anchors along the faces of the quarter, then

$$\begin{aligned}\text{c-vor}(V_P) \quad &< \text{c-vor}_0(V_P) + (1 - \text{dih}(Q)/(2\pi))\,\text{crown}(|v|/2)\\ &+ \text{anc}(|v|, |v'|, |v - v'|) + \text{anc}(|v|, |v''|, |v - v''|).\end{aligned}$$

In general, when there are multiple anchors around the same enclosed vertex v, we add a term $(2-k)$ anc for each anchor, where $k \in \{0, 1, 2\}$ is the number of quarters bounded by the face formed by the anchor. We must be cautious (see Condition 2 in Definition 9.2 in the use of this formula. If the circumradius of $\{0, v, v', v''\}$ is less than $\eta_0(|v|/2)$, the Rogers simplices used to define the terms anc() at v' and v'' overlap. When this occurs, the geometric decomposition on which the correction terms anc() are based is no longer valid. In this case, other methods must be used.

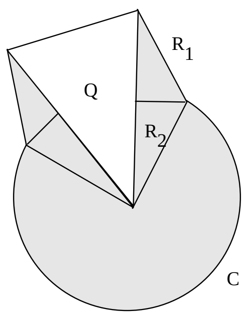

Figure 10.3. *The terms* anc *near an upright quarter.*

If (P, D) is a mixed quad cluster, let (P, D') be the new quad cluster obtained by removing all the enclosed vertices. We define a V-cell $V(P, D')$ of (P, D') and the truncation of $V(P, D')$ at t_0. We take its score $\mathrm{vor}_{0,P}(D')$ as we do for standard clusters. (P, D') does not contain any quarters.

Lemma 10.15. *If (P, D) is a mixed quad cluster, $\sigma_P(D') < \mathrm{vor}_{0,P}(D)$.*

Remark 10.16. *The special case of the proof where an upright quarter has context $c(Q) = (2, 1)$ will be applied in Section 11.2 in situations other than mixed quad clusters.*

Proof. Suppose there exists an enclosed vertex that has context $(2, 1)$; that is, there is a single upright quarter $Q = S(y_1, y_2, \ldots, y_6)$ and no additional anchors. In this context $\sigma(Q) = \mu(Q)$. Let v be the enclosed vertex. To compare $\sigma_P(D)$ with $\mathrm{vor}_{0,P}(D')$, consider the V-cell near Q. The quarter Q cuts a wedge of angle $\mathrm{dih}(Q)$ from the crown at v. There is an anchor term for the two anchors of v along the faces of Q. Let V_P^v be the truncation at height t_0 of V_P near v and under the four Rogers simplices stemming from the two anchors. (Figure 10.3 shades the truncated parts of the quad cluster.) As a consequence

$$\text{c-vor}(V_P) < (1-\mathrm{dih}(Q)/(2\pi))\,\mathrm{crown}(y_1/2)+\mathrm{anc}(y_1, y_2, y_6)+\mathrm{anc}(y_1, y_3, y_5)+\text{c-vor}(V_P^v). \tag{10.5}$$

Combining this inequality with calculations[21], we find

$$\text{c-vor}(V_P) + \mu(Q) < \text{c-vor}(V_P^v) + \text{s-vor}_0(Q). \tag{10.6}$$

Now suppose there is an enclosed vertex v with context $(3, 1)$. Let the quad cluster have corners v_1, v_2, v_3, v_4, ordered consecutively. Suppose the two quarters along v are $Q_1 = \{0, v, v_1, v_2\}$ and $Q_2 = \{0, v, v_2, v_3\}$. We consider two cases.
Case 1: $\mathrm{dih}(Q_1) + \mathrm{dih}(Q_2) < \pi$ or $\mathrm{rad}(0, v, v_1, v_3) \geq \eta(|v|, 2, 2t_0)$. In this case, the use of correction terms to the crown are legitimate as in Definition 9.2. Proceeding as in context $(2, 1)$, we find that

$$\text{c-vor}(V_P) < (1-(\mathrm{dih}(Q_1)+\mathrm{dih}(Q_2))/(2\pi))\,\mathrm{crown}(|v|/2)+\mathrm{anc}(F_1)+\mathrm{anc}(F_2)+\text{c-vor}(V_P^v). \tag{10.7}$$

Here V_P^v is defined by the truncation at height t_0 under the V-face determined by v and under the Rogers simplices stemming from the side of F_i that occur in the definition of anc. Also, $\mathrm{anc}(F_i) = \mathrm{anc}(y_i, y_j, y_k)$ for a face F_i with edges y_i along an upright quarter. By a calculation[22] applied to both Q_1 and Q_2, we have

$$\text{c-vor}(V_P) + \sum_{i=1}^{2} \sigma(Q_i) < \text{c-vor}(V_P^v) + \sum_{i=1}^{2} \text{s-vor}_0(Q_i). \tag{10.8}$$

That is, by truncating near v, and changing the scoring of the quarters to s-vor_0, we obtain an upper bound on the score.

[21] CALC-906566422, CALC-703457064, and CALC-175514843
[22] CALC-554253147

Case 2: $\mathrm{dih}(Q_1) + \mathrm{dih}(Q_2) \geq \pi$ and $\mathrm{rad}(0, v, v_1, v_3) \leq \eta_0(|v|/2)$. The anchor terms cannot be used here. In the mixed case, $\sqrt{8} < |v_1 - v_3|$, so

$$\sqrt{2} < \frac{1}{2}|v_1 - v_3| \leq \mathrm{rad} \leq \eta_0(|v|/2),$$

and this implies $|v| \geq 2.696$. We have[23]

$$\sum_{i=1}^{2} \sigma(Q_i) < \sum_{i=1}^{2} \text{s-vor}_0(Q_i) + \sum_{i=1}^{2} 0.01(\pi/2 - \mathrm{dih}(Q_i)) < \sum_{i=1}^{2} \text{s-vor}_0(Q_i).$$

Inequality 10.8 holds, for $V_P^v = V_P$.

In the general case, we run over all enclosed vertices v and truncate around each vertex. For each vertex we obtain Inequality 10.6 or 10.8. These inequalities can be coherently combined over multiple enclosed vertices because the V-faces were associated with different vertices v and none of the Rogers simplices used in the terms anc() overlap. More precisely, if Z is a set of enclosed vertices, set $V_P^Z = \cap_{v \in Z} V_P^v$, and $V_P^{v,Z} = V_P^Z \cap V_P^v$. Coherence means that we obtain valid inequalities by adding the superscript Z to V_P and V_P^v in Inequalities 10.6 and 10.8, if $v \notin Z$. In sum, $\sigma_P(D) < \mathrm{vor}_{0,P}(D)$. □

[23] CALC-855677395

Paper IV

Sphere Packings IV. Detailed Bounds

This paper contains the technical heart of the proof of the Kepler conjecture. Its primary purpose is to obtain good bounds on the score $\sigma_R(D)$ when R is an arbitrary standard region of a decomposition star D. This is particularly challenging, because we have no *a priori* restrictions on the combinatorial type of the standard region R. It is not known to be bounded by a simple polygon. It is not known to be simply connected. Moreover, there are multitudes of possible geometrical configurations of upright and flat quarters, each scored by a different rule. This paper will deal with these complexities and will bound the score $\sigma_R(D)$ in a way that depends on a simple numerical invariant $n(R)$ of R. When R is bounded by a simple polygon, the numerical invariant is simply the number of sides of the polygon. This bound on the score of a standard region represents the turning point of the proof, in the sense that it caps the complexity of a contravening decomposition star, and restrains the combinatorial possibilities. Later in the proof, it will be instrumental in the complete enumeration of the plane graphs attached to contravening stars.

The first section will prove a series of approximations for the score of upright quarters. The strategy is to limit the number of geometrical configurations of upright quarters by showing that a common upper bound (to the scoring function) can be found for quite disparate geometrical configurations of upright quarters. When a general upper bound can be found that is independent of the geometrical details of upright quarters, we say that the upright quarters can be *erased.* (A precise definition of what it means to erase an upright quarter appears below.) There are some upright quarters that cannot be treated in this manner; and this adds some complications to the proofs in this paper

The second section states the main result of the paper (Theorem 12.1). An initial reduction reduces the proof to the case that the boundary of the given standard region is a polygon. A further argument is presented to reduce the proof to a convex polygon.

The third section completes the proof of the main theorem. This part of the proof relies on a new geometrical decomposition of the part of a V-cell over a standard region. The pieces in this decomposition are called *truncated corner cells.*

A final section in this paper collects miscellaneous further bounds that will be needed in later parts of the proof of the Kepler conjecture.

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Section 11

Upright Quarters

11.1 Erasing Upright Quarters

Definition 11.1. *A standard region is said to be exceptional if it is not a triangle or a quadrilateral. The pair (D, R) consisting of a decomposition star and an exceptional standard region is said to be an exceptional cluster. The vertices of the packing of height at most $2t_0$ that are contained in the closed cone over the standard region are called its corners.*

Fix an exceptional cluster R. Throughout this paper, we assume that R lies on a star of score at least $8\,pt$. It is to be understood, when we say that a standard region does not exist, that we mean that there exists no such region on any star scoring more than $8\,pt$.

In Section 11, we discuss how to eliminate many cases of upright diagonals. The results are summarized in Section 11.9.

If R is a standard region, we write $V_R(t)$ for the intersection of the local V-cell $V_R = \mathrm{VC}(0) \cap C(R)$ with a ball $B(t)$, centered at the origin, of radius t. We usually take $t = t_0$. If $\{0, v\}$, of length between $2t_0$ and $2\sqrt{2}$, is not the diagonal of an upright quarter in the Q-system, then v does not affect the truncated cell $V_R(t_0)$ and may be disregarded. For this reason we confine our attention to upright diagonals that lie along an upright quarter in the Q-system.

We say that an upright diagonal $\{0, v\}$ can be *erased with penalty* $\pi_0 \geq 0$, if we have, in terms of the decomposition of Section 9,

$$\sum_Q \sigma(Q) + \sum_S \sigma(V_S(t_S)) - 4\delta_{oct}\mathrm{vol}(\delta_P(v)) < \pi_0 + \sum_Q \text{s-vor}_0(Q) + \sum_S \text{s-vor}_0(S).$$

Here the sum over Q runs over the upright quarters around $\{0, v\}$. The scores $\sigma(Q)$ are context-dependent (see Section 7). The second sum runs over simplices S along $\{0, v\}$ of type C in the $\mathcal{S}$-system. We define their score $\sigma(V_S(t_S))$ as in Section 9. Also, $\delta_P(v)$ is the piece of the decomposition defined in Section 9. The right-hand side is scored by the truncation function in Section 7 Formula 7.13. When we erase without mention of a penalty, $\pi_0 = 0$ is assumed.

If the diagonal can be erased, an upper bound on the score is obtained by ignoring the upright diagonal and all of the structures around it coming from the decomposition of Section 9, and switching to the truncation at t_0. Section 11 shows that various vertices can be erased, and this will greatly reduce the number combinatorial possibilities for an exceptional cluster.

11.2 Contexts

Each upright diagonal has a context (p, q), with p the number of anchors and $p - q$ the number of quarters around the diagonal (Definition 7.1). The dihedral angle of a quarter is less than[24] π, so the context $(2, 0)$ is impossible. There is at least one quarter, so $p \geq q + 1$, $p \geq 2$.

The context $(2, 1)$ is treated in Section 10.4. Lemma 10.15 shows that by removing the upright diagonal, and scoring the surrounding region by a truncated function vor_0, an upper bound on the score is obtained. In the remaining contexts, $p \geq 3$. We start with contexts satisfying $p = 3$. The context $(3, 0)$ is to be regarded as two quasi-regular tetrahedra sharing a face rather than as three quarters along a diagonal. In particular, by Definition 4.8, the upright quarters do not belong to the Q-system.

We recall that the score of an upright quarter is given by

$$\sigma(Q, v) = (\mu(Q, v) + \mu(Q, \hat{v}) + \text{s-vor}_0(Q, v) - \text{s-vor}_0(Q, \hat{v}))/2,$$

except in the contexts $(2, 1)$ and $(4, 0)$. Define $\nu(Q)$ to be the right-hand side of this equation. The context $(2, 1)$ has been treated, and the context $(4, 0)$ does not occur in exceptional clusters. Thus, for the remainder of this section, the scoring rule $\sigma(Q) = \nu(Q)$ will be used.

We have several different variants on the score depending on the truncation, analytic continuation, and so forth. If f is any of the functions

$$\text{s-vor}_0,\ \text{s-vor},\ \Gamma,\ \nu,$$

we set τ_0, τ_V, τ_Γ, τ_ν, respectively, to

$$\tau_* = -f(S) + \mathrm{sol}(S)\zeta pt.$$

We set $\tau(S, t) = -\,\text{s-vor}(S, t) + \mathrm{sol}(S)\zeta pt$. The family of functions τ_* measure what is squandered by a simplex. We say that Q has *compression type* or *Voronoi type* according to the scoring of $\mu(Q)$. (See Section 7.1.)

Crowns and anchor correction terms are used in Section 10.4 to erase upright quarters. We imitate those methods here. The functions crown and anc are defined and discussed in Section 10.4. If $S = S(y_1, \ldots, y_6)$ is a simplex along $\{0, v\}$, set

$$\kappa(S(y_1, \ldots, y_6)) = \mathrm{crown}(y_1/2)\,\mathrm{dih}(S)/(2\pi) + \mathrm{anc}(y_1, y_2, y_6) + \mathrm{anc}(y_1, y_3, y_5).$$

[24] CALC-971555266

$\kappa(S)$ is a bound on the difference in the score resulting from truncation around v. Assume that S is the simplex formed by $\{0, v\}$ and two consecutive anchors around $\{0, v\}$. Assume further that the circumradius of S is at least $\eta_0(y_1/2)$. Then we have

$$\kappa(S) = -4\delta_{oct}\mathrm{vol}(\delta_P(W^e)),$$

where W^e is the extended wedge constructed in Section 9.2. To see this, it is a matter of interpreting the terms in κ. The function *crown* enters the volume through the region over the spherical cap D_0 of Section 9.2, lying outside $B(t_0)$. By multiplying by $\mathrm{dih}(S)/(2\pi)$, we select the part of the spherical cap over the unextended wedge W between the anchors. The terms *anc* adjust for the four Rogers simplices lying above the extension W^e.

11.3 Three anchors

Lemma 11.2. *The upright diagonal can be erased in the context* $(3, 2)$.

Proof. Let v_1 and v_2 be the two anchors of the upright diagonal $\{0, v\}$ along the quarter. Let the third anchor be v_3.

Assume first that $|v| \geq 2.696$. If Q is of compression type, then[25] the score is dominated by the truncated function s-vor$_0$. Assume Q is of Voronoi type. If $|v_1|$, $|v_2| \leq 2.45$, then a calculation[26] gives the result. Take $|v_2| \geq 2.45$. By symmetry, $|v-v_1|$ or $|v-v_2| \geq 2.45$. The case $|v-v_1| \geq 2.45$ is treated by another calculation.[27] We take $|v-v_2| \geq 2.45$. Let $S = \{0, v, v_2, v_3\}$. If S is of type C, the result follows.[28] S is of type C, if and only if $y_4 \leq 2.77$, (because $\eta_{456} \geq \eta(2.45, 2, 2.77) > \sqrt{2}$.) If S is not of type C, we argue as follows. The function $h^2(\eta(2h, 2.45, 2.45)^{-2} - \eta_0(h)^{-2})$ is a quadratic polynomial in h^2 with negative values for $2h \in [2.696, 2\sqrt{2}]$. From this we find

$$\mathrm{rad}(S) \geq \eta(2h, 2.45, 2.45) \geq \eta_0(h), \quad \text{where } 2h = |v|,$$

and this justifies the use of κ (see Section 9.2 Case (2)). That the truncated function dominates the score now follows from a calculation.[29]

Now assume that $|v| \leq 2.696$. If the simplices $\{0, v, v_1, v_3\}$ and $\{0, v, v_2, v_3\}$ are of type C, the bound follows from a calculation.[30] [31] If say $S = \{0, v, v_2, v_3\}$ is not of type C, then

$$\mathrm{rad}(S) \geq \sqrt{2} > \eta_0(2.696/2) \geq \eta_0(h),$$

[25] CALC-73974037
[26] CALC-764978100
[27] CALC-764978100
[28] CALC-764978100
[29] CALC-618205535
[30] CALC-73974037
[31] CALC-764978100

justifying the use of κ. The bound follows from further calculations.[32] [33] [34] ($\Gamma + \kappa <$ octavor$_0$, etc.) □

Lemma 11.3. *The upright diagonal can be erased in the context* $(3,1)$*, provided the three anchors do not form a flat quarter at the origin.*

Proof. In the absence of a flat quarter, truncate, score, and remove the vertex v as in the context $(3,1)$ of Lemma 10.15. If there is a flat quarter, by the rules of Definition 4.8, v is enclosed over the flat quarter. We do nothing further with them for now. This unerased case appears in the summary at the end of the section (11.9). See Lemma 11.27. □

11.4 Six anchors

Lemma 11.4. *An upright diagonal has at most five anchors.*

Proof. The proof relies on constants and inequalities from two calculations.[35] [36] If between two anchors there is a quarter, then the angle is greater than 0.956, but if there is not, the angle is greater than 1.23. So if there are k quarters and at least six anchors, they squander more than

$$k(1.01104) - [2\pi - (6-k)1.23]0.78701 > (4\pi\zeta - 8)\,pt,$$

for $k \geq 0$. □

11.5 Anchored simplices

Let $\{0, v\}$ be an upright diagonal, and let $v_1, v_2, \ldots, v_k = v_1$ be its anchors, ordered cyclically around $\{0, v\}$. This cyclic order gives dihedral angles between consecutive anchors around the upright diagonal. We define the dihedral angles so that their sum is 2π, even though this will lead us to depart from our usual conventions by assigning a dihedral angle greater than π when all the anchors are concentrated in some half-space bounded by a plane through $\{0, v\}$. When the dihedral angle of $S = \{0, v, v_i, v_{i+1}\}$ is at most π, we say that S is an *anchored simplex* if $|v_i - v_{i+1}| \leq 3.2$. (The constant 3.2 appears throughout this section.) All upright quarters are anchored simplices. If an upright diagonal is completely surrounded by anchored simplices, the upright diagonal is sometimes called a *loop*. If $|v_i - v_{i+1}| > 3.2$ and

[32] CALC-618205535
[33] CALC-73974037
[34] CALC-764978100
[35] CALC-729988292
[36] CALC-83777706

the angle is less than π, we say there is a *large gap* around $\{0, v\}$ between v_i and v_{i+1}.

To understand how anchored simplices overlap we need a bound satisfied by vertices enclosed over an anchored simplex.

Lemma 11.5. *A vertex w of height between 2 and $2\sqrt{2}$, enclosed in the cone over an anchored simplex $\{0, v, v_1, v_2\}$ with diagonal $\{0, v\}$ satisfies $|w - v| \le 2t_0$. In particular, if $|w| \le 2t_0$, then w is an anchor.*

Proof. As in Lemma 4.16, the vertex w cannot lie inside the anchored simplex. If $|v_1 - v_2| \le 2\sqrt{2}$, the result follows from Lemma 5.16. In fact, if $|w| \le 2\sqrt{2}$, the Voronoi cells at 0 and w meet, so that Lemma 5.16 forces $\{0, v_1, v_2, w\}$ to be a quarter. (This observation gives a second proof of Lemma 4.34.)

Assume that a figure exists with $|v_1 - v_2| > 2\sqrt{2}$. Suppose for a contradiction that $|v - w| > 2t_0$. Pivot v_1 around $\{0, v_2\}$ until $|v - v_1| = 2t_0$ and v_2 around $\{0, v_1\}$ until $|v - v_2| = 2t_0$. Rescale w so that $|w| = 2\sqrt{2}$. Set $x = |v_1 - v_2|$. If, through geometric considerations, w is not deformed into the plane of $\{0, v_2, v_1\}$, then we are left with the one-dimensional family $|w'| = |w' - w| = 2$, for $w' = v_2, v_1$, $|v - w| = |v| = |v_1 - v| = |v_2 - v| = 2t_0$, depending on x. This gives a contradiction

$$\begin{aligned} \pi &\ge \mathrm{dih}(v_2, v_1, 0, v) + \mathrm{dih}(v_2, v_1, v, w) \\ &= 2\,\mathrm{dih}(S(x, 2, 2t_0, 2t_0, 2t_0, 2)) > \pi, \end{aligned}$$

for $x > 2\sqrt{2}$. (Equality is attained if $x = 2\sqrt{2}$.)

Thus, we may assume that w lies in the plane $P = \{0, v_1, v_2\}$. Take the circle in P at distance $2t_0$ from v. The vertices 0 and w lie on or outside the circle. The vertices v_1 and v_2 lie on the circle, so the diameter is at least $x > 2\sqrt{2}$. The distance from v to P is less than $x_0 = \sqrt{2t_0^2 - 2}$. The edge $\{0, w\}$ cannot pass through the center of the circle, because $|w|$ is less than the diameter. Reflect v through P to get v'. Then $|v - v'| < 2x_0$. Swapping v_1 and v_2 as necessary, we may assume that w is enclosed over $\{0, v, v', v_2\}$. The desired bound $|v - w| \le 2t_0$ now follows from geometric considerations and the contradiction

$$2\sqrt{2} = |w| > \mathcal{E}(S(2, 2t_0, 2t_0, 2x_0, 2t_0, 2t_0), 2, 2t_0, 2t_0) = 2\sqrt{2}.$$

□

Corollary 11.6. *A vertex of height at most $2t_0$ is never enclosed over an anchored simplex.*

Proof. If so, it would be an anchor to the upright diagonal, contrary to the assumption that the anchored simplex is formed by consecutive anchors. □

11.6 Anchored simplices do not overlap

Definition 11.7. *Consider an upright diagonal that is not a loop. Let R be the standard region that contains the upright diagonal and its surrounding quarters. Assume we are in the context $(4,1)$ or $(5,1)$. In the context $(4,1)$, suppose that 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, we say that the context is* 3*-crowded. We call the context* $(5,1)$ *a* 4*-crowded upright diagonal. Sections 11.3 and 11.4 reduce everything to contexts with four or five anchors around each vertex. If there are* 5 *anchors, Lemma 11.14 (and Remark 11.13) show that we can assume at most one large gap. This gives contexts* $(5,0)$ *and* $(5,1)$*. If there are four anchors, then Lemma 11.21 will dismiss all contexts except* $(4,0)$ *and* $(4,1)$*. Thus, every upright diagonal is exactly one of the following: a loop,* 3*-unconfined,* 3*-crowded, or* 4*-crowded.*

Definition 11.8. *The Cayley-Menger determinant expresses the volume of a simplex $S(y1,\ldots,y_6)$ in the form $\sqrt{\Delta(x_1,\ldots,x_6)}/12$, where $x_i = y_i^2$, and Δ is a polynomial with integer coefficients. The polynomial Δ will be used frequently.*

This lemma is a consequence of the two others that follow. The context of the lemma is the set of anchored simplices that have not been erased by previous reductions.

Lemma 11.9. *Anchored simplices do not overlap.*

The remaining contexts have four or five anchors. Let w and the anchored simplex $S = \{0, v, v_1, v_2\}$ be as in Section 11.5. Our object is to describe the local geometry when an upright diagonal is enclosed over an anchored simplex. If $|v_1 - v_2| \le 2\sqrt{2}$, we have seen in Lemma 4.32 that there can be no enclosed upright diagonal with ≥ 4 anchors over the anchored simplex S.

Assume $|v_1 - v_2| > 2\sqrt{2}$. Let $w_1, \ldots, w_k$, $k \ge 4$, be the anchors of $\{0, w\}$, indexed consecutively. The anchors of $\{0, w\}$ do not lie in $C(S)$, and the triangles $\{0, w, w_i\}$ and $\{0, v, v_j\}$ do not overlap. Thus, the plane $\{0, v_1, v_2\}$ separates w from $\{w_1, \ldots, w_k\}$. Set $S_i = \{0, w, w_i, w_{i+1}\}$. By a calculation[37]

$$\pi \ge \mathrm{dih}(S_1) + \cdots + \mathrm{dih}(S_{k-1}) \ge (k-1)0.956.$$

Thus, $k = 4$. The common upright diagonal of the three simplices $\{S_i\}$ is 3-*crowded*. We claim that $\{v_1, v_2\} = \{w_1, w_4\}$. Suppose to the contrary that, after reindexing as necessary, $S_0 = \{0, w, w_1, v_1\}$ is a simplex, with $v_1 \ne w_1$, that does not overlap $S_1, \ldots, S_3$. Then $\pi \ge \mathrm{dih}(S_0) + \cdots + \mathrm{dih}(S_3)$. So $0.28 \ge \pi - 3(0.956) \ge \mathrm{dih}(S_0)$. A calculation[38] now implies that $|w - v_1| \ge 2\sqrt{2}$.

Assume that $\{0, w, v_1, v_2\}$ are coplanar. Disregard the other vertices. We

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minimize $|v_1 - v_2|$ when

$$|w| = 2\sqrt{2}, \quad |v_2| = |v_1| = |w - v_2| = 2, \quad |w - v_1| = 2\sqrt{2}.$$

This implies $3.2 \geq |v_1 - v_2| \geq x$, where x is the largest positive root of the polynomial $\Delta(8, 4, 4, x^2, 4, 8)$. But $x \approx 3.36$, a contradiction.

Since $\{0, w, v_1, v_2\}$ cannot be coplanar vertices, geometric considerations apply and

$$2\sqrt{2} \geq |w| \geq \mathcal{E}(S(2, 2, 2, 2, 2, 3.2), 2\sqrt{2}, 2, 2) > 2\sqrt{2}.$$

This contradiction establishes that $v_1 = w_1$.

Lemma 11.10. *Around a 3-crowded upright diagonal, all of the anchored simplices are quarters.*

Proof. The proof makes use of constants and inequalities from several different calculations.[39] [40] [41] The dihedral angles are at most $\pi - 2(0.956) < 1.23$. This forces $y_4 \leq 2t_0$, for each simplex S. So they are all quarters. □

Lemma 11.11. *If there is 3-crowded upright diagonal, then the three anchored simplices squander more than* 0.5606 *and score at most* −0.4339.

Proof. The proof makes use of constants and inequalities from several different calculations.[42] [43] [44] The three anchored simplices squander at least

$$3(1.01104) - \pi(0.78701) > 0.5606.$$

The bound on score follows similarly from $\nu < -0.9871 + 0.80449\,\mathrm{dih}$. □

Lemma 11.12. *If a simplex at a 3-crowded upright diagonal overlaps an anchored simplex, the decomposition star does not contravene.*

Proof. Suppose that $\{0, v, v_1, v_2\}$ is an anchored simplex that another anchored simplex overlaps, with $\{0, v\}$ the upright diagonal. Let $\{0, w\}$ be a 3-crowded upright diagonal. We score the two simplices $S_i' = \{0, v, w, v_i\}$ by truncation at $\sqrt{2}$. Truncation at $\sqrt{2}$ is justified by face-orientation arguments or by geometric considerations:

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

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[43] CALC-83777706
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A calculation[45] gives

$$\tau_V(S_1', \sqrt{2}) + \tau_V(S_2', \sqrt{2}) \geq 2(0.13) + 0.2(\mathrm{dih}(S_1') + \mathrm{dih}(S_2') - \pi) > 0.26.$$

Together with the three simplices around the 3-crowded upright diagonal that squander at least 0.5606, we obtain the stated bound. □

11.7 Five anchors

When there are five anchors of an upright diagonal, each dihedral angle around the diagonal is at most $2\pi - 4(0.956) < \pi$.

Remark 11.13. *There are at most two large gaps by the calculation*[46]

$$3(1.65) + 2(0.956) > 2\pi.$$

Lemma 11.14. *If an upright diagonal has five anchors with two large gaps, then the three anchored simplices squander* $> (4\pi\zeta - 8)\,pt$.

Proof. By a calculation,[47] the anchored simplices are all quarters, $1.23 + 2(1.65) + 2(0.956) > 2\pi$. The dihedral angle is less than $2\pi - 2(1.65)$. The linear programming bound based on various inequalities[48] is greater than $0.859 > (4\pi\zeta - 8)\,pt$. □

Definition 11.15. *Define a masked flat quarter to be a flat quarter that is not in the Q-system because it overlaps an upright quarter in the Q-system. They can only occur in a very special setting.*

Lemma 11.16. *Let $\{0, v\}$ be an upright diagonal with at least four anchors. If Q is a flat quarter that overlaps an anchored simplex along $\{0, v\}$, then the vertices of Q are the origin and three consecutive anchors of $\{0, v\}$.*

Proof. For there to be overlap, the diagonal $\{w_1, w_2\}$ of Q must pass through the face $\{0, v, v_1\}$ formed by some anchor v_1 (see Lemma 4.19). By Lemma 4.24, w_1 and w_2 are anchors of $\{0, v\}$. By Lemma 4.32, w_2, v_1, and w_1 are consecutive anchors. If v_1 is a vertex of Q we are done. Otherwise, let $w_3 \neq 0, w_1, w_2$ be the remaining vertex of Q. The edges $\{v, v_1\}$ and $\{v_1, 0\}$ do not pass through the face $\{w_1, w_2, w_3\}$ by Lemma 4.19. Likewise, the edges $\{w_2, w_3\}$ and $\{w_3, w_1\}$ do not pass through the face $\{0, v, v_1\}$. Thus, v is enclosed over the quarter Q.

Let $w_3' \neq w_1, v_1, w_2$ be a fourth anchor of $\{0, v\}$. By Lemma 4.19, we have $w_3' = w_3$. □

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Corollary 11.17. *(of proof) If v is enclosed over a flat quarter, then $\{0, v\}$ has at most four anchors.*

When we are unable to erase the upright diagonal with five anchors and a large gap, we are able to obtain strong bounds on the score.

Lemma 11.18. *Suppose an upright diagonal in a decomposition star has five anchors and one large gap. The four anchored simplices score at most -0.25. The four anchored simplices squander at least 0.4. If any of the four anchored simplices is not an upright quarter then the decomposition star does not contravene.*

Proof. A list of inequalities[49] together with[50] $\mathrm{dih} > 1.65$ give the bound -0.25. Further inequalities [51] give the bound 0.4. To get the final statement of the lemma, we again use a series of inequalities.[52] [53] $\square$

Corollary 11.19. *There is at most one 4-crowded upright diagonal in a contravening decomposition star.*

Proof. The crown along the large gap, with the bound of the lemma, gives[54] $0.4 - \kappa \geq 0.4 + 0.02274$ squandered by the upright quarters around a 4-crowded upright diagonal. The rest squanders a positive amount (see Lemma 9.20). If there are two 4-crowded upright diagonals, use $2(0.4 + 0.02274) > (4\pi\zeta - 8)\,pt$. $\square$

Definition 11.20. *We set $\xi_\Gamma = 0.01561$, $\xi_V = 0.003521$, $\xi'_\Gamma = 0.00935$, $\xi_\kappa = -0.029$, $\xi_{\kappa,\Gamma} = \xi_\kappa + \xi_\Gamma = -0.01339$.*

The first two constants appear in calculations[55] [56] as penalties for erasing upright quarters of compression type, and Voronoi type, respectively. ξ'_Γ is an improved bound on the penalty for erasing when the upright diagonal is at least 2.57. Also, ξ_κ is an upper bound[57] on κ, when the upright diagonal is at most 2.57. If the upright diagonal is at least 2.57, then we still obtain the bound[58] $\xi_{\kappa,\Gamma} = -0.02274 + \xi'_\Gamma$ on the sum of κ with the penalty from erasing an upright quarter.

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[51] CALC-729988292
[52] CALC-628964355
[53] CALC-187932932
[54] CALC-618205535
[55] CALC-73974037
[56] CALC-764978100
[57] CALC-618205535
[58] CALC-618205535

11.8 Four anchors

Lemma 11.21. *If there are at least two large gaps around an upright diagonal with four anchors, then it can be erased.*

Proof. There are at least as many large gaps as upright quarters. Each large gap drops us by ξ_κ and each quarter lifts us by at most[59] [60] [61] ξ_Γ. We have $\xi_{\kappa,\Gamma} < 0$. □

Remark 11.22. *Let $\{0, v\}$ be an enclosed vertex over a flat quarter. Then*

$$|v| \geq \mathcal{E}(2, 2, 2, 2t_0, 2t_0, 2\sqrt{2}, 2, 2, 2) > 2.6.$$

If an edge of the flat quarter is sufficiently short, say $y_6 \leq 2.2$, then

$$|v| \geq \mathcal{E}(2, 2, 2, 2.2, 2t_0, 2\sqrt{2}, 2, 2, 2) > 2.7.$$

The two dihedral angles on the gaps are > 1.65. If the two quarters mask a flat quarter, we use the scoring of 11.9.2.c. We have $0.0114 < -2\xi_{\kappa,\Gamma}$.

When there is one large gap, we may erase with a penalty $\pi_0 = 0.008$.

Lemma 11.23. *Let v be an upright diagonal with four anchors. Assume that there is one large gap. The anchored simplices can be erased with penalty $\pi_0 = 0.008$. If any of the anchored simplices around v is not an upright quarter then we can erase with penalty $\pi_0 = 0.00222$.*

Moreover, if there is a flat quarter overlapping an upright quarter, then (1) or (2) holds.

1. *The truncated function* s-vor_0 *exceeds the score by at least* 0.0063. *The diagonal of the flat is at least* 2.6, *and the edge opposite the diagonal is at least* 2.2.
2. *The truncated function exceeds the score by at least* 0.0114. *The diagonal of the flat is at least* 2.7, *and the edge opposite the diagonal is at most* 2.2.

Definition 11.24. *Let a 3-unconfined upright diagonal be an upright diagonal that has four anchors and one large gap in a situation where there is no masked flat quarter.*

Proof. The constants and inequalities used in this proof can be found in a series of calculations.[62] [63] [64]

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[62] CALC-618205535
[63] CALC-73974037
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First we establish the penalty 0.008. The truncated function s-vor$_0$ is an upper bound on the score of an anchored simplex that is not a quarter. By these inequalities, the result follows if the diagonal satisfies $y_1 \ge 2.57$.

Take $y_1 \le 2.57$. If any of the upright quarters are of Voronoi type, the result follows from $(\xi_{\kappa,\Gamma} + \xi_\Gamma < 0.008)$. If the edges along the large gap are less than 2.25, the result follows from $(-0.03883 + 3\xi_\Gamma = 0.008)$. If all but one edge along the large gap are less than 2.25, the result follows from $(-0.0325 + 2\xi_\Gamma + 0.00928 = 0.008)$.

If there are at least two edges along the large gap of length at least 2.25, we consider two cases according to whether they lie on a common face of an upright quarter. The same group of inequalities gives the result. The bound 0.008 is now fully established.

Next we prove that we can erase with penalty 0.00222, when one of the anchored simplices is not a quarter. If $|v| \ge 2.57$, then we use

$$2\xi_\Gamma + \xi_V + \xi_\kappa \le 0.00935 + 0.003521 - 0.2274 \le 0.$$

If $|v| \le 2.57$, we use

$$2(0.01561) - 0.029 \le 0.00222.$$

Let $v_1 \ldots, v_4$ be the consecutive anchors of the upright diagonal $\{0, v\}$ with $\{v_1, v_4\}$ the large gap. Suppose $|v_1 - v_3| \le 2\sqrt{2}$.

We claim the upright diagonal $\{0, v\}$ is not enclosed over $\{0, v_1, v_2, v_3\}$. Assume the contrary. The edge $\{v_1, v_3\}$ passes through the face $\{0, v, v_4\}$. Disregarding the vertex v_2, by geometric considerations, we arrive at the rigid figure

$$\begin{array}{ll} |v| & = 2\sqrt{2},\ |v_1| = |v_1 - v| = |v - v_3| = |v_3| = |v_3 - v_4| = 2 \\ |v - v_4| & = |v_4| = 2t_0,\ |v_1 - v_4| = 3.2. \end{array}$$

The dihedral angles of $\{0, v, v_1, v_4\}$ and $\{0, v, v_3, v_4\}$ are

$$\mathrm{dih}(S(2\sqrt{2}, 2, 2t_0, 3.2, 2t_0, 2)) > 2.3,\ \mathrm{dih}(S(2\sqrt{2}, 2, 2t_0, 2, 2t_0, 2)) > 1.16$$

The sum is greater than π, contrary to the claim that the edge $\{v_1, v_3\}$ passes through the face $\{0, v, v_4\}$. (This particular conclusion leads to the corollary cited at the end of the proof.) Thus, $\{v_1, v_3\}$ passes through $\{0, v, v_2\}$ so that the simplices $\{0, v, v_1, v_2\}$ and $\{0, v, v_2, v_3\}$ are of Voronoi type.

To complete the proof of the lemma, we show that when there is a masked flat quarter, either (1) or (2) holds. Suppose we mask a flat quarter $Q' = \{0, v_1, v_2, v_3\}$. We have established that $\{v_1, v_3\}$ passes through the face $\{0, v, v_2\}$. To establish (1) assume that $|v_2| \ge 2.2$. The remark before the lemma gives

$$|v_1 - v_3| \ge \mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2t_0, 2t_0), 2, 2, 2) > 2.6.$$

The bound 0.0063 comes from

$$\xi_{\kappa,\Gamma} + 2\xi_V < -0.0063$$

To establish (2) assume that $|v_2| \le 2.2$. The remark gives

$$|v_1 - v_3| \ge \mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2.2, 2t_0), 2, 2, 2) > 2.7.$$

If the simplex $\{0, v, v_3, v_4\}$ is of Voronoi type, then

$$\xi_\kappa + 3\xi_V < -0.0114$$

Assume that $\{0, v, v_3, v_4\}$ is of compression type. We have

$$-0.004131 + \xi_{\kappa,\Gamma} + \xi_V \leq -0.0114.$$

□

Corollary 11.25. *(of proof) If there are four anchors and if the upright diagonal is enclosed over a flat quarter, then there are four anchored simplices and at least three quarters around the upright diagonal.*

11.9 Summary

The following index summarizes the cases of upright quarters that have been treated in Section 11. If the number of anchors is the number of anchored simplices (no large gaps), the results appear in Section 13.12. Every other possibility has been treated.

- 0,1,2 anchors Sec. 11.2
- 3 anchors Sec. 11.3
  - context $(3, 0)$
  - context $(3, 1)$
  - context $(3, 2)$
  - context $(3, 3)$
- 4 anchors Sec. 11.8
  - 0 gaps (Section 13.12)
  - 1 gap
  - 2 or more gaps
- 5 anchors Sec. 11.7
  - 0 gaps (Section 13.12)
  - 1 gap (4-crowded)
  - 2 or more gaps
- 6 or more anchors Sec. 11.4

By truncation and various comparison lemmas, we have entirely eliminated upright diagonals except when there are between three and five anchors. We may assume that there is at most one large gap around the upright diagonal.

1. Consider an anchored simplex Q around a remaining upright diagonal. The score of is $\nu(Q)$ if Q is a quarter, the analytic function s-vor(Q) if the simplex is of type C (Section 9.4), and the truncated function s-vor$_0(Q)$ otherwise.

2. Consider a flat quarter Q in an exceptional cluster. An upper bound on the score is obtained by taking the maximum of all of the following functions that satisfy the stated conditions on Q. Let y_4 denote the length of the diagonal and y_1 be the length of the opposite edge.

(a) The function $\mu(Q)$.

(b) s-vor$_0(Q) - 0.0063$, if $y_4 \geq 2.6$ and $y_1 \geq 2.2$. (Lemma 11.23)

(c) s-vor$_0(Q) - 0.0114$, if $y_4 \geq 2.7$ and $y_1 \leq 2.2$. (Lemma 11.23)

(d) $\nu(Q_1)+\nu(Q_2)+$s-vor$_x(S)$, if there is an enclosed vertex v over Q of height between $2t_0$ and $2\sqrt{2}$ that partitions the convex hull of (Q, v) into two upright quarters Q_1, Q_2 and a third simplex S. Here s-vor$_x$ = s-vor if S is of type C, and s-vor$_x$ = s-vor$_0$ otherwise. (Lemma 11.3)

(e) s-vor$(Q, 1.385)$ if the simplex is of type B (Section 9.4).

(f) s-vor$_0(Q)$ if the simplex is an isolated quarter with $\max(y_2, y_3) \geq 2.23$, $y_4 \geq 2.77$, and $\eta_{456} \geq \sqrt{2}$.

3. If S is a simplex is of type A, its score is s-vor(S). (Section 9.4.)

4. Everything else is scored by the truncation vor$_0$. Formula 7.13 is used on these remaining pieces. On top of what is obtained for the standard cluster by summing all these terms, there is a penalty $\pi_0 = 0.008$ each time a 3-unconfined upright diagonal is erased.

5. The remaining upright diagonals that are not completely surrounded by anchored simplices are 3-unconfined, 3-crowded, or 4-crowded from Section 11.6, 11.7, and 11.8.

11.10 Some flat quarters

Recall that $\xi_V = 0.003521$, $\xi_\Gamma = 0.01561$, $\xi'_\Gamma = 0.00935$. They are the penalties that result from erasing an upright quarter of Voronoi type, an upright quarter of compression type, and an upright quarter of compression type with diagonal ≥ 2.57. (See calculations.[65] [66]

In the next lemma, we score a flat quarter by any of the functions on the given domains

$$\hat{\sigma} = \begin{cases} \Gamma, & \eta_{234}, \eta_{456} \leq \sqrt{2}, \\ \text{s-vor}, & \eta_{234} \geq \sqrt{2}, \\ \text{s-vor}_0, & y_4 \geq 2.6, y_1 \geq 2.2, \\ \text{s-vor}_0, & y_4 \geq 2.7, \\ \text{s-vor}_0, & \eta_{456} \geq \sqrt{2}. \end{cases}$$

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Lemma 11.26. *$\hat{\sigma}$ is an upper bound on the functions in Section 11.9.2(a)–(f). That is, each function in Section 11.9.2 is dominated by some choice of $\hat{\sigma}$.*

Proof. The only case in doubt is the function of 3.10(d):

$$\nu(Q_1) + \nu(Q_2) + \text{s-vor}_x(S).$$

This is established by the following lemma. □

We consider the context $(3,1)$ that occurs when two upright quarters in the Q-system lie over a flat quarter. Let $\{0, v\}$ be the upright diagonal, and assume that $\{0, v_1, v_2, v_3\}$ is the flat quarter, with diagonal $\{v_2, v_3\}$. Let σ denote the score of the upright quarters and other anchored simplex lying over the flat quarter.

Lemma 11.27. $\sigma \le \min(0, \text{s-vor}_0)$.

Proof. The bound of 0 is established in Theorem 8.4.

By a calculation[67], if $|v| \ge 2.69$, then the upright quarters satisfy

$$\nu < \text{s-vor}_0 + 0.01(\pi/2 - \text{dih})$$

so the upright quarters can be erased. Thus we assume without loss of generality that $|v| \le 2.69$.

We have

$$|v| \ge \mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 2\sqrt{2}), 2, 2, 2) > 2.6.$$

If $|v_1 - v_2| \le 2.1$, or $|v_1 - v_3| \le 2.1$, then

$$|v| \ge \mathcal{E}(S(2, 2, 2, 2.1, 2t_0, 2\sqrt{2}), 2, 2, 2) > 2.72,$$

contrary to assumption. So take $|v_1 - v_2| \ge 2.1$ and $|v_1 - v_3| \ge 2.1$. Under these conditions we have the interval calculation[68] $\nu(Q) < \text{s-vor}_0(Q)$ where Q is the upright quarter. □

Remark 11.28. *If we have an upright diagonal enclosed over a masked flat quarter in the context $(4,1)$, then there are three upright quarters. By the same argument as in the lemma, the two quarters over the masked flat quarter score $\le \text{s-vor}_0$. The third quarter can be erased with penalty ξ_V.*

Define the *central vertex* v of a flat quarter to be the vertex for which $\{0, v\}$ is the edge opposite the diagonal.

Lemma 11.29. $\mu < \text{s-vor}_0 + 0.0268$ *for all flat quarters. If the central vertex has height ≤ 2.17, then* $\mu < \text{s-vor}_0 + 0.02$.

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Proof. This is an interval calculation.[69] □

We measure what is squandered by a flat quarter by $\hat{\tau} = \mathrm{sol}\,\zeta pt - \hat{\sigma}$.

Lemma 11.30. *Let v be a corner of an exceptional cluster at which the dihedral angle is at most 1.32. Then the vertex v is the central vertex of a flat quarter Q in the exceptional region. Moreover, $\hat{\tau}(Q) > 3.07\,pt$. If $\hat{\sigma} = \text{s-vor}_0$ (and if $\eta_{456} \geq \sqrt{2}$), we may use the stronger constant $\tau_0(Q) > 3.07\,pt + \xi_V + 2\xi'_\Gamma$.*

Proof. Let $S = S(y_1, \ldots, y_6)$ be the simplex inside the exceptional cluster centered at v, with $y_1 = |v|$. The inequality $\mathrm{dih} \leq 1.32$ gives the interval calculation $y_4 \leq 2\sqrt{2}$, so S is a quarter. The result now follows by interval arithmetic.[70] □

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Section 12

Bounds in Exceptional Regions

12.1 The main theorem

Let (R, D) be a standard cluster. Let U be the set of corners, that is, the set of vertices in the cone over R that have height at most $2t_0$. Consider the set E of edges of length at most $2t_0$ between vertices of U. We attach a multiplicity to each edge. We let the multiplicity be 2 when the edge projects radially to the interior of the standard region, and 0 when the edge projects radially to the complement of the standard region. The other edges, those bounding the standard region, are counted with multiplicity 1.

Let n_1 be the number of edges in E, counted with multiplicities. Let c be the number of classes of vertices under the equivalence relation $v \sim v'$ if there is a sequence of edges in E from v to v'. Let $n(R) = n_1 + 2(c-1)$. If the standard region under R is a polygon, then $n(R)$ is the number of sides.

Theorem 12.1. *Let D be a contravening decomposition star. $\tau_R(D) > t_n$, where $n = n(R)$ and*

$$\begin{aligned} t_4 &= 0.1317, \quad t_5 = 0.27113, \quad t_6 = 0.41056, \\ t_7 &= 0.54999, \quad t_8 = 0.6045. \end{aligned}$$

The decomposition star scores less than $8\,pt$, if $n(R) \geq 9$, for some standard cluster R. The scores satisfy $\sigma_R(D) < s_n$, for $5 \leq n \leq 8$, where

$$s_5 = -0.05704, \quad s_6 = -0.11408, \quad s_7 = -0.17112, \quad s_8 = -0.22816.$$

Sometimes, it is convenient to calculate these bounds as a multiple of pt. We have

$$\begin{aligned} t_4 &> 2.378\,pt, \quad t_5 > 4.896\,pt, \quad t_6 > 7.414\,pt, \\ t_7 &> 9.932\,pt, \quad t_8 > 10.916\,pt. \end{aligned}$$

$$s_5 < -1.03\,pt, \quad s_6 < -2.06\,pt, \quad s_7 < -3.09\,pt, \quad s_8 < -4.12\,pt.$$

Corollary 12.2. *Every standard region is a either a polygon or one shown in Figure 12.1*

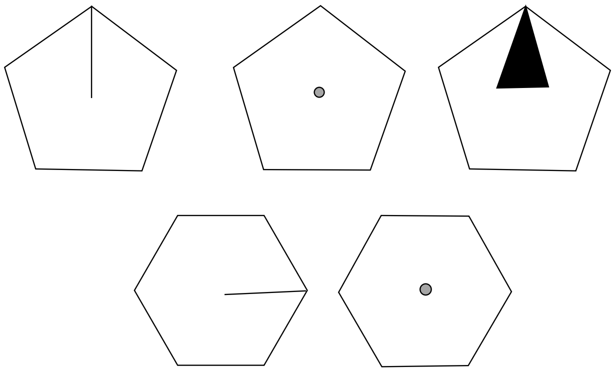

Figure 12.1.

In the cases that are not (simple) polygons, we call the *polygonal hull* the polygon obtained by removing the internal edges and vertices. We have $m(R) \leq n(R)$, where the constant $m(R)$ is the number of sides of the polygonal hull.

Proof. By the theorem, if the standard region is not a polygon, then $8 \geq n_1 \geq m \geq 5$. (Quad clusters and quasi-regular tetrahedra have no enclosed vertices. See Lemma 10.4 and Lemma 5.13.) If $c > 1$, then $8 \geq n = n_1 + 2(c-1) \geq 5 + 2(c-1)$, so $c = 2$, and $n_1 = 5, 6$ (frames 2 and 5 of the figure).

Now take $c = 1$. Then $8 \geq n \geq 5 + (n - m)$, so $n - m \leq 3$. If $n - m = 3$, we get frame 3. If $n - m = 2$, we have $8 \geq m + 2 \geq 5 + 2$, so $m = 5, 6$ (frames 1, 4).

But $n - m = 1$ cannot occur, because a single edge that does not bound the polygonal hull has even multiplicity. Finally, if $n - m = 0$, we have a polygon. □

Corollary 12.3. *If the type of a vertex of a decomposition star is* $(7, 0)$*, then it does not contravene.*

Proof. By Theorem 12.1, if there is a non-triangular region, we have

$$\tau(D) \geq \tau_{\rm LP}(7, 0) + t_4 > (4\pi\zeta - 8)\,pt.$$

Assume that all standard regions are triangular. If there is a vertex that does not lie on one of seven triangles, we have by Lemma 10.5:

$$\tau(D) \geq \tau_{\rm LP}(7, 0) + 0.55\,pt > (4\pi\zeta - 8)\,pt.$$

Thus, all vertices lie on one of the seven triangles. The complement of these seven triangles is a region triangulation by five standard regions. There is some vertex of these five that does not lie on any of the other four standard regions in the complement. That vertex has type $(3, 0)$, which is contrary to Lemma 10.9. □

12.2 Nonagons

A few additional comments are needed to eliminate $n = 9$ and 10, even after the bounds t_9, t_{10} are established.

Lemma 12.4. *Let F be a set of one or more 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. Suppose that $n = 9$, and that R squanders at least t_9 and scores less than s_9. This bound is already sufficient to conclude that there are no other standard clusters except quasi-regular tetrahedra ($t_9 + t_4 > (4\pi\zeta - 8)\,pt$). There are no vertices of type $(4, 0)$ or $(6, 0)$: $t_9 + 4.14\,pt > (4\pi\zeta - 8)\,pt$ by Lemma 10.5. So all vertices not over the exceptional cluster are of type $(5, 0)$. Suppose that there are ℓ vertices of type $(5, 0)$. The polygonal hull of R has $m \le 9$ edges. There are $m - 2 + 2\ell$ quasi-regular tetrahedra. If $\ell \le 3$, then by Lemma 10.6, the score is less than

$$s_9 + (m - 2 + 2\ell)\,pt - 0.48\ell\,pt < 8\,pt.$$

If on the other hand, $\ell \ge 4$, the decomposition star squanders more than

$$t_9 + 4(0.55)\,pt > (4\pi\zeta - 8)\,pt.$$

□

The bound s_9 will be established as part of the proof of Theorem 12.1.

The case $n = 10$ is similar. If $\ell = 0$, the score is less than $(m - 2)\,pt \le 8\,pt$, because the score of an exceptional cluster is strictly negative, Theorem 8.4. If $\ell > 0$, we squander at least $t_{10} + 0.55\,pt > (4\pi\zeta - 8)\,pt$ (Lemma 10.6).

12.3 Distinguished edge conditions

Take an exceptional cluster. We prepare the cluster by erasing upright diagonals, including those that are 3-unconfined, 3-crowded, or 4-crowded. The only upright diagonals that we leave unerased are loops. When the upright diagonal is erased, we score with the truncated function vor_0 away from flat quarters. Flat quarters are scored with the function $\hat{\sigma}$. The exceptional clusters in Sections 12 and 13 are assumed to be prepared in this way.

A simplex S is *special* if the fourth edge has length at least $2\sqrt{2}$ and at most 3.2, and the others have length at most $2t_0$. The fourth edge will be called its diagonal.

We draw a system of edges between vertices. Each vertex will have height at most $2t_0$. The radial projections of the edges to the unit sphere will divide the standard region into subregions. We call an edge *nonexternal* if the radial projection of the edge lies entirely in the (closed) exceptional region.

1. Draw all nonexternal edges of length at most $2\sqrt{2}$ except those between nonconsecutive anchors of a remaining upright diagonal. These edges do not cross (Lemma 4.30). These edges do not cross the edges of anchored simplices (Lemma 4.22 and Lemma 4.24).

2. Draw all edges of (remaining) anchored upright simplices that are opposite the upright diagonal, except when the edge gives a special simplex. The anchored simplices do not overlap (Lemma 11.9), so these edges do not cross. These edges are nonexternal (Lemma 11.5 and Lemma 4.19).

3. Draw as many additional nonexternal edges as possible of length at most 3.2 subject to not crossing another edge, not crossing any edge of an anchored simplex, and not being the diagonal of a special simplex.

We fix once and for all a maximal collection of edges subject to these constraints. Edges in this collection are called *distinguished* edges. The radial projection of the distinguished edges to the unit sphere gives the bounding edges of regions called the *subregions*. Each standard region is a union of subregions. The vertices of height at most $2t_0$ and the vertices of the remaining upright diagonals are said to form a *subcluster*.

By construction, the special simplices and anchored simplices around an upright quarter form a subcluster. Flat quarters in the Q-system, flat quarters of an isolated pair, and simplices of type A and B are subclusters. Other subclusters are scored by the function vor_0. For these subclusters, Formula 7.13 extends without modification.

12.4 Scoring subclusters

The terms of Formula 7.13 defining $\mathrm{vor}_{0,P}(D) = \mathrm{vor}_P(D, t_0)$ have a clear geometric interpretation as quoins, wedges of t_0-cones, and solid angles (see Section 7). There is a quoin for each Rogers simplex. There is a somewhat delicate point that arises in connection with the geometry of subclusters. It is not true in general that the Rogers simplices entering into the truncation $\mathrm{vor}_{0,P}(D)$ of (P, D) lie in the cone over P. Formula 7.13 should be viewed as an analytic continuation that has a nice geometric interpretation when things are nice, and which always gives the right answer when summed over all the subclusters in the cluster, but which may exhibit unusual behavior in general. The following lemma shows that the simple geometric interpretation of Formula 7.13 is valid when the subregion is not triangular.

Lemma 12.5. *If a subregion is not a triangle and is not the subregion containing the anchored simplices around an upright diagonal, the cone of arcradius*

$$\psi = \arccos(|v|/(2t_0))$$

centered along $\{0, v\}$, *where* v *is a corner of the subcluster, does not cross out of the subregion.*

Proof. For a contradiction, let $\{v_1, v_2\}$ be a distinguished edge that the cone crosses. If both edges $\{v, v_1\}$ and $\{v, v_2\}$ have length less than $2t_0$, there can be no enclosed vertex w of height at most $2t_0$, unless its distance from v_1 and v_2 is less than $2t_0$:

$$\mathcal{E}(S(2,2,2,2t_0,2t_0,3.2),2t_0,2,2) > 2t_0.$$

In this case, we can replace $\{v_1, v_2\}$ by an edge of the subregion closer to v, so without loss of generality we may assume that there are no enclosed vertices when both edges $\{v, v_1\}$ and $\{v, v_2\}$ have length less than $2t_0$.

The subregion is not a triangle, so $|v - v_1| \geq 2t_0$, or $|v - v_2| \geq 2t_0$, say $|v - v_1| \geq 2t_0$. Also $|v - v_2| \geq 2$. Pivot so that $|v_1 - v_2| = 3.2$, $|v - v_1| = 2t_0$, $|v - v_2| = 2$. (The simplex $\{0, v_1, v_2, v\}$ cannot collapse ($\Delta \neq 0$) as we pivot. For more details about why $\Delta \neq 0$, see Inequality 12.2 in Section 12.7.) Then use[71] $\beta_\psi \leq \mathrm{dih}_3$. ☐

As a consequence, in nonspecial standard regions, the terms in the Formula 7.13 for vor_0 retain their interpretations as quoins, Rogers simplices, t_0-cones, and solid angles, all lying in the cone over the standard region.

12.5 Proof

The proof of the theorem occupies the rest of the section. The inequalities for triangular and quadrilateral regions have already been proved. The bounds on t_3, t_4, s_3, and s_4 are found in Lemma 10.1, Section 11.1, Lemma 8.10, and Theorem 8.4, respectively. Thus, we may assume throughout the proof that the standard region is exceptional

We begin with a slightly simplified account of the method of proof. Set $t_9 = 0.6978$, $t_{10} = 0.7891$, $t_n = (4\pi\zeta - 8)\,pt$, for $n \geq 11$. Set $D(n,k) = t_{n+k} - 0.06585\,k$, for $0 \leq k \leq n$, and $n + k \geq 4$. This function satisfies

$$D(n_1,k_1) + D(n_2,k_2) \geq D(n_1+n_2-2, k_1+k_2-2). \tag{12.1}$$

In fact, this inequality unwinds to $t_r + 0.13943 \geq t_{r+1}$, $D(3,2) = 0.13943$, and $t_n = (0.06585)2 + (n-4)D(3,2)$, for $n = 4,5,6,7$. These hold by inspection.

Call an edge between two vertices of height at most $2t_0$ *long* if it has length greater than $2t_0$. Add the distinguished edges to break the standard regions into subregions. We say that a subregion has *edge parameters* (n,k) if there are n bounding edges, where k of them are long. (We count edges with multiplicities as in Section 12.1, if the subregion is not a polygon.) Combining two subregions of edge parameters (n_1,k_1) and (n_2,k_2) along a long edge e gives a union with edge parameters (n_1+n_2-2, k_1+k_2-2), where we agree not to count the internal edge e that no longer bounds. Inequality 12.1 localizes the main theorem to what

[71] CALC-193836552

is squandered by subclusters. Suppose we break the standard cluster into groups of subregions such that if the group has edge parameters (n, k), it squanders at least $D(n, k)$. Then by superadditivity (Sec. 12.5, Formula 12.1), the full standard cluster R must squander $D(n, 0) = t_n$, $n = n(R)$, giving the result.

Similarly, define constants $s_4 = 0$, $s_9 = -0.1972$, $s_n = 0$, for $n \geq 10$. Set $Z(n, k) = s_{n+k} - k\epsilon$, for $(n, k) \neq (3, 1)$, and $Z(3, 1) = \epsilon$, where[72] $\epsilon = 0.00005$. The function $Z(n, k)$ is subadditive:

$$Z(n_1, k_1) + Z(n_2, k_2) \leq Z(n_1 + n_2 - 2, k_1 + k_2 - 2).$$

In fact, this easily follows from $s_a + s_b \leq s_{a+b-4}$, for $a, b \geq 4$, and $\epsilon > 0$. It will be enough in the proof of Theorem 12.1 to show that the score of a union of subregions with edge parameters (n, k) is at most $Z(n, k)$.

12.6 Preparation of the standard cluster

Fix a standard cluster. We return to the construction of subregions and distinguished edges, to describe the penalties. Take the penalty of 0.008 for each 3-unconfined upright diagonal. Take the penalty $0.03344 = 3\xi_\Gamma + \xi_{\kappa,\Gamma}$ for 4-crowded upright diagonals. Take the penalty $0.04683 = 3\xi_\Gamma$ for 3-crowded upright diagonals. Set $\pi_{\max} = 0.06688$. The penalty in the next lemma refers to the combined penalty from erasing all 3-unconfined, 3-crowded, and 4-crowded upright diagonals in the decomposition star. The upright quarters that completely surround an upright diagonal (loops) are not erased.

Lemma 12.6. *The total penalty from a contravening decomposition star is at most* $\pi_{\max}$.

Proof. Before any upright quarters are erased, each quarter squanders[73] > 0.033, so the star squanders $> (4\pi\zeta - 8)\,pt$ if there are ≥ 25 quarters. Assume there are at most 24 quarters. If the only penalties are 0.008, we have $8(0.008) < \pi_{\max}$. If we have the penalty 0.04683, there are at most seven other quarters $(0.5606+8(0.033) > (4\pi\zeta-8)\,pt)$ (Lemma 11.6), and no other penalties from this type or from 4-crowded upright diagonals, so the total penalty is at most $2(0.008)+0.04683 < \pi_{\max}$. Finally, if there is one 4-crowded upright diagonal, there are at most twelve other quarters (Section 11.7), and erasing gives the penalty $0.03344 + 4(0.008) < \pi_{\max}$. ∎

The remaining upright diagonals are surrounded by anchored simplices. If the edge opposite the diagonal in an anchored simplex has length $\geq 2\sqrt{2}$, then there may be an adjacent special simplex whose diagonal is that edge. Section 13.12 will give bounds on the aggregate of these anchored simplices and special simplices. In all other contexts, the upright quarters have been erased with penalties.

Break the standard cluster into subclusters as in Section 12.3. If the subregion is a triangle, we refer to the bounds of 13.8. Sections 12.7–13.11 give bounds for

[72] Compare CALC-193836552.
[73] CALC-148776243

subregions that are not triangles in which all the upright quarters have been erased. We follow the strategy outlined in Section 12.5, although the penalties will add certain complications.

We now assume that we have a subcluster without quarters and whose region is not triangular. The truncated function vor_0 is an upper bound on the score. Penalties are largely disregarded until Section 13.4.

We describe a series of deformations of the subcluster that increase $\mathrm{vor}_{0,P}(D)$ and decrease $\tau_{0,P}(D)$. These deformations disregard the broader geometric context of the subcluster. Consequently, we cannot claim that the deformed subcluster exists in any decomposition star D. As the deformation progresses, an edge $\{v_1, v_2\}$, not previously distinguished, can emerge with the properties of a distinguished edge. If so, we add it to the collection of distinguished edges, use it if possible to divide the subcluster into smaller subclusters, and continue to deform the smaller pieces. When triangular regions are obtained, they are set aside until Section 13.8.

12.7 Reduction to polygons

By deformation, we can produce subregions whose boundary is a polygon. Let U be the set of vertices over the subregion of height $\le 2t_0$. As in Section 12.1, the distinguished edges partition U into equivalence classes. Move the vertices in one equivalence class U_1 as a rigid body preserving heights until the class comes sufficiently close to form a distinguished edge with another subset. Continue until all the vertices are interconnected by paths of distinguished edges. vor_0 and τ_0 are unchanged by these deformations.

If some vertex v is connected to three or more vertices by distinguished edges, it follows from the connectedness of the open subregion that there is more than one connected component U_i (by paths of distinguished edges) of $U \setminus \{v\}$. Move $U_1 \cup \{v\}$ rigidly preserving heights and keeping v fixed until a distinguished edge forms with another component. Continue until the distinguished edges break the subregions into subregions with polygon boundaries. Again vor_0 and τ_0 are unchanged.

By the end of Section 12, we will deform all subregions into convex polygons.

Remark 12.7. *We will deform in such a way that the edges $\{v_1, v_2\}$ will maintain a length of at least 2. The proof that distances of at least 2 are maintained is given in Section 12.13.*

We will deform in such a way that no vertex crosses a boundary of the subregion passing from outside to inside.

Edge length constraints prevent a vertex from crossing a boundary of the subregion from the inside to outside. In fact, if v is to cross the edge $\{v_1, v_2\}$, the simplex $S = \{0, v_1, v, v_2\}$ attains volume 0. We may assume, by the argument of the proof of Lemma 12.4, that there are no vertices enclosed over S. Because we are assuming that the subregion is not a triangle, we may assume that $|v - v_1| > 2t_0$. We have $|v| \in [2, 2t_0]$. If v is to cross $\{v_1, v_2\}$, we may assume that the dihedral angles of S along $\{0, v_1\}$, and $\{0, v_2\}$ are acute. Under these constraints, by the explicit formulas of [Hal97a, Sec. 8], the vertex v cannot cross out of the subregion

$$\Delta(S) \geq \Delta(2t_0^2, 4, 4, 3.2^2, 4, 2t_0^2) > 0. \tag{12.2}$$

We say that a corner v_1 is *visible* from another v_2 if $\{v_1, v_2\}$ lies over the subregion. A deformation may make v_1 visible from v_2, making it a candidate for a new distinguished edge. If $|v_1 - v_2| \leq 3.2$, then as soon as the deformation brings them into visibility (obstructed until then by some v), then Inequality 12.2 shows that $|v_1 - v|, |v_2 - v| \leq 2t_0$. So v_1, v, v_2 are consecutive edges on the polygonal boundary, and $|v_1 - v_2| \geq 2\sqrt{4 - t_0^2} > \sqrt{8}$. By the distinguished edge conditions for special simplices, $\{v_1, v_2\}$ is too long to be distinguished. In other words, there can be no potentially distinguished edges hidden behind corners. They are always formed in full view.

12.8 Some deformations

Definition 12.8. *Consider three consecutive corners v_3, v_1, v_2 of a subcluster R such that the dihedral angle of R at v_1 is greater than π. We call such an corner concave. (If the angle is less than π, we call it convex.) Similarly, the angle of a subregion is said to be convex or concave depending on whether it is less than or greater than π.*

Let $S = S(y_1, \ldots, y_6) = \{0, v_1, v_2, v_3\}$, $y_i = |v_i|$. Suppose that $y_6 > y_5$. Let $x_i = y_i^2$.

Lemma 12.9. *At a concave vertex, $\partial \operatorname{vor}_0 / \partial x_5 > 0$ and $\partial \tau_0 / \partial x_5 < 0$.*

Proof. As x_5 varies, $\operatorname{dih}_i(S) + \operatorname{dih}_i(R)$ is constant for $i = 1, 2, 3$. The part of Formula 7.13 for vor_0 that depends on x_5 can be written

$$-B(y_1)\operatorname{dih}(S) - B(y_2)\operatorname{dih}_2(S) - B(y_3)\operatorname{dih}_3(S) - 4\delta_{oct}(\operatorname{quo}(R_{135}) + \operatorname{quo}(R_{315})),$$

where $B(y_i) = A(y_i/2) + \phi_0$, $R_{135} = R(y_1/2, b, t_0)$, $R_{315} = R(y_3/2, b, t_0)$, $b = \eta(y_1, y_3, y_5)$, and $A(h) = (1 - h/t_0)(\phi(h, t_0) - \phi_0)$. Set $u_{135} = u(x_1, x_3, x_5)$, and $\Delta_i = \partial\Delta/\partial x_i$. (The notation comes from [Hal97a, Sec. 8] and Section 7.) We have

$$\frac{\partial \operatorname{quo}(R(a, b, c))}{\partial b} = \frac{-a(c^2 - b^2)^{3/2}}{3b(b^2 - a^2)^{1/2}} \leq 0$$

and $\partial b / \partial x_5 \geq 0$. Also, $u \geq 0$, $\Delta \geq 0$ (see [Hal97a, Sec. 8]). So it is enough to show

$$V_0(S) = u_{135}\Delta^{1/2} \frac{\partial}{\partial x_5}(B(y_1)\operatorname{dih}(S) + B(y_2)\operatorname{dih}_2(S) + B(y_3)\operatorname{dih}_3(S)) < 0.$$

By the explicit formulas of [Hal97a, Sec. 8], we have

$$V_0(S) = -B(y_1)y_1\Delta_6 + B(y_2)y_2u_{135} - B(y_3)y_3\Delta_4.$$

For τ_0, we replace B with $B - \zeta pt$. It is enough to show that

$$V_1(S) = -(B(y_1) - \zeta pt)y_1\Delta_6 + (B(y_2) - \zeta pt)y_2 u_{135} - (B(y_3) - \zeta pt)y_3\Delta_4 < 0.$$

The lemma now follows from an interval calculation. We note that the polynomials V_i are linear in x_4, and x_6, and this may be used to reduce the dimension of the calculation. □

We give a second form of the lemma when the dihedral angle of R is less than π, that is, at a convex corner.

Lemma 12.10. *At a convex corner,* $\partial\,\mathrm{vor}_0/\partial x_5 < 0$ *and* $\partial\tau_0/\partial x_5 > 0$*, if* $y_1, y_2, y_3 \in [2, 2t_0]$*,* $\Delta \geq 0$*, and (i)* $y_4 \in [2\sqrt{2}, 3.2]$*,* $y_5, y_6 \in [2, 2t_0]$*, or (ii)* $y_4 \geq 3.2, y_5, y_6 \in [2, 3.2]$.

Proof. We adapt the proof of the previous lemma. Now $\mathrm{dih}_i(S) - \mathrm{dih}_i(R)$ is constant, for $i = 1, 2, 3$, so the signs change. vor_0 depends on x_5 through

$$\sum B(y_i)\,\mathrm{dih}_i(S) - 4\delta_{oct}(\mathrm{quo}(R_{135}) + \mathrm{quo}(R_{315})).$$

So it is enough to show that

$$V_0 - 4\delta_{oct}\Delta^{1/2}u_{135}\frac{\partial}{\partial x_5}(\mathrm{quo}(R_{135}) + \mathrm{quo}(R_{315})) < 0.$$

Similarly, for τ_0, it is enough to show that

$$V_1 - 4\delta_{oct}\Delta^{1/2}u_{135}\frac{\partial}{\partial x_5}(\mathrm{quo}(R_{135}) + \mathrm{quo}(R_{315})) < 0.$$

By an interval calculation[74]

$$\begin{array}{lll} -4\delta_{oct}u_{135}\frac{\partial}{\partial x_5}(\mathrm{quo}(R_{135}) + \mathrm{quo}(R_{315})) & < 0.82, & \text{on } [2, 2t_0]^3, \\ & < 0.5, & \text{on } [2, 2t_0]^3, y_5 \geq 2.189. \end{array}$$

The result now follows from the inequalities.[75] □

Return to the situation of concave corner v_1. Let v_2, v_3 be the adjacent corners. By increasing x_5, the vertex v_1 moves away from every corner w for which $\{v_1, w\}$ lies outside the region. This deformation then satisfies the constraint of Remark 12.7. Stretch the shorter of $\{v_1, v_2\}$, $\{v_1, v_3\}$ until $|v_1 - v_2| = |v_1 - v_3| = 3.07$ (or until a new distinguished edge forms, etc.). Do this at all concave corners.

By stopping at 3.07, we prevent a corner crossing an edge from outside-in. Let w be a corner that threatens to cross a distinguished edge $\{v_1, v_2\}$ as a result of the motion at a nonconvex vertex. To say that the crossing of the edge is from the outside-in implies more precisely that the vertex being moved is an endpoint, say

[74] CALC-984628285
[75] CALC-984628285

v_1, of the distinguished edge. At the moment of crossing the simplex $\{0, v_1, v_2, w\}$ degenerates to a planar arrangement, with the radial projection of w lying over the geodesic arc connecting the radial projections of v_1 and v_2. To see that the crossing cannot occur, it is enough to note that the volume of a simplex with opposite edges of lengths at most $2t_0$ and 3.07 and other edges at least 2 cannot be planar. The extreme case is

$$\Delta(2^2, 2^2, (2t_0)^2, 2^2, 2^2, 3.07^2) > 0.$$

If $|v_1| \geq 2.2$, we can continue the deformations even further. We stretch the shorter of $\{v_1, v_2\}$ and $\{v_1, v_3\}$ until $|v_1 - v_2| = |v_1 - v_3| = 3.2$ (or until a new distinguished edge forms, etc.). Do this at all concave corners v_1 for which $|v_1| \geq 2.2$. To see that corners cannot cross an edge from the outside-in, we argue as in the previous paragraph, but replacing 3.07 with 3.2. The extreme case becomes

$$\Delta(2.2^2, 2^2, (2t_0)^2, 2^2, 2^2, 3.2^2) > 0.$$

12.9 Truncated corner cells

Because of the arguments in the Section 12.8, we may assume without loss of generality that we are working with a subregion with the following properties. If v is a concave vertex and w is not adjacent to v, and yet is visible from v, then $|v - w| \geq 3.2$. If v is a concave corner, then $|v - w| \geq 3.07$ for both adjacent corners w. If v is a concave corner and $|v| \geq 2.2$, then $|v - w| \geq 3.2$ for both adjacent corners w. These hypotheses will remain in force through the end of Section 12.

Recall from Definition 12.8 that we call a spherical region *convex* if its interior angles are all less than π. The case where the subregion is a convex triangle will be treated in Section 13.8. Hence, we may also assume in Sections 12.9 through 12.12 that the subregion is not a convex triangle.

We construct a *corner cell* at each corner. It depends on a parameter $\lambda \in [1.6, 1.945]$. In all applications, we take $\lambda = 1.945 = 3.2 - t_0$, $\lambda = 1.815 = 3.07 - t_0$, or $\lambda = 1.6 = 3.2/2$.

To construct the cell around the corner v, place a triangle along $\{0, v\}$ with sides $|v|$, t_0, λ (with λ opposite the origin). Generate the solid of rotation around the axis $\{0, v\}$. Extend to a cone over 0. Slice the solid by the perpendicular bisector of $\{0, v\}$, retaining the part near 0. Intersect the solid with a ball of radius t_0. The cones over the two boundary edges of the subregion at v make two cuts in the solid. Remove the slice that lies outside the cone over the subcluster. What remains is the corner cell at v with parameter λ.

Corner cells at corners separated by a distance less than 2λ may overlap. We define a truncation of the corner cell that has the property that the *truncated corner cells* at adjacent corners do not overlap. Let $\{0, v_i, v_j\}^\perp$ denote the plane perpendicular to the plane $\{0, v_i, v_j\}$ passing through the origin and the circumcenter of $\{0, v_i, v_j\}$.

Let v_1, v_2, v_3 be consecutive corners of a subcluster. Take the corner cell with parameter λ at the corner v_2. Slice it by the planes $\{0, v_1, v_2\}^\perp$ and $\{0, v_2, v_3\}^\perp$, and retain the part along the edge $\{0, v_2\}$. This is the truncated corner cell (tcc).

By construction tccs at adjacent corners are separated by a plane $(0,\cdot,\cdot)^\perp$. Tccs at nonadjacent corners do not overlap if the corners are $\ge 2\lambda$ apart. Tccs will only be used in subregions satisfying this condition. It will be shown in Section 12.11 that tccs lie in the cone over the subregion (for suitable λ).

12.10 Formulas for Truncated corner cells

We will assign a score to truncated corner cells, in such a way that the score of the subcluster can be estimated from the scores of the corner cells.

We write C_0 for a truncated corner cell. We write C_0^u for the corresponding untruncated corner cell. (Although we call this the untruncated corner cell to distinguish it from the corner cell, it is still truncated in the sense that it lies in the ball at the origin of radius t_0. It is untruncated in the sense that it is not cut by the planes $(\ldots)^\perp$.)

For any solid body X, we define the *geometric* truncated function by

$$\mathrm{vor}_0^g(X) = 4(-\delta_{oct}\mathrm{vol}(X) + \mathrm{sol}(X)/3)$$

the counterpart for squander

$$\tau_0^g(X) = \zeta pt\,\mathrm{sol}(X) - \mathrm{vor}_0^g(X).$$

The solid angle is to be interpreted as the solid angle of the cone formed by all rays from the origin through nonzero points of X. We may apply these definitions to obtain formulas for $\mathrm{vor}_0^g(C_0)$, and so forth.

The formula for the score of a truncated corner cell differs slightly according to the convexity of the corner. We start with a convex corner v, and let v_1, v, and v_2 be consecutive corners in the subregion.

Let $S = \{0, v, v_1, v_2\}$ be a simplex with $|v_1 - v_2| \ge 3.2$. The formula for the score of a tcc $C_0(S)$ simplifies if the face of C_0 cut by $\{0, v, v_1\}^\perp$ does not meet the face cut by $\{0, v, v_2\}^\perp$. We make that assumption in this subsection. Set $\chi_0(S) = \mathrm{vor}_0^g(C_0(S))$. (The function χ_0 is unrelated to the function χ that was introduced in Definition 5.14 to measure the orientation of faces.)

$$\begin{aligned}
\psi \quad &= \mathrm{arc}(y_1, t_0, \lambda), \quad h = y_1/2,\\
R'_{126} \quad &= R(y_1/2, \eta_{126}, y_1/(2\cos\psi)), \quad R_{126} = R(y_1/2, \eta_{126}, t_0),\\
\mathrm{sol}'(y_1, y_2, y_6) \quad &= +\,\mathrm{dih}(R'_{126})(1-\cos\psi) - \mathrm{sol}(R'_{126}),\\
\chi_0(S) \quad &= \mathrm{dih}(S)(1-\cos\psi)\phi_0\\
&\quad - \mathrm{sol}'(y_1, y_2, y_6)\phi_0 - \mathrm{sol}'(y_1, y_3, y_5)\phi_0\\
&\quad + A(h)\,\mathrm{dih}(S) - 4\delta_{oct}(\mathrm{quo}(R_{126}) + \mathrm{quo}(R_{135})).
\end{aligned}$$

In the three lines giving the formula for χ_0, the first line represents the score of the cone before it is cut by the planes $\{0, v, v_i\}^\perp$ and the perpendicular bisector of $\{0, v\}$. The second line is the correction resulting from cutting the tcc along the planes $\{0, v, v_i\}^\perp$. The face of the Rogers simplex R'_{126} lies along the plane $\{0, v, v_1\}^\perp$. The third line is the correction from slicing the tcc with the perpendicular bisector of $\{0, v\}$. This last term is the same as the term appearing for a similar reason in the formula for vor_0 in Formula 7.13. In this formula R is the usual Rogers simplex and $\mathrm{quo}(R_{ijk})$ is the quoin coming from a Rogers simplex along the face with edges (ijk).

The formula for the untruncated corner cell is obtained by setting "sol′" and "quo" to "0" in the expression for χ_0. Thus,

$$\mathrm{vor}^g(C_0^u) = \mathrm{dih}(S)[(1-\cos\psi)\phi_0 + A(h)]$$

The formula depends only on λ, the dihedral angle, and the height $|v|$. We write $C_0^u = C_0^u(|v|, \mathrm{dih})$, and suppress λ from the notation. The dependence on $\mathrm{dih}(S)$ is linear:

$$\tau_0^g(C_0^u(|v|, \mathrm{dih})) = (\mathrm{dih}/\pi)\tau_0^g(C_0^u(|v|, \pi)).$$

The dependence of χ_0 on the fourth edge $y_4 = |v_1 - v_2|$ comes through a term proportional to $\mathrm{dih}(S)$. Since the dihedral angle is monotonic in y_4, so is χ_0. Thus, under the assumption that $|v_1 - v_2| \geq 3.2$, we obtain an upper bound on χ_0 at $y_4 = 3.2$. Our deformations will fix the lengths of the other five variables, and monotonicity gives us the sixth. Thus, the tccs lead to an upper bound on vor_0^g (and a lower bound on τ_0^g) that does not require interval arithmetic.

At a concave vertex, the formula is similar. Replace "$\mathrm{dih}(S)$" with "$(2\pi - \mathrm{dih}(S))$" in the given expression for χ_0. We add a superscript $-$ to the name of the function at concave vertices, to denote this modification: $\chi_0^-(C_0)$.

12.11 Containment of Truncated corner cells

The assumptions made at the beginning of Section 12.9 remain in force.

Lemma 12.11. *Let v be a concave vertex with $|v| \geq 2.2$. The truncated corner cell at v with parameter $\lambda = 1.945$ lies in the truncated V-cell over R.*

Proof. Consider a corner cell at v and a distinguished edge $\{v_1, v_2\}$ forming the boundary of the subregion. The corner cell with parameter $\lambda = 1.945$ is contained in a cone of arcradius $\theta = \mathrm{arc}(2, t_0, \lambda) < 1.21 < \pi/2$ (in terms of the function *arc* of Section 9.7). Take two corners w_1, w_2, visible from v, between which the given bounding edge appears. (We may have $w_i = v_i$). The two visible edges, $\{v, w_i\}$, have length ≥ 3.2. (Recall that the distinguished edges at v have been deformed to length 3.2.) They have arc-length at least $\mathrm{arc}(2t_0, 2t_0, 3.2) > 1.38$. The segment of the distinguished edge $\{v_1, v_2\}$ visible from v has arc-length at most $\mathrm{arc}(2, 2, 3.2) < 1.86$.

We check that the corner cell cannot cross the visible portion of the edge $\{v_1, v_2\}$. Consider the spherical triangle formed by the edges $\{v, w_1\}$, $\{v, w_2\}$ (extended as needed) and the visible part of $\{v_1, v_2\}$. Let C be the radial projection of v and AB be the radial projection of the visible part of $\{v_1, v_2\}$. Pivot A and B toward C until the edges AC and BC have arc-length 1.38. The perpendicular from C to AB has length at least

$$\arccos(\cos(1.38)/\cos(1.86/2)) > 1.21 > \theta.$$

This proves that the corner cell lies in the cone over the subregion. □

Lemma 12.12. *Let v be a concave vertex. The truncated corner cell at v with parameter $\lambda = 1.815$ lies in the truncated V-cell over R.*

Proof. The proof proceeds along the same lines as the previous lemma, with slightly different constants. Replace 1.945 with 1.815, 1.38 with 1.316, 1.21 with 1.1. Replace 3.2 with 3.07 in contexts giving a lower bound to the length of an edge at v, and keep it at 3.2 in contexts calling for an upper bound on the length of a distinguished edge. The constant 1.86 remains unchanged. □

Lemma 12.13. *The truncated corner cells with parameter* 1.6 *in a subregion do not overlap.*

Proof. We may assume that the corners are not adjacent. If a nonadjacent corner w is visible from v, then $|w - v| \geq 3.2$, and an interior point intersection p is incompatible with the triangle inequality: $|p - v| \leq 1.6$, $|p - w| < 1.6$. If w is not visible, we have a chain $v = v_0, v_1, \ldots, v_r = w$ such that v_{i+1} is visible from v_i. Imagine a taut string inside the subregion extending from v to w. The radial projections of v_i are the corners of the string's path. The string bends in an angle greater than π at each v_i, so the angle at each intermediate v_i is greater than π. That is, they are concave. Thus, by our deformations $|v_i - v_{i+1}| \geq 3.07$. The string has arc-length at least $r\,\mathrm{arc}(2t_0, 2t_0, 3.07) > r(1.316)$. But the corner cells lie in cones of arcradius $\mathrm{arc}(2, t_0, \lambda) < 1$. So $2(1.0) > r(1.316)$, or $r = 1$. Thus, w is visible from v. □

Lemma 12.14. *The corner cell for $\lambda \leq 1.815$ does not overlap the t_0-cone wedge around another corner w.*

Proof. We take $\lambda = 1.815$. As in the previous proof, if there is overlap along a chain, then

$$\mathrm{arc}(2, t_0, \lambda) + \mathrm{arc}(2, t_0, t_0) > r\,\mathrm{arc}(2t_0, 2t_0, 3.07),$$

and again $r = 1$. So each of the two vertices in question is visible from the other. But overlap implies $|p - v| \leq 1.815$ and $|p - w| < t_0$, forcing the contradiction $|w - v| < 3.07$. □

Lemma 12.15. *The corner cell for $\lambda \leq 1.945$ at a corner v satisfying $|v| \geq 2.2$ does not overlap the t_0-cone wedge around another corner w.*

Proof. We take $\lambda = 1.945$. As in the previous proof, if there is overlap along a chain, then

$$\mathrm{arc}(2, t_0, \lambda) + \mathrm{arc}(2, t_0, t_0) > r\,\mathrm{arc}(2t_0, 2t_0, 3.2),$$

and again $r = 1$. Then the result follows from

$$|w - v| \le |p - v| + |p - w| < 1.945 + t_0 = 3.2.$$

□

Definition 12.16. *(By penalty-free score, we mean the part of the scoring bound that does not include any of the penalty terms. We will sometimes call the full score, including the penalty terms, the penalty-inclusive score.)*

Lemma 12.4 was stated in the context of a subregion before deformation, but a cursory inspection of the proof shows that the geometric conditions required for the proof remain valid by our deformations. (This assumes that the subregion is not a triangle, which we assumed at the beginning of Section 12.9.) In more detail, there is a solid CP_0 contained in the ball of radius of t_0 at the origin, and lying over the cone of the subregion P such that a bound on the penalty-free subcluster score is $\mathrm{vor}_0^g(CP_0)$ and squander $\tau_0^g(CP_0)$.

Let $\{y_1, \ldots, y_r\}$ be a decomposition of the subregion into disjoint regions whose union is X. Then if we let $CP_0(y_i)$ denote the intersection of $CP_0(y_i)$ with the cone over y_i, we can write

$$\tau_0^g(CP_0) = \sum_i \tau_0^g(CP_0(y_i)).$$

These lemmas allow us to express bounds on the score (and squander) of a subcluster as a sum of terms associated with individual (truncated) corner cells. By Lemmas 12.11 through 12.15, these objects do not overlap under suitable conditions. Moreover, by the interpretation of terms provided by Section 12.4, the cones over these objects do not overlap, when the objects themselves do not. In other words, under the various conditions, we can take the (truncated) corner cells to be among the sets $CP_0(y_i)$.

To work a typical example, let us place a truncated corner cell with parameter $\lambda = 1.6$ at each concave corner. Place a t_0-cone wedge X_0 at each convex corner. The cone over each object lies in the cone over the subregion. By Lemma 12.5 and Lemma 9.20 (see the proof), the t_0-cone wedge X_0 squanders a positive amount. The part P' of the subregion outside all truncated corner cells and outside the t_0-cone wedges squanders

$$\mathrm{sol}(P')(\zeta pt - \phi_0) > 0.$$

where $\mathrm{sol}(P')$ is the part of the solid angle of the subregion lying outside the tccs. Dropping these positive terms, we obtain a lower bound on the penalty-free squander:

$$\tau_0^g(CP_0) \ge \sum_{C_0} \tau_0^g(C_0).$$

There is one summand for each concave corner of the subregion. Other cases proceed similarly.

12.12 Convexity

Lemma 12.17. *There are at most two concave corners.*

Proof. Use the parameter $\lambda = 1.6$ and place a truncated corner cell C_0 at each concave corner v. Let $C_0^u(|v|, \mathrm{dih})$ denote the corresponding untruncated cell. The Formula of Section 12.10 gives

$$\tau_0^g(C_0) = \tau_0^g(C_0^u(|v|, \mathrm{dih})) - \mathrm{sol}'(y_1, y_2, y_6)\phi_0' - \mathrm{sol}'(y_1, y_3, y_5)\phi_0',$$

where $\phi_0' = \zeta pt - \phi_0 < 0.6671$. (The conditions $y_5 \geq 3.07$ and $y_6 \geq 3.07$ force the faces along the these edges to have circumradius greater than t_0, and this causes the "quo" terms in the formula to be zero.)

By monotonicity in dih, a lower bound on $\tau_0^g(C_0^u)$ is obtained at $\mathrm{dih} = \pi$. $\tau_0(C_0^u(|v|, \pi))$ is an explicit monotone decreasing rational function of $|v| \in [2, 2t_0]$, which is minimized for $|v| = 2t_0$. We find

$$\tau_0(C_0^u(|v|, \mathrm{dih})) \geq \tau_0(C_0^u(2t_0, \pi)) > 0.32.$$

The term $\mathrm{sol}'(y_1, y_3, y_5)$ is maximized when $y_3 = 2t_0$, $y_5 = 3.07$, so that $\mathrm{sol}' < 0.017$. (This was checked with interval arithmetic in Mathematica.) Thus,

$$\tau_0(C_0(v)) \geq 0.32 - 2(0.017)\phi_0' > 0.297.$$

If there are three or more concave corners, then the penalty-free corner cells squander at least $3(0.297)$. The penalty is at most $\pi_{\max}$ (Section 12.6). So the penalty-inclusive squander is more than $3(0.297) - \pi_{\max} > (4\pi\zeta - 8)\,pt$. □

Lemma 12.18. *There are no concave corners of height at most* 2.2.

Proof. Suppose there is a corner of height at most 2.2. Place an untruncated corner cell $C_0^u(|v|, \mathrm{dih})$ with parameter $\lambda = 1.815$ at that corner and a t_0-cone wedge at every other corner. The subcluster squanders at least $\tau_0(C_0(|v|, \pi)) - \pi_{\max}$. This is an explicit monotone decreasing rational function of one variable. The penalty-inclusive squander is at least

$$\tau_0(C_0^u(2t_0, \pi)) - \pi_{\max} > (4\pi\zeta - 8)\,pt.$$

□

By the assumptions at the beginning of Section 12.9, the lemma implies that each concave corner has distance at least 3.2 from every other visible corner.

As in the previous lemma, when $\lambda = 1.945$, a lower bound on what is squandered by the corner cell is obtained for $|v| = 2t_0$, $\mathrm{dih} = \pi$. The explicit formulas give penalty-free squander > 0.734. Two disjoint corner cells give penalty-inclusive squander $> (4\pi\zeta - 8)\,pt$. Suppose two at v_1, v_2 overlap. The lowest bound is obtained when $|v_1 - v_2| = 3.2$, the shortest distance possible.

We define a function $f(y_1, y_2)$ that measures what the union of the overlapping corner cells squander. Set $y_i = |v_i|$, $\ell = 3.2$, and

$$\begin{aligned}
\alpha_1 &= \mathrm{dih}(y_1, t_0, y_2, \lambda, \ell, \lambda),\\
\alpha_2 &= \mathrm{dih}(y_2, t_0, y_1, \lambda, \ell, \lambda),\\
\mathrm{sol} &= \mathrm{sol}(y_2, t_0, y_1, \lambda, \ell, \lambda),\\
\phi_i &= \phi(y_i/2, t_0), \quad i = 1, 2,\\
\lambda &= 3.2 - t_0 = 1.945,\\
f(y_1, y_2) &= 2(\zeta pt - \phi_0)\,\mathrm{sol} + 2\textstyle\sum_1^2 \alpha_i(1 - y_i/(2t_0))(\phi_0 - \phi_i)\\
&\quad + \textstyle\sum_1^2 \tau_0(C(y_i, \lambda, \pi - 2\alpha_i)).
\end{aligned}$$

An interval calculation[76] gives $f(y_1, y_2) > (4\pi\zeta - 8)\,pt + \pi_{\max}$, for $y_1, y_2 \in [2, 2t_0]$.

We conclude that there is at most one concave corner. Let v be such a corner. If we push v toward the origin, the solid angle is unchanged and vor_0 is increased. Following this by the deformation of Section 12.8, we maintain the constraints $|v - w| = 3.2$, for adjacent corners w, while moving v toward the origin. Eventually $|v| = 2.2$. This is impossible by Lemma 12.18.

We verify that this deformation preserves the constraint $|v - w| \geq 2$, for all corners w such that $\{v, w\}$ lies entirely outside the subregion. If fact, every corner is visible from v, so that the subregion is star convex at v. We leave the details to the reader.

We conclude that all subregions can be deformed into convex polygons.

12.13 Proof that Distances Remain at least 2

Remark 12.19. *In Section 12.7, to allow for more flexible deformations, we drop all constraints on the lengths of (undistinguished) edges $\{v_1, v_2\}$ that cross the boundary of the subregion. We deform in such a way that the edges $\{v_1, v_2\}$ will maintain a length of at least 2.*

Recall that we say that a vertex of a subregion is *convex* if its angle is less than π, and otherwise that is *concave* (Definition 12.8). In general, if P is a subregions and p_1 and p_2 are two vertices of P, there is a minimal curve joining p_1 and p_2 inside P. This curve is a finite sequence $e_1, \ldots, e_r$ of spherical geodesics. We refer to this sequence as the *sequence of arcs* from p_1 to p_2. The endpoint of each spherical arc is a vertex of P. All endpoints except possible p_1 and p_2 are nonconvex. These endpoints are the radial projections of corners of P: $v_0, v_1, \ldots, v_{r+1}$, with $p(v_0) = p_1$ and $p(v_{r+1}) = p_2$. The vertex p_1 is visible from p_2 if and only if $r = 1$.

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Lemma 12.20. *This deformation of a subregion at a concave corner v maintains a distance of at least 2 to every other corner w.*

Proof. The proof is by contradiction. We may assume that $|v - w| < \sqrt{8}$. We may assume that v and w are the first corners to violate the condition of being at least 2 apart, so that distances between other pairs of corners are at least 2. A distinguished edge connects v and w, if w is visible from v. So assume that w is not visible. Let $e(v_1, v_2)$ be the first distinguished edge crossed by the geodesic arc g from $p(v)$ to $p(w)$. Let p_0 be the intersection of $e(v_1, v_2)$ and g. By construction, the deformation moves v into the subregion, and the subregion P is concave at the corner v, so that the arc from $p(v)$ to $p(w)$ begins in P, then crosses out at $e(v_1, v_2)$.

Geometric considerations show that $|v_1 - v_2| \geq 2.91$. In fact, geometric considerations show that the shortest possible distance for $|v_1 - v_2|$ under the condition that $|v - w| \leq 2$ is the length of the segment passing through the triangle of sides $2, 2t_0, 2t_0$ with both endpoints at distance exactly two from all three vertices of the triangle. This distance is greater than 2.91.

Let $e_1, \ldots, e_r$ be the sequence of arcs from $p(v)$ to $p(v_1)$, and let $f_1, \ldots, f_s$ be the sequence of arcs from $p(v)$ to $p(v_2)$. Since this sequence forms a minimal curve, the sum of the lengths of e_i is at most the sum of the lengths of $e(v, p_0)$ and $e(p_0, v_1)$, and the sum of the lengths of f_i is at most the sum of the lengths of $e(v, p_0)$ and $e(p_0, v_2)$.

Note that if $r + s \leq 4$, then one of the edge-lengths must be at least 3.2, for otherwise the sequence of arcs are all distinguished or diagonals of specials, and this would not permit the existence of a corner w. That is, we can fully enumerate the corners of the subregion, and each projects radially to an endpoint in the sequence of arcs, or is a vertex of a special simplex. None of these corners is separated from v by the plane $\{0, v_1, v_2\}$.

We have $r + s \leq 3$ by the following calculations. Here $y \in [2, 2t_0]$.

$$5\,\mathrm{arc}(2t_0, 2t_0, 2) > \mathrm{arc}(2, 2, 3.2) + 2\,\mathrm{arc}(2, 2, 2).$$

$$3\,\mathrm{arc}(2t_0, 2t_0, 2) + \mathrm{arc}(2t_0, y, 3.2) > \mathrm{arc}(y, 2, 3.2) + 2\,\mathrm{arc}(2, 2, 2).$$

$$3\,\mathrm{arc}(2t_0, 2t_0, 2) + \mathrm{arc}(2t_0, y, 3.2) > \mathrm{arc}(2, 2, 3.2) + 2\,\mathrm{arc}(y, 2, 2).$$

First we prove the lemma in the special case that the distance from v to one of the endpoints, say v_1, of $\{v_1, v_2\}$ is at least 3.2. In this special case, we claim that the constraints on the edge-lengths creates an impossible geometric configuration. The constraints are as follows. There are five points: $0, v_1, w, v, v_2$. The plane $\{0, v_1, v_2\}$ separates the point w from v. The distance constraints are as follows:

$$2 \leq |u| \leq 2t_0,$$

for $u = v_1, w, v, v_2$, $|v - v_1| \geq 3.2$, $|v - w| \leq 2$, $|v - v_2| \geq 2$, $|w - v_1| \geq 2$, $|w - v_2| \geq 2$, $2 \leq |v_1 - v_2| \leq 3.2$.

If the segment $\{v, w\}$ passes through the triangle $\{0, v_1, v_2\}$, then the desired impossibility proof follows by geometric considerations. Again, if the segment $\{v_1, v_2\}$ passes through the triangle $\{0, v, w\}$, then the desired impossibility proof follows by geometric considerations, provided that $\{0, v_1, v_2, w\}$ are not coplanar. Assume for a contradiction that $\{0, v_1, v_2, w\}$ lie in the plane P. We move back to the nonplanar case if $|v_2 - v|$ is not 2 (pivot v_2 around $\{0, w\}$ toward v), if $|v_1 - v|$ is not 3.2 (pivot v_1 around $\{0, w\}$ toward v), if $|w - v|$ is not 2 (pivot w around $\{v_1, v_2\}$ away from v), or v is not $2t_0$ (pivot v and w simultaneously preserving $|w - v|$ around $\{v_1, v_2\}$). Therefore, we may assume without loss of generality that $|v_2 - v| = 2$, $|v_1 - v| = 3.2$, $|w - v| = 2$, and $|v| = 2t_0$.

Let p be the orthogonal projection of v to the plane P. Let $h = |v - p|$. The distances from p to $u \in P$ is $f(|v - u|, h) = \sqrt{|v - u|^2 - h^2}$. We consider two cases depending on whether we can find a line in P through p dividing the plane into a half-plane containing v_1, 0, and v_2, or into a half-plane containing v_1, w, and v_2. In the first case we have

$$\begin{aligned} 0 = \operatorname{arc}(|p - v_1|, |p|, |v_1|)+ \\ \operatorname{arc}(|p - v_2|, |p|, |v_2|) - \operatorname{arc}(|p - v_1|, |p - v_2|, |v_1 - v_2|) \\ \geq \operatorname{arc}(f(3.2, h), f(2t_0, h), 2)+ \\ \operatorname{arc}(f(2, h), f(2t_0, h), 2) - \operatorname{arc}(f(3.2, h), f(2, h), 3.2) \end{aligned} \tag{12.3}$$

The function arc is monotonic in the arguments and from this it follows easily that this function of h is positive on its domain $0 \leq h \leq \sqrt{3}$. This is a contradiction. (The upper bound $\sqrt{3}$ is determined by the condition that the triangle $\{w, v_1, v\}$, which is equilateral in the extreme case, exist under the given edge constraints.) In the second case, we obtain the related contradiction

$$\begin{aligned} 0 = \operatorname{arc}(|p - v_1|, |p - w|, |v_1 - w|) + \operatorname{arc}(|p - v_2|, |p - w|, |v_2 - w|)- \\ \operatorname{arc}(|p - v_1|, |p - v_2|, |v_1 - v_2|) \\ \geq \operatorname{arc}(f(3.2, h), f(2, h), 2)+ \\ \operatorname{arc}(f(2, h), f(2, h), 2) - \operatorname{arc}(f(3.2, h), f(2, h), 3.2) \\ > 0 \end{aligned} \tag{12.4}$$

Now assume that the distances from v to the vertices v_1 and v_2 are at most 3.2.

If $r + s = 2$, then v_1 and v_2 are visible from v. Thus, they are distinguished or diagonals of special simplices. As $\{v_1, v_2\}$ is also distinguished, the corners of P are fully enumerated: v, v_1, v_2, and the vertices of special simplices. Since none of these are w, we conclude that w does not exist in this case.

If $r + s = 3$, then say $r = 1$ and $s = 2$. We have $\{v, v_1\}$ is distinguished or the diagonal of a special simplex. Let $p(v), p(u)$ be the endpoints of f_1, for some corner u. We have $|u - v_1| \geq \sqrt{8}$ because $\{u, v_1\}$ is not distinguished, and $\max(|u - v|, |u - v_1|) \geq 3.2$, because otherwise we enumerate all vertices of P as in the case $r + s = 2$, and find that w is not among them. But now geometric considerations lead to a contradiction: there does not exist a configuration of five points 0, u, v, v_1, v_2, with all distances at least 2 satisfying these constraints. (This can be readily solved by geometric considerations.) □

Section 13

Convex Polygons

13.1 Deformations

We divide the bounding edges over the polygon according to length $[2, 2t_0]$, $[2t_0, 2\sqrt{2}]$, $[2\sqrt{2}, 3.2]$. The deformations of Section 12.8 contract edges to the lower bound of the intervals ($2, 2t_0$, or $2\sqrt{2}$) unless a new distinguished edge is formed. By deforming the polygon, we assume that the bounding edges have length $2, 2t_0$, or $2\sqrt{2}$. (There are a few instances of triangles or quadrilaterals that do not satisfy the hypotheses needed for the deformations. These instances will be treated in Sections 13.8 and 13.9.)

Lemma 13.1. *Let $S = S(y_1, \ldots, y_6)$ be a simplex, with $x_i = y_i^2$, as usual. Let $y_4 \geq 2$, $\Delta \geq 0$, $y_5, y_6 \in \{2, 2t_0, 2\sqrt{2}\}$. Fixing all the variables but x_1, let $f(x_1)$ be one of the functions* $\text{s-vor}_0(S)$ *or* $-\tau_0(S)$. *We have $f''(x_1) > 0$ whenever $f'(x_1) = 0$.*

Proof. This is an interval calculation.[77] □

The lemma implies that f does not have an interior point local maximum for $x_1 \in [2^2, 2t_0^2]$. Fix three consecutive corners, v_0, v_1, v_2 of the convex polygon, and apply the lemma to the variable $x_1 = |v_1|^2$ of the simplex $S = \{0, v_0, v_1, v_2\}$. We deform the simplex, increasing f. If the deformation produces $\Delta(S) = 0$, then some dihedral angle is π, and the arguments for nonconvex regions bring us eventually back to the convex situation. Eventually y_1 is 2 or $2t_0$. Applying the lemma at each corner, we may assume that the height of every corner is 2 or $2t_0$. (There are a few cases where the hypotheses of the lemma are not met, and these are discussed in Sections 13.8 and 13.9.)

Lemma 13.2. *The convex polygon has at most seven sides.*

Proof. Since the polygon is convex, its perimeter on the unit sphere is at most a

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great circle 2π. If there are eight sides, the perimeter is at least $8\,\mathrm{arc}(2t_0, 2t_0, 2) > 2\pi$. $\square$

13.2 Truncated corner cells

The following lemma justifies using tccs at the corners as an upper bound on the score (and lower bound on what is squandered). We fix the truncation parameter at $\lambda = 1.6$.

Lemma 13.3. *Take a convex subregion that is not a triangle. Assume edges between adjacent corners have lengths* $\in \{2, 2t_0, 2\sqrt{2}, 3.2\}$. *Assume nonadjacent corners are separated by distances* ≥ 3.2. *Then the truncated corner cell at each vertex lies in the cone over the subregion.*

Proof. Place a tcc at v_1. For a contradiction, let $\{v_2, v_3\}$ be an edge that the tcc overlaps. Assume first that $|v_1 - v_i| \geq 2t_0$, $i = 2, 3$. Pivot so that $|v_1 - v_2| = |v_1 - v_3| = 2t_0$. Write $S(y_1, \ldots, y_6) = \{0, v_1, v_2, v_3\}$. Set $\psi = \mathrm{arc}(y_1, t_0, 1.6)$. A calculation[78] gives $\beta_\psi(y_1, y_2, y_6) < \mathrm{dih}_2(S)$.

Now assume $|v_1 - v_2| < 2t_0$. By the hypotheses of the lemma, $|v_1 - v_2| = 2$. If $|v_1 - v_3| < 3.2$, then $\{0, v_1, v_2, v_3\}$ is triangular, contrary to hypothesis. So $|v_1 - v_3| \geq 3.2$. Pivot so that $|v_1 - v_3| = 3.2$. Then[79]

$$\beta_\psi(y_1, y_2, y_6) < \mathrm{dih}_2(S),$$

where $\psi = \mathrm{arc}(y_1, t_0, 1.6)$, provided $y_1 \in [2.2, 2t_0]$. Also, if $y_1 \in [2.2, 2t_0]$

$$\mathrm{arc}(y_1, t_0, 1.6) < \mathrm{arc}(y_1, y_2, y_6).$$

If $y_1 \leq 2.2$, then $\Delta_1 \geq 0$, so $\partial\,\mathrm{dih}_2/\partial x_3 \leq 0$. Set $x_3 = 2t_0^2$. Also, $\Delta_6 \geq 0$, so $\partial\,\mathrm{dih}_2/\partial x_4 \leq 0$. Set $x_4 = 3.2^2$.

Let c be a point of intersection of the plane $\{0, v_1, v_2\}^\perp$ with the circle at distance $\lambda = 1.6$ from v_1 on the sphere centered at the origin of radius t_0. The angle along $\{0, v_2\}$ between the planes $\{0, v_2, v_1\}$ and $\{0, v_2, c\}$ is

$$\mathrm{dih}(R(y_2/2, \eta_{126}, y_1/(2\cos\psi))).$$

This angle is less[80] than $\mathrm{dih}_2(S)$. Also, $\Delta_1 \geq 0$, $\partial\,\mathrm{dih}_3/\partial x_2 \leq 0$, so set $x_2 = 2t_0^2$. Then $\Delta_5 < 0$, so $\mathrm{dih}_2 > \pi/2$. This means that $\{0, v_1, v_2\}^\perp$ separates the tcc from the edge $\{v_2, v_3\}$. $\square$

[78] CALC-193836552
[79] CALC-193836552
[80] CALC-193836552

13.3 Analytic continuation

In this subsection we assume that $\lambda = 1.6$ and that the truncated corner cell under consideration lies at a convex vertex.

Assume that the face cut by $\{0, v, v_1\}^\perp$ meets the face cut by $\{0, v, v_2\}^\perp$. Let c_i be the point on the plane $\{0, v, v_i\}^\perp$ satisfying $|c_i - v| = 1.6$, $|c_i| = t_0$. (Pick the root within the wedge between v_1 and v_2.) The overlap of the two faces is represented in Figure 13.1.

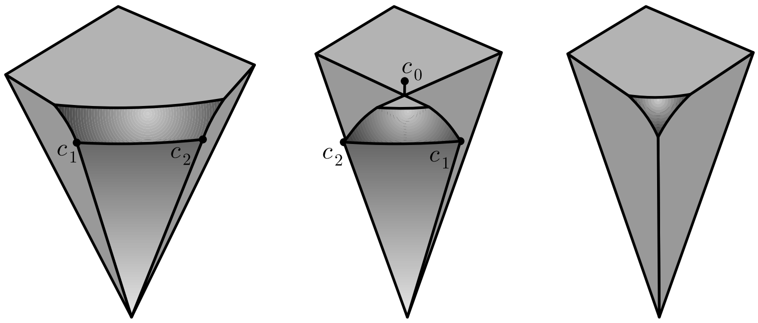

Figure 13.1. *Different forms of truncated corner cells are shown. The structure shown in the middle frame cannot occur.*

We let c_0 be the point of height t_0 on the intersection of the planes $\{0, v, v_1\}^\perp$ and $\{0, v, v_2\}^\perp$. We claim that c_0 lies over the truncated spherical region of the tcc, rather than the wedges of t_0-cones or the Rogers simplices along the faces $\{0, v, v_1\}$ and $\{0, v, v_2\}$. (This implies that c_0 cannot protrude beyond the corner cell as depicted in the second frame of the figure.) To see the claim, consider the tcc as a function of $y_4 = |v_1 - v_2|$. When y_4 is sufficiently large the claim is certainly true. Contract y_4 until $c_0 = c_0(y_4)$ meets the perpendicular bisector of $\{0, v\}$. Then c_0 is equidistant from $0, v, v_1$ and v_2 so it is the circumcenter of $\{0, v, v_1, v_2\}$. It has distance t_0 from the origin, so the circumradius is t_0. This implies that $y_4 \le 2t_0$.

The tcc is defined by the constraints represented in the third frame. The analytic continuation of the function $\chi_0(S) = \chi_0^{\mathrm{an}}(S)$, defined above, acquires a volume X, counted with negative sign, lying under the spherical triangle (c_0, c_1, c_2). Extending our notation, we have an analytically defined function χ_0^{an} and a geometrically defined function χ_0^{g},

$$\begin{aligned} \chi_0^{\mathrm{an}}(S) &= \chi_0^{\mathrm{g}}(S) - \text{c-vor}_0(X), \text{ where} \\ \text{c-vor}_0(X) &= 4(-\delta_{oct}\mathrm{vol}(X) + \mathrm{sol}(X)/3) = \phi_0\,\mathrm{sol}(X) < 0. \end{aligned}$$

So $\chi_0^{\mathrm{an}} > \chi_0^{\mathrm{g}}$, and we may always use $\chi_0(S) = \chi_0^{\mathrm{an}}(S)$ as an upper bound on the score of a tcc.

For example, with $\lambda = 1.6$ and $S = S(2.3, 2.3, 2.3, 2.9, 2, 2)$, we have

$$\chi_0^{\mathrm{an}}(S) \approx -0.103981, \quad \chi_0^{\mathrm{g}}(S) \approx -0.105102.$$

Or, if $S = S(2, 2, 2t_0, 3.2, 2, 2t_0)$, then

$$\chi_0^{\mathrm{an}}(S) \approx -0.0718957, \quad \chi_0^{\mathrm{g}}(S) \approx -0.0726143.$$

13.4 Penalties

In Section 12.6, we determined the bound of $\pi_{\max} = 0.06688$ on penalties. In this section, we give a more thorough treatment of penalties. Until now a penalty has been associated with a given standard region, but by taking the worst case on each subregion, we can move the penalties to the level of subregions. Roughly, each subregion should incur the penalties from the upright quarters that were erased along edges of that subregion. Each upright quarter of the original standard region is attached at an edge between adjacent corners of the standard cluster. The edges have lengths between 2 and $2t_0$. The deformations shrink the edges to length 2. We attach the penalty from the upright quarter to this edge of this subregion. In general, we divide the penalty evenly among the upright quarters along a common diagonal, without trying to determine a more detailed accounting. For example, the penalty 0.008 in Lemma 11.23 comes from three upright quarters. Thus, we give each of three edges a penalty of 0.008/3. Or, if there are only two upright quarters around the 3-unconfined upright diagonal, then each of the two upright quarters is assigned the penalty 0.00222/2 (see Lemma 11.23).

The penalty $0.04683 = 3\xi_\Gamma$ in Section 12.6 comes from three upright quarters around a 3-crowded upright diagonal. Each of three edges is assigned a penalty of ξ_Γ. The penalty $0.03344 = 3\xi_\Gamma + \xi_{\kappa,\Gamma}$ comes from a 4-crowded upright diagonal of Section 11.7. It is divided among 4 edges. These are the only upright quarters that take a penalty when erased. (The case of two upright quarters over a flat quarter as in Lemma 11.3, are treated by a separate argument in Section 13.8. Loops will be discussed in Section 13.12.)

The penalty can be reduced in various situations involving a masked flat quarter. For example, around a 3-crowded upright diagonal, if there is a masked flat quarter, two of the upright quarters are scored by the analytic function s-vor, so that the penalty plus adjustment is only[81] [82] $0.034052 = 2\xi_V + \xi_\Gamma + 0.0114$. The adjustment 0.0114 reflects the scoring rules for masked flat quarters (Lemma 11.23). This we divide evenly among the three edges that carried the upright quarters. If e is an edge of the subregion R, let $\pi_0(R, e)$ denote the penalty and score adjustment along edge e of R.

In summary, we have the penalties,

$$\xi_\kappa, \xi_V, \xi_\Gamma, \ 0.008,$$

combined in various ways in the upright diagonals that are 3-unconfined, 3-crowded, or 4-crowded. There are score adjustments

$$0.0114 \quad \text{and} \quad 0.0063$$

[81] CALC-73974037
[82] CALC-764978100

from Section 11.9 for masked flat quarters. If the sum of these contributions is s, we set $\pi_0(R,e) = s/n$, for each edge e of R originating from an erased upright quarter of $\mathbf{S}_n^{\pm}$.

13.5 Penalties and Bounds

Recall that the bounds for flat quarters we wish to establish from Section 12.5 are $Z(3,1) = 0.00005$ and $D(3,1) = 0.06585$. Flat quarters arise in two different ways. Some flat quarters are present before the deformations begin. They are scored by the rules of Section 11.9. Others are formed by the deformations. In this case, they are scored by vor_0. Since the flat quarter is broken away from the subregion as soon as the diagonal reaches $2\sqrt{2}$, and then is not deformed further, the diagonal is fixed at $2\sqrt{2}$. Such flat quarters can violate our desired inequalities. For example,

$$Z(3,1) < \text{s-vor}_0(S(2,2,2,2\sqrt{2},2,2)) \approx 0.00898, \quad \tau_0(S(2,2,2,2\sqrt{2},2,2)) \approx 0.0593.$$

On the other hand, as we will see, the adjacent subregion satisfies the inequality by a comfortable margin. Therefore, we define a transfer ϵ from flat quarters to the adjacent subregion. (In an exceptional region, the subregion next to a flat quarter along the diagonal is not a flat quarter.)

For a flat quarter Q, set

$$\epsilon_\tau(Q) = \begin{cases} 0.0066, & \text{(deformation)},\\ 0, & \text{(otherwise)}.\end{cases}$$

$$\epsilon_\sigma(Q) = \begin{cases} 0.009, & \text{(deformation)},\\ 0, & \text{(otherwise)}.\end{cases}$$

The nonzero value occurs when the flat quarter Q is obtained by deformation from an initial configuration in which Q is not a quarter. The value is zero when the flat quarter Q appears already in the undeformed standard cluster. Set

$$\begin{aligned} \pi_\tau(R) &= \textstyle\sum_e \pi_0(R,e) + \sum_e \pi_0(Q,e) + \sum_Q \epsilon_\tau(Q),\\ \pi_\sigma(R) &= \textstyle\sum_e \pi_0(R,e) + \sum_e \pi_0(Q,e) + \sum_Q \epsilon_\sigma(Q).\end{aligned}$$

The first sum runs over the edges of a subregion R. The second sum runs over the edges of the flat quarters Q that lie adjacent to R along the diagonal of Q.

The edges between corners of the polygon have lengths 2, $2t_0$, or $2\sqrt{2}$. Let k_0, k_1, and k_2 be the number of edges of these three lengths respectively. By Lemma 13.2, we have $k_0 + k_1 + k_2 \le 7$. Let $\tilde\sigma$ denote any of the functions of Section 11.9.2(a)–(f). Let $\tilde\tau = \mathrm{sol}\,\zeta pt - \tilde\sigma$.

To prove Theorem 12.1, refining the strategy proposed in Section 12.5, we must show that for each flat quarter Q and each subregion R that is not a flat quarter, we have

$$\begin{aligned} \tilde\tau(Q) &> D(3,1) - \epsilon_\tau(Q),\\ \tau_0(Q) &> D(3,1) - \epsilon_\tau(Q), \quad \text{if } y_4(Q) = 2\sqrt{2},\\ \tau_V(R) &> D(3,2), \quad \text{(type } A),\\ \tau_0(R) &> D(k_0+k_1+k_2, k_1+k_2) + \pi_\tau(R), \end{aligned} \tag{13.1}$$

where $D(n, k)$ is the function defined in Section 12.5. The first of these inequalities follows.[83] [84] [85] In general, we are given a subregion without explicit information about what the adjacent subregions are. Similarly, we have discarded all information about what upright quarters have been erased. Because of this, we assume the worst, and use the largest feasible values of π_τ.

Lemma 13.4. *We have* $\pi_\tau(R) \le 0.04683 + (k_0 + 2k_2 - 3)0.008/3 + 0.0066k_2$.

Proof. The worst penalty $0.04683 = 3\xi_\Gamma$ per edge comes from a 3-crowded upright diagonal. The number of penalized edges not on a simplex around a 3-crowded upright diagonal is at most $k_0 + 2k_2 - 3$. For every three edges, we might have one 3-unconfined upright diagonal. The other cases such as 4-crowded upright diagonals or situations with a masked flat quarter are readily seen to give smaller penalties. □

For bounds on the score, the situation is similar. The only penalties we need to consider are 0.008 from Lemma 11.23. If either of the other configurations of 3-crowded or 4-crowded upright diagonals occur, then the score of the standard cluster is less than $s_8 = -0.228$, by Sections 11.6 and 11.7. This is the desired bound. So it is enough to consider subregions that do not have these upright configurations. Moreover, the penalty 0.008 does not occur in connection with masked flats. So we can take $\pi_\sigma(R)$ to be

$$(k_0 + 2k_2)0.008/3 + 0.009k_2.$$

If $k_0 + 2k_2 < 3$, we can strengthen this to $\pi_\sigma(R) = 0.009k_2$. Let $\tilde\sigma$ be any of the functions of Section 11.9.2 parts (a)–(f). To prove Theorem 12.1, we will show

$$\begin{array}{ll} \tilde\sigma(Q) & < Z(3,1) + \epsilon_\sigma(Q), \\ \text{s-vor}_0(Q) & < Z(3,1) + \epsilon_\sigma(Q), \quad \text{if } y_4(Q) = 2\sqrt{2}, \\ \text{vor}_0(R) & < Z(3,2), \quad (\text{type } A), \\ \text{vor}_0(R) & < Z(k_0 + k_1 + k_2, k_1 + k_2) - \pi_\sigma(R). \end{array} \tag{13.2}$$

The first of these inequalities follows.[86] [87] [88]

13.6 Penalties

Erasing an upright quarter of compression type gives a penalty of at most ξ_Γ and one of Voronoi type gives at most ξ_V. We take the worst possible penalty. It is at most $n\xi_\Gamma$ in an n-gon. If there is a masked flat quarter, the penalty is at most $2\xi_V$ from the two upright quarters along the flat quarter. We note in this connection that both edges of a polygon along a flat quarter lie on upright quarters, or neither does.

[83] CALC-193836552
[84] CALC-148776243
[85] CALC-163548682
[86] CALC-193836552
[87] CALC-148776243
[88] CALC-163548682

If an upright diagonal appears enclosed over a flat quarter, the flat quarter is part of a loop with context $(n, k) = (4, 1)$, for a penalty at most $2\xi'_\Gamma + \xi_V$. This is smaller than the bound on the penalty obtained from a loop with context $(n, k) = (4, 1)$, when the upright diagonal is not enclosed over the flat quarter:

$$\xi_\Gamma + 2\xi_V.$$

So we calculate the worst-case penalties under the assumption that the upright diagonals are not enclosed over flat quarters.

A loop of context $(n, k) = (4, 1)$ gives $\xi_\Gamma + 2\xi_V$ or $3\xi_\Gamma$. A loop of context $(n, k) = (4, 2)$ gives $2\xi_\Gamma$ or $2\xi_V$.

If we erase a 3-unconfined upright diagonal, there is a penalty of 0.008 (or 0 if it masks a flat quarter.) This is dominated by the penalty $3\xi_\Gamma$ of context $(n, k) = (4, 1)$.

Suppose we have an octagonal standard region. We claim that a loop does not occur in context $(n, k) = (4, 2)$. If there are at most three vertices that are not corners of the octagon, then there are at most twelve quasi-regular tetrahedra, and the score is at most

$$s_8 + 12\,pt < 8\,pt.$$

Assume there are more than three vertices that are not corners over the octagon. We squander

$$t_8 + \delta_{loop}(4, 2) + 4\tau_{\mathrm{LP}}(5, 0) > (4\pi\zeta - 8)\,pt.$$

As a consequence, context $(n, k) = (4, 2)$ does not occur.

So there are at most two upright diagonals and at most six quarters, and the penalty is at most $6\xi_\Gamma$. Let f be the number of flat quarters This leads to

$$\pi_F = \begin{cases} 6\xi_\Gamma, & f = 0, 1, \\ 4\xi_\Gamma + 2\xi_V, & f = 2, \\ 2\xi_\Gamma + 4\xi_V, & f = 3, \\ 0, & f = 4. \end{cases}$$

The 0 is justified by a parity argument. Each upright quarter occurs in a pair at each masked flat quarter. But there is an odd number of quarters along the upright diagonal, so no penalty at all can occur.

Suppose we have a heptagonal standard region. Three loops are a geometric impossibility. Assume there are at most two upright diagonals. If there is no context $(n, k) = (4, 2)$, then we have the following bounds on the penalty

$$\pi_F = \begin{cases} 6\xi_\Gamma, & f = 0, \\ 4\xi_\Gamma + 2\xi_V, & f = 1, \\ 3\xi_\Gamma, & f = 2, \\ \xi_\Gamma + 2\xi_V, & f = 3. \end{cases}$$

If an upright diagonal has context $(n, k) = (4, 2)$, then

$$\pi_F = \begin{cases} 5\xi_\Gamma, & f = 0, 1, \\ 3\xi_\Gamma + 2\xi_V, & f = 2, \\ \xi_\Gamma + 4\xi_V, & f = 3. \end{cases}$$

This gives the bounds used in the diagrams of cases.

13.7 Constants

Theorem 12.1 now results from the calculation of a host of constants. Perhaps there are simpler ways to do it, but it was a routine matter to run through the long list of constants by computer. What must be checked is that the Inequalities 13.1 and 13.2 of Section 13.5 hold for all possible convex subregions. Call these inequalities the D and Z inequalities. This section describes in detail the constants to check.

We begin with a subregion given as a convex n-gon, with at least four sides. The heights of the corners and the lengths of edges between adjacent edges have been reduced by deformation to a finite number of possibilities (lengths 2, $2t_0$, or lengths 2, $2t_0$, $2\sqrt{2}$, respectively). By Lemma 13.2, we may take $n = 4, 5, 6, 7$. Not all possible assignments of lengths correspond to a geometrically viable configuration. One constraint that eliminates many possibilities, especially heptagons, is that of Section 13.1: the perimeter of the convex polygon is at most a great circle. Eliminate all length-combinations that do not satisfy this condition. When there is a special simplex it can be broken from the subregion and scored[89] separately unless the two heights along the diagonal are 2. We assume in all that follows that all specials that can be broken off have been. There is a second condition related to special simplices. We have $\Delta(2t_0^2, 2^2, 2^2, x^2, 2^2, 2^2) < 0$, if $x > 3.114467$. This means that if the cluster edges along the polygon are $(y_1, y_2, y_3, y_5, y_6) = (2t_0, 2, 2, 2, 2)$, the simplex must be special ($y_4 \in [2\sqrt{2}, 3.2]$).

The easiest cases to check are those with no special simplices over the polygon. In other words, these are subregions for which the distances between nonadjacent corners are at least 3.2. In this case we approximate the score (and what is squandered) by tccs at the corners. We use monotonicity to bring the fourth edge to length 3.2. We calculate the tcc constant bounding the score, checking that it is less than the constant $Z(k_0 + k_1 + k_2, k_1 + k_2) - \pi_\sigma$, from the Z inequalities. The D inequalities are verified in the same way.

When $n = 5, 6, 7$, and there is one special simplex, the situation is not much more difficult. By our deformations, we decrease the lengths of edges $2, 3, 5, 6$ of the special to 2. We remove the special by cutting along its fourth edge e (the diagonal). We score the special with weak bounds.[90] Along the edge e, we then apply deformations to the $(n-1)$-gon that remains. If this deformation brings e to length $2\sqrt{2}$, then the $(n-1)$-gon may be scored with tccs as in the previous paragraph. But there are other possibilities. Before e drops to $2\sqrt{2}$, a new distinguished edge

[89] CALC-148776243
[90] CALC-148776243

of length 3.2 may form between two corners (one of the corners will be a chosen endpoint of e). The subregion breaks in two. By deformations, we eventually arrive at $e = 2\sqrt{2}$ and a subregion with diagonals of length at least 3.2. (There is one case that may fail to be deformable to $e = 2\sqrt{2}$, a pentagonal cases discussed further in Section 13.10.) The process terminates because the number of sides to the polygon drops at every step. A simple recursive computer procedure runs through all possible ways the subregion might break into pieces and checks that the tcc-bound gives the D and Z inequalities. The same argument works if there is a special simplex that overlaps each of the other special simplices in the subcluster.

When $n = 6, 7$ and there are two nonoverlapping special simplices, a similar argument can be applied. Remove both specials by cutting along the diagonals. Then deform both diagonals to length $2\sqrt{2}$, taking into account the possible ways that the subregion can break into pieces in the process. In every case the D and Z inequalities are satisfied.

There are a number of situations that arise that escape this generic argument and were analyzed individually. These include the cases involving more than two special simplices over a given subregion, two special simplices over a pentagon, or a special simplex over a quadrilateral. Also, the deformation lemmas are insufficient to bring all of the edges between adjacent corners to one of the three standard lengths $2, 2t_0, 2\sqrt{2}$ for certain triangular and quadrilateral regions. These are treated individually.

The next few sections describe the cases treated individually. The cases not mentioned in the sections that follow fall within the generic procedure just described.

13.8 Triangles

With triangular subregions, there is no need to use any of the deformation arguments because the dimension is already sufficiently small to apply interval arithmetic directly to obtain our bounds. There is no need for the tcc-bound approximations.

Flat quarters and simplices of type A are treated by a computer calculation.[91] Other simplices are scored by the truncated function s-vor$_0$. We break the edges between corners into the cases $[2, 2t_0)$, $[2t_0, 2\sqrt{2})$, $[2\sqrt{2}, 3.2]$. Let k_0, k_1, and k_2, with $k_0 + k_1 + k_2 = 3$, be the number of edges in the respective intervals.

If $k_2 = 0$, we can improve the penalties,

$$\pi_\tau = \pi_\sigma = 0.$$

To see this, first we observe that there can be no 3-crowded or 4-crowded upright diagonals. By placing ≥ 3 quarters around an upright diagonal, if the subregion is triangular, the upright diagonal becomes surrounded by anchored simplices, a case deferred until Section 13.12.

If $k_0 = k_1 = k_2 = 1$, we can take $\pi'_\tau = \xi_\Gamma + 2\xi_V + 0.0114 = 0.034052$. A few cases are needed to justify this constant. If there are no 3-crowded upright

[91] CALC-163548682

diagonals, π'_τ is at most

$$\begin{array}{ll} & [\xi_\Gamma + 2\xi_V + \xi_{\kappa,\Gamma}]3/4 < 0.0254, \\ \text{or} & [\xi_\Gamma + 2\xi_V + \xi_{\kappa,\Gamma}]2/4 + 0.008/3 < 0.0254 \end{array}$$

If there are at most two edges in the subregion coming from an 3-crowded upright diagonal,

$$(\xi_\Gamma + 2\xi_V + 0.0114)2/3 + 0.008/3 < 0.0254.$$

If three edges come from the simplices of a 3-crowded upright diagonal, we get 0.034052. To get somewhat sharper bounds, we consider how the edge k_2 was formed. If it is obtained by deformation from an edge in the standard region of length ≥ 3.2, then it becomes a distinguished edge when the length drops to 3.2. If the edge in the standard region already has length ≤ 3.2, then it is distinguished before the deformation process begins, so that the subregion can be treated in isolation from the other subregions. We conclude that when $\pi'_\tau = 0.034052$ we can take $y_4 \geq 2.6$ or $y_5 = 3.2$ (Remark 11.22).

The D and Z inequalities now follow.[92] [93]

13.9 Quadrilaterals

We introduce some notation for the heights and edge lengths of a convex polygon. The heights will generally be 2 or $2t_0$, the edge lengths between consecutive corners will generally be 2, $2t_0$, or $2\sqrt{2}$. We represent the edge lengths by a vector

$$(a_1, b_1, a_2, b_2, \ldots, a_n, b_n),$$

if the corners of an n-gon, ordered cyclically have heights a_i and if the edge length between corner i and $i+1$ is b_i. We say two vectors are equivalent if they are related by a different cyclic ordering on the corners of the polygon, that is, by the action of the dihedral group.

The vector of a polygon with a special simplex is equivalent to one of the form

$$(2, 2, a_2, 2, 2, \ldots).$$

If $a_2 = 2t_0$, then what we have is necessarily special (Section 13.7). However, if $a_2 = 2$, it is possible for the edge opposite a_2 to have length greater than 3.2.

Turning to quadrilateral regions, we use tcc scoring if both diagonals are greater than 3.2. Suppose that both diagonals are between $[2\sqrt{2}, 3.2]$, creating a pair of overlapping special simplices. The deformation lemma requires a diagonal longer than 3.2, so although we can bring the quadrilateral to the form

$$(a_1, 2, 2, 2, 2, 2, a_4, b_4),$$

[92] CALC-852270725
[93] CALC-819209129

the edges a_1, a_4, b_4 and the diagonal vary[94] continuously. We have bounds[95] on the score

$$\begin{array}{lll} \tau_0 & > 0.235, & \mathrm{vor}_0 < -0.075, \text{ if } b_4 \in [2t_0, 2\sqrt{2}], \\ \tau_0 & > 0.3109, & \mathrm{vor}_0 < -0.137, \text{ if } b_4 \in [2\sqrt{2}, 3.2], \end{array}$$

We have $D(4,1) = 0.2052$, $Z(4,1) = -0.05705$. When $b_4 \in [2t_0, 2\sqrt{2}]$, we can take $\pi_\tau = \pi_\sigma = 0$. (We are excluding loops here.) When $b_4 \in [2\sqrt{2}, 3.2]$, we can take

$$\begin{array}{ll} \pi_\tau & = \pi_{\max} + 0.0066, \\ \pi_\sigma & = 0.008(5/3) + 0.009. \end{array}$$

It follows that the D and Z Inequalities are satisfied.

Suppose that one diagonal has length $[2\sqrt{2}, 3.2]$ and the other has length at least 3.2. The quadrilateral is represented by the vector

$$(2, 2, a_2, 2, 2, b_3, a_4, b_4).$$

The hypotheses of the deformation lemma hold, so that $a_i \in \{2, 2t_0\}$ and $b_j \in \{2, 2t_0, 2\sqrt{2}\}$. To avoid quad clusters, we assume $b_4 \geq \max(b_3, 2t_0)$. These are one-dimensional with a diagonal of length $[2\sqrt{2}, 3.2]$ as parameter. The required verifications[96] have been made by interval arithmetic.

13.10 Pentagons

Some extra comments are needed when there is a special simplex. The general argument outlined above removes the special, leaving a quadrilateral. The quadrilateral is deformed, bringing the edge that was the diagonal of the special to $2\sqrt{2}$. This section discusses how this argument might break down.

Suppose first that there is a special and that both diagonals on the resulting quadrilateral are at least 3.2. We can deform using either diagonal, keeping both diagonals at least 3.2. The argument breaks down if both diagonals drop to 3.2 before the edge of the special reaches $2\sqrt{2}$ and both diagonals of the quadrilateral lie on specials. When this happens, the quadrilateral has the form

$$(2, 2, 2, 2, 2, 2, 2, b_4),$$

where b_4 is the edge originally on the special simplex. If both diagonals are 3.2, this is rigid, with $b_4 = 3.12$. We find its score to be

$$\begin{array}{l} \text{s-vor}_0(S(2,2,2,b_4,3.2,2)) + \text{s-vor}_0(S(2,2,2,3.2,2,2)) + 0.0461 < -0.205, \\ \tau_0(S(2,2,2,b_4,3.2,2)) + \tau_0(S(2,2,2,3.2,2,2))2 > 0.4645. \end{array}$$

So the D and Z Inequalities hold easily.

If there is a special and there is a diagonal on resulting quadrilateral ≤ 3.2, we have two nonoverlapping specials. It has the form

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, b_5).$$

[94] CALC-148776243
[95] CALC-128523606
[96] CALC-874876755

The edges a_2 and a_4 lie on the special. If $b_5 > 2$, cut away one of the special simplices. What is left can be reduced to a triangle, or a quadrilateral case and then treated[97] by computer. Assume $b_5 = 2$. We have a pentagonal standard region. We may assume that there is no 3-crowded or 4-crowded upright diagonal, for otherwise Theorem 12.1 follows trivially from the bounds in Section 9. A pentagon can then have at most a 3-unconfined upright diagonal for a penalty of 0.008.

If $a_2 = 2t_0$ or $a_4 = 2t_0$, we again remove a special simplex and produce triangles, quadrilaterals, or the special cases treated by computer.[98] We may impose the condition $a_2 = a_4 = b_5 = 2$. We score this full pentagonal arrangement by computer,[99] using the edge lengths of the two diagonals of the specials as variables. The inequalities follow.

13.11 Hexagons and heptagons

We turn to hexagons. There may be three specials whose diagonals do not cross. Such a subcluster is represented by the vector

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, 2, a_6, 2).$$

The heights a_{2i} are 2 or $2t_0$. Draw the diagonals between corners 1, 3, and 5. This is a three-dimensional configuration, determined by the lengths of the three diagonals, which is treated by computer.[100]

There is one case with a special simplex that did not satisfy the generic computer-checked inequalities for what is to be squandered. Its vector is

$$(a_1, 2, 2, 2, 2, 2, 2, b_4, 2, 2, 2, 2),$$

with $a_1 = b_4 = 2t_0$. A vertex of the special simplex has height $a_1 = 2t_0$ and all other corners have height 2. The subregion is a hexagon with one edge longer than 2. We have $D(6, 1) = 0.48414$. This is certainly obtained if the subregion contains a 3-crowded upright diagonal, squandering 0.5606. But if this configuration does not appear, we can decrease π_τ to $0.03344 + (2/3)0.008$, a constant coming from 4-crowded upright diagonals in Section 12.6. With this smaller penalty the inequality is satisfied.

Now turn to heptagons.The bound 2π on the perimeter of the polygon, eliminates all but one equivalence class of vectors associated with a polygon that has two or more potentially specials simplices. The vector is

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, 2, a_6, 2, a_7, 2),$$

$a_2 = a_4 = a_6 = a_7 = 2t_0$. In other words, the edges between adjacent corners are 2 and four heights are $2t_0$. There are two specials. This case is treated by the procedure outlined for subregions with two specials whose diagonals do not cross.

[97] CALC-874876755
[98] CALC-874876755
[99] CALC-692155251
[100] CALC-692155251

13.12 Loops

We now return to a collection of anchored simplices that surround the upright diagonal. This is the last case needed to complete the proof of Theorem 12.4. There are four or five anchored simplices around the upright diagonal. There are linear inequalities[101] [102] [103] [104] [105] [106] satisfied by the anchored simplices, broken up according to type: upright, type C, opposite edge > 3.2, etc. The anchored simplices are related by the constraint that the sum of the dihedral angles around the upright diagonal is 2π. We run a linear program in each case based on these linear inequalities, subject to this constraint to obtain bounds on the score and what is squandered by the anchored simplices.

When the edge opposite the diagonal of an anchored simplex has length $\in [2\sqrt{2}, 3.2]$ and the simplex adjacent to the anchored simplex across that edge is a special simplex, we use inequalities[107] [108] that run parallel to the similar system[109] [110] It is not necessary to run separate linear programs for these. It is enough to observe that the constants for what is squandered improve on those from the similar system[111] and that the constants for the score in one system[112] differ with those of the other[113] by no more than 0.009.

When the dihedral angle of an anchored simplex is greater than 2.46, the simplex is dropped, and the remaining anchored simplices are subject to the constraint that their dihedral angles sum to at most $2\pi - 2.46$. There can not be an anchored simplex with dihedral angle greater than 2.46 when there are five anchors: $2.46 + 4(0.956) > 2\pi$. There cannot[114] be two anchored simplices with dihedral angle greater than 2.46: $2(2.46 + 0.956) > 2\pi$.

The following table summarizes the linear programming results.

(n,k)	$\mathrm{D}_{\mathrm{LP}}(n,k)$	$D(n,k)$	$\mathrm{Z}_{\mathrm{LP}}(n,k)$	$Z(n,k)$
$(4,0)$	0.1362	0.1317	0	0
$(4,1)$	0.208	0.20528	-0.0536	-0.05709
$(4,2)$	0.3992	0.27886	-0.2	-0.11418
$(4,3)$	0.6467	0.35244	-0.424	-0.17127
$(5,0)$	0.3665	0.27113	-0.157	-0.05704
$(5,1)$	0.5941	0.34471	-0.376	-0.11413
$(5,\geq 2)$	0.9706	$(4\pi\zeta - 8)\,pt$	$*$	$*$

[101] CALC-815492935
[102] CALC-729988292
[103] CALC-531888597
[104] CALC-628964355
[105] CALC-934150983
[106] CALC-187932932
[107] CALC-485049042
[108] CALC-209361863
[109] CALC-531888597
[110] CALC-628964355
[111] CALC-531888597
[112] CALC-485049042
[113] CALC-531888597
[114] CALC-83777706

The bound for $D(4,0)$ comes from Lemma 10.8. A few more comments are needed for $Z(4,1)$. Let $S = S(y_1, \ldots, y_6)$ be the anchored simplex that is not a quarter. If $y_4 \geq 2\sqrt{2}$ or $\operatorname{dih}(S) \geq 2.2$, the linear programming bound is $< Z(4,1)$. With this, if $y_1 \leq 2.75$, we have[115] $\sigma(S) < Z(4,1)$. But if $y_1 \geq 2.75$, the three upright quarters along the upright diagonal satisfy

$$\nu < -0.3429 + 0.24573 \,\mathrm{dih}\,.$$

With this stronger inequality, the linear programming bound becomes $< Z(4,1)$. This completes the proof of Theorem 12.1.

Lemma 13.5. *Consider an upright diagonal that is a loop. Let R be the standard region that contains the upright diagonal and its surrounding simplices. Then the following contexts (m,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 $\tau_R(D)$ when R contains one loop of that context.*

$n = n(R)$	(m,k)	σ	τ
4			
	$(4,0)$	-0.0536	0.1362
5			
	$(4,1)$	s_5	0.27385
	$(5,0)$	-0.157	0.3665
6			
	$(4,1)$	s_6	0.41328
	$(4,2)$	-0.1999	0.5309
	$(5,1)$	-0.37595	0.65995
7			
	$(4,1)$	s_7	0.55271
	$(4,2)$	-0.25694	0.67033
8			
	$(4,1)$	s_8	0.60722
	$(4,2)$	-0.31398	0.72484

Proof. In context (m,k), and if $n = n(R)$, we have

$$\sigma_R(D) < s_n + \mathrm{Z_{LP}}(m,k) - Z(m,k) \quad \tau_R(D) > t_n + \mathrm{D_{LP}}(m,k) - D(m,k).$$

The result follows. $\square$

In the context $(n,k) = (4,3)$, the standard region R must have at least seven sides $n(R) \geq 7$. Then

$$\begin{aligned} \tau(D) &\geq t_7 + \delta_{loop}(4,3) \\ &> (4\pi\zeta - 8)\, pt. \end{aligned}$$

[115] CALC-855294746

Thus, we may assume that this context does not occur.

If the context $(5, 1)$ appears in an octagon, we have

$$\tau(D) > \delta_{loop}(5, 1) + t_8 > (4\pi\zeta - 8)\,pt.$$

If this appears in a heptagon, we have

$$\tau(D) > \delta_{loop}(5, 1) + t_7 + 0.55\,pt > (4\pi\zeta - 8)\,pt,$$

because there must be a vertex that is not a corner of the heptagon. It cannot appear on a pentagon.

Section 14

Further Bounds in Exceptional Regions

14.1 Small dihedral angles

Recall that Section 12.1 defines an integer $n(R)$ that is equal to the number of sides if the region is a polygon. Recall that if the dihedral angle along an edge of a standard cluster is at most 1.32, then there is a flat quarter along that edge (Lemma 11.30).

Lemma 14.1. *Let R be an exceptional cluster with a dihedral angle ≤ 1.32 at a vertex v. Then R squanders $> t_n + 1.47\,pt$, where $n = n(R)$.*

Proof. In most cases we establish the stronger bound $t_n + 1.5\,pt$. In the proof of Theorem 12.1, we erase all upright diagonals, except those completely surrounded by anchored simplices. The contribution to t_n from the flat quarter Q at v in that proof is $D(3,1)$ (Sections 12.5 and Inequalities 13.1). Note that $\epsilon_\tau(Q) = 0$ here because there are no deformations. If we replace $D(3,1)$ with $3.07\,pt$ from Lemma 11.30, then we obtain the bound. Now suppose the upright diagonal is completely surrounded by anchored simplices. Analyzing the constants of Section 13.12, we see that $\mathrm{D_{LP}}(n,k) - D(n,k) > 1.5\,pt$ except when $(n,k) = (4,1)$.

Here we have four anchored simplices around an upright diagonal. Three of them are quarters. We erase and take a penalty. Two possibilities arise. If the upright diagonal is enclosed over the flat quarter, its height is ≥ 2.6 by geometric considerations and the top face of the flat quarter has circumradius at least $\sqrt{2}$. The penalty is $2\xi'_\Gamma + \xi_V$, so the bound holds by the last statement of Lemma 11.30.

If, on the other hand, the upright diagonal is not enclosed over the flat diagonal, the penalty is $\xi_\Gamma + 2\xi_V$. In this case, we obtain the weaker bound $1.47\,pt + t_n$:

$$3.07\,pt > D(3,1) + 1.47\,pt + \xi_\Gamma + 2\xi_V.$$

□

Remark 14.2. *If there are r nonadjacent vertices with dihedral angles ≤ 1.32, we find that R squanders $t_n + r(1.47)\,pt$.*

In fact, in the proof of the lemma, each $D(3,1)$ is replaced with $3.07\,pt$ from Lemma 11.30. The only questionable case occurs when two or more of the vertices are anchors of the same upright diagonal (a loop). Referring to Section 13.12, we have the following observations about various contexts.

- $(4,1)$ can mask only one flat quarter and it is treated in the lemma.
- $(4,2)$ can mask only one flat quarter and $\mathrm{D_{LP}}(4,2) - D(4,2) > 1.47\,pt$.
- $(5,0)$ can mask two flat quarters. Erase the five upright quarters, and take a penalty $4\xi_V + \xi_\Gamma$. We get

$$D(3,2) + 2(3.07)\,pt > t_5 + 4\xi_V + \xi_\Gamma + 2(1.47)\,pt.$$

- $(5,1)$ can mask two flat quarters, and $\mathrm{D_{LP}}(5,1) - D(5,1) > 2(1.47)\,pt$.

14.2 A particular 4-circuit

This subsection bounds the score 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 14.1 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 $(p_1, \ldots, p_5)$.

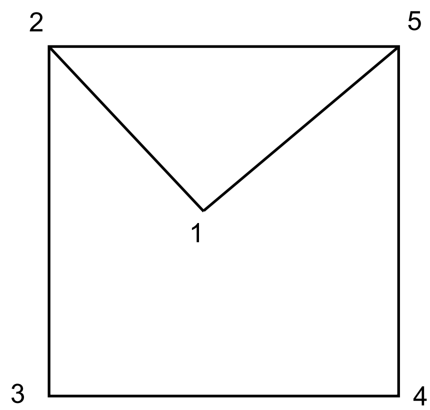

Figure 14.1. *A 4-circuit*

Suppose that D is a decomposition star whose associate graph contains such triangular and pentagonal standard regions. Recall that D determines a set $U(D)$ of vertices in Euclidean 3-space of distance at most $2t_0$ from the origin, and that each vertex p_i can be realized geometrically as a point on the unit sphere at the origin, obtained as the radial projection of some $v_i \in U(D)$.

Lemma 14.3. *One of the edges $\{v_1, v_3\}$, $\{v_1, v_4\}$ has length less than $2\sqrt{2}$. Both of the them have lengths less than 3.02. Also, $|v_1| \geq 2.3$.*

Proof. This is a standard exercise in geometric considerations as introduced in Section 4.2. (The reader should review that section for the framework of the following argument.) We deform the figure using pivots to a configuration $v_2, \ldots, v_5$ at height 2, and $|v_i - v_j| = 2t_0$, $(i, j) = (2,3), (3,4), (4,5), (5,2)$. We scale v_1 until $|v_1| = 2t_0$. We can also take the distance from v_1 to v_5 and to v_2 to be 2. If we have $|v_1 - v_3| \geq 2\sqrt{2}$, then we stretch the edge $|v_1 - v_4|$ until $|v_1 - v_3| = 2\sqrt{2}$. The resulting configuration is rigid. Pick coordinates to find that $|v_1 - v_4| < 2\sqrt{2}$. If we have $|v_1 - v_3| \geq 2t_0$, follow a similar procedure to reduce to the rigid configuration $|v_1 - v_3| = 2t_0$, to find that $|v_1 - v_4| < 3.02$. The estimate $|v_1| \geq 2.3$ is similar. □

There are restrictive bounds on the dihedral angles of the simplices $\{0, v_1, v_i, v_j\}$ along the edge $\{0, v_1\}$. The quasi-regular tetrahedron has a dihedral angle of at most[116] 1.875. The dihedral angles of the simplices $\{0, v_1, v_2, v_3\}$, $\{0, v_1, v_5, v_4\}$ adjacent to it are at most[117] 1.63. The dihedral angle of the remaining simplex $\{0, v_1, v_3, v_4\}$ is at most[118] 1.51. This leads to lower bounds as well. The quasi-regular tetrahedron has a dihedral angle that is at least $2\pi - 2(1.63) - 1.51 > 1.51$. The dihedral angles adjacent to the quasi-regular tetrahedron is at least $2\pi - 1.63 - 1.51 - 1.875 > 1.26$. The remaining dihedral angle is at least $2\pi - 1.875 - 2(1.63) > 1.14$.

A decomposition star D determines a set of vertices $U(D)$ that are of distance at most $2t_0$ from the center of D. Three consecutive vertices p_1, p_2, and p_3 of a standard region are determined as the projections to the unit sphere of three corners v_1, v_2, and v_3, respectively in $U(D)$. By Lemma 11.30, if the interior angle of the standard region is less than 1.32, then $|v_1 - v_3| \leq \sqrt{8}$.

Lemma 14.4. *These two standard regions $F = \{R_1, R_2\}$ give $\tau_F(D) \geq 11.16\,pt$.*

Proof. Let dih denote the dihedral angle of a simplex along a given edge. Let S_{ij} be the simplex $\{0, v_1, v_i, v_j\}$, for $(i, j) = (2,3), (3,4), (4,5), (2,5)$. We have $\sum_{(4)} \mathrm{dih}(S_{ij}) = 2\pi$. Suppose one of the edges $\{v_1, v_3\}$ or $\{v_1, v_4\}$ has length $\geq 2\sqrt{2}$. Say $\{v_1, v_3\}$.

We have[119]

$$\begin{array}{ll}
\tau(S_{25}) & -0.2529\,\mathrm{dih}(S_{25}) > -0.3442,\\
\tau_0(S_{23}) & -0.2529\,\mathrm{dih}(S_{23}) > -0.1787,\\
\hat{\tau}(S_{45}) & -0.2529\,\mathrm{dih}(S_{45}) > -0.2137,\\
\tau_0(S_{34}) & -0.2529\,\mathrm{dih}(S_{34}) > -0.1371.
\end{array}$$

[116] CALC-984463800
[117] CALC-821707685
[118] CALC-115383627
[119] CALC-572068135, CALC-723700608, CALC-560470084, and CALC-535502975

We have a penalty ξ_Γ for erasing, so that

$$\begin{aligned}\tau(D) &\ge \textstyle\sum_{(4)} \tau_x(S_{ij}) - 5\xi_\Gamma\\ &> 2\pi(0.2529) - 0.3442\\ &\qquad -0.1787 - 0.2137 - 0.1371 - 5\xi_\Gamma\\ &> 11.16\,pt,\end{aligned}$$

where $\tau_x = \tau, \hat{\tau}, \tau_0$ as appropriate.

Now suppose $\{v_1, v_3\}$ and $\{v_1, v_4\}$ have length $\le 2\sqrt{2}$. If there is an upright diagonal that is not enclosed over either flat quarter, the penalty is at most $3\xi_\Gamma+2\xi_V$. Otherwise, the penalty is smaller: $4\xi'_\Gamma + \xi_V$. We have

$$\begin{aligned}\tau(D) &\ge \textstyle\sum_{(4)} \tau(S_{ij}) - (3\xi_\Gamma + 2\xi_V)\\ &> 2\pi(0.2529) - 0.3442\\ &\qquad -2(0.2137) - 0.1371 - (3\xi_\Gamma + 2\xi_V)\\ &> 11.16\,pt.\end{aligned}$$

□

14.3 A particular 5-circuit

Lemma 14.5. *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. Since -0.4339 is less than this the lower bound, a 3-crowded upright diagonal does not occur. Similarly, since -0.25 is less than the lower bound, a 4-crowded upright diagonal does not occur (Lemma 11.18 and Lemma 11.7).

Suppose that there is a loop in context $(n,k) = (4,2)$. Again by Lemma 13.5 (with $n(R) = 7$),

$$\sigma_R(D) < -0.2345.$$

We conclude that all loops have context $(n,k) = (4,1)$.

Case 1. *The vertex $v = v_{12}$ has distance at least $2t_0$ from the five corners of $U(D)$ over the pentagon.*

The penalty to switch the pentagon to a pure vor_0 score is at most $5\xi_\Gamma$ (see Section 12.6). There cannot be two flat quarters because then

$$|v_{12}| > \mathcal{E}(S(2,2,2,2t_0,2\sqrt{2},2\sqrt{2}),2t_0,2t_0,2t_0) > 2t_0.$$

(Case 1-a) Suppose there is one flat quarter, $|v_1 - v_4| \le 2\sqrt{2}$. There is a lower bound of 1.2 on the dihedral angles of the simplices $\{0, v_{12}, v_i, v_{i+1}\}$. This is obtained as follows. The proof relies on the convexity of the quadrilateral region. We leave it to the reader to verify that the following pivots can be made to preserve convexity. Disregard all vertices except $v_1, v_2, v_3, v_4, v_{12}$. We give the argument that $\mathrm{dih}(0, v_{12}, v_1, v_4) > 1.2$. The others are similar. Disregard the length $|v_1 - v_4|$. We show that

$$\begin{aligned} sd \;&:= \mathrm{dih}(0, v_{12}, v_1, v_2) + \mathrm{dih}(0, v_{12}, v_2, v_3) \\ &\quad + \mathrm{dih}(0, v_{12}, v_3, v_4) < 2\pi - 1.2. \end{aligned}$$

Lift v_{12} so $|v_{12}| = 2t_0$. Maximize sd by taking $|v_1 - v_2| = |v_2 - v_3| = |v_3 - v_4| = 2t_0$. Fixing v_3 and v_4, pivot v_1 around $\{0, v_{12}\}$ toward v_4, dragging v_2 toward v_{12} until $|v_2 - v_{12}| = 2t_0$. Similarly, we obtain $|v_3 - v_{12}| = 2t_0$. We now have $sd \le 3(1.63) < 2\pi - 1.2$, by a calculation.[120]

Return to the original figure and move v_{12} without increasing $|v_{12}|$ until each simplex $\{0, v_{12}, v_i, v_{i+1}\}$ has an edge (v_{12}, v_j) of length $2t_0$. Interval calculations[121] show that the four simplices around v_{12} squander

$$2\pi(0.2529) - 3(0.1376) - 0.12 > (4\pi\zeta - 8)\,pt + 5\xi_\Gamma.$$

(Case 1-b) Assume there are no flat quarters. By hypothesis, the perimeter satisfies

$$\sum |v_i - v_{i+1}| \le 11.407.$$

We have $\mathrm{arc}(2,2,x)'' = 2x/(16 - x^2)^{3/2} > 0$. The arclength of the perimeter is therefore at most

$$2\,\mathrm{arc}(2,2,2t_0) + 2\,\mathrm{arc}(2,2,2) + \mathrm{arc}(2,2,2.387) < 2\pi.$$

There is a well-defined interior of the spherical pentagon, a component of area $< 2\pi$. If we deform by decreasing the perimeter, the component of area $< 2\pi$ does not get swapped with the other component.

Disregard all vertices but $v_1, \ldots, v_5, v_{12}$. If a vertex v_i satisfies $|v_i - v_{12}| > 2t_0$, deform v_i as in Section 12.8 until $|v_{i-1} - v_i| = |v_i - v_{i+1}| = 2$, or $|v_i - v_{12}| = 2t_0$. If at any time, four of the edges realize the bound $|v_i - v_{i+1}| = 2$, we have reached an impossible situation, because it leads to the contradiction[122]

$$2\pi = \sum^{(5)} \mathrm{dih} < 1.51 + 4(1.16) < 2\pi.$$

[120] CALC-821707685
[121] CALC-467530297 and CALC-135427691
[122] CALC-115383627 and CALC-603145528

(This inequality relies on the observation, which we leave to the reader, that in any such assembly, pivots can by applied to bring $|v_{12} - v_i| = 2t_0$ for at least one edge of each of the five simplices.)

The vertex v_{12} may be moved without increasing $|v_{12}|$ so that eventually by these deformations (and reindexing if necessary) we have $|v_{12} - v_i| = 2t_0$, $i = 1, 3, 4$. (If we have $i = 1, 2, 3$, the two dihedral angles along $\{0, v_2\}$ satisfy[123] $< 2(1.51) < \pi$, so the deformations can continue.)

There are two cases. In both cases $|v_i - v_{12}| = 2t_0$, for $i = 1, 3, 4$.

$$\begin{array}{ll} (i) & |v_{12} - v_2| = |v_{12} - v_5| = 2t_0, \\ (ii) & |v_{12} - v_2| = 2t_0, \quad |v_4 - v_5| = |v_5 - v_1| = 2, \end{array}$$

Case (i) follows from interval calculations[124]

$$\sum \tau_0 \geq 2\pi(0.2529) - 5(0.1453) > 0.644 + 7\xi_\Gamma.$$

In case (ii), we have again

$$2\pi(0.2529) - 5(0.1453).$$

In this interval calculation we have assumed that $|v_{12} - v_5| < 3.488$. Otherwise, setting $S = (v_{12}, v_4, v_5, v_1)$, we have

$$\Delta(S) < \Delta(3.488^2, 4, 4, 8, (2t_0)^2, (2t_0)^2) < 0,$$

and the simplex does not exist. ($|v_4 - v_1| \geq 2\sqrt{2}$ because there are no flat quarters.) This completes Case 1.

Case 2. *The vertex v_{12} has distance at most $2t_0$ from the vertex v_1 and distance at least $2t_0$ from the others.*

Let $\{0, v_{13}\}$ be the upright diagonal of a loop $(4, 1)$. The vertices of the loop are not $\{v_2, v_3, v_4, v_5\}$ with v_{12} enclosed over $\{0, v_2, v_5, v_{13}\}$ by Lemma 11.5. The vertices of the loop are not $\{v_2, v_3, v_4, v_5\}$ with v_{12} enclosed over $\{0, v_1, v_2, v_5\}$ because this would lead to a contradiction

$$y_{12} \geq \mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 3.2), 2t_0, 2t_0, 2) > 2t_0,$$

or

$$y_{12} \geq \mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 3.2), 2, 2t_0, 2) > 2t_0.$$

We get a contradiction for the same reasons unless $\{v_1, v_{12}\}$ is an edge of some upright quarter of every loop of type $(4, 1)$.

We consider two cases. (2-a) There is a flat quarter along an edge other than $\{v_1, v_{12}\}$. That is, the central vertex is v_2, v_3, v_4, or v_5. (Recall that the *central vertex* of a flat quarter is the vertex other than the origin that is not an endpoint of the diagonal.) (2-b) Every flat quarter has central vertex v_1.

[123] CALC-115383627
[124] CALC-312132053

Case 2-a. We erase all upright quarters including those in loops, taking penalties as required. There cannot be two flat quarters by geometric considerations

$$\begin{array}{ll}\mathcal{E}(S(2,2,2,2\sqrt{2},2\sqrt{2},2t_0),2t_0,2t_0,2) & > 2t_0 \\ \mathcal{E}(S(2,2,2,2\sqrt{2},2\sqrt{2},2t_0),2,2t_0,2t_0) & > 2t_0\end{array}$$

The penalty is at most $7\xi_\Gamma$. We show that the region (with upright quarters erased) squanders $> 7\xi_\Gamma + 0.644$. We assume that the central vertex is v_2 (case 2-a-i) or v_3 (case 2-a-ii). In case 2-a-i, we have three types of simplices around v_{12}, characterized by the bounds on their edge lengths. Let $\{0, v_{12}, v_1, v_5\}$ have type A, $\{0, v_{12}, v_5, v_4\}$ and $\{0, v_{12}, v_4, v_3\}$ have type B, and let $\{0, v_{12}, v_3, v_1\}$ have type C. In case 2-a-ii there are also three types. Let $\{0, v_{12}, v_1, v_2\}$ and $\{0, v_{12}, v_1, v_5\}$ have type A, $\{0, v_{12}, v_5, v_4\}$ type B, and $\{0, v_{12}, v_2, v_4\}$ type D. (There is no relation here between these types and the types of simplices A, B, C defined in Section 9.) Upper bounds on the dihedral angles along the edge $\{0, v_{12}\}$ are given as calculations[125]. These upper bounds come as a result of a pivot argument similar to that establishing the bound 1.2 in Case 1-a.

These upper bounds imply the following lower bounds. In case 2-a-i,

$$\begin{array}{lll}\mathrm{dih} & > 1.33 & (A), \\ \mathrm{dih} & > 1.21 & (B), \\ \mathrm{dih} & > 1.63 & (C),\end{array}$$

and in case 2-a-ii,

$$\begin{array}{lll}\mathrm{dih} & > 1.37 & (A), \\ \mathrm{dih} & > 1.25 & (B), \\ \mathrm{dih} & > 1.51 & (D),\end{array}$$

In every case the dihedral angle is at least 1.21. In case 2-a-i, the inequalities give a lower bound on what is squandered by the four simplices around $\{0, v_{12}\}$. Again, we move v_{12} without decreasing the score until each simplex $\{0, v_{12}, v_i, v_{i+1}\}$ has an edge satisfying $|v_{12} - v_j| \le 2t_0$. Interval calculations[126] give

$$\begin{array}{ll}\sum_{(4)} \tau_0 & > 2\pi(0.2529) - 0.2391 - 2(0.1376) - 0.266 \\ & > 0.808.\end{array}$$

In case 2-a-ii, we have[127]

$$\begin{array}{ll}\sum_{(4)} \tau_0 & > 2\pi(0.2529) - 2(0.2391) - 0.1376 - 0.12 \\ & > 0.853.\end{array}$$

So we squander more than $7\xi_\Gamma + 0.644$, as claimed.

Case 2-b. We now assume that there are no flat quarters with central vertex $v_2, \ldots, v_5$. We claim that v_{12} is not enclosed over $\{0, v_1, v_2, v_3\}$ or $\{0, v_1, v_5, v_4\}$. In

[125] CALC-821707685, CALC-115383627, CALC-576221766, and CALC-122081309
[126] CALC-644534985, CALC-467530297, and CALC-603910880
[127] CALC-135427691

fact, if v_{12} is enclosed over $\{0, v_1, v_2, v_3\}$, then we reach the contradiction[128]

$$\begin{aligned}\pi &< \mathrm{dih}(0, v_{12}, v_1, v_2) + \mathrm{dih}(0, v_{12}, v_2, v_3)\\ &< 1.63 + 1.51 < \pi.\end{aligned}$$

We claim that v_{12} is not enclosed over $\{0, v_5, v_1, v_2\}$. Let $S_1 = \{0, v_{12}, v_1, v_2\}$, and $S_2 = \{0, v_{12}, v_1, v_5\}$. We have by hypothesis,

$$y_4(S_1) + y_4(S_2) = |v_1 - v_2| + |v_1 - v_5| < 4.804.$$

An interval calculation[129] gives

$$\begin{aligned}\textstyle\sum_{(2)} \mathrm{dih}(S_i) &\le \textstyle\sum_{(2)} (\mathrm{dih}(S_i) + 0.5(0.4804/2 - y_4(S_i)))\\ &< \pi.\end{aligned}$$

So v_{12} is not enclosed over $\{0, v_1, v_2, v_5\}$.

Erase all upright quarters, taking penalties as required. Replace all flat quarters with s-vor$_0$-scoring taking penalties as required. (Any flat quarter has v_1 as its central vertex.) We move v_{12} keeping $|v_{12}|$ fixed and not decreasing $|v_{12} - v_1|$. The only effect this has on the score comes through the quoins along $\{0, v_1, v_{12}\}$. Stretching $|v_{12} - v_1|$ shrinks the quoins and increases the score. (The sign of the derivative of the quoin with respect to the top edge is computed in the proof of Lemma 12.9.)

If we stretch $|v_{12} - v_1|$ to length $2t_0$, we are done by case 1 and case 2-a. (If deformations produce a flat quarter, use case 2-a, otherwise use case 1.) By the claims, we can eventually arrange (reindexing if necessary) so that

$$\begin{array}{ll}(i) & |v_{12} - v_3| = |v_{12} - v_4| = 2t_0, \quad \text{or}\\ (ii) & |v_{12} - v_3| = |v_{12} - v_5| = 2t_0.\end{array}$$

We combine this with the deformations of Section 12.8 so that in case (i) we may also assume that if $|v_5 - v_{12}| > 2t_0$, then $|v_4 - v_5| = |v_5 - v_1| = 2$ and that if $|v_2 - v_{12}| > 2t_0$, then $|v_1 - v_2| = |v_2 - v_3| = 2$. In case (ii) we may also assume that if $|v_4 - v_{12}| > 2t_0$, then $|v_3 - v_4| = |v_4 - v_5| = 2$ and that if $|v_2 - v_{12}| > 2t_0$, then $|v_1 - v_2| = |v_2 - v_3| = 2$.

Break the pentagon into subregions by cutting along the edges (v_{12}, v_i) that satisfy $|v_{12} - v_i| \le 2t_0$. So for example in case (i), we cut along (v_{12}, v_3), (v_{12}, v_4), (v_{12}, v_1), and possibly along (v_{12}, v_2) and (v_{12}, v_5). This breaks the pentagon into triangular and quadrilateral regions.

In case (ii), if $|v_4 - v_{12}| > 2t_0$, then the argument used in Case 1 to show that $|v_4 - v_{12}| < 3.488$ applies here as well. In case (i) or (ii), if $|v_{12} - v_2| > 2t_0$, then for similar reasons, we may assume

$$\Delta(|v_{12} - v_2|^2, 4, 4, 8, (2t_0)^2, |v_{12} - v_1|^2) \ge 0.$$

[128] CALC-821707685 and CALC-115383627

[129] CALC-69064028

This justifies the hypotheses for the calculations[130] that we use. We conclude that

$$\sum \tau_0 \geq 2\pi(0.2529) - 3(0.1453) - 2(0.2391) > 0.6749.$$

If the penalty is less than $0.067 = 0.6749 - 0.6079$, we are done.

We have ruled out the existence of all loops except $(4,1)$. Note that a flat quarter with central vertex v_1 gives penalty at most 0.02 by Lemma 11.29. If there is at most one such a flat quarter and at most one loop, we are done:

$$3\xi_\Gamma + 0.02 < 0.067.$$

Assume there are two loops of context $(n,k) = (4,1)$. They both lie along the edge $\{v_1, v_{12}\}$, which precludes any unmasked flat quarters. If one of the upright diagonals has height ≥ 2.696, then the penalty is at most $3\xi_\Gamma + 3\xi_V < 0.067$. Assume both heights are at most 2.696. The total interior angle of the exceptional face at v_1 is at least four times the dihedral angle of one of the flat quarters along $\{0, v_1\}$, or $4(0.74)$ by an interval calculation[131]. This is contrary to the hypothesis of an interior angle < 2.89. This completes Case 2. This shows that heptagons with pentagonal hulls do not occur. $\square$

Lemma 14.6. *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. *No two vertices in V are adjacent.*
2. *No two vertices in V lie on a common quadrilateral.*
3. *If $v \in V$, then there are five standard regions at v.*
4. *If $v \in V$, then the corner over v is a central vertex of a flat quarter in the cone over R.*
5. *If $v \in V$, then $p_v \geq 3$. That is, at least three of the five standard regions at v are triangular.*
6. *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.*
7. *If $(p_v, q_v) = (3,1)$, then the internal angle at v of the exceptional region is at most 1.32.*

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

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

[130] CALC-312132053 and CALC-644534985
[131] CALC-751442360

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

$$\sum_F \tau_F(D) > \sum_{v\in V} (p_v d(3) + q_v d(4) + a(p_v))\, pt.$$

Proof. We erase all upright diagonals in the Q-system, except for those that carry a penalty: loops, 3-unconfined, 3-crowded, and 4-crowded diagonals.

We assume that if $(p_v, q_v) = (3, 1)$, then the internal angle is at most 1.32. Because of this, if we score the flat quarter by vor_0, then the flat quarter Q satisfies (Lemma 11.30)

$$\mathrm{vor}_0(Q) > 3.07\, pt > 1.4\, pt + D(3,1) + 2\xi_V + \xi_\Gamma. \tag{14.1}$$

Every flat quarter that is masked by a remaining upright quarter in the Q-system has $y_4 \geq 2.6$. Moreover, $y_1 \geq 2.2$ or $y_4 \geq 2.7$. Let $\pi_v = 2\xi_V + \xi_\Gamma$ if the flat quarter is masked, and $\pi_v = 0$ otherwise.

We claim that the flat quarter (scored by vor_0) together with the triangles and quadrilaterals at a given vertex v squander at least

$$(p_v d(3) + q_v d(4) + a(p_v))\, pt + D(3,1) + \pi_v \tag{14.2}$$

If $p_v = 4$, this is CALC-314974315. If $p_v = 3$, we may assume by the preceding remarks that there are two exceptional regions at v. If the internal angle of R at v is at most 1.32, then we use Inequality 14.1. If the angle is at least 1.32, then by hypothesis, the angle R' at v is at least 1.32. We then appeal to the calculations CALC-675785884 and CALC-193592217.

To complete the proof of the lemma, it is enough to show that we can erase the upright quarters masking a flat quarter at v without incurring a penalty greater than π_v. For then, by summing the Inequality 14.2 over v, we obtain the result.

If the upright diagonal is enclosed over the masked flat quarter, then the upright quarters can be erased with penalty at most ξ_V (by Remark 11.28). Assume the upright diagonal is not enclosed over the masked flat quarter.

If there are at most three upright quarters, the penalty is at most $2\xi_V + \xi_\Gamma$. Assume four or more upright quarters. If the upright diagonal is not a loop, then it must be 4-crowded. This can be erased with penalty

$$2\xi_V + 2\xi_\Gamma - \kappa < 2\xi_V + \xi_\Gamma.$$

Finally, assume that the upright quarter is a loop with four or more upright quarters. Lemma 13.5 limits the possibilities to parameters $(5, 0)$ or $(5, 1)$. In the case of a loop $(5, 1)$, there is no need to erase because $|V| \leq 3$ and by Lemma 13.5, the hexagonal standard region squanders at least

$$t_6 + 3a(p_v)\, pt$$

as required by the lemma. In the case of a loop $(5, 0)$ in a pentagonal region, if $|V| = 1$ then there is no need to erase (again we appeal to Lemma 13.5). If $|V| = 2$, then the two vertices share a penalty of $4\xi_V + \xi_\Gamma$, with each receiving

$$2\xi_V + \xi_\Gamma/2 < 2\xi_V + \xi_\Gamma.$$

□

Paper V

Sphere Packings V. Pentahedral Prisms – Ferguson

Introduction

This paper is the fifth in a series of papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing.

In this paper, we prove that decomposition stars associated with the plane graph of arrangements we term pentahedral prisms do not contravene. Recall that a contravening decomposition star is a potential counterexample to the Kepler conjecture. We use interval arithmetic methods to prove particular linear relations on components of any such contravening decomposition star. These relations are then combined to prove that no such contravening stars exist.

Pentahedral prisms come remarkably close to achieving the optimal score of 8 *pt*, that achieved by the decomposition stars of the face-centered cubic lattice packing. In this sense, we consider pentahedral prisms to be "worst case" decomposition stars.

Pentahedral prisms constituted a counterexample to an early version of Hales's approach to a proof of the Kepler conjecture, and have always been a somewhat thorny obstacle to the proof of the conjecture. Relations required to treat pentahedral prisms are delicate in contrast to the more general bounds which suffice to treat other decomposition stars.

This paper is a revised version of the author's PhD thesis at the University of Michigan. The author wishes to thank Tom Hales, Jeff Lagarias and the referees for their many contributions to this revision.

Section 15

Pentahedral Prisms

Recall that a *contravening decomposition star* is a potential counterexample to the Kepler conjecture. The subject of this paper is a particular class of potentially contravening decomposition stars.

We use the term *pentahedral prisms* to refer to this class of potentially contravening decomposition stars, and refer to a decomposition star in this class as a *pentahedral prism.* This class is defined by the plane graph in Figure 15.1.

An example of an arrangement with such a graph is depicted in Figure 15.2.

A pentahedral prism is characterized by the arrangement and combinatorics of its standard regions. It is composed of ten triangular standard regions, and five quadrilateral standard regions.

The ten triangles are arranged in two *pentahedral caps*, five triangles arranged around a common vertex. The five quadrilaterals lie in a band between the two caps. See Figure 15.3.

Recall that the standard cluster attached to a triangular standard region is a quasi-regular tetrahedron. Likewise, the standard cluster attached to a quadrilateral is a quad cluster. We use the term pentahedral cap to refer to both the standard regions and the quasi-regular tetrahedrons which comprise it.

15.1 The Main Theorem

We begin by recalling various definitions from Paper II, Formulation. The constant pt is introduced in Definition 3.6. Similarly, *score* is defined in Theorem 3.5, as well as Definition 7.8 and Remark 7.20. We denote the score of a region R by $\sigma(R)$.

Theorem 15.1. *Each pentahedral prism P satisfies*

$$\sigma(P) \leq (8 - \epsilon_0)\ pt$$

for $\epsilon_0 = 10^{-8}$. Hence there are no contravening pentahedral prisms.

The next section will introduce a series of propositions which will prove the

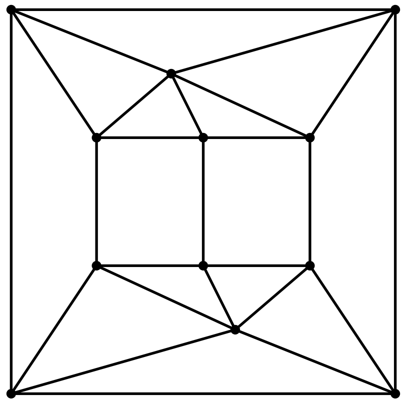

Figure 15.1. *The plane graph of a pentahedral prism.*

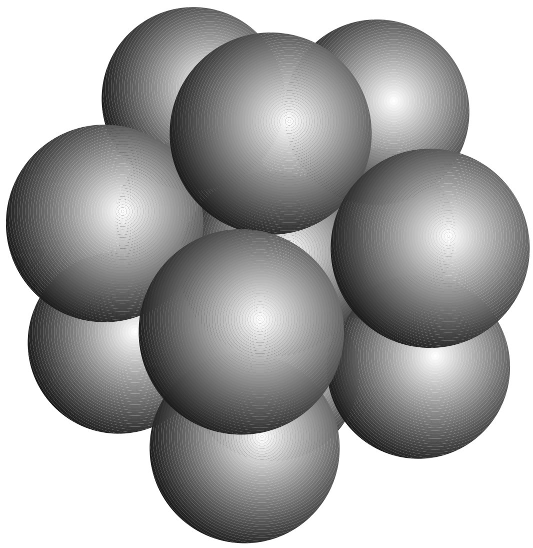

Figure 15.2. *Spheres in a pentahedral prism arrangement.*

main theorem. The first proposition will restrict our attention to a set of potentially contravening pentahedral prisms. Subsequent propositions will provide a collection of relations which we will use to prove the main theorem.

15.2 Propositions

The function $sol(\cdot)$ is introduced in Definition 7.5. The function $dih(\cdot)$ is introduced in Definition 4.12.

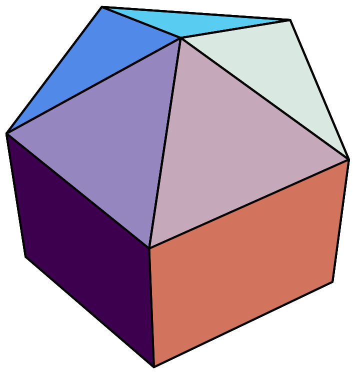

Figure 15.3. *The faces of a pentahedral prism.*

We present computations using auxiliary bounds which imply the main result of the paper, that the score of any pentahedral prism is strictly less than 8 *pt*.

Recall from Section 7.4 that the score decomposition for a decomposition star S takes the form

$$\sigma(S) = \sum_R \sigma(R)$$

where R runs over the standard clusters in S.

In the case of a pentahedral prism P, the score $\sigma(P)$ decomposes as

$$\sigma(P) = \sum_{i=1}^{10} \sigma(T_i) + \sum_{j=1}^{5} \sigma(Q_j)$$

with the triangular regions T_i numbered so that the two pentahedral caps C_i consist of $\{T_i : 1 \le i \le 5\}, \{T_i : 6 \le i \le 10\}$ and Q_j denote the quad clusters. Thus

$$\sigma(C_1) = \sum_{i=1}^{5} \sigma(T_i), \qquad \sigma(C_2) = \sum_{i=6}^{10} \sigma(T_i).$$

The following proposition gives basic inequalities which we will use to form a restricted set of pentahedral prisms.

Proposition 15.1. *A pentahedral prism P satisfies the bound*

$$\sigma(P) \le (8 - \epsilon_0)\ pt$$

for $\epsilon_0 = 10^{-8}$ provided that any one of the following conditions holds:

1. *P contains a tetrahedron T such that*

$$\sigma(T) \le -0.52\ pt$$

2. *P contains a quad cluster Q such that*

$$\sigma(Q) \leq -1.04 \ pt$$

3. *P contains a pentahedral cap C such that*

$$\sigma(C) \leq 3.48 \ pt$$

Proof. We use the following scoring bounds proved earlier for any admissible decomposition star.

First, Lemma 8.10 states that any quasi-regular tetrahedron T satisfies

$$\sigma(T) \leq 1 \ pt.$$

Theorem 8.4 states that any quad cluster Q satisfies

$$\sigma(Q) \leq 0.$$

Next, a pentahedral cap C consists of five quasi-regular tetrahedra T_i sharing a common distinguished edge. At one end of the distinguished edge is the distinguished vertex $v = 0$ which is the center of the decomposition star P. Each T_i has context $c_i = (5, 0)$. Lemma 10.6 (with $k = 1$ and $r = 5$) and Lemma 10.7 state that any pentahedral cap C_i satisfies

$$\sigma(C_i) = \sum_{i=1}^{5} \sigma(T_i, c_i, v) \leq (4.52 - \epsilon_0) \ pt$$

with $\epsilon_0 = 10^{-8}$.

1. Suppose that some $\sigma(T) \leq -0.52 \ pt$, with T contained in a pentahedral cap C_1. Then the inequalities above give

$$\begin{aligned} \sigma &\leq -0.52 \ pt + 4(1 \ pt) + \sigma(C_2) + \sum_{j=1}^{5} \sigma(Q_j) \\ &\leq 3.48 \ pt + (4.52 - \epsilon_0) \ pt + 5(0) = (8 - \epsilon_0) \ pt \end{aligned}$$

2. Suppose that some quad cluster $\sigma(Q_j) \leq -1.04 \ pt$. Then

$$\begin{aligned} \sigma(P) &\leq \sigma(C_1) + \sigma(C_2) + (-1.04 \ pt) + 4(0) \\ &\leq 2((4.52 - \epsilon_0) \ pt) - (1.04 \ pt) = (8 - 2\epsilon_0) \ pt \end{aligned}$$

3. Suppose that some pentahedral cap C_1 has $\sigma(C_1) \leq 3.48 \ pt$. Then the inequalities above give

$$\sigma(P) \leq (3.48 \ pt) + (4.52 - \epsilon_0) \ pt + 5(0) = (8 - \epsilon_0) \ pt$$

This completes the proof. □

Definition 15.1.

A PC pentahedral prism *is a pentahedral prism such that*

1. *All tetrahedra T have $\sigma(T) \geq -0.52$ pt*
2. *All quad clusters have $\sigma(Q) \geq 1.04$ pt*
3. *All pentahedral caps have $\sigma(C) \geq 3.48$ pt*

and the configuration arises as a pointwise limit of configurations in which (1), (2), (3) hold with strict inequality. A strict PC pentahedral prism *is one in which (1), (2), (3) each hold with strict inequality.*

All remaining propositions will apply to PC pentahedral prisms. This restriction improves the quality of the bounds which we are able to prove on components of a pentahedral prism.

The following two propositions contain linear relations which will imply the main theorem. We defer their proofs to the next section.

Proposition 15.2. *For a quasi-regular tetrahedron T in a PC pentahedral prism, the following linear inequality holds between $\sigma(T)$, the spherical angle* $\mathrm{sol}(T)$ *(at the central vertex common to the five tetrahedra in the pentahedral cap), and the dihedral angle* $\mathrm{dih}(T)$ *associated with the first edge of the tetrahedron (that is, the edge common to the five tetrahedra in a pentahedral cap):*

$$\sigma(T) + m\,\mathrm{sol}(T) + a(\mathrm{dih}(T) - \frac{2\pi}{5}) - b_c \leq 0$$

Here $a = 0.0739626$, $b_c = 0.253095$, and $m = 0.3621$.

Proposition 15.3. *For a quad cluster Q in a PC pentahedral prism, the following linear inequality holds between $\sigma(Q)$ and the spherical angle* $\mathrm{sol}(Q)$*:*

$$\sigma(Q) + m\,\mathrm{sol}(Q) - b_q \leq 0,$$

Here $b_q = 0.49246$ and again $m = 0.3621$.

From Propositions 15.2 and 15.3 we can deduce the following theorem.

Theorem 15.2. *Each PC pentahedral prism P satisfies the score bound*

$$\sigma(P) \leq 7.9997 \ pt$$

.

Proof. Propositions 15.2 and 15.3 provide linear relations on all of the standard clusters in a PC pentahedral prism P. We combine these relations to prove the required score bound.

Invoking Proposition 15.2 for the five quasi-regular tetrahedrons $\{T_i : i = 1 \dots 5\}$ from a pentahedral cap, we find

$$\sum_{i=1}^{5} \sigma(T_i) + m \sum_{i=1}^{5} \mathrm{sol}(T_i) + a \sum_{i=1}^{5} (\mathrm{dih}(T_i) - \frac{2\pi}{5}) - 5b_c \leq 0.$$

Summing over both pentahedral caps and using the relation that the sum of the five dihedral angles in a pentahedral cap is 2π,

$$\sum_{i=1}^{5} \mathrm{dih}(T_i) = 2\pi,$$

we find

$$\sum_{i=1}^{10} \sigma(T_i) + m \sum_{i=1}^{10} \mathrm{sol}(T_i) - 10b_c \leq 0.$$

We represent the tetrahedra from the second pentahedral cap by the indices $i = 6 \dots 10$.

Invoking Proposition 15.3 for the five quad clusters $\{Q_i : i = 11 \dots 15\}$, and using the fact that the sum of the solid angles is 4π,

$$\sum_{i=1}^{10} \mathrm{sol}(Q_i) + \sum_{j=11}^{15} \mathrm{sol}(Q_j) = 4\pi$$

we find

$$\sum_{i=1}^{10} \sigma(T_i) + \sum_{j=11}^{15} \sigma(Q_j) + 4\pi m - 5b - 10b_c \leq 0.$$

Therefore,

$$\sigma(P) \leq 5b + 10b_c - 4\pi m.$$

Substituting the values of $b, b_c, m,$ and pt, we find that the score of a PC pentahedral prism is less than 7.9997 pt. □

Assuming Proposition 15.1 and Theorem 15.2 we can prove Theorem 15.1.

Proof. Given a pentahedral prism P, it is either PC or it is not. In the former case, its score is bounded by 7.9997 pt. In the latter case, its score is bounded by $(8 - 10^{-8})$ pt. In both cases, its score is bounded by $(8 - 10^{-8})$ pt. □

Remark 15.1. *The score bound in Theorem 15.1 is weaker than what is possible to prove. In the interest of simplifying the exposition as well as the required computations, we establish this weaker bound which suffices for this part of the proof of the Kepler conjecture.*

Section 16

The Main Propositions

In the first section, we recall the definition of score, and introduce some local notation. In the next section, we recall the notion of dimension reduction, and prove its validity for some relevant cases. In the following section, we prove Proposition 15.2. In the remaining sections we prove Proposition 15.3.

16.1 Scoring

The development of a scoring function is central to the proof of the Kepler conjecture. Its definition is therefore somewhat complicated. Fortunately, in our treatment of the pentahedral prism we are able to restrict our attention to only a few cases in the scoring system.

Recall that *score* is defined in Theorem 3.5, as well as Definitions 7.6 and 7.8 and Remark 7.20. See Remark 7.23 for a simplified version of the scoring function for quarters.

In our context, the score $\sigma(\cdot)$ breaks into four different scoring types: $gma(\cdot)$, $vor(\cdot)$, $octavor(\cdot)$, and Voronoi.

$gma(\cdot)$ applies to quasi-regular tetrahedrons and quarters, and is introduced as $\Gamma(\cdot)$ in Definition 7.6. We frequently use the term *compression* as an alias for gma$(\cdot)$. This alias was introduced in Section 7.6.

$vor(\cdot)$ is the score determined by the analytic continuation of the Voronoi volume associated with the distinguished vertex of a tetrahedron, and corresponds to $s\text{-}vor(\cdot)$ in Definition 7.6.

We let $octavor(\cdot)$ denote the score of an upright quarter in context (4,0) which is not scored by compression. In this case, $octavor(\cdot)$ is the average of two $vor(\cdot)$ scores.

Voronoi scoring, which we also refer to as pure Voronoi scoring, is $vor_R(D)$ from Remark 7.20.

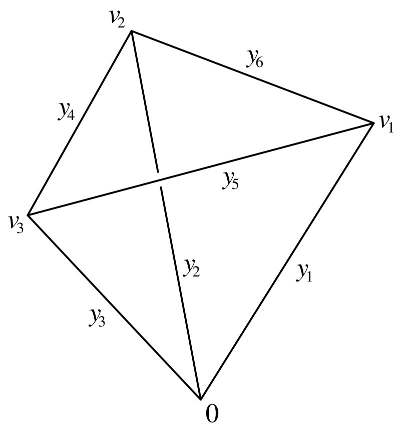

Figure 16.1. *Tetrahedron with distinguished vertex and labeled edges.*

16.2 Dimension Reduction

The relations on tetrahedra required for the scoring bound on decomposition stars are typically six-dimensional, as they are formulated in terms of the edge lengths of a tetrahedron. For a quad cluster, they can be even higher-dimensional. For high-dimensional relations, the method of subdivision becomes very expensive, computationally speaking.

We define a simplification which reduces the dimension of the required computations. This simplification therefore reduces the computational expense of the verification of a relation.

We refer to this simplification as dimension-reduction. We will apply this simplification for three different scoring types: compression, vor analytic, and Voronoi. These scoring functions are introduced in Definitions 7.6 and 7.8. See Remark 7.23 for a simplified version of the scoring function for quarters.

Theorem 16.1. *(Dimension-reduction) Given a tetrahedron T with a fixed scoring type (one of compression, vor analytic, or Voronoi), the deformation consisting of moving a vertex v_i along the edge $(0, v_i)$ towards the origin increases the score of the tetrahedron.*

Note that this deformation holds the solid angle at the origin fixed. See Figure 16.1. Since the reduction may be performed until either a scoring system or an edge-length constraint is met, this argument reduces the number of free parameters for the verification, thus reducing the dimension and complexity of the verification of a relation.

Proof. There are three cases to consider: compression scoring, vor analytic scoring and Voronoi scoring. This technique was introduced in Proposition 8.7.1 of [Hal97a] for compression-scoring, and is proved there in the compression case.

Next we consider vor analytic-scored tetrahedra. The validity of the same reduction for vor analytic-scored tetrahedra is obvious if the tip of the Voronoi cell does not protrude. If the tip does protrude, we must use the analytic continuation for the Voronoi volume. In this case, the validity of the reduction is not obvious.

The geometric constraint of moving a vertex along an edge can easily be stated analytically in terms of the original edge lengths, $(y_1, y_2, y_3, y_4, y_5, y_6)$. This action depends on a single parameter, the distance of the vertex v_1 from the origin, which we call t. The new edge lengths are given by

$$(t, y_2, y_3, y_4, \sqrt{t^2 + {y_3}^2 - \frac{t\ ({y_1}^2 + {y_3}^2 - {y_5}^2)}{y_1}}, \sqrt{t^2 + {y_2}^2 - \frac{t\ ({y_1}^2 + {y_2}^2 - {y_6}^2)}{y_1}}).$$

Recall from Section 8.6.3 of [Hal97a] that the formula for the analytic Voronoi volume is a rational function of χ, u, $\sqrt{\Delta}$, and x_i, where $x_i = y_i^2$. Further recall that χ, u, and Δ are all polynomial functions in x_i that are defined in Sections 8.1 and 8.2 of [Hal97a].

Substituting the computed edge lengths in the formula for the analytic Voronoi volume, taking the partial derivative with respect to t, replacing t with y_1, multiplying by the positive term

$$8\sqrt{\Delta}u(x_1, x_3, x_5)u(x_1, x_2, x_6)/y_1,$$

and then simplifying, we end up with a large homogeneous polynomial in x_i of degree 6, which is too ugly to exhibit here (having 91 terms).

Evaluating this polynomial over all possible quasi-regular tetrahedrons and quarters, we find that it is positive.

Therefore the volume is increasing in t, so to increase the score, we should push the vertex in along the edge. The verification of the sign of the polynomial is found in Calculation 17.4.5.1. This completes the case of vor analytic-scored tetrahedra.

The final case is Voronoi scoring. The deformation does not change the solid angle of the tetrahedron. The only term of the Voronoi score that changes is a negative constant times a volume. The contraction of the tetrahedron decreases this volume, and increases the score. The validity of a similar reduction argument for Voronoi scoring of a tetrahedron is now obvious. $\square$

16.3 Proof of Proposition 15.2

It suffices to prove Proposition 15.2 for strict PC pentahedral prisms. Each non-strict PC pentahedral prism is a pointwise limit of strict ones of the same combinatorial type, so the inequality in the conclusion of the proposition will hold for non-strict PC pentahedral prisms by continuity.

We use three separate computations to construct and prove Proposition 15.2. First, we prove a relation between dihedral angle and score. We then show that if the dihedral angle of a tetrahedron in a pentahedral cap exceeds a certain bound, then the associated pentahedral prism is not a strict PC pentahedral prism. We call such a bound a *dihedral cutoff*. This cutoff allows us to prove the final bound.

In the following discussion, $\mathrm{dih}(T)$ refers to the dihedral angle associated with the first edge of a quasi-regular tetrahedron T, $\sigma(T)$ refers to the compression score of the tetrahedron, and $\mathrm{sol}(T)$ refers to the solid angle at the distinguished vertex. We restrict our attention to quasi-regular tetrahedrons whose score exceeds $-0.52\ pt$, as otherwise the associated pentahedral prism cannot contravene.

The first relation is

$$\sigma(T) \leq a_1 \,\mathrm{dih}(T) - a_2 \tag{16.1}$$

where $a_1 = 0.3860658808124052$ and $a_2 = 0.4198577862$. Calculation 17.4.1.1 provides the verification of this relation.

Lemma 16.1. *If a pentahedral prism has a pentahedral cap that contains a quasi-regular tetrahedron T with dihedral angle $\mathrm{dih}(T) \geq d_0$, where $d_0 = 1.4674$, then it is not a strict PC pentahedral prism.*

Proof. Applying relation (16.1) to four quasi-regular tetrahedrons T_i forming part of a strict PC pentahedral prism, we find

$$\sum_{i=1}^{4} \sigma(T_i) \leq a_1 \sum_{i=1}^{4} \mathrm{dih}(T_i) - 4a_2 \tag{16.2}$$

Applying the relation

$$\mathrm{dih}(T_5) = 2\pi - \sum_{i=1}^{4} \mathrm{dih}(T_i) \tag{16.3}$$

and adding $\sigma(T_5)$ to both sides of relation (16.2), we find

$$\sum_{i=1}^{5} \sigma(T_i) \leq \sigma(T_5) + a_1(2\pi - \mathrm{dih}(T_5)) - 4a_2 \tag{16.4}$$

The left-hand side represents the score of the pentahedral cap. If the right-hand side does not exceed $3.48\ pt$, then the pentahedral prism is not a strict PC pentahedral prism.

We assert that if $\mathrm{dih}(T) \geq d_0$, the right-hand side

$$\sigma(T_5) + a_1(2\pi - \mathrm{dih}(T_5)) - 4a_2$$

does not exceed $3.48\ pt$. Equivalently, we prove that $\mathrm{dih}(T) \geq d_0$ implies

$$\sigma(T) - a_1 \,\mathrm{dih}(T) \leq 3.48\ pt - 2\pi a_1 + 4a_2$$

which is verified in Calculation 17.4.1.2.

We conclude that if $\mathrm{dih}(T) \geq d_0$ then the pentahedral prism cannot be a strict PC pentahedral prism.

□

Hence we may restrict our attention to quasi-regular tetrahedrons whose dihedral angle does not exceed the dihedral cutoff d_0.

Using the dihedral cutoff, we establish the final relation,

$$\sigma(T) + m\,\mathrm{sol}(T) + a(\mathrm{dih}(T) - \frac{2\pi}{5}) - b_c \leq 0$$

via Calculation 17.4.1.3. This completes the proof of Proposition 15.2.

16.4 Proof of Proposition 15.3: Top level

It suffices to prove Proposition15.3 for strict PC pentahedral prisms, by a similar argument to that used for Proposition 15.2.

Recall from Definition 7.15 that a quad cluster is a standard region that is a quadrilateral. Quad clusters can be classified as follows:

1. Flat quad clusters
2. Octahedra
3. Pure Voronoi quad clusters
4. Mixed quad clusters

We will subdivide (3) into acute and obtuse types. See Section 10.4 for a discussion on the classification of quad clusters. By Lemma 10.14, the score of a mixed quad cluster is less than -1.04 *pt*. A PC pentahedral prism therefore cannot contain a mixed quad cluster, so the bound of Proposition 15.3 holds trivially for this class.

We treat the remaining classes in the following sections.

16.5 Proof of Proposition 15.3: Flat quad clusters

Recall that a *flat* quarter is a quarter whose long edge is opposite its distinguished vertex.

Lemma 16.2. *Given a flat quarter Q with $\sigma(Q) \geq -1.04$ pt, the relation*

$$\sigma(Q) \leq -m\,\mathrm{sol}(Q) + b/2 \qquad (16.5)$$

holds.

Proof. Label the diagonal of a flat quarter y_6.

Flat quarters may be scored using either compression or vor scoring. We treat each case separately.

First, suppose that we wish to prove the bound for compression scored quarters. This means that the circumradii of the two faces adjacent to the long diagonal do not exceed $\sqrt{2}$. We subdivide the verification into Calculation 17.4.2.1, a computation where we apply dimension-reduction and partial derivative information, and Calculation 17.4.2.2, a boundary verification, where we restrict our attention to cells which lie on the boundary between compression and vor scoring.

Second, we treat the vor-scoring case. In this case we prove the bound for vor-scored quarters. This means that at least one of the circumradii of the two faces adjacent to the long diagonal is at least $\sqrt{2}$. This verification is somewhat more complex than the compression case. We subdivide the verification into

1. Verification that the first three partials are negative on a small cell containing the corner (Calculation 17.4.2.3).

2. Verification of the bound on that small cell containing the corner, using the property that the first three partials are negative (Calculation 17.4.2.4).

3. A computation where we apply dimension-reduction and partial derivative reduction, omitting the corner cell (Calculation 17.4.2.5).

4. A boundary verification, where we restrict our attention to cells which lie on the boundary between compression and vor scoring, again omitting the corner cell (Calculation 17.4.2.6).

These calculations complete the proof of Lemma 16.2. $\square$

We are now prepared to prove Proposition 15.3 for flat quad clusters.

Flat quad clusters are composed of two flat quarters, whose common face includes the long edge.

By Proposition 15.1, we restrict our attention to flat quarters whose score exceeds $-1.04\ pt$, recalling the fact that the score of flat quarters is nonpositive.

Invoking Lemma 16.2 for each flat quarter and adding the relations, we arrive at the desired bound for flat quad clusters. This completes the proof.

16.6 Proof of Proposition 15.3: Octahedra

Recall that quartered octahedra, a type of quad cluster, are composed of four upright quarters arrayed around their common long edge (called the *diagonal*) so that each face containing the common edge is shared by two quarters.

We are required to prove a relation of the form

$$\sigma(H) + m\,\mathrm{sol}(H) - b \le 0,$$

where $\sigma(H)$ denotes the score of an octahedron H, $\mathrm{sol}(H)$ denotes the solid angle associated with the distinguished vertex, and m and b are positive constants. By Proposition 15.1, we restrict our attention to octahedra whose score exceeds $-1.04\ pt$.

Our treatment of octahedra, as usual, is comprised of a number of auxiliary computations. We prove bounds on upright quarters which are part of an octahedron, and then combine these bounds to deduce the required bound on octahedra in general.

The scoring function $\sigma(\cdot)$ for upright quarters is either compression (denoted by $\mathrm{gma}(\cdot)$) or an average of two $\mathrm{vor}(\cdot)$ scores, which we will continue to refer to as vor-scoring. See Remark 7.23 for a simplified version of the scoring rules.

Due to the complex nature of octahedra, we consider a number of sub-cases. These cases are partitioned according to the length of the diagonal and the scoring system applied to the upright quarters.

Using a dihedral summation argument, we will eliminate octahedra whose diagonal lies in the range $[2.51, 2.716]$.

Next, we will treat the case where the diagonal lies in the range $[2.716, 2\sqrt{2}]$. Using a dihedral correction term, we will prove the bound for octahedra which are completely compression-scored, and octahedra which are completely vor-scored.

The remaining cases will consist of octahedra which contain either two or three vor-scored quarters. (Since a quarter is vor-scored if one of the faces containing the diagonal has circumradius $\sqrt{2}$ or greater, it is not possible for an octahedron to contain only one vor-scored quarter.) We treat these cases using an additional correction term.

In all computations involving octahedra, we label the diagonal y_1.

In order to simplify the computations, we first prove an auxiliary cutoff bound. This first bound reduces the size of the cell over which we must conduct our search, as per Proposition 15.1.

Lemma 16.3. *If an upright quarter contains an edge numbered 2, 3, 5, or 6 whose length is not less than* 2.2*, its score is less than or equal to* -0.52 *pt.*

Proof. This is Calculation 17.4.3.1. □

Since such an edge is shared by another upright quarter in the same octahedron, the score of the associated octahedron must fall below -1.04 *pt*.

We restrict our search accordingly.

Lemma 16.4. *The score of an octahedron* H *with upright diagonal in the range* $[2.51, 2.716]$ *is less than or equal to* -1.04 *pt.*

Proof. In Calculation 17.4.3.2, we prove a bound of the form

$$\sigma(S) + c\,\mathrm{dih}(S) \leq d$$

on upright quarters S, where $c = 0.1533667634670977$, and $d = 0.2265$. Adding the bound for four quarters S_i forming an octahedron, we find

$$\sum_{i=1}^{4} \sigma(S_i) + c \sum_{i=1}^{4} \mathrm{dih}(S_i) \leq 4d.$$

Using the fact that the sum of the dihedral angles is 2π, we find that

$$\sigma(H) \leq -2\pi c + 4d$$

for such an octahedron H.

A computation involving the constants c and d shows that the score is less than -1.04 *pt*. $\square$

Again invoking Proposition 15.1, we need only consider octahedra whose diagonal lies in the range $[2.716, 2\sqrt{2}]$.

Using this assumption, we prove bounds of the form

$$\sigma(S) + m\,\mathrm{sol}(S) + \alpha\,\mathrm{dih}(S) \leq \frac{b}{4} + \alpha\frac{\pi}{2} \tag{16.6}$$

and

$$\sigma(S) + m\,\mathrm{sol}(S) + \alpha\,\mathrm{dih}(S) + \beta x_1 \leq \frac{b}{4} + \alpha\frac{\pi}{2} + 8\beta, \tag{16.7}$$

where $\mathrm{dih}(S)$ refers to the dihedral angle associated with the diagonal, $\sigma(S)$ refers to the scoring scheme appropriate for a particular upright quarter S, and x_1 refers to the square of the length of the diagonal. We choose α and β according to the scoring scheme.

Appropriate values for the correction terms involving α and β were determined by experimentation.

Choosing $\alpha = 0.14$, we prove (16.6) for compression-scored quarters with diagonal in the interval $[2.716, 2\sqrt{2}]$ (Calculation 17.4.3.3). Using the same α, we prove (16.6) for vor-scored quarters with diagonal in the range $[2.716, 2.81]$ (Calculation 17.4.3.4).

Choosing $\alpha = 0.054$, $\beta = 0.00455$, we prove (16.7) for compression-scored quarters with diagonal in $[2.81, 2\sqrt{2}]$ (Calculation 17.4.3.5). Choosing the same α, but $\beta = -0.00455$, we prove (16.7) for vor-scored quarters with diagonal in $[2.81, 2\sqrt{2}]$ (Calculation 17.4.3.6).

Note that for vor-scored quarters, the first inequality is a relaxation of the second, since β is negative.

The verification of each of these inequalities involves a computation where we apply dimension-reduction and partial derivative information, and a boundary verification, where we restrict our attention to cells which lie on the boundary between compression and vor analytic scoring. Note that the dimension-reduction step for relation (16.7) is complicated by the presence of the βx_1 term.

Lemma 16.5. *Proposition 15.3 holds for octahedra with upright diagonals in the range* $[2.716, 2\sqrt{2}]$.

Proof. Summing inequality (16.6) over the four quarters S_i of an octahedron, we find

$$\sum_{i=1}^{4}\sigma(S_i) + m\sum_{i=1}^{4}\mathrm{sol}(S_i) + \alpha\sum_{i=1}^{4}\mathrm{dih}(S_i) \leq b + 2\alpha\pi.$$

Using the fact that the dihedral angles sum to 2π, we find

$$\sigma(H) + m\,\mathrm{sol}(H) \le b,$$

so octahedra H with diagonals in the range $[2.716, 2.81]$ satisfy the requisite bound.

Summing inequality (16.6) over a consistently scored octahedron (either all compression or all vor) with diagonal in the range $[2.81, 2\sqrt{2}]$, we again arrive at the desired bound.

The remaining cases involve octahedra which contain both compression and vor-scored quarters, and whose diagonals lie in the range $[2.81, 2\sqrt{2}]$. For this case, we use inequality (16.7).

The summation involving inequality (16.7) is identical to inequality (16.6) save for the presence of the β terms. If there are two vor-scored quarters and two compression-scored quarters, the beta terms cancel, giving the relation as before.

If there are three vor-scored quarters and one compression-scored quarter, we note that the same relation for vor-scored quarters holds if we replace β by $\beta/3$ (since we have now relaxed the bound). Summing the inequalities, the term involving β vanishes again, leaving the desired inequality. $\square$

Lemmas 16.4 and 16.5 prove Proposition 15.3 for octahedra.

16.7 Proof of Proposition 15.3: Pure Voronoi quad clusters

The next class of quad clusters which we treat are the pure Voronoi quad clusters. We will define a truncation operation on these quad clusters. Truncation will simplify the geometry of the quad clusters, and will provide a convenient scoring bound. We will divide our treatment of pure Voronoi quad clusters into two cases in order to simplify the analysis and numerical verifications as much as possible.

Recall from the classification of quad clusters that a pure Voronoi quad cluster consists of the intersection of a V-cell at the origin with the cone at the origin over a quadrilateral standard region. We refer to the restriction of the V-cell to the cone over the quadrilateral as either the V-cell or the Voronoi cell of the quad cluster. Figure 16.2 describes the geometry of a simple V-cell.

In addition, recall that a vertex lying in the cone over a pure Voronoi quad cluster must have height greater than $2\sqrt{2}$. Such vertices can significantly complicate the geometry of the V-cell, affecting its shape and volume.

We remove the effect of vertices lying above a pure Voronoi quad cluster by removing all points from the V-cell which have height greater than $\sqrt{2}$. We call this operation *truncation at* $\sqrt{2}$. Truncation decreases the volume of the quad cluster. This decrease in volume increases the score of the quad cluster, bringing it closer to the proposed bound.

We refer to truncated pure Voronoi quad clusters as *truncated* quad clusters.

We define a scoring operation on pure Voronoi quad clusters which we call *truncated Voronoi* scoring. This operation consists of truncation at $\sqrt{2}$, followed by the usual Voronoi scoring.

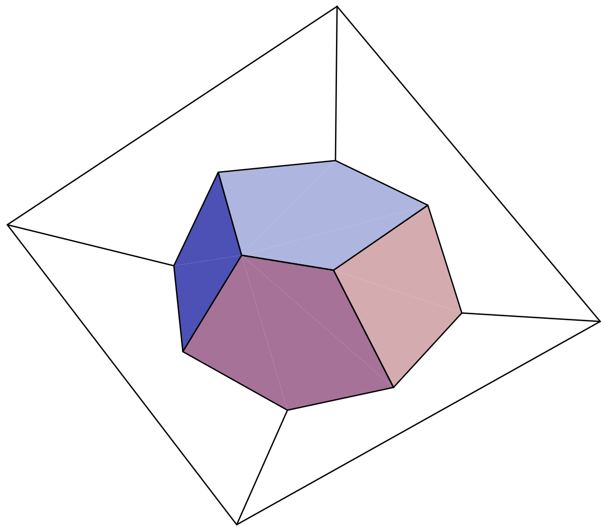

Figure 16.2. *A pure Voronoi quad cluster.*

Each diagonal across the face of a cluster must have length greater than $2\sqrt{2}$, otherwise we could form two flat quarters, contradicting the decomposition. We choose the shorter of the two possible diagonals, and will consider that diagonal in the analysis which follows.

We decompose the cluster into two tetrahedrons along the chosen diagonal. The face dividing the tetrahedrons is either acute or it is obtuse. We treat each case separately.

We must prove

$$\sigma(Q) + m\,\mathrm{sol}(Q) - b \leq 0,$$

where $\sigma(Q)$ denotes the score of a pure Voronoi quad cluster Q, $\mathrm{sol}(Q)$ denotes the solid angle associated with the distinguished vertex, and m and b are positive constants. We call this relation a *bound* on the solid angle and score of a quad cluster. Invoking Proposition 15.1, we restrict our attention to quad clusters whose score exceeds $-1.04\ pt$.

16.8 Pure Voronoi quad clusters: acute case

Lemma 16.6. *If an acute quad cluster is divided along an acute separating face, then the score of each half is nonpositive.*

Proof. This is a consequence of the arguments of Theorem 8.4. □

We therefore restrict our attention to halves whose score exceeds $-1.04\ pt$, by Proposition 15.1.

If the separating face is acute, we prove

$$\sigma(S_i) + m\,\mathrm{sol}(S_i) - b/2 \leq 0 \tag{16.8}$$

for each half S_i independently, and deduce the desired bound by adding the bounds for each half.

Lemma 16.7. *Let T_0 denote the tetrahedron with edge lengths $(2, 2, 2, 2, 2, 2\sqrt{2})$. Let $\mathrm{sol}(T_0)$ denote the solid angle of the tetrahedron T_0. Given a tetrahedron T, if $\mathrm{sol}(T) < \mathrm{sol}(T_0)$, then relation (16.8) holds.*

Proof. If $\mathrm{sol}(T) < \mathrm{sol}(T_0)$, then $m\,\mathrm{sol}(T) < m\,\mathrm{sol}(T_0)$, hence

$$m\,\mathrm{sol}(T) - b/2 < m\,\mathrm{sol}(T_0) - b/2 \leq 0,$$

and

$$\sigma(T) + m\,\mathrm{sol}(T) - b/2 < \sigma(T) \leq 0,$$

by Lemma 16.6. □

We therefore may restrict our attention to halves whose solid angle is at least $\mathrm{sol}(T_0)$. In addition, we restrict our attention to halves for which the dividing face is acute.

Lemma 16.8. *The relation*

$$\sigma(T) + m\,\mathrm{sol}(T) - b/2 \leq 0$$

holds for a tetrahedron T forming half of an acute quad cluster with score exceeding -1.04 pt.

Proof. The required verifications for each half of an acute quad cluster are somewhat difficult to achieve directly, so we subdivide into a number of different cases in an attempt to reduce the complexity of the calculations. First, we show that the bound holds for all halves whose diagonal is at least 2.84 (Calculation 17.4.4.1). Using this information, we then prove the bound everywhere but in a small corner cell (Calculation 17.4.4.2). We then restrict our attention to the small corner cell (Calculation 17.4.4.3). These computations involve the use of partial derivative information, and include the required boundary computations. □

Invoking Lemma 16.8 for each half and adding them proves Proposition 15.3 for the acute case.

16.9 Pure Voronoi quad clusters: obtuse case

If the separating face is obtuse, the analysis becomes significantly harder. It is no longer possible to prove the desired bound on each half independently. The dimension of the full bound, even using the usual dimension-reduction techniques,

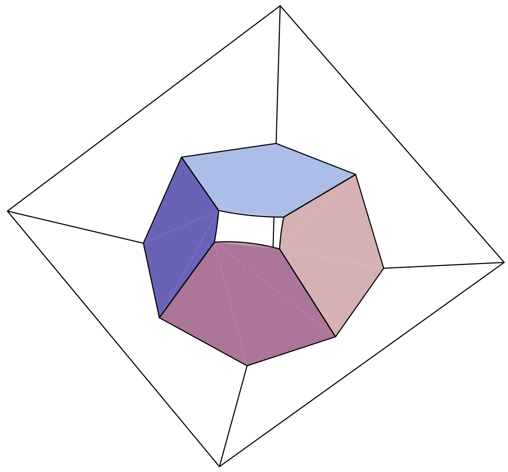

Figure 16.3. *A typical truncated quad cluster.*

is too high to make the verification tractable numerically. Therefore we adopt a different approach.

Using the dimension-reduction technique, we push each vertex along its edge until the distance from each vertex to the origin is 2. We call the resulting quad cluster a *squashed* cluster. Observe that the solid angle of the cluster is unchanged, while the volume of the Voronoi cell has decreased, thereby increasing the score of the cluster.

Since the central face is still obtuse, the length of the diagonal after this perturbation must still exceed $2\sqrt{2}$. Note, however, that the other edge lengths in the quad cluster can be as small as $4/2.51$.

The geometry of the V-cell of a squashed cluster, assuming that there is no truncation from vertices of the packing lying above the quad cluster, is that of Figure 16.2. When the V-cell is truncated at $\sqrt{2}$ from the origin, two potential arrangements arise. In the first arrangement, the truncated region is connected, as in Figure 16.3. In second potential arrangement, the truncated region is formed of two disjoint pieces, as in Figure 16.4.

Lemma 16.9. *The disjoint case cannot arise for squashed quad clusters.*

Proof. Suppose that it could. Pick an untruncated point along the central ridge of the V-cell (see Figure 16.4). The distance of this point from the origin is then less than $\sqrt{2}$, but due to its location on the central ridge, it is equidistant from the two nearest vertices and the origin. This implies that the circumradius of the resulting triangle must be less than $\sqrt{2}$, which contradicts the fact that the diagonals have length at least $2\sqrt{2}$. ∎

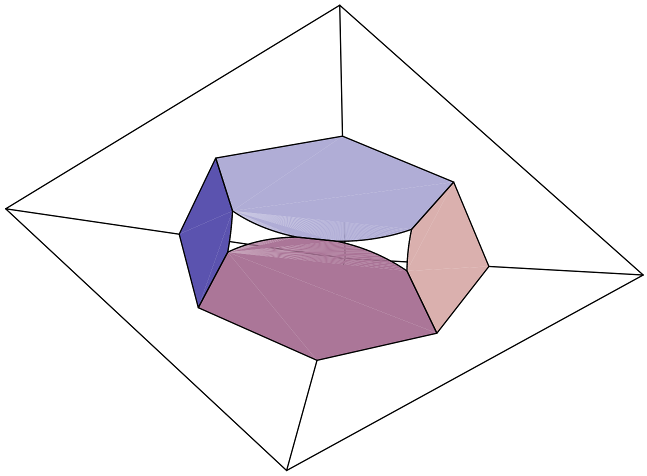

Figure 16.4. *An impossible arrangement.*

16.9.1 A geometric argument

We introduce a simplification which will reduce the complexity of the obtuse case. This simplification will consist of a perturbation of the upper edge lengths of a squashed quad cluster. This perturbation will increase the score while holding the solid angle of the quad cluster fixed.

This simplification is based on a geometric decomposition of the truncated Voronoi cell. We will describe the decomposition, and then describe a construction which will ultimately simplify the analysis.

While our arguments will extend to treat a general squashed and truncated Voronoi cell associated with a general standard cluster, we restrict our attention to truncated Voronoi cells associated with quad clusters.

To begin, we consider the decomposition of a truncated Voronoi cell into its fundamental components. A truncated Voronoi cell is formed of three elements: a central spherical section (formed by the truncation), *wedges* of a right circular cone, and tetrahedrons called *Rogers simplices*.

We choose a representation of a truncated quad cluster composed of the radial projection of each element to a plane passing close to the four corners of the quad cluster. This decomposition is represented in Figure 16.5.

16.9.2 Rogers simplices

We now consider the geometry of the Rogers simplices.

Consider a face with edge lengths $(2, 2, t)$ associated with a side of a truncated quad cluster. Let b represent the circumradius of the face, and let r represent the orthogonal extension of a Rogers simplex from the face, as in Figure 16.6.

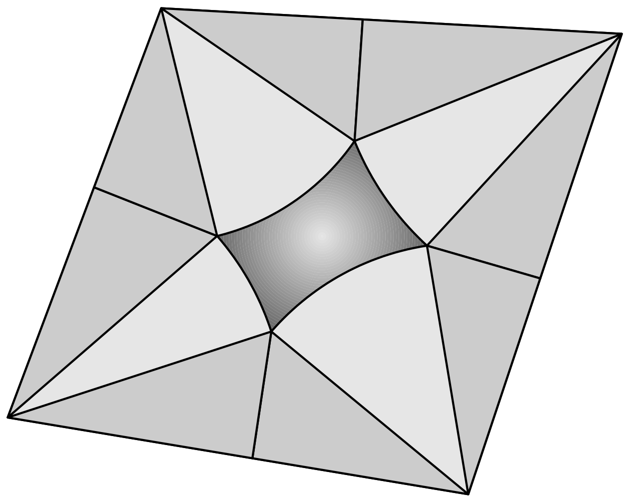

Figure 16.5. *A representation of a truncated quad cluster.*

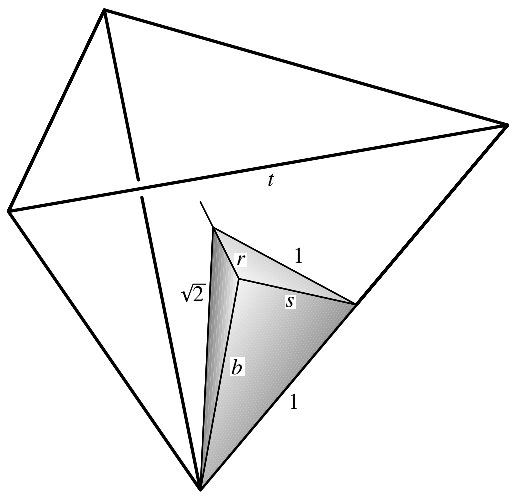

Figure 16.6. *Detail of truncated Voronoi decomposition.*

Then

$$b = \frac{4}{\sqrt{16 - t^2}}$$

$$r = \sqrt{2 - b^2} = \sqrt{\frac{16 - 2t^2}{16 - t^2}},$$

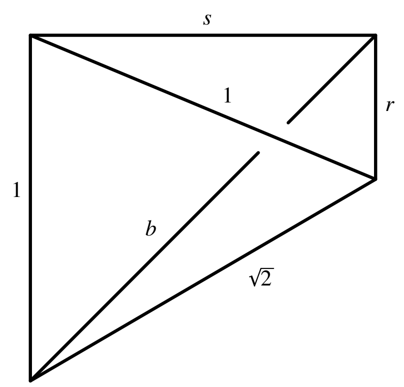

Figure 16.7. *Detail of Rogers simplex.*

and

$$s = \sqrt{b^2 - 1} = \frac{t}{\sqrt{16 - t^2}}.$$

See Figure 16.7.

16.9.3 The geometric construction

We now present the geometric construction which will imply the simplification.

We represent the geometry of the truncated Voronoi cell associated with one half of a quad cluster in Figure 16.8.

We can simplify the representation by extending the wedges to enclose the Rogers simplices. See Figure 16.9. This process adds an extra volume term.

The overlap between the wedges is slightly complicated. We simplify the overlap as follows. Take the cone over the overlap. Intersect it with a ball of radius $\sqrt{2}$ at the origin. We call the spherical sections produced by this construction *flutes*. This construction is represented in Figure 16.10. Figure 16.11 is a planar representation of this construction.

To form each flute, we have added two extra pieces of volume (per flute) to our construction. We call these pieces *quoins*. We attach each quoin to a Rogers simplex. See Figure 16.12.

16.9.4 A solid angle invariant

We now require some notation for the volumes which enter into this construction. Let c denote the volume of the central spherical angle. Let r denote the volume of the Rogers simplices. Let w denote the volume of the wedges. Let w' denote the volume of the extended wedges. Let q denote the volume of the quoins. Let f denote the volume of the flutes. Finally, let v denote the volume of the truncated Voronoi cell.

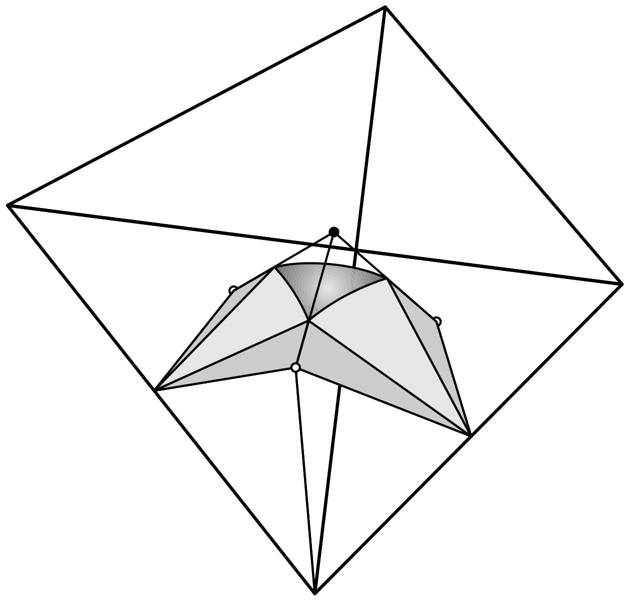

Figure 16.8. *Decomposition of a truncated Voronoi cell.*

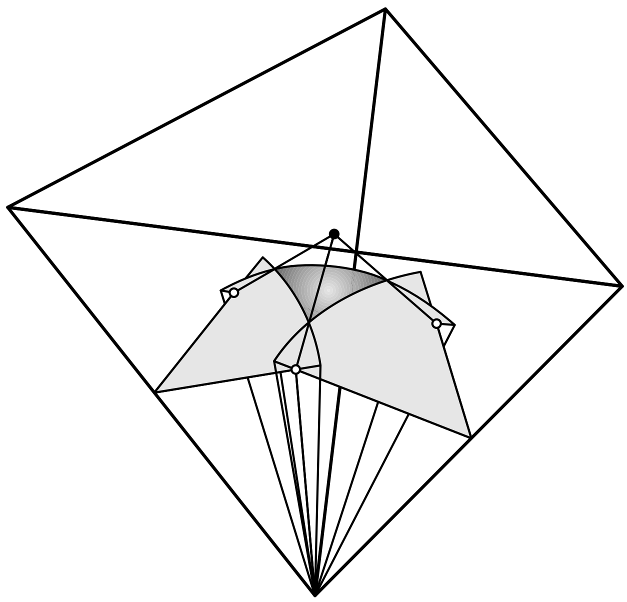

Figure 16.9. *Wedges extended to include the Rogers simplices.*

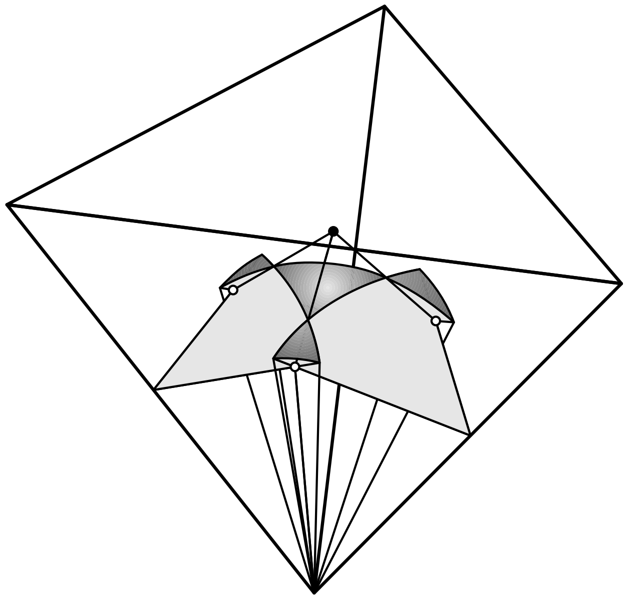

Figure 16.10. *Decomposition with flutes.*

Lemma 16.10. *If we hold the solid angle fixed, the volume of a truncated squashed Voronoi cell depends only on q, the volume of the quoins.*

Proof. By the original decomposition,

$$v = c + r + w.$$

By our construction,

$$v = c + w' + q - f.$$

Recall that the solid angle s of the quad cluster is the sum of the dihedral angles minus 2π. The dihedral angles to which we refer are those associated with the edges between each corner of the quad cluster and the origin.

Our perturbation will hold the solid angle s of the quad cluster fixed. Therefore, the sum of the dihedral angles must also be fixed. This fixes w'.

Take the cone over each extended wedge and intersect it with a ball of radius $\sqrt{2}$ centered at the origin. Let t denote the sum of these volumes. Since the sum of the dihedral angles is fixed, t is also fixed.

Further, note that

$$\frac{2\sqrt{2}}{3}s = c + t - f.$$

This relation implies that $c - f$ is fixed. Combining this with the previous relations, we find that if we hold the solid angle fixed, the volume of the truncated Voronoi cell depends only on q, the volume of the quoins. $\square$

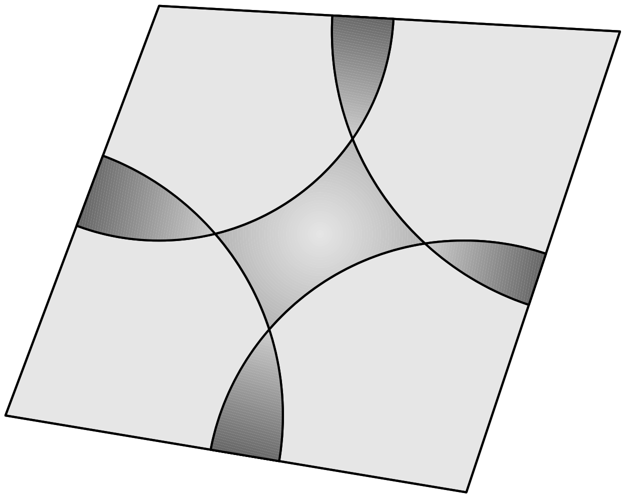

Figure 16.11. *Planar representation with flutes.*

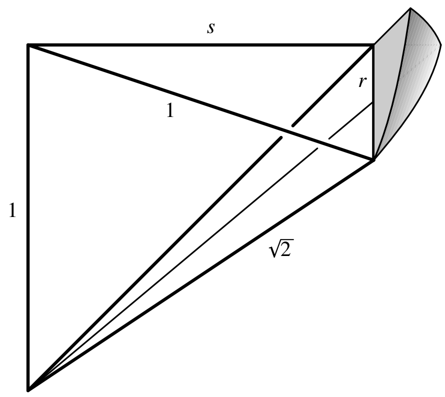

Figure 16.12. *Detail of Rogers simplex with quoin.*

16.9.5 Variation of the volume of a quoin

Consider a face $(2, 2, t)$ of a truncated quad cluster. Two Rogers simplices are associated with this face, as suggested in Figure 16.6. Observe that the volume of the quoin associated with one of these Rogers simplices is increasing in $r = \sqrt{\frac{16-2t^2}{16-t^2}}$. Next, observe that r is in turn decreasing in t. Therefore increasing t decreases the volume of the squashed quad cluster, if we hold the solid angle fixed (by varying the length of another edge of the squashed quad cluster).

Each half of a squashed quad cluster has two variable edge lengths (not counting the shared diagonal). We label the variable edge lengths of one half of the squashed quad cluster y_1 and y_2. We label the length of the diagonal d. Holding the solid angle fixed, we may perturb one half by shrinking the larger and increasing the shorter length. We wish to establish the following lemma, that increasing the short length reduces the volume of the truncated Voronoi cell more than decreasing the longer length increases the volume.

Lemma 16.11. *Holding the solid angle fixed for one half of a squashed quad cluster, shrinking the longer upper edge (while increasing the shorter edge appropriately) reduces the volume of the squashed quad cluster (increasing the score).*

To prove Lemma 16.11, we establish a variational formula for the volume of a quoin.

We then verify that the volume of the quoin associated with the shorter edge is decreasing faster under this perturbation than the volume of the quoin associated with the longer edge is increasing.

In other words, we wish to show that $y_1 < y_2$ implies that $V(y_1) + V(y_2(y_1))$ is decreasing in y_1, or equivalently,

$$V_t(y_1) + V_t(y_2(y_1))\frac{dy_2}{dy_1} < 0$$

where $V(t)$ is the volume of the quoin, $V_t(t)$ is the derivative of the volume, and y_2 is an implicit function of y_1.

We construct the volume of a quoin by integrating the area of a slice. We place the quoin in a convenient coordinate system. See Figures 16.13 and 16.14. The truncating sphere has equation $x^2 + y^2 + z^2 = 2$. At the base of the quoin, $z = 1$, so $x = \sqrt{1 - y^2}$ gives the location of the right-boundary of the quoin. The plane forming the left face of the quoin is given by the equation $x = sz$, so the ridge of the quoin is given by the curve (su, y, u), where $u = \sqrt{\frac{2-y^2}{1+s^2}}$.

Hence the area of a slice parallel to the x-z plane is given by the formula

$$A(t, y) = \frac{1}{2}(su - s)(u - 1) + \int_{su}^{\sqrt{1-y^2}} (\sqrt{2 - x^2 - y^2} - 1)\, dx.$$

The volume of a quoin is therefore given by the formula

$$V(t) = \int_0^r A(t, y)\, dy.$$

We actually only need to compute $V_t(t)$, which is fortunate, since the explicit formula for $V(t)$ is somewhat complicated. We have

$$V_t(t) = \int_0^r A_t(t, y)\, dy + A(t, r)r_t,$$

but $A(t, r) = 0$, so

$$V_t(t) = \int_0^r A_t(t, y)\, dy.$$

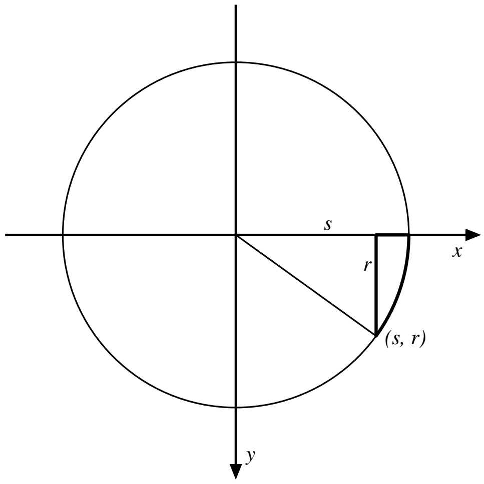

Figure 16.13. *Top view of quoin.*

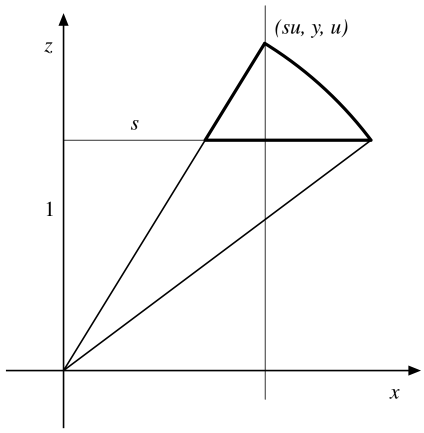

Figure 16.14. *Side view of quoin.*

So in addition, we only need $A_t(t, y)$,

$$A_t(t, y) = (\frac{s}{2}(u^2 + 1) - \sqrt{1 - y^2} + \int_{\frac{t}{4}\sqrt{2-y^2}}^{\sqrt{1-y^2}} \sqrt{2 - x^2 - y^2}\, dx)_t,$$

so

$$A_t(t, y) = (\frac{s}{2}(u^2 + 1))_t - \sqrt{2 - \frac{t^2}{16}(2 - y^2) - y^2}\,\frac{1}{4}\sqrt{2 - y^2}$$

which simplifies to

$$A_t(t,y) = \frac{8}{(16-t^2)^{3/2}} - \frac{2-y^2}{2\sqrt{16-t^2}}.$$

Hence

$$V_t(t) = \frac{8r}{(16-t^2)^{3/2}} - \frac{r}{\sqrt{16-t^2}} + \frac{r^3}{6\sqrt{16-t^2}},$$

which simplifies to

$$V_t(t) = \frac{-2\sqrt{2}(8-t^2)^{3/2}}{3(16-t^2)^2}.$$

We are now prepared to prove Lemma 16.11.

Proof. Holding the solid angle fixed, y_2 is an implicit function of y_1. We wish to prove that $y_1 < y_2$ implies

$$V_t + V_t fracdy_2dy_1 0. \tag{16.9}$$

We derive a formula for $\frac{dy_2}{dy_1}$, using the solid angle constraint

$$\mathrm{sol}(2,2,2,y_1,y_2,d) = c, \tag{16.10}$$

where c is a constant. Using formulas from [Hal97a], (16.10) becomes

$$2\arctan(\frac{\sqrt{\Delta}}{2a}) = c.$$

Let $x_1 = y_1^2$, $x_2 = y_2^2$, and $b = d^2$. Then

$$\Delta = -4b^2 - 4(x_1 - x_2)^2 + b(x_1(8-x_2) + 8x_2),$$

and

$$a = 32 - d - x_1 - x_2.$$

So

$$\frac{-4b^2 - 4(x_1-x_2)^2 + b(x_1(8-x_2)+8x_2)}{(32-d-x_1-x_2)^2} = c_1.$$

Therefore

$$\frac{dx_2}{dx_1} = -\frac{(16-x_2)(x_2+b-x_1)}{(16-x_1)(x_1+b-x_2)},$$

and

$$\frac{dy_2}{dy_1} = \frac{y_1}{y_2}\frac{dx_2}{dx_1},$$

hence

$$\frac{dy_2}{dy_1} = -\frac{y_1(16-x_2)(x_2+b-x_1)}{y_2(16-x_1)(x_1+b-x_2)}. \tag{16.11}$$

We substitute the formula for $\frac{dy_2}{dy_1}$ into (16.9). Letting $x_i = y_i^2$, and noting that all the denominators are positive, we obtain on clearing denominators that the desired relation (16.9) is equivalent to

$$
\begin{aligned}
&-(8-x_1)^{3/2}(16-x_2)y_2(x_1+b-x_2)+\\
&\qquad(8-x_2)^{3/2}(16-x_1)y_1(x_2+b-x_1)<0,
\end{aligned}
$$

or

$$
\begin{aligned}
&(16-x_1)^2x_1(8-x_2)^3(b-x_1+x_2)^2<\\
&\qquad(16-x_2)^2x_2(8-x_1)^3(b+x_1-x_2)^2.
\end{aligned}
$$

If we define

$$g(x_1,x_2)=(16-x_1)^2x_1(8-x_2)^3(b-x_1+x_2)^2,$$

then the desired inequality is equivalent to $g(x_1,x_2)<g(x_2,x_1)$ for $x_1<x_2$. There are several ways to prove this monotonicity relation. One is to prove that the polynomial

$$\frac{g(x_1,x_2)-g(x_2,x_1)}{8(x_1-x_2)}$$

is positive for all allowable values for x_1, x_2, and b. Unfortunately, the resulting polynomial has degree six, so the verification is somewhat unwieldy, although easy enough using interval methods.

A simpler method involves a factorization of g into g_1 and g_2. We show that g_1 and g_2 each satisfy the monotonicity relation, and the relation then follows for g.

Define

$$g_1(x_1,x_2)=(16-x_1)x_1(8-x_2)(b-x_1+x_2),$$

and

$$g_2(x_1,x_2)=(16-x_1)(8-x_2)^2(b-x_1+x_2).$$

Clearly $g=g_1g_2$. We then construct the polynomials

$$p_1=\frac{g_1(x_1,x_2)-g_1(x_2,x_1)}{x_1-x_2}$$

and

$$p_2=\frac{g_2(x_1,x_2)-g_2(x_2,x_1)}{x_1-x_2}.$$

Simplifying p_1 and p_2, we find that

$$
\begin{aligned}
p_1=&128b-128x_1-8bx_1+8x_1^2-128x_2\\
&+32x_1x_2+bx_1x_2-x_1^2x_2+8x_2^2-x_1x_2^2
\end{aligned}
$$

and

$$
\begin{aligned}
p_2=&-2048+192b+320x_1-16bx_1-16x_1^2+320x_2\\
&-16bx_2-32x_1x_2+bx_1x_2+x_1^2x_2-16x_2^2+x_1x_2^2.
\end{aligned}
$$

These polynomials are quadratic in x_1 and x_2, and linear in b. The coefficient of b in p_1 is

$$128 - 8x_1 - 8x_2 + x_1x_2.$$

The coefficient of b in p_2 is

$$192 - 16x_1 - 16x_2 + x_1x_2.$$

Both coefficients are positive for x_1 and x_2 in $[16/2.51^2, 2.51^2]$. Therefore, the minimum values of p_1 and p_2 occur when b is at a minimum, $b = 8$.

The minimum value of each polynomial for values of x_1 and x_2 in the range $[16/2.51^2, 2.51^2]$ is now easily computed. Making the appropriate computations, we find that each polynomial is indeed positive. Hence the desired relation follows. □

16.9.6 Final simplification

Lemma 16.12. *Obtuse quad clusters satisfy the bound of Proposition 15.3.*

Proof. We begin with a squashed quad cluster with consecutive upper edge lengths (y_1, y_2, y_3, y_4) and diagonal d adjacent to the first two upper edges.

Recall that we chose the diagonal of the quad cluster to be the shorter of the two possible diagonals. We refer to the other possible diagonal as the *cross-diagonal*. Recall that the reduction fixes the length of the diagonal.

If the length of the cross-diagonal does not drop to $2\sqrt{2}$ under the perturbation of Lemma 16.11, we arrive at the configuration with edge lengths (y_1', y_1', y_2', y_2') with diagonal d.

If the length of the cross-diagonal does drop to $2\sqrt{2}$, then stop the perturbation. This gives a quadrilateral (y_1', y_2', y_3', y_4') with diagonal $2\sqrt{2}$. Applying the perturbation to each half independently, we find that the score of each half is maximized by the configuration $(y_1'', y_1'', y_2'', y_2'')$ with diagonal $2\sqrt{2}$. We verify the relation for this arrangement in Calculation 17.4.4.5.

If the length of the cross-diagonal did not drop to $2\sqrt{2}$, switch to the cross-diagonal and repeat the process. If the (new) cross-diagonal does not drop to $2\sqrt{2}$, we have arrived at the configuration (y, y, y, y) with diagonal d'. Choose a new diagonal d'' to be the shorter of the two possible diagonals. We verify the desired relation for this arrangement in Calculation 17.4.4.4.

Finally, we make a few comments about extra constraints in the verifications.

Since the score of a quad cluster is nonpositive, and $m(2\,\mathrm{sol}(T_0)) - b \le 0$ where $\mathrm{sol}(T_0) = \mathrm{sol}(2, 2, 2, 2, 2, 2\sqrt{2})$, we need only consider quad clusters for which the solid angle exceeds $2\,\mathrm{sol}(T_0)$.

The maximum length of the diagonal is $2.51\sqrt{2}$, since otherwise the triangles in the quadrilateral would be obtuse, forcing the cross-diagonal to be shorter than the diagonal. This would contradict our original choice of the shortest diagonal.

In Calculation 17.4.4.4, we assume that d is the shortest diagonal. Adding this constraint directly is tedious, since the formula for the cross-diagonal of the quad cluster is somewhat complicated. We apply a simpler but weaker constraint, that the diagonal d of a planar quadrilateral with edge lengths (y, y, y, y) is shorter than d', the other planar diagonal. The constraint $d \le d'$ gives the constraint $d^2 \le 2y^2$. Since the cross-diagonal of the quad cluster is shorter than the cross-diagonal of the planar quadrilateral, this constraint is weaker. $\square$

Lemmas 16.8 and 16.12 prove Proposition 15.3 for pure Voronoi quad clusters.

Section 17

Calculations

The verifications of the relations required in this paper appear intractable using traditional methods. Therefore, we use a relatively new proof technique, interval arithmetic via floating-point computer calculations.

17.1 Interval Arithmetic

We review the basic notions of interval arithmetic.

Suppose that the value of a function $f(x)$ lies in the interval $[a, b]$. Further, suppose that $g(x)$ lies in the interval $[c, d]$. Then $f(x)+g(x)$ must lie in $[a+c, b+d]$. While it may be the case that we could produce better bounds than this for the function $f + g$, these interval bounds give crude control over the behavior of the function. Interval arithmetic provides a mechanism for formalizing arithmetic on these bounds.

We represent an interval t as $\left[\underline{t}, \overline{t}\right]$. Then for intervals a and b,

$$a + b = \left[\underline{a} + \underline{b}, \overline{a} + \overline{b}\right].$$

Likewise,

$$a - b = \left[\underline{a} - \overline{b}, \overline{a} - \underline{b}\right].$$

Multiplication is somewhat more complicated. Define

$$C = \{\underline{a}\underline{b}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b}\}.$$

Then

$$a * b = [\min(C), \max(C)].$$

Division is similar, as long as the dividing interval does not contain zero.

Similarly, we can define the operation of a monotonic function on an interval. For example,

$$\arctan(a) = [\arctan(\underline{a}), \arctan(\overline{a})].$$

Using interval arithmetic, we can produce rigorous bounds for polynomials evaluated on intervals. Likewise, we can produce rigorous bounds for rational functions evaluated on intervals. Finally, we add the composition of monotonic functions. This allows us to produce interval bounds for functions such as $\mathrm{sol}(\cdot)$ and $\mathrm{vor}(\cdot)$ over quasi-regular tetrahedrons, quarters, or quad clusters.

17.2 The Method of Subdivision

The relations on tetrahedra and quad clusters required for our approach typically have the form $g(y) \leq 0$ for $y \in I$, where I is a product of closed intervals. As g is usually continuous, the existence of a maximum is trivial. However, bounds on the behavior of g over all of I computed directly via interval arithmetic are generally poor.

We define a *cell* to be a product of closed intervals. By subdividing I into sufficiently small cells, the quality of the computed bounds on each cell usually improves enough to prove the relation for each cell, and hence for the original domain I.

If in fact $g(y) \leq c < 0$, this approach works very well. However, if the bound is tight at a point y_0, i.e., $g(y_0) = 0$, then pure subdivision will usually fail, since the computed upper bound on g over any cell containing y_0 will typically be positive.

If y_0 is not an interior maximum, we turn to the partial derivatives of g. If we can show that the partials of g on a small cell containing y_0 have fixed sign (bounded away from zero), then the maximum value of g on that cell is easily computed. It is typically the case that a cell must be very small before we can determine the sign of the partials via interval arithmetic bounds.

17.3 Numerical Considerations

Most real numbers are not representable in computer floating-point format. However, floating-point intervals may be found which contain any real number. Although the magnitude of real numbers representable in fixed-length floating-point format is finite, the format also provides for $\pm\infty$, which allows for interval containment of all reals. These intervals may be added, multiplied, etc., and the resulting intervals will contain the result of the operation applied to the real numbers which they represent.

Since floating-point arithmetic is not exact, interval arithmetic conducted using floating-point arithmetic is not optimal, in the sense that the interval resulting from an operation will usually be larger than the true resultant interval, due to roundoff. However, barring hardware or software errors (implementation errors, not roundoff errors), floating-point interval arithmetic, unlike floating-point arithmetic, is correct, in the sense that it provides correct interval bounds on the value of a computation, while floating-point arithmetic alone only provides an approximation to the correct value of a computation. We may therefore use interval arithmetic to prove mathematical results. Floating-point arithmetic alone, in the absence of rigorous error analysis, cannot constitute a proof.

We implement floating-point interval arithmetic routines via the IEEE 754 Standard for floating-point arithmetic [IEEE].

Implementation of interval arithmetic is straightforward using directed rounding. In addition to arithmetic functions, we require interval implementations of the square root and arctangent functions. Fortunately, the IEEE standard provides the square root function. However, the arctangent function is somewhat problematic, since the standard math libraries do not provide explicit error bounds for their implementations of the arctangent function. In theory, they should provide an accuracy for the arctangent routine of 0.7 ulps, meaning that the error is less than one unit in the last place. I add interval padding of the form $[v-\epsilon, v+\epsilon]$, where v is the computed value, and $\epsilon = 2^{-49}$. This should be sufficient to guarantee proper interval containment, assuming that the library routines are correctly implemented.

Armed with standard interval arithmetic and interval arithmetic implementations of *sqrt* and *arctan*, we can implement interval arithmetic versions of all the special functions required for proving the sphere packing relations.

Evaluating these functions on cells, we get bounds. Unfortunately, these bounds are not very good. The bounds which we get from interval versions of the partial derivative functions are even worse. This means that cells have to be very small before we can draw conclusions about the signs of the partials. These bad bounds are due to the inherent nature of interval arithmetic–it produces worst-case results by design.

These bad bounds increase the complexity of the verifications tremendously. Some verifications, using these bounds, require the consideration of billions or trillions of cells, or worse. Therefore, we needed a method for producing better bounds than those which direct interval methods could provide.

The method which we eventually discovered is to use Taylor series. We compute explicit second (mixed) partial bounds for the major special functions, and use these bounds to produce very good interval bounds. These bounds are computed in Calculations 17.4.6.1 through 17.4.6.8. Essentially, the Taylor method postpones the error bound until the end of the computation, eliminating the error bound explosion which occurs with a straightforward interval method implementation.

17.4 Calculations

The following inequalities have been proved by computer using interval methods. Let $S = S(y) = S(y_1, \ldots, y_6)$ denote a tetrahedron parametrized by the edge lengths $(y_1, \ldots, y_6)$. In addition, we often parametrize by the squares of the edge lengths, $(x_1, \ldots, x_6)$.

Recall from Section 15.1 that $m = 0.3621$, $b = 0.49246$, $a = 0.0739626$ and $b_c = 0.253095$.

Recall that for our purposes, the scoring function $\sigma(\cdot)$ is given by one of four functions: $\mathrm{gma}(\cdot)$, $\mathrm{vor}(\cdot)$, $\mathrm{octavor}(\cdot)$, or truncated Voronoi. See Remark 7.23 for a simplified version of the scoring function.

The scoring rules depend on $\eta(\cdot)$, the circumradius of a face, introduced in Definition 4.20.

17.4.1 Quasi-regular Tetrahedra

Define $C = [2, 2.51]^6$, and recall

$$a_1 = 0.3860658808124052, a_2 = 0.4198577862, d_0 = 1.4674.$$

Calculation 17.4.1.1. *Either*

$$\mathrm{gma}(S) \le a_1 \,\mathrm{dih}(S) - a_2$$

or

$$\mathrm{gma}(S) \le -0.52\ pt$$

for $y \in C$, using dimension-reduction.

Calculation 17.4.1.2. *Either*

$$\mathrm{gma}(S) - a_1 \,\mathrm{dih}(S) \le 3.48\ pt - 2\pi a_1 + 4a_2$$

or

$$\mathrm{dih}(S) < d_0$$

or

$$\mathrm{gma}(S) \le -0.52\ pt$$

for $y \in C$, using dimension-reduction.

Calculation 17.4.1.3. *Either*

$$\mathrm{gma}(S) + m \,\mathrm{sol}(S) + a(\mathrm{dih}(S) - \frac{2\pi}{5}) - b_c \le 0$$

or

$$\mathrm{dih}(S) > d_0$$

or

$$\mathrm{gma}(S) \le -0.52\ pt$$

for $y \in C$, using dimension-reduction.

17.4.2 Flat Quad Clusters

Define $I = [2, 2.51]^5[2.51, 2\sqrt{2}]$, and define the corner cell

$$C = [2, 2 + 0.51/16]^5[2\sqrt{2} - (2\sqrt{2} - 2.51)/16, 2\sqrt{2}].$$

Calculation 17.4.2.1. *Either*

$$\mathrm{gma}(S) + m \,\mathrm{sol}(S) \le b/2$$

or

$$\eta(y_1, y_2, y_6)^2 > 2$$

or

$$\eta(y_4, y_5, y_6)^2 > 2$$

or

$$\mathrm{gma}(S) \leq -1.04\ pt$$

for $y \in I$, using dimension reduction.

Calculation 17.4.2.2. *Either*

$$\mathrm{gma}(S) + m\,\mathrm{sol}(S) \leq b/2$$

or

$$\eta(y_1, y_2, y_6)^2 = 2 \text{ with } \eta(y_4, y_5, y_6)^2 \leq 2,$$

or

$$\eta(y_4, y_5, y_6)^2 = 2 \text{ with } \eta(y_1, y_2, y_6)^2 \leq 2,$$

or

$$\mathrm{gma}(S) \leq -1.04\ pt$$

for $y \in I$, not using dimension-reduction.

Calculation 17.4.2.3. $\frac{d}{dy_i}\mathrm{vor}(S) < 0$ *for $i = 1, 2, 3$ and $y \in C$.*

Calculation 17.4.2.4. *This computation is somewhat tricky, since the scoring constraint depends on both faces. The partial derivative information gives $y_3 = 2$. The rest of the analysis depends on which face is assumed to be large.*

If the (y_1, y_2, y_6) face is large, the partial derivative information implies that the face constraint is tight, so $\eta(y_1, y_2, y_6)^2 = 2$. Therefore solve for y_1 in terms of y_2 and y_6. Apply partial derivative information for y_4 and y_5. In this case,

$$\mathrm{vor}(S) + m\,\mathrm{sol}(S) \leq b/2$$

for $y_3 = 2$, $y \in C$.

If the (y_4, y_5, y_6) face is large, assume that $y_1 = y_2 = 2$. Then either

$$\mathrm{vor}(S) + m\,\mathrm{sol}(S) \leq b/2$$

or

$$\eta(y_4, y_5, y_6)^2 < 2$$

for $y_1 = y_2 = y_3 = 2$, $y \in C$.

Calculation 17.4.2.5. *Either*

$$\mathrm{vor}(S) + m\,\mathrm{sol}(S) \leq b/2,$$

or

$$\eta(y_1, y_2, y_6)^2 < 2 \text{ and } \eta(y_4, y_5, y_6)^2 < 2,$$

or

$$\mathrm{vor}(S) \le -1.04\ pt$$

for $y \in I$, $y \notin C$, using dimension-reduction and partial derivative information.

Calculation 17.4.2.6. *Either*

$$\mathrm{vor}(S) + m\,\mathrm{sol}(S) \le b/2,$$

with

$$\eta(y_1, y_2, y_6)^2 = 2 \text{ or } \eta(y_4, y_5, y_6)^2 = 2,$$

or

$$\mathrm{vor}(S) \le -1.04\ pt$$

for $y \in I$, $y \notin C$, not using dimension-reduction.

17.4.3 Octahedra

Calculation 17.4.3.1. *$\sigma(S) \le -0.52\ pt$, for each (appropriately scored) upright quarter with edge lengths in the cell $[2.51, 2\sqrt{2}][2.2, 2.51][2, 2.51]^4$.*

Calculation 17.4.3.2. *Recall $c = 0.1533667634670977$, and $d = 0.2265$. Either*

$$\mathrm{gma}(S) + c\,\mathrm{dih}(S) \le d$$

or

$$\mathrm{gma}(S) \le -1.04\ pt$$

for $y \in [2.51, 2.716][2, 2.2]^5$, using dimension-reduction Note that for both faces adjacent to the diagonal,

$$\max \eta^2 = \eta(2.2, 2.2, 2.716)^2 < 2,$$

so all quarters in this cell are compression-scored.

Calculation 17.4.3.3. *Either*

$$\mathrm{gma}(S) + m\,\mathrm{sol}(S) + \alpha\,\mathrm{dih}(S) \le \frac{b}{4} + \alpha\frac{\pi}{2}$$

or

$$\mathrm{gma}(S) \le -1.04\ pt$$

for all compression-scored quarters $S(y)$, where $\alpha = 0.14$,

$$y \in [2.716, 2\sqrt{2}][2, 2.2]^2[2, 2.51][2, 2.2]^2,$$

using dimension-reduction.

Calculation 17.4.3.4. *Either*

$$\mathrm{octavor}(S) + m\,\mathrm{sol}(S) + \alpha\,\mathrm{dih}(S) \le \frac{b}{4} + \alpha\frac{\pi}{2}$$

or

$$\mathrm{octavor}(S) \le -1.04\ pt$$

for all vor analytic-scored quarters $S(y)$*, where* $\alpha = 0.14$*,*

$$y \in [2.716, 2.81][2, 2.2]^2[2, 2.51][2, 2.2]^2.$$

Calculation 17.4.3.5. *Either*

$$\mathrm{gma}(S) + m\,\mathrm{sol}(S) + \alpha\,\mathrm{dih}(S) + \beta x_1 \le \frac{b}{4} + \alpha\frac{\pi}{2} + 8\beta$$

or

$$\mathrm{gma}(S) \le -1.04\ pt$$

for all compression-scored quarters $S(y)$*, where* $\alpha = 0.054$*,* $\beta = 0.00455$*,* $x_1 = y_1^2$*, and*

$$y \in [2.81, 2\sqrt{2}][2, 2.2]^2[2, 2.51][2, 2.2]^2,$$

using some dimension-reduction.

Calculation 17.4.3.6. *Either*

$$\mathrm{octavor}(S) + m\,\mathrm{sol}(S) + \alpha\,\mathrm{dih}(S) + \beta x_1 \le \frac{b}{4} + \alpha\frac{\pi}{2} + 8\beta$$

or

$$\mathrm{octavor}(S) \le -1.04\ pt$$

for all vor analytic-scored quarters $S(y)$*, where* $\alpha = 0.054$*,* $\beta = -0.00455$*,* $x_1 = y_1^2$*, and*

$$y \in [2.81, 2\sqrt{2}][2, 2.2]^2[2, 2.51][2, 2.2]^2.$$

17.4.4 Pure Voronoi Quad Clusters

Recall $\mathrm{sol}(T_0)$ denotes the solid angle of the tetrahedron $(2, 2, 2, 2, 2, 2\sqrt{2})$.

Define the corner cell $C = [2, 2 + 0.51/8]^5[2\sqrt{2}, 2.84]$. We denote truncated Voronoi scoring by σ. The constraint that the dividing face be acute translates into $x_1 + x_2 - x_6 \ge 0$. In each computation we apply dimension-reduction.

We begin with the acute case.

Calculation 17.4.4.1. *Either*

$$\sigma(S) + m\,\mathrm{sol}(S) - b/2 \le 0$$

or

$$\mathrm{sol}(S) < \mathrm{sol}(T_0)$$

or

$$x_1 + x_2 - x_6 < 0$$

or

$$\sigma(S) \le -1.04\ pt$$

for $y \in [2, 2.51]^5[2.84, 4]$.

Calculation 17.4.4.2. *Either*

$$\sigma(S) + m\,\mathrm{sol}(S) - b/2 \le 0$$

or

$$\mathrm{sol}(S) < \mathrm{sol}(T_0)$$

or

$$x_1 + x_2 - x_6 < 0$$

or

$$\sigma(S) \le -1.04\ pt$$

for $y \in [2, 2.51]^5[2\sqrt{2}, 2.84]$ *with* $y \notin C$.

Calculation 17.4.4.3. *Either*

$$\sigma(S) + m\,\mathrm{sol}(S) - b/2 \le 0$$

or

$$\mathrm{sol}(S) < \mathrm{sol}(T_0)$$

or

$$x_1 + x_2 - x_6 < 0,$$

$y \in C$.

Finally, we consider the obtuse case.

Calculation 17.4.4.4. *Either*

$$\sigma(S) + m\,\mathrm{sol}(S) - b/2 \le 0$$

or

$$\mathrm{sol}(S) < \mathrm{sol}(T_0)$$

or

$$\sigma(S) \le -0.52\ pt$$

or

$$2y^2 < d^2$$

for a symmetric pure Voronoi quad cluster composed of two copies of S, where

$$S = (2, 2, 2, y, y, d),$$

$y \in [4/2.51, 2.51]$ *and* $d \in [2\sqrt{2}, 2.51\sqrt{2}]$.

Calculation 17.4.4.5. *Either*

$$\sigma(S_1) + \sigma(S_2) + m(\mathrm{sol}(S_1) + \mathrm{sol}(S_2)) - b \leq 0$$

or

$$\sigma(S_1) + \sigma(S_2) \leq -1.04\ pt$$

or

$$\mathrm{sol}(S_1) + \mathrm{sol}(S_2) < 2\,\mathrm{sol}(T_0)$$

for a pure Voronoi quad cluster composed of two tetrahedrons S_1 and S_2, where

$$S_i = (2, 2, 2, y_i, y_i, 2\sqrt{2}),$$

$y_i \in [4/2.51, 2.51]$.

17.4.5 Dimension Reduction

Calculation 17.4.5.1. *The polynomial derived for the dimension-reduction argument is positive for* $x \in [4, 2.51^2]^6$ *and* $x \in [4, 2.51^2]^5[4, 8]$.

17.4.6 Second Partial Bounds

We compute all second partials $\frac{d^2}{dx_i dx_j}$ in terms of x_i, the squares of the edge lengths. We do each computation twice, once for quasi-regular tetrahedrons and once for quarters. We compute the second partials of $\mathrm{dih}(\cdot)$, $\mathrm{sol}(\cdot)$, compression volume, and Voronoi volume (the vor analytic volume). Since the scoring functions are linear combinations of $\mathrm{sol}(\cdot)$ and the volume terms, we may derive second partial bounds for $\mathrm{gma}(\cdot)$ and $\mathrm{vor}(\cdot)$ from these.

With the application of additional computer power, these bounds could be improved. These bounds were computed using 16 subdivisions. While using 32 subdivisions would improve the bounds by a factor of 2, perhaps, the time required for the computations increases by a factor of 64.

Calculation 17.4.6.1. *For quasi-regular tetrahedrons T, the second partials of* $\mathrm{dih}(T)$ *lie in*

$$[-0.0926959464, 0.0730008897].$$

Calculation 17.4.6.2. *For quarters Q, the second partials of* $\mathrm{dih}(Q)$ *lie in*

$$[-0.2384125007, 0.169150875].$$

Calculation 17.4.6.3. *For quasi-regular tetrahedrons T, the second partials of* $\mathrm{sol}(T)$ *lie in*

$$[-0.0729140255, 0.088401996].$$

Calculation 17.4.6.4. *For quarters Q, the second partials of* $\mathrm{sol}(Q)$ *lie in*

$$[-0.1040074557, 0.1384785805].$$

Calculation 17.4.6.5. *For quasi-regular tetrahedrons T, the second partials of* $\mathrm{gma}(T)$ *volume lie in*

$$[-0.0968945273, 0.0512553817].$$

Calculation 17.4.6.6. *For quarters Q, the second partials of* $\mathrm{gma}(Q)$ *volume lie in*

$$[-0.1362100221, 0.1016538923].$$

Calculation 17.4.6.7. *For quasi-regular tetrahedrons T, the second partials of* $\mathrm{vor}(T)$ *volume lie in*

$$[-0.1856683356, 0.1350478467].$$

Calculation 17.4.6.8. *For quarters Q, the second partials of* $\mathrm{vor}(Q)$ *volume lie in*

$$[-0.2373892383, 0.1994181009].$$

The computed $\mathrm{gma}(\cdot)$ second partials then lie in

$$[-0.2119591984, 0.2828323141],$$

for quasi-regular tetrahedrons and quarters.

Likewise, the computed $\mathrm{vor}(\cdot)$ second partials then lie in

$$[-0.7137209962, 0.8691765157],$$

for quasi-regular tetrahedrons and quarters.

Paper VI

Sphere Packings VI. Tame Graphs and Linear Programs

This paper is the last in the series of paper devoted to the proof of the Kepler conjecture. The first several sections prove a result that asserts that "all contravening graphs are tame." A contravening graph is one that is attached to a potential counterexample to the Kepler conjecture. Contravening graphs by nature are elusive and are studied by indirect methods. In contrast, the defining properties of tame graphs lend themselves to direct examination. (By definition, tame graphs are planar graphs such that the degree of every vertex is at least two and at most six, the length of every face is at least 3 and at most 8, and such that other similar explicit properties hold true.)

It is no coincidence that contravening graphs all turn out to be tame. The definition of tame graph has been tailored to suit the situation at hand. We set out to prove explicit properties of contravening graphs, and when we are satisfied with what we have proved, we brand a graph with these properties a tame graph.

The first section of this paper gives the definition of tame graph. The second section gives the classification of all tame graphs. There are several thousand such graphs. The classification was carried out by computer. This classification is one of the main uses of a computer in the proof of the Kepler conjecture. A detailed description of the algorithm that is used to find all tame graphs is presented in this section.

The third section of this paper gives a review of results from earlier parts of the paper that are relevant to the study of tame plane graphs. In the abridged version of the proof [Hal05a], the results cited in this section are treated as axioms. This section thus serves as a guide to the results that are proved in this volume, but not in the abridged version of the proof.

This section also contains a careful definition of what it means to be a contravening plane graph. The first approximation to the definition is that it is the combinatorial plane graph associated with the net of edges on the unit sphere bounding the standard regions of a contravening decomposition star. The precise definition is somewhat more subtle because we wish ensure that every face of a contravening plane graph is a simple polygon. To guarantee that this property holds, we simplify the net of edges on the unit sphere whenever necessary.

The fourth and fifth sections of this paper contain the proof that all contravening plane graphs are tame. These sections complete the first half of this paper.

The second half of this paper is about linear programming. Linear programs are used to prove that with the exception of three tame graphs (those attached to the face-centered cubic packing, the hexagonal-close-packing, and the pentahedral prism), a tame graph cannot be a contravening graph. This result reduces the proof of the Kepler conjecture to a close examination of three graphs. Pentahedral prism graphs are treated in Paper V. The face-centered cubic and hexagonal-close packing graphs are treated in Section 8 of Paper III. The linear programming results together with these earlier results complete the proof of the Kepler conjecture.

The sixth section of this paper describes how to attach a linear program to a tame plane graph. The output from this linear program is an upper bound on the score of all decomposition stars associated with the given tame plane graph. The seventh section of this paper shows how to use linear programs to eliminate what are called the *aggregate* tame plane graphs. The *aggregates* are those cases where the net of edges formed by the edges of standard regions was simplified to ensure that every face of a contravening plane graph is a polygon. By the end of this section, we have a proof that every standard region in a contravening decomposition star is bounded by a simple polygon.

The final section of this paper gives a long list of special strategies that are used when the output from the linear program in the sixth section does not give conclusive results. The general strategy is to partition the original linear program into a collection of refined linear programs with the property that the score is no greater than the maximum of the outputs from the linear programs in the collection. These branch and bound strategies are described in this final section. Linear programming shows that every decomposition star with a tame plane graph (other than the three mentioned above) has a score less than that of the decomposition stars attached to the face-centered cubic packing. This and earlier results imply the Kepler conjecture.

Section 18

Tame Graphs

This section defines a class of plane graphs. Graphs in this class are said to be *tame*. In the next section, 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.

18.1 Basic Definitions

Definition 18.1. *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 18.2. *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 18.3. *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 three 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 18.1. 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.*

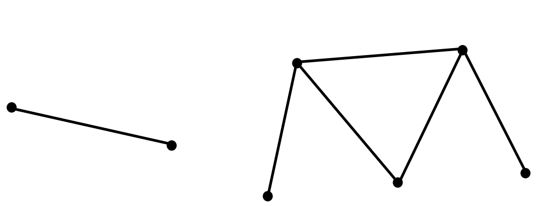

Figure 18.1. *Some examples of graphs that are excluded from the narrow definition of plane graph, as defined in this section.*

Definition 18.4. *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* $\mathrm{tri}(v)$ *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 18.5. *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 18.6. *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).*

18.2 Weight Assignments

We call the constant 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 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.

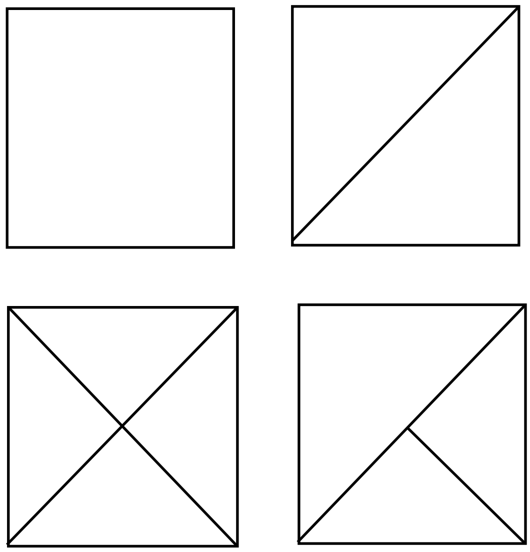

Figure 18.2. *Tame* 4-*circuits*

18.3 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 18.2.

4. The degree of every vertex is at least two and at most six.

5. If a vertex is contained in an exceptional face, then the degree of the vertex is at most five.

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

7. There exists an admissible weight assignment of total weight less than the target, 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 18.7. *We pause to review the strategy of the proof of the Kepler conjecture as described in Section 3.2. The decomposition stars that violate the main inequality $\sigma(D) \geq 8\,pt$ 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 section will give a classification of tame plane graphs. (There are several thousand.) Section 20 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.

Section 19

Classification of tame plane graphs

19.1 Statement of the Theorem

A list of several thousand plane graphs appears at [Hal05b]. The following theorem is listed as one of the central claims in the proof in Section 3.3.

Theorem 19.1. *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 19.1.

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.

19.2 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 19.2. *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 two.

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^{op} and in which no other vertex of P' is a vertex of G. Then

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

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 19.1). (It is immediate that the Condition 19.2 in the definition of partial plane graphs is maintained by this process.) There are n distinct proper ways of identifying F_1 with F^{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 $\phi : F_1 \mapsto F^{op}$).

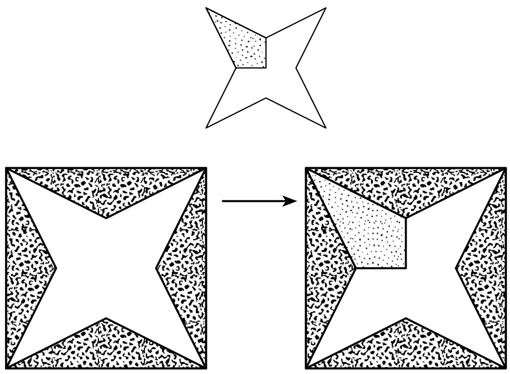

Figure 19.1. *Patching a plane graph*

19.3 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 19.1 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:

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

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 19.3. *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 $F_1 = F^{op}$ 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 19.4. *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.*

19.4 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 18.3, 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 19.3.)
- 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 $b(p, q) <$ 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 19.2.) 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.

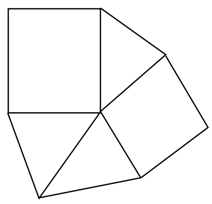

Figure 19.2. *States $I_{3,2}$ and $I'_{3,2}$*

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

Lemma 19.5. *Let A and B be triangular or quadrilateral faces that have at least two 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 19.3. Some properties that are particularly useful for the exercise are Properties 2 and 3 of tameness, and Property 2 of admissibility. $\square$

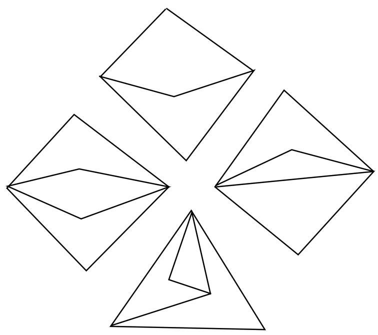

Figure 19.3. *Some impossibilities*

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 19.1 is proved.

Section 20

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 $|v-w| \le 2t_0$. 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 Section 18.

The purpose of this section 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 Section 18. These plane graphs are called contravening plane graphs, or simply contravening graphs.

20.1 A Review of Earlier 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:

$$\tau_R(D) = \mathrm{sol}(R)\zeta pt - \sigma_R(D) \tag{20.1}$$

and

$$\tau(D) = \sum \tau_R(D) = 4\pi\zeta pt - \sigma(D). \tag{20.2}$$

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

$$\tau(D) \le 4\pi\zeta pt - 8\,pt = (4\pi\zeta - 8)pt. \tag{20.3}$$

The constant $(4\pi\zeta - 8)\,pt$ (and its upper bound $\mathrm{tgt}\,pt$ 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

$$\sigma_F(D) = \sum_R \sigma_R(D), \quad \tau_F(D) = \sum_R \tau_R(D), \tag{20.4}$$

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

$$\sigma(D) = \sum \sigma_R(D), \quad \tau(D) = \sum \tau_R(D). \tag{20.5}$$

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 20.1. *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 20.1.*

Proof. This is Theorem 12.1 and Corollary 12.2. □

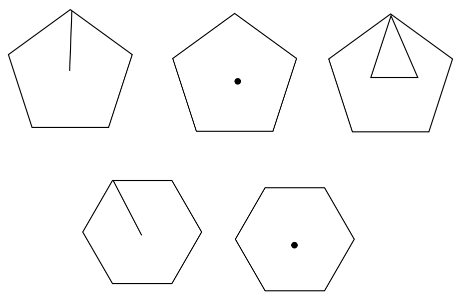

Figure 20.1. *Non-polygonal standard regions ($n(R) = 7, 7, 8, 8, 8$)*

Lemma 20.2. *Let R be a standard region. We have $\tau_R(D) \geq t_n$, where $n = n(R)$, and*

$$t_3 = 0, \quad t_4 = 0.1317, \quad t_5 = 0.27113, \quad t_6 = 0.41056 \quad t_7 = 0.54999, \quad t_8 = 0.6045.$$

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

$$s_3 = 1\,pt, \quad s_4 = 0, \quad s_5 = -0.05704, \quad s_6 = -0.11408, \quad s_7 = -0.17112, \quad s_8 = -0.22816.$$

Proof. This is Theorem 12.1. □

Lemma 20.3. *Let F be a set of standard regions bounded by a simple polygon with at most nine edges. Assume that*

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

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

Proof. This is Section 12.2. □

Lemma 20.4. *Let (R, D) be a standard cluster. If R is a triangular region, then*

$$\sigma_R(D) \le 1\,pt.$$

If R is not a triangular region, then

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

Proof. See Lemma 8.10 and Theorem 8.4. □

Lemma 20.5. $\tau_R(D) \ge 0$, *for all standard clusters R.*

Proof. This is Lemma 10.1. □

Recall that v has *type* (p, q) if every standard region with a vertex at v is a triangle or a quadrilateral, and if there are exactly p triangular faces and q quadrilateral faces that meet at v (see Definition 18.6). We write (p_v, q_v) for the type of v. Define constants $\tau_{\rm LP}(p, q)/pt$ by Table 20.6. The entries marked with an asterisk will not be needed.

$\tau_{\rm LP}(p,q)/pt$	$q = 0$	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	*	*	*	*	*

(20.6)

Lemma 20.6. *Let $S_1, \ldots, S_p$ and $R_1, \ldots, R_q$ be the tetrahedra and quad clusters around a vertex of type (p, q). Consider the constants of Table 20.6. Now,*

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

Proof. This is Lemma 10.5. □

Lemma 20.7. *Let $v_1, \dots, v_k$, for some $k \le 4$, be distinct vertices of type $(5,0)$. Let $S_1, \dots, S_r$ be quasi-regular tetrahedra around the edges $(0, v_i)$, for $i \le k$. Then*

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

and

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

Proof. This is Lemma 10.6. □

Lemma 20.8. *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. This is Lemma 10.10 and Lemma 12.3. □

Lemma 20.9. *A triangular standard region does not contain any enclosed vertices.*

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

Lemma 20.10. *A quadrilateral region does not enclose any vertices of height at most $2t_0$.*

Proof. This is Lemma 10.13. □

Lemma 20.11. *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 20.12. *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 20.2.*

Then

$$\tau_F(D) \geq 11.16\, pt.$$

Proof. This is Lemma 14.4. □

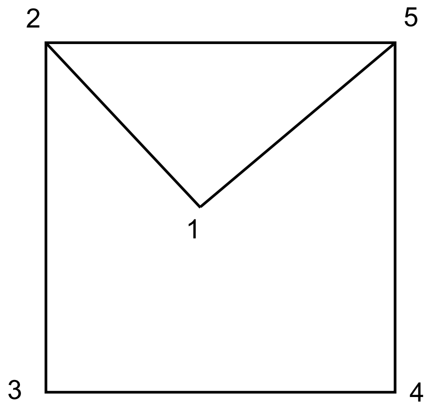

Figure 20.2. *A* 4*-circuit*

Lemma 20.13. *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*

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

Proof. This is Remark 14.2. □

Lemma 20.14. *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 20.15. *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 20.16. *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. This is Lemma 11.30. □

20.2 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 $|v_1|, |v_2|, |v_1 - v_2| \leq 2t_0$, we obtain a plane graph that breaks the unit sphere into standard regions. (The arcs do not meet except at endpoints by Lemma 4.19.)

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 20.17. *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 20.1 (see Lemma 20.1).*

Remark 20.18. *Observe that one case of Figure 20.1 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 20.3), which is a union of two standard regions (a triangle and an eight-sided region).*

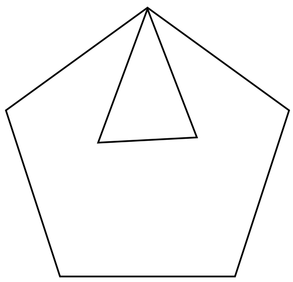

Figure 20.3. *An aggregate forming a pentagon*

Remark 20.19. *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 20.4. (It will be shown in Lemma 21.11 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.)*

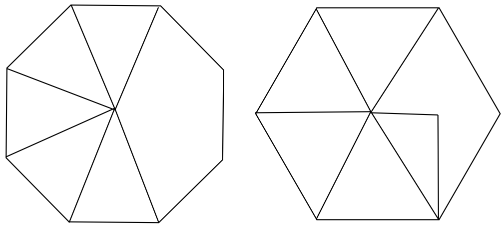

Figure 20.4. *Degree six aggregates*

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 20.18 and 20.19 occur. We 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 21.1 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 18.3, 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 20.20. *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 3.3. Its proof occupies Sections 21 and 22. In Theorem 19.1, the tame graphs are classified up to isomorphism. As a corollary, we have an explicit list of graphs that contains all contravening plane graphs.

Section 21

Contravention is tame

This section begins the proof of Theorem 20.20 (contravening graphs are tame). To prove Theorem 20.20, 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 Section 22. This section verifies all the properties of tameness, except for the last one (weight assignments).

21.1 First Properties

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

Proposition 21.1. *The construction of Section 20.2 associates a (nonempty) 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 Sections 4 and 5 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

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

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

Equation 20.5 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 8.4 that $\sigma_R \leq 0$, 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 20.18 and 20.19), there certainly remain at least two faces. □

Proposition 21.2. *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 eight edges is Lemma 20.1. Note that the aggregates of Remarks 20.19 and 20.18 have between five and eight edges. ∎

Proposition 21.3. *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 20.18 and 20.19 do not produce any new 3-circuits. (See the accompanying figures.) The result is Lemma 20.9. ∎

Proposition 21.4. *Contravening graphs satisfy Property 4 of tameness: The degree of every vertex is at least two and at most six.*

Proof. The statement that degrees are at least two 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 seven or more is found in Lemma 20.8. If the type is (p, q, r), with $r \geq 1$, then Lemma 20.14 shows that the interior angles of the standard regions cannot sum to 2π:

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

∎

Proposition 21.5. *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]. ∎

21.2 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 section, we rely on some inequalities that are not proved in this paper. Recall from Section 8.3 that there is an archive of hundreds of inequalities that have been proved by computer. This full archive appears in [Hal05b]. 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[132] that give lower bounds on $\tau_R(D)$ when R is a triangle or a quadrilateral. To obtain lower 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[133] a lower bound $\tau_{\mathrm{LP}}(p,q,d)$ to this minimization problem. This gives a lower bound to the corresponding constrained sum of nonlinear functions τ_R.

Similarly, another group of inequalities[134] yields upper bounds $\sigma_{\mathrm{LP}}(p,q,d)$ 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.

21.3 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 20.19 and 20.18.

Lemma 21.6. *The plane graph of a contravening decomposition star satisfies Property 6 of tameness:*

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

Proof. We will show that

$$c(\mathrm{len}(F))\, pt \geq \sigma_F(D). \tag{21.1}$$

[132] The sequence of five inequalities starting with CALC-927432550, Lemma 20.5, and for quads CALC-310151857, CALC-655029773, CALC-73283761, CALC-15141595, CALC-574391221, CALC-396281725

[133] Although they are closely related, the function τ_{LP} of three arguments introduced here is distinct from the function of two variables of the same name that is introduced in Section 20.1.

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

Assuming this, the result follows for contravening stars D:

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

We consider three cases for Inequality 21.1. In the first case, assume that the face F corresponds to exactly one standard region in the decomposition star. In this case, Inequality 21.1 follows directly from the bounds of Lemma 20.2:

$$\sigma_F(D) \leq s_n \leq c(n)\,pt.$$

In the second case, assume the context of a pentagon F formed in Remark 20.18. Then, again by Theorem 20.2, we have

$$\sigma_F(D) \leq s_3 + s_8 \leq (c(3) + c(8))\,pt \leq c(5)\,pt.$$

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

In the third case, we consider the situation of Remark 20.19. The six standard regions give

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

The constant 1.153 comes from Lemma 20.14. □

Proposition 21.7. *Let F be a face of a contravening plane graph $G(D)$. Then*

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

Proof. Similar. □

Lemma 21.8. *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.

($k \leq 2$) 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 20.14.)

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

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

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

($k = 5$) 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 $t_7 + \tau_{\mathrm{LP}}(5, 0, 2\pi - 1.153) > (4\pi\zeta - 8)\,pt$.

If the standard region is a hexagon, then $\tau(D)$ is at least $t_6 + \tau_{\mathrm{LP}}(5, 0, 2\pi - 1.153) > t_9$. Also, $s_6 + \sigma_{\mathrm{LP}}(5, 0, 2\pi - 1.153) < s_9$. The aggregate of the six standard regions is 9-sided. Lemma 20.3 gives the bound of $8\,pt$. $\square$

Lemma 21.9. *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 21.1.*

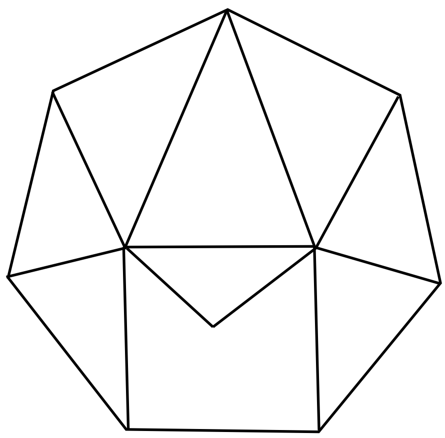

Figure 21.1. *Non-adjacent vertices of degree six on a pentagon*

Proof. We begin with the first part of the lemma. The sum $\tau_F(D)$ over these six standard regions is at least
$$t_5 + \tau_{\mathrm{LP}}(5, 0, 2\pi - 1.153) > t_8.$$
Similarly,
$$s_5 + \sigma_{\mathrm{LP}}(5, 0, 2\pi - 1.153) < s_8.$$
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:
$$t_8 + t_5 > (4\pi\zeta - 8)\,pt.$$

Such a second vertex on the octagonal aggregate leads to one of the following constants greater than $(4\pi\zeta - 8)\,pt$. 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.

$$\begin{array}{ll} t_8 & +\tau_{\mathrm{LP}}(4, 0, 2\pi - 1.32 - 0.8638), \quad \text{or} \\ t_8 & +1.47\,pt + \tau_{\mathrm{LP}}(4, 0, 2\pi - 1.153 - 0.8638), \quad \text{or} \\ t_8 & +\tau_{\mathrm{LP}}(5, 0, 2\pi - 1.153). \end{array}$$

(The relevant constants are found at Lemma 20.13 and Lemma 20.14.)
□

21.4 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 20.2 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 4.19. If an interior angle of the quadrilateral is less than 1.32, then by Lemma 20.16, $|v_1 - v_3| \le \sqrt{8}$. Thus, we assume in the following lemma, that all interior angles of the quadrilateral aggregate are at least 1.32.

Lemma 21.10. *A decomposition star that contains this configuration does not contravene.*

Proof. Let P denote the quadrilateral aggregate of these two standard regions. By Lemma 20.12, we have $\tau_P(D) \ge 11.16\,pt$. There are no other exceptional faces, because $11.16\,pt + t_5 > (4\pi\zeta - 8)\,pt$. Every vertex not on P has type $(5, 0)$, by Lemma 20.6. 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

$$11.16\,pt + \tau_{\mathrm{LP}}(5, 0, 2\pi - 1.32) > (4\pi\zeta - 8)\,pt.$$

There are at least three triangles at every vertex of P, otherwise we contradict Lemma 20.9 or Lemma 20.11.

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

$$\tau_F(D) \ge 2(1.5)\,pt.$$

There are two additional vertices of type $(5,0)$ whose tetrahedra are distinct from these eight quasi-regular tetrahedra. They give an additional $2(0.55)\,pt$. Now $(11.16 + 2(1.5) + 2(0.55))\,pt > (4\pi\zeta - 8)\,pt$ by Lemma 20.7. The result follows. ∎

Lemma 21.11. *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 five.*

Proof. An exceptional standard region with a vertex of degree six must be pentagonal by Lemma 21.9. If that pentagonal region has two or more such vertices, then by the same lemma, it must be the arrangement shown in Figure 21.1. This arrangement does not appear on a contravening graph by Lemma 21.10. ∎

Remark 21.12. *We have now fully justified the claim made in Remark 20.19: 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 $G(D)$.*

21.5 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 20.11 asserts that either the interior or the exterior has at most one 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 one vertex. With this choice, we have the following proposition.

Proposition 21.13. *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 20.6 show that the graph cannot be contravening.

If v is connected to two adjacent vertices in the 4-cycle, then we appeal to Lemma 21.10 to conclude that the graph does not contravene.

If v is connected to at most one vertex, then we appeal to Lemma 20.10. This completes the proof. ∎

Section 22

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 22.1. *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

$$F \mapsto w(F) = \tau_F(D)/pt.$$

Since D contravenes,

$$\begin{aligned} \textstyle\sum_F w(F) &= \textstyle\sum_F \tau_F(D)/pt \\ &= \tau(D)/pt \leq (4\pi\zeta - 8)\, pt/pt \\ &< \mathrm{tgt} = 14.8. \end{aligned}$$

The challenge of the theorem will be to prove that w, when defined by this formula, is admissible.

22.1 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 22.2. *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 21.7. □

Lemma 22.3. *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 20.6. □

Lemma 22.4. *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 20.7. □

The following proposition establishes the final property that $w(F)$ must satisfy to make it admissible. *Separated sets* are defined in Section 18.2.

Proposition 22.5. *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 section. 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 22.3.

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.

22.2 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 20.18 and 20.19.

Lemma 22.6. *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 20.7. 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 20.6
$(0, q, r \geq 1)$	$t_5 + 4t_4 \approx 14.41\,pt$	
$(1, 4, 0)$	$17.62\,pt$	Lemma 20.6
$(1, 3, 1)$	$t_5 + 12.58\,pt$	(τ_{LP})
$(1, 2, 2)$	$2t_5 + 7.53\,pt$	(τ_{LP})
$(1, q, r \geq 3)$	$3t_5 + t_4$	

∎

Lemma 22.7. *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 $e + \mathrm{tri}(v) \leq 5$.

The constants $0.55\,pt$ and $0.48\,pt$ used throughout the proof come from Lemma 20.7. The constants t_n comes from Lemma 20.2.

($e = 3$): First, assume that there are three exceptional faces around vertex v. They must all be pentagons ($2t_5 + t_6 > (4\pi\zeta - 8)\,pt$). The aggregate of the five faces is an m-gon (some $m \leq 11$). If there is a vertex not on this aggregate, use $3t_5 + 0.55\,pt > (4\pi\zeta - 8)\,pt$. So there are at most nine triangles away from the aggregate, and

$$\sigma(D) \leq 9\,pt + (3s_5 + 2\,pt) < 8\,pt.$$

The argument is the same if there is a quad, a pentagon, or a hexagon ($t_4 + t_6 = 2t_5$, $s_4 + s_6 = 2s_5$).

($e = 2$): 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 $m \leq 10$). There must be a vertex not on the aggregate of five faces, for otherwise we have

$$\sigma(D) \leq 8\,pt + (2s_5 + 2\,pt) < 8\,pt.$$

The interior angle of one of the pentagons is at most 1.32. For otherwise, $\tau_{\mathrm{LP}}(2, 1, 2\pi - 2(1.32)) + 2t_5 + 0.55\,pt > (4\pi\zeta - 8)\,pt$.

Lemma 20.13 shows that any pentagon R with an interior angle less than 1.32 yields $\tau_R(D) \geq t_5 + (1.47\,pt)$. If both pentagons have an interior angle < 1.32 the lemma follows easily from this calculation: $2(t_5 + 1.47\,pt)\,pt + \tau_{\rm LP}(2, 1, 2\pi - 2(1.153)) + 0.55\,pt > (4\pi\zeta - 8)\,pt$. If there is one pentagon with angle > 1.32, we then have $t_5 + (1.47\,pt) + \tau_{\rm LP}(2, 1, 2\pi - 1.153 - 1.32) + t_5 + 0.55\,pt > (4\pi\zeta - 8)\,pt$.

$(e = 1)$: Assume finally that there is one exceptional face at the vertex. If it is a hexagon (or more), we are done: $t_6 + \tau_{\rm LP}(2, 2, 2\pi - 1.153) > (4\pi\zeta - 8)\,pt$. Assume it is a pentagon. The aggregate of the five faces at the vertex is bounded by an m-circuit (some $m \leq 9$). If there are no more than nine quasi-regular tetrahedra outside the aggregate, then $\sigma(D)$ is at most $(9 - 2(0.48))\,pt + s_5 + \sigma_{\rm LP}(2, 2, 2\pi - 1.153) < 8\,pt$ (Lemma 20.7). 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,

$$\tau_{\rm LP}(2, 2, 2\pi - 1.32) + 3(0.55)\,pt + t_5 > (4\pi\zeta - 8)\,pt;$$

if it is less than 1.32, by Lemma 20.13

$$\tau_{\rm LP}(2, 2, 2\pi - 1.153) + 3(0.55)pt + 1.47\,pt + t_5 > (4\pi\zeta - 8)\,pt.$$

□

Lemma 22.8. *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

$$t_5,\ s_5,\ 1.47\,pt$$

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. □

22.3 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 20.18 and 20.19. 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 22.9. *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 the inequality 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 22.10. *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*

$$\tau_{\mathrm{LP}}(p', q', \alpha) > (p' d(3) + q' d(4) + a(p))\, pt$$

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

$$\sum_{1}^{m} (wF_i(D) - d(\mathrm{len}(F_i))) > a(p).$$

Clearly, the inequality for V is the sum of this inequality, the inequality for V', and $d(n) \ge 0$. □

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 22.11. *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

$$\tau_F(D) > \sum_{v \in V} (p_v d(3) + q_v d(4) + a(p_v))\, pt.$$

Proof. If $(p_v, q_v) = (3,1)$ and the internal angle of R at v is at least 1.32, then we use

$$\tau_{\mathrm{LP}}(3, 1, 2\pi - 1.32) > 1.4\, pt + t_4.$$

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 now follows from Lemma 14.6. □

Lemma 22.12. *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 22.2 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

$$\tau_{\mathrm{LP}}(3, 1, 2\pi - 1.32) > 1.4\, pt + t_4. \tag{22.1}$$

This gives the bound in the sense of Lemma 22.10 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 20.16 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 20.16, the interior angles of the exceptional regions at v are at least 1.32. It follows[135] that

$$\tau_{\mathrm{LP}}(p_v, q_v, \alpha) > (p_v d(3) + q_v d(4) + a(p_v))\, pt. \tag{22.2}$$

[135] CALC-551665569, CALC-824762926, and CALC-325738864

Thus, by Lemma 22.10, 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 20.16, 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 22.11, 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. $\square$

22.4 Weight Assignments for Aggregates

Lemma 22.13. *Consider a separated set of vertices V on an aggregated face F as in Remark 20.18. Then Inequality 4 holds (in the definition of admissible weight assignments):*

$$\sum_{V \cap F \neq \emptyset} (w(F) - d(\text{len}(F))) \geq \sum_{v \in V} a(\text{tri}(v)).$$

Proof. We may assume that $\text{tri}(v) \in \{3, 4\}$.

First consider the aggregate of Remark 20.18 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:

$$t_8 + t_5 > (4\pi\zeta - 8)\,pt.$$

A separated set of vertices V on F has cardinality at most 2. This gives the desired bound

$$t_8 > t_5 + 2(1.5)\,pt.$$

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

$$t_8 > t_6 + k(1.5)\,pt.$$

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 22.10 and Inequalities 22.1 and 22.2). 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 4.14.)

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:

$$t_7 + t_5 > (4\pi\zeta - 8)\,pt.$$

The result follows from

$$t_7 > t_5 + 2(1.5)\,pt.$$

□

Lemma 22.14. *Consider a separated set of vertices V on an aggregate face of a contravening plane graph as in Remark 20.19. Inequality 4 holds in the definition of admissible weight assignments.*

Proof. There is at most one exceptional face in the plane graph:

$$t_8 + t_5 > (4\pi\zeta - 8)\,pt.$$

Assume first that an aggregate face is an octagon (Figure 20.4). 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 22.10 and the estimate

$$\tau_{\mathrm{LP}}(4, 0, 2\pi - 2(0.8638)) > 1.5\,pt.$$

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 $a(4) = 1.5\,pt$ can be estimated at this vertex in the same way it is done for a non-aggregated case in Section 22.3.

Now consider the case of an aggregate face that is a hexagon (Figure 20.4). The argument is the same: we reduce to V containing a single vertex, and argue that this vertex can be treated as in Section 22.3. (Alternatively, use the fact that the pentagon-triangle combination in this aggregate has been eliminated by Lemma 21.10.) □

The proof that contravening plane graphs are tame is complete.

Section 23

Linear Program Estimates

We have completed a major portion of the proof of the Kepler conjecture by proving that every contravening plane graph is tame.

The final portion 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 8.1, and the case G_{pent} is treated in Paper V.

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 $\sigma(D) < 8\,pt$. 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 19.1, 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 section.

Theorem 23.1. *If the plane graph of a contravening decomposition star is isomorphic to one in the list [Hal05b], 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 3.3 that lead to the proof of the Kepler conjecture.

23.1 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 $A\,x \le b$, 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

$$\max(c \cdot x : A\,x \le b).$$

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 $A\,x \le b$ of the linear program are *satisfied* under the interpretation I if for all $p \in |I|$,

$$A\,x^I(p) \le b.$$

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. $f(p) \le c \cdot x^I(p)$, for all $p \in |I|$.

Lemma 23.2. *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. □

Remark 23.3. *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 [Hal05b].

Remark 23.4. *There is a second method of establishing the satisfaction of inequalities under an interpretation. Suppose we wish to show that the inequality $e \cdot x \leq b'$ is satisfied under the interpretation I. Suppose that we have already established that a system of inequalities $A\,x \leq b$ is satisfied under the interpretation I. We solve the linear programming problem* $\max(e \cdot x : A\,x \leq b)$. *If this maximum is at most b', then the inequality $e \cdot x \leq b'$ is satisfied under the interpretation I. We will refer to $e \cdot x \leq b'$ as an* LP*-derived inequality (with respect to the system $A\,x \leq b$).*

23.2 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 23.5. *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 $8\,pt$.*
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 $8\,pt$. 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.

Remark 23.6. *The paper [Hal03, Section 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 23.7. *If a tame graph G is not isomorphic to G_{fcc}, G_{hcp}, or G_{pent}, then it is not contravening.*

Proof. This follows immediately from Theorem 23.5 and Lemma 23.2. □

23.3 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 [Hal05b].

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

$$\begin{array}{ll} \sigma[F]^I & = \sigma_F(D), \\ \mathrm{sol}[F]^I & = \mathrm{sol}(F^I), \\ \tau[F]^I & = \tau_F(D). \end{array}$$

The objective function for the optimization problems is

$$\max : \quad \sum_{F \in \texttt{FACE}} \sigma[F].$$

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

$$\begin{array}{ll} 0 \le y[v] \le 2t_0, & v \in \texttt{VERTEX}, \\ 0 \le e[v,w] \le 2t_0, & (v,w) \in \texttt{EDGE}, \\ 0 \le \alpha[v,F] \le 2\pi, & (v,F) \in \texttt{ANGLE}, \\ 0 \le \mathrm{sol}[F] \le 4\pi & F, \in \texttt{FACE}. \end{array}$$

There are other linear relations that are suggested directly by the definitions or the geometry. Here, v belongs to VERTEX.

$$\begin{array}{ll} \tau[F] & = \mathrm{sol}[F]\zeta pt - \sigma[F], \\ 2\pi & = \sum_{F:v\in F} \alpha[v,F], \\ \mathrm{sol}[F] & = \sum_{v\in F} \alpha[v,F] - (\mathrm{len}(F) - 2)\pi. \end{array}$$

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 [Hal05b].

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 20.2.

23.4 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 23.3. 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.[136]

[136] 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

We present an informal analysis of the floating-point errors. For each quasi-regular tetrahedron S_i we have a nonnegative variable $x_i = pt - \sigma(S_i)$. For each quad cluster R_k, we have a nonnegative variable $x_k = -\sigma(R_k)$. A bound on $\sigma(D)$ is $p\,pt - \sum_{i\in I} x_i$, 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 $p\,pt + z \cdot b < 7.9999\,pt$, and if $\epsilon < 10^{-8}$, then $\sigma(D)$ is less than $8\,pt$. 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 $p \le 2(N-2) \le 116$ is the number of triangular faces,

$$\begin{aligned}
\sigma(D) &\le p\,pt + c \cdot x \le p\,pt + \left(\tfrac{z}{1+\epsilon}\right) Ax + \tfrac{\epsilon}{1+\epsilon} \textstyle\sum_{j\in J} x_j \\
&\le p\,pt + \tfrac{z\cdot b}{1+\epsilon} + \tfrac{\epsilon}{1+\epsilon} 2\pi N \\
&\le \left[p\,pt + z \cdot b + \epsilon(p\,pt + 2\pi N)\right]/(1+\epsilon) \\
&\le \left[7.9999\,pt + 10^{-8}(116\,pt + 500)\right]/(1 + 10^{-8}) < 8\,pt.
\end{aligned}$$

In practice, we used $0.4429 < 0.79984\,pt$ as our cutoff, and $N \le 14$ in the interesting cases, so that much tighter error estimates are possible.

Section 24

Elimination of Aggregates

The proof of the following theorem occupies the entire section. It eliminates all the pathological cases that we have had to carry along until now.

Theorem 24.1. *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 20.1 is not contravening.)*

24.1 Triangle and Quad Branching

Section 25 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 Section 25. This is a branching on triangular and quadrilateral faces.

We divide triangular faces with corners v_1, v_2, v_3 into two cases:

$$\begin{aligned} e[v_1,v_2]+e[v_2,v_3]+e[v_3,v_1] &\le 6.25,\\ e[v_1,v_2]+e[v_2,v_3]+e[v_3,v_1] &\ge 6.25, \end{aligned}$$

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.

24.2 A pentagonal hull with $n = 8$

The next few sections treat the nonpolygonal standard regions described in Remark 20.18. In this subsection, there is an aggregate of the octagonal region and a triangle has a pentagonal hull. Let P denote this aggregate.

Lemma 24.2. *Let G be a contravening plane graph with the aggregate of Remark 20.18. 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

$$t_8 + \sum_{(4)} \tau_{\mathrm{LP}}(4, 0, 2\pi - 2(1.153)) > (4\pi\zeta - 8)\, pt,$$

so that the graph does not contravene. □

For a general contravening plane graph with this aggregate, we have bounds

$$\begin{aligned} \sigma_F(D) &\leq pt + s_8, \\ \tau_F(D) &\geq t_8. \end{aligned}$$

We add the inequalities $\tau[F] > t_8$ and $\sigma[F] < pt + s_8$ to the exceptional face. There is no other exceptional face, because $t_8 + t_5 > (4\pi\zeta - 8)\, pt$. We run the linear programs for all tame graphs with the property asserted by Lemma 24.2. Every upper bound is less than $8\, pt$, so that there are no contravening decomposition stars with this configuration.

24.3 $n = 8$, hexagonal hull

We treat the two cases from Remark 20.18 that have a hexagonal hull (Figure 20.1). 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 24.2. 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 $8\, pt$.

24.4 $n = 7$, pentagonal hull

We treat the two cases illustrated in Figure 20.1 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 $t_5 + t_7 > (4\pi\zeta - 8)\,pt$. 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 eleven 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 23.4) $y[v_i] \le 2.168$, 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 24.1, 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 24.3. *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 is Lemma 14.5. □

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.

24.5 Type $(p, q, r) = (5, 0, 1)$

We return briefly to the case of six standard regions around a vertex discussed in Remark 20.19. 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 20.4 contains a pentagon-triangle combination that was ruled out by Lemma 21.10.

24.6 Summary

Lemma 24.4. *None of the aggregates of Remark 20.19 and Remark 20.18 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.*

Proof. The proof is the main result of this section. □

Section 25

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 that appear in unpublished (but publicly available) computer logs, this section is more technical than the others. The purpose of the section 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.

The first branching strategy has already been described in Section 24.1. 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 24 that eliminate the most unpleasant types of configurations.

25.1 Review of Internal Structures

For the past several sections, it has not been necessary to refer to the internal structure of the standard clusters. This section 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[137] 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 Section 11.5.

In every case, the simplices around a given upright diagonal lie in the cone over a single standard region.

Lemma 25.1. *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.*

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	$0.72484.$

[137]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.

Proof. This is Lemma 13.5. □

25.2 3-crowded and 4-crowded upright diagonals

Definition 25.2. *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 Section 11.9 for a proof of these facts and for further details.*

Lemma 25.3. *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 Lemmas 11.11 and 11.18. □

Lemma 25.4. *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 $(0.5606 + t_5 > (4\pi\zeta - 8)\,pt)$. 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 25.5. *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.[138] 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 25.6. *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 $8\,pt$. ☐

25.3 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 25.1).

Lemma 25.7. *Let D be a contravening decomposition star. Then there are no loops with context* $(5,1)$ *in D.*

Proof. By Lemma 25.1, 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 $8\,pt$. ☐

25.4 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* certain loops and 3-unconfined upright diagonals. There is a *penalty* for doing so. Let D be a decomposition star with an

[138] CALC-161665083

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 6.1) 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 25.8. *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 25.9. *A function $\hat{\sigma}$ has been defined in Section 11.10. 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*

$$\hat{\tau}(Q) = \mathrm{sol}(Q)\zeta pt - \hat{\sigma}(Q).$$

Remark 25.10. *At times, we work with various upper bounds to $\sigma_R(D)$, say,*

$$\sigma_R(D) \leq f_R(D).$$

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

$$f_R(D) \leq f_{R'}(D') + \pi_R.$$

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

$$\sum_i f_{R_i}(D) \leq \sum_\ell \hat{\sigma}(Q_j) = \mathrm{vor}_{R',0}(D) + \pi_R.$$

If the upright diagonal is not a loop, we include in the set R all regions along the "gaps" around the upright diagonal.

Sections 13.4 and 13.6 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[139] in Section 11.7 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 25.11. *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 Section 11.9. □

25.5 Pent and Hex Branching

If a single linear program does not yield the bound $\sigma(D) < 8\,pt$, 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.

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 25.4. Details about the size of the penalties can be found in Section 13.6.

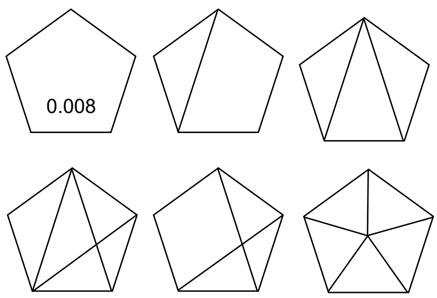

Figure 25.1. *Pentagonal face refinements*

[139] CALC-751772680 and CALC-310679005

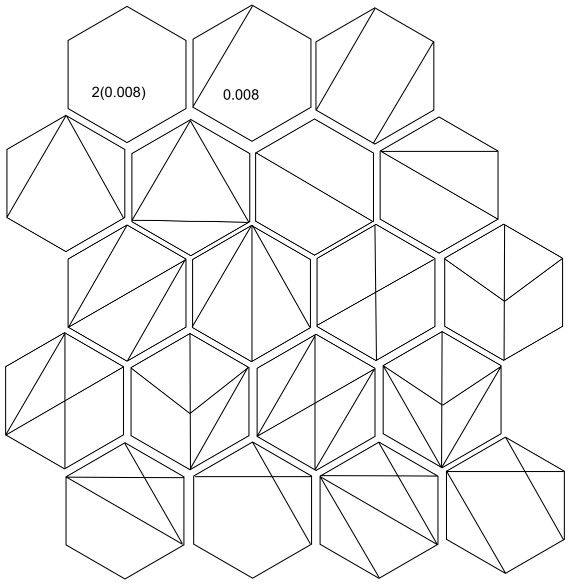

Figure 25.2. *Hexagonal face refinements. The only figures with a penalty are the first two on the top row and those on the bottom row. The first two on the top row have penalties* 2(0.008) *and* 0.008*. Those on the bottom row have penalties* $3\xi_\Gamma$, $3\xi_\Gamma$, $\xi_\Gamma + 2\xi_V$, *and* $\xi_\Gamma + 2\xi_V$.

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 1-1 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 25.1 and 25.2.

25.6 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.

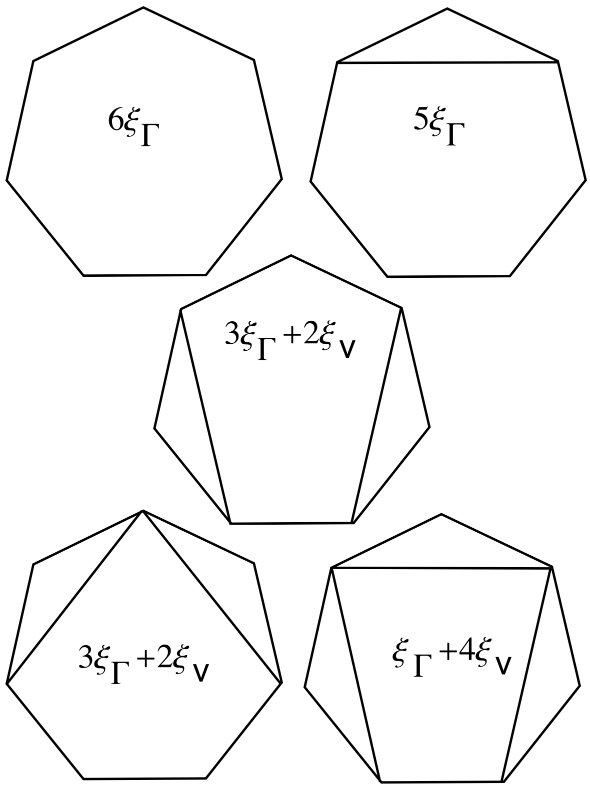

Figure 25.3. *Hept face refinements*

In the cases where 3-confined upright diagonals or loops have been erased, a number indicating a penalty accompanies the diagram (Figures 25.3 and 25.4. These penalties are derived in Sections 13.6 and 13.4.

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.

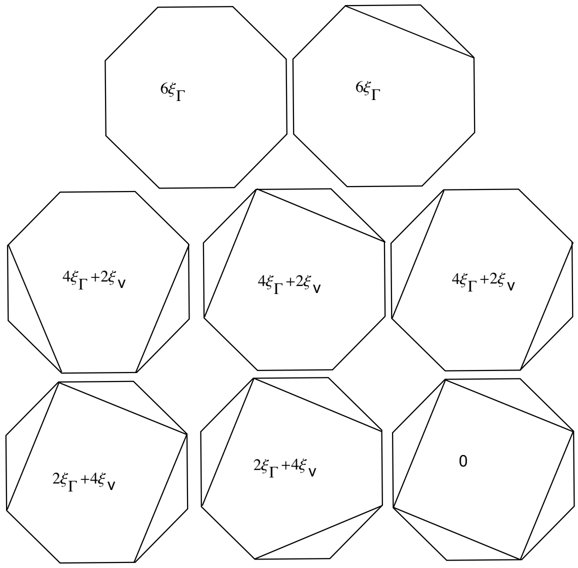

Figure 25.4. *Oct face refinements*

25.6.1 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 Section 11.10 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. $\sigma_R(D) < (\hat{\sigma}(Q) - Z(3,1)) + s_{n(R)}$.

25.6.2 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 Section 11.10 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 25.1. If, on the other hand, there is no loop of context $(n,k) = (4,2)$, then we have the upper bound

$$\sigma_R(D) \le (\hat{\sigma}(Q_1) - Z(3,1)) + (\hat{\sigma}(Q_2) - Z(3,1)) + s_{n(R)} + 2(\xi_\Gamma + 2\xi_V),$$

where $n(R) \in \{7,8\}$.

25.7 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 $|w| \ge 2.45$ or $|v-w| \ge 2.45$. (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 $|w| \le 2.45$ and $|v-w| \le 2.45$.

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 7.8) and the diagonal has height at least 2.696, then[140]

$$\sigma(Q) < \text{s-vor}_0(Q).$$

(If there are masked flat quarters, they become scored by $\hat{\sigma}$.) If an upright quarter has Voronoi type and the anchors w satisfy $|w| \le 2.45$ and $|v-w| \le 2.45$, then the quarter can be erased[141]

$$\sigma(Q) < \text{s-vor}_0(Q)$$

In general, we only have the weaker inequality[142]

$$\sigma(Q) < \text{s-vor}_0(Q) + 0.003521.$$

[140] CALC-214637273.
[141] CALC-378432183.
[142] CALC-310679005.

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

$$\text{octavor} < \text{octavor}_0 - 0.008, \tag{25.1}$$

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[143] 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 $8\,pt$.

25.8 Branching on Flat Quarters

We make a few general remarks about flat quarters.

Remark 25.12. *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 Section 22.3 show that the union* F *of the four quasi-regular tetrahedra and exceptional region give* $\tau_F(D) \geq 1.5\,pt$*. If there is no flat quarter with central vertex* v*, then the union* F *of four quasi-regular tetrahedra along* $\{0, v\}$ *give* $\tau_F(D) \geq 1.5\,pt$*. We can make similar improvements when* $\mathrm{tri}(v) = 3$*.*

Remark 25.13. *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 7.1). 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

[143] See, for example, CALC-867513567-*

and diagonal is at most $\eta(2.14, 2.14, 2.77) < \sqrt{2}$. This allows us to branch combine into three cases.

Lemma 25.14. *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, $\eta(y_4, y_5, y_6) \ge \sqrt{2}$, *and* $\sigma(Q) \le \text{s-vor}_0(Q)$.
3. *The diagonal has length* ≥ 2.7 *and* $\sigma(Q) \le \text{s-vor}_0(Q)$.

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 $\eta(y_4, y_5, y_6) \ge \sqrt{2}$ and $\sigma(Q) \le \text{s-vor}_0(Q)$. If Q is not in the Q-system, then $\text{s-vor}_0(Q)$ is an upper bound Lemma 11.26. 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 25.11.) In this case, we use the upper bound $\text{s-vor}_0(Q)$. $\square$

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.

25.9 Branching on Simplices that are not Quarters

Lemma 25.15. *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 $\min(y_5, y_6) \le 2.77$. Then one of the following is true.*

1. *The edges have lengths* $y_5, y_6 \in [2t_0, 2.77]$, $\eta_{456} \ge \sqrt{2}$, *and* $\sigma(S) \le \text{s-vor}_0(S)$.
2. $y_5, y_6 \in [2t_0, 2.77]$, *and* $\sigma(S) \le \text{s-vor}(S)$ *(the analytic Voronoi function).*
3. *An edge (say y_6) has length* $y_6 \ge 2.77$ *and* $\sigma(S) \le \text{s-vor}_0(S)$.

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 Section 9.6. $\square$

There are linear programming inequalities that are tailored to each case.

25.10 Branching on Quadrilateral subregions

One of the inequalities of holds for a quadrilateral subregion, if certain conditions are satisfied. One of the conditions is $y_4 \in [2\sqrt{2}, 3.0]$, where y_4 is a diagonal of the subregion. Since this diagonal is not one of the linear-programming variables, these bounds cannot be verified directly from the linear program. Instead we use an inequality which relates the desired bound $y_4 \leq 3$ to the linear-programming variables $\alpha[v, F]$, y_2, y_3, y_5, and y_6.

25.11 Implementation Details for Branching

We will now make a detailed examination of the internal structure of exceptional regions.

A *refinement* $\tilde{F}$ of a face F of a plane graph G is a set $\tilde{F}$ of faces such that

1. The intersection of the vertex set of G with that of $\tilde{F}$ is the set F.

2. $\tilde{F} \cup \{F^{op}\}$ is a plane graph.

We use refinements of faces to describe the internal structure of faces.

We introduce indexing sets $\texttt{FACE-}\tilde{F}$, $\texttt{VERTEX-}\tilde{F}$, $\texttt{ANGLE-}\tilde{F}$, $\texttt{EDGE-}\tilde{F}$, the sets of faces, vertices, angles, and edges in $\tilde{F}$, respectively, analogous to those introduced for G.

We create variables $\pi[\tilde{F}]$, and indexed variables

$$\begin{array}{lll} \mathrm{sol}\{\texttt{FACE-}\tilde{F}\}, & \mathrm{sc}\{\texttt{FACE-}\tilde{F}\} & \tau\mathrm{sc}\{\texttt{FACE-}\tilde{F}\}, \\ \alpha\{\texttt{ANGLE-}\tilde{F}\}, & y\{\texttt{VERTEX-}\tilde{F}\}, & e\{\texttt{EDGE-}\tilde{F}\}. \end{array}$$

(Variables with names "$y[v]$" and "$e[v, w]$" were already created for some $v, w \in \texttt{VERTEX-}\tilde{F} \cap \texttt{VERTEX}$. In these cases, we use the variables already created.)

Each vertex v in the refinement will be interpreted either as a vertex $v^I \in U(D)$, or as the endpoint of an upright diagonal lying over the standard region F^I. We will interpret the faces of the refinement in terms of the geometry of the decomposition star D variously as flat quarters, upright quarters, anchored simplices, and the other constructs of Paper IV. This interpretation depends on the context, and will be described in greater detail below.

Once the interpretation of faces is fixed, the interpretations are as before for the variable names introduced already: y, e, α, sol. The lower and upper bounds for α and sol are as before. The lower and upper bounds for $y[v]$ are 2 and $2t_0$ if $v^I \in U(D)$, but if $(0, v^I)$ is an upright diagonal, then the bounds are $[2t_0, 2\sqrt{2}]$. The lower and upper bounds for e will depend on the context.

25.12 Variables related to score

The variables sc are a stand-in for the score σ on a face. We do not call them σ because the sum of these variables will not in general equal the variable $\sigma[F]$, when $\tilde{F}$ is a refinement of F:

$$[\sum_{F' \in \tilde{F}} \mathrm{sc}[F'] \neq \sigma[F]].$$

We will use have a weaker relation:

$$\sigma[F] \le \sum_{F' \in \tilde{F}} \mathrm{sc}[F'] + \pi[\tilde{F}].$$

The variable $\pi[\tilde{F}]$ is called the penalty associated with the refinement $\tilde{F}$. (Penalties are discussed at length in Sections 13.6 and 13.4.) The interpretations of sc and $\pi[\tilde{F}]$ are rather involved, and will be discussed on a case-by-case basis below. The interpretation of τsc follows from the identity:

$$\tau\mathrm{sc}[F'] = \mathrm{sol}[F']\zeta pt - \mathrm{sc}[F'], \quad \forall F' \in \tilde{F}.$$

The interpretation of variables that follows might appear to be hodge-podge at first. However, they are obtained in a systematic way. We analyze the proofs and approximations in Part IV, and define $\mathrm{sc}[F]^I$ as the best penalty-free scoring approximation that is consistent with the given face refinement. here are the details.

If the subregion is a flat quarter, the interpretation of sc$[F]$ is the function $\hat{\sigma}$, defined in 11.10. If the subregion is an upright quarter Q, the interpretation of sc$[F]$ is the function $\sigma(Q)$ from Section 7. If the subregion is an anchored simplex that is not an upright quarter, sc$[F]$ is interpreted as the analytic Voronoi function vor if the simplex has type C or C', and as vor_0 otherwise. (The types A, B, C and C' are defined in Section 9.4.) Whether or not the simplex has type C, the inequality $\mathrm{sc}[F] \le 0$ is satisfied. In fact, if vor_0 scoring is used, we note that there are no quoins, and $\phi(1, t_0) < 0$.

If the subregion is triangular, if no vertex represents an upright diagonal, and if the subregion is not a quarter, then sc$[F]$ is interpreted as vor or vor_0 depending on whether the simplex has type A. In either case, the inequality $\mathrm{sc}[F] \le \mathrm{vor}_0$ is satisfied.

In most other cases, the interpretation of sc$[F]$ is vor_0. However, if R is a heptagon or octagon, and F has ≥ 4 sides, then sc$[F]$ is interpreted as vor_0 except on simplices of type A, where it becomes the analytic Voronoi function.

If R is a pentagon or hexagon, and F is a quadrilateral that is not adjacent to a flat quarter, and if there are no penalties in the region, then the interpretation of sc$[F]$ is the actual score of the subregion over the subregion. In this case, the score σ_R has a well-defined meaning for the quadrilateral, because it is not possible for an upright quarter in the Q-system to straddle the quadrilateral region and an adjacent region. Consequently, any erasing that is done can be associated with the subregion without ambiguity. By the results of Sections 8.4 and 8.5, we have $\mathrm{sc}[F] \le 0$. We also have $\mathrm{sc}[F] \le \mathrm{vor}_0$.

One other bound that we have not explicitly mentioned is the bound $\sigma_R(D) < s_n$. For heptagons and octagons that are not aggregates, this is a better bound than the one used in the definition of tameness (Property 6). In heptagons and octagons that are not aggregates, if we have a subregion with four or more sides, then $\mathrm{sc}[F] < Z(n,k)$ and $\tau\mathrm{sc}[F] > D(n,k)$. (See Section 13.5, Equations 13.1 and 13.2.

The variables are subject to a number of compatibility relations that are evident from the underlying definitions and geometry.

$$\begin{array}{ll} \mathrm{sol}[F'] = \sum_{v\in F'} \alpha[v,F'] - (len[F']-2)\pi, & \forall F' \\ \sum_{F':v\in F', F'\in \texttt{FACE-}\tilde{F}} \alpha[v,F'] = \alpha[v,F], & \forall v \end{array}$$

Assume that a face $F_1 \in \tilde{F}$ has been interpreted as a subregion $R = F_1^I$ of a standard region. Assume that each vertex of F_1 is interpreted as a vertex in $U(D)$ or as the endpoint of an upright diagonal over F^I. One common interpretation of sc is $\mathrm{vor}_{0,F}(U(D))$, the truncated Voronoi function. When this is the interpretation, we introduce further variables:

$$\begin{array}{ll} \mathrm{quo}[v,s(v,F_1)] & \forall v \in F_1, \\ \mathrm{quo}[s(v,F_1),v] & \forall v \in F_1, \\ \mathrm{Adih}[v,F_1] & \forall v \in F_1, \end{array}$$

We interpret the variables as follows. If $w = s(v)$, and the triangle $(0, v^I, w^I)$ has circumradius η at most t_0, then

$$\begin{array}{ll} \mathrm{quo}[v,w]^I & = \mathrm{quo}(R(|v^I|/2,\eta,t_0)), \\ \mathrm{quo}[w,v]^I & = \mathrm{quo}(R(|w^I|/2,\eta,t_0)). \end{array}$$

If the circumradius is greater than t_0, we take

$$\mathrm{quo}[v,w]^I = \mathrm{quo}[w,v]^I = 0.$$

The variable Adih has the following interpretation:

$$\mathrm{Adih}[v,F_1]^I = \begin{cases} A(|v^I|/2)\alpha(v^I,F_1^I) & |v^I| \le 2t_0, \\ 0 & \text{otherwise.} \end{cases}$$

Under these interpretations, the following identity is satisfied:

$$\begin{array}{ll} \mathrm{sc}[F_1] & = \mathrm{sol}[F_1]\phi_0 + \sum_{v\in F_1} \mathrm{Adih}[v,F_1] \\ & \quad -4\delta_{oct} \sum \mathrm{quo}[v,w]. \end{array}$$

The final sum runs over all pairs (v,w), where $v = s(w,F_1)$ or $w = s(v,F_1)$.

For this to be useful, we need good inequalities governing the individual variables. Such inequalities for Adih$[v,F]$ and quo$[v,w]$ are found in Calculations CALC-815275408 and CALC-349475742. To make of use these inequalities, it is necessary to have lower and upper bounds on $\alpha[v,F]$ and $y[v]$. We obtain such bounds as LP-derived inequalities in the sense of Remark 23.4.

25.13 Appendix Hexagonal Inequalities

There are a number of inequalities that have been particularly designed for standard regions that are hexagons. This appendix describes those inequalities. They are generally inequalities involving more than six variables, and because of current technological limitations on interval arithmetic, we were not able to prove these inequalities directly with interval arithmetic.

Instead we give various lemmas that deduce the inequalities from inequalities in a smaller number of variables (small enough to prove by interval arithmetic.)

25.13.1 Statement of results

There are a number of inequalities that hold in special situations when there is a hexagonal region. Although these inequalities do not appear in the main text of the proof of the Kepler conjecture, they are used in the linear programs.

After stating all of them, we will turn to the proofs.

1. If there are no flat quarters and no upright quarters (so that there is a single subregion F), then

$$\mathrm{vor}_0 < -0.212 \tag{25.2}$$
$$\tau_0 > 0.54525. \tag{25.3}$$

2. If there is one flat quarter and no upright quarters, there is a pentagonal subregion F. It satisfies

$$\begin{array}{ll} \mathrm{vor}_0 & < -0.221 \\ \tau_0 & > 0.486. \end{array}$$

3. If there are two flat quarters and no upright quarters, there is a quadrilateral subregion F. It satisfies

$$\begin{array}{ll} \mathrm{vor}_0 & < -0.168, \\ \tau_0 & > 0.352. \end{array}$$

These are twice the constants appearing in 11;

4. If there is an edge of length between $2t_0$ and $2\sqrt{2}$ running between two opposite corners of the hexagonal cluster, and if there are no flat or upright quarters on one side, leaving a quadrilateral region F, then F satisfies

$$\begin{array}{ll} \mathrm{vor}_0 & < -0.075, \\ \tau_0 & > 0.176. \end{array}$$

5. If the hexagonal cluster has an upright diagonal with context $(4, 2)$, and if there are no flat quarters (Figure 25.5), then the hexagonal cluster R satisfies

$$\begin{array}{ll} \sigma_R & < -0.297, \\ \tau_R & > 0.504. \end{array}$$

6. If the hexagonal cluster has an upright diagonal with context $(4, 2)$, and if there is one unmasked flat quarter (Figure 25.6, let $\{F\}$ be the set of four subregions around the upright diagonal. (That is, take all subregions except for the flat quarter.) In the following inequality and Inequality 7, let σ_R^+ be defined as σ_R on quarters, and vor_x on other anchored simplices. τ_R^+ is the adapted squander function.

$$\begin{array}{ll} \sum_{(4)} \sigma_R^+ & < -0.253, \\ \sum_{(4)} \tau_R^+ & > 0.4686. \end{array}$$

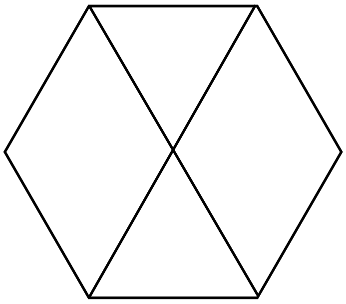

Figure 25.5. *A hexagonal cluster with context* $(4, 2)$.

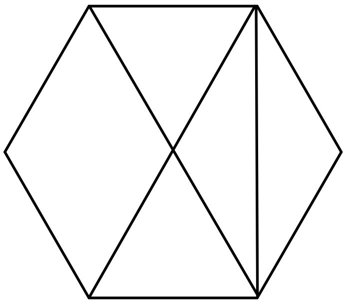

Figure 25.6. *A hexagonal cluster with context* $(4, 2)$.

7. If the hexagonal cluster has an upright diagonal with context $(4, 2)$, and if there are two unmasked flat quarters (Figure 25.7), let $\{F\}$ be the set of four subregions around the upright diagonal. (That is, take all subregions except for the flat quarters.)

$$\begin{array}{ll} \sum_{(4)} \sigma_R^+ & < -0.2, \\ \sum_{(4)} \tau_R^+ & > 0.3992. \end{array}$$

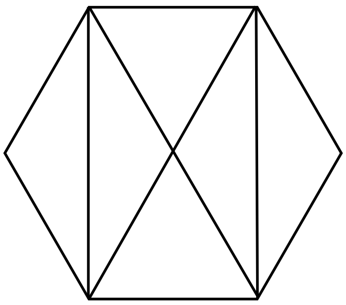

Figure 25.7. *A hexagonal cluster with context* $(4, 2)$.

8. If the hexagonal cluster has an upright diagonal in context $(4, 1)$, and if there are no flat quarters, let $\{F\}$ be the set of four subregions around the upright diagonal. Assume that the edge opposite the upright diagonal on the anchored simplex has length at least $2\sqrt{2}$. (See Figure 25.8.)

$$\begin{array}{ll} \mathrm{vor}_{0,R}(D) + \sum_{(3)} \sigma(Q) & < -0.2187 \\ \tau_{0,R}(D) + \sum_{(3)} \tau(Q) & > 0.518. \end{array}$$

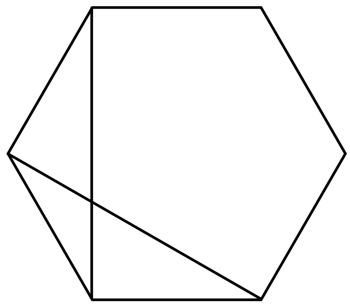

Figure 25.8. *A hexagonal cluster with context* $(4, 1)$.

9. In this same context, let F be the pentagonal subregion along the upright diagonal. It satisfies

$$\mathrm{vor}_0 < -0.137, \tag{25.4}$$
$$\tau_0 > 0.31. \tag{25.5}$$

10. If the hexagonal cluster has an upright diagonal in context $(4, 1)$, and if there is one unmasked flat quarter, let $\{F\}$ be the set of four subregions around the upright diagonal. Assume that the edge opposite the upright diagonal on the anchored simplex has length at least $2\sqrt{2}$. (There are five subregions, shown in Figure 25.9.)

$$\begin{array}{ll} \mathrm{vor}_{0,R}(D) + \sum_{(3)} \sigma(Q) & < -0.1657, \\ \tau_{0,R}(D) + \sum_{(3)} \tau(Q) & > 0.384. \end{array}$$

11. In this same context, let F be the quadrilateral subregion in Figure 25.9. It satisfies

$$\begin{array}{ll} \mathrm{vor}_0 & < -0.084, \\ \tau_0 & > 0.176. \end{array}$$

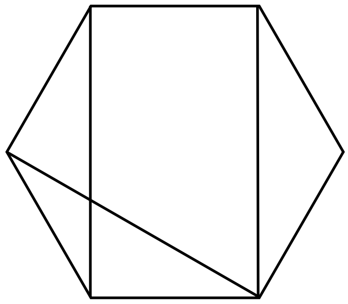

Figure 25.9. *A hexagonal cluster with context* $(4, 1)$.

25.13.2 Proof of inequalities

Proposition 25.16. *Inequalities 1 –11 are valid.*

We prove the inequalities in reverse order 11– 1. The bounds[144] $\mathrm{vor}_0 < 0.009$ and $\tau_0 > 0.05925$ for what a flat quarters with diagonal $\sqrt{8}$ will be used repeatedly. Some of the proofs will make use of tcc-bounds, which are described in 12.9.

Proof. (*Inequality 10 and Inequality 11.*) Break the quadrilateral cluster into two simplices S and S' along the long edge of the anchored simplex S. The anchored simplex S satisfies $\tau(S) \geq 0$, $\sigma(S) \leq 0$. The other simplex satisfies $\tau_0(S') > 0.176$ and $\mathrm{vor}_0(S') < -0.084$ by an interval calculation.[145] This gives Inequality 11. For Inequality 10, we combine these bounds with the linear programming bound on the four anchored simplices around the upright diagonal. From a series of inequalities[146] we find that they score < -0.0817 and squander > 0.208. Adding these to the bounds from Inequality 11, we obtain Inequality 10. $\square$

Proof. *(Inequality (8) and (9).)* The pentagon is a union of an anchored simplex and a quadrilateral region. LP-bounds similar to those in the previous paragraph and based on the inequalities of Section 13.12 show that the loop scores at most -0.0817 and squanders at least 0.208. If we show that the quadrilateral satisfies

$$\mathrm{vor}_0 < -0.137, \tag{25.6}$$
$$\tau_0 \quad > 0.31, \tag{25.7}$$

then Inequalities (8) and (9) follow. If by deformations a diagonal of the quadrilateral drops to $2\sqrt{2}$, then the result follows interval calculations.[147] By this we may

[144] CALC-148776243
[145] CALC-938091791
[146] CALC-815492935, CALC-187932932, CALC-485049042, CALC-835344007
[147] CALC-148776243,CALC-468742136

now assume that the quadrilateral has the form

$$(a_1, 2, a_2, 2, a_3, 2, a_4, b_4), \quad a_2, a_3 \in \{2, 2t_0\}.$$

If the diagonals drop under 3.2 and $\max(a_2, a_3) = 2t_0$, again the result follows from interval calculations.[148] If the diagonals drop under 3.2 and $a_2 = a_3 = 2$, then the result follows from further interval calculations.[149] So finally we attain by deformations $b_4 = 2\sqrt{2}$ with both diagonals greater than 3.2. But this does not exist, because

$$\Delta(4, 4, 4, 3.2^2, 4, 8, 3.2^2) < 0.$$

□

Proof. *(Inequality 5, Inequality 6, and Inequality 7.)* Inequalities 7 are derived in Section 13.12. Inequalities 5, 6 are LP-bounds based on interval calculations.[150] □

Proof. *(Inequality 4.)* Deform as in Section 12. If at any point a diagonal of the quadrilateral drops to $2\sqrt{2}$, then the result follows from interval calculations[151] and Inequality 11:

$$\begin{array}{ll} \mathrm{vor}_0 & < 0.009 - 0.084 = -0.075, \\ \tau_0 & > 0 + 0.176 = 0.176, \end{array}$$

Continue deformations until the quadrilateral has the form

$$(a_1, 2, a_2, 2, a_3, 2, a_4, b_4), \quad a_2, a_3 \in \{2, 2t_0\}.$$

There is necessarily a diagonal of length ≤ 3.2, because

$$\Delta(4, 4, 3.2^2, 8, 4, 3.2^2) < 0.$$

Suppose the diagonal between vertices v_2 and v_4 has length at most 3.2. If $a_2 = 2t_0$ or $a_3 = 2t_0$, the result follows from interval calculations[152] and Inequality 11. Take $a_2 = a_3 = 2$. Inequality 4 now follows from interval calculations.[153] □

Proof. *(Inequality 3).* We prove that the quadrilateral satisfies

$$\begin{array}{ll} \mathrm{vor}_0 & < -0.168 \\ \tau_0 & > 0.352. \end{array}$$

[148] calc148776243,CALC-468742136
[149] CALC-128523606
[150] CALC-815492935, CALC-187932932, CALC-485049042
[151] CALC-148776243
[152] CALC-148776243
[153] CALC-128523606

There are two types of quadrilaterals. In (a), there are two flat quarters whose central vertices are opposite corners of the hexagon. In (b), the flat quarters share a vertex. We consider case (a) first.

Case (a). We deform the quadrilateral as in Section 12.If at any point there is a diagonal of length at most 3.2, the result follows from Inequality 10 and Inequality 11. Otherwise, the deformations give us a quadrilateral

$$(a_1, 2, a_2, 2t_0, a_3, 2, a_4, 2), \quad a_i \in \{2, 2t_0\}.$$

The tcc approximation now gives the result (see Section 12.10).

Case (b). Label the vertices of the quadrilateral $v_1, \ldots, v_4$, where (v_1, v_2) and (v_1, v_4) are the diagonals of the flat quarter. Again, we deform the quadrilateral. If at any point of the deformation, we find that $|v_1 - v_3| \leq 3.2$, the result follows from Inequalities 10, 11. If during the deformation $|v_2 - v_4| \leq 2\sqrt{2}$, the result follows from interval calculations.[154] If the diagonal (v_2, v_4) has length at least 3.2 throughout the deformation, we eventually obtain a quadrilateral of the form

$$(a_1, 2t_0, a_2, 2, a_3, 2, a_4, 2t_0), \quad a_i \in \{2, 2t_0\}.$$

But this does not exist:

$$\Delta(4, 4, 3.2^2, (2t_0)^2, (2t_0)^2, 3.2^2) < 0.$$

We may assume that $|v_2 - v_4| \in [2\sqrt{2}, 3.2]$. The result now follows from interval calculations.[155] □

Proof. *(Inequality 2).* This case requires more effort. We show that

$$\begin{array}{ll} \mathrm{vor}_0 & < -0.221 \\ \tau_0 & > 0.486 \end{array}$$

Label the corners $(v_1, \ldots, v_5)$ cyclically with (v_1, v_5) the diagonal of the flat quarter in the hexagonal cluster. We use the deformation theory of Section 12. The proof appears in steps $(1), \ldots, (6)$.

(1) If during the deformations, $|v_1 - v_4| \leq 3.2$ or $|v_2 - v_5| \leq 3.2$, the result follows from Inequalities 25.13.2 and 11. We may assume this does not occur.

(2) If an edge (v_1, v_3), (v_2, v_4), or (v_3, v_5) drops to $2\sqrt{2}$, continue with deformations that do not further decrease this diagonal. If $|v_1 - v_3| = |v_3 - v_5| = 2\sqrt{2}$, then the result follows from interval calculations.[156]

If we have $|v_1 - v_3| = 2\sqrt{2}$, deform the figure to the form

$$(a_1, 2, a_2, 2, a_3, 2, a_4, 2, a_5, 2t_0), \quad a_2, a_4, a_5 \in \{2, 2t_0\}.$$

Once it is in this form, break the flat quarter $(0, v_1, v_2, v_3)$ from the cluster and deform v_3 until $a_3 \in \{2, 2t_0\}$. The result follows from an interval calculation.[157]

[154] CALC-148776243, CALC-315678695
[155] CALC-315678695
[156] CALC-148776243, CALC-673399623
[157] CALC-297256991

We handle a boundary case of the preceding calculation separately. After breaking the flat quarter off, we have the cluster

$$(a_1, 2\sqrt{2}, a_3, 2, a_4, 2, a_5, 2t_0), \quad a_3, a_4, a_5 \in \{2, 2t_0\}.$$

If $|v_1 - v_4| = 3.2$, we break the quadrilateral cluster into two pieces along this diagonal and use interval calculations[158] to conclude the result. This completes the analysis of the case $|v_1 - v_3| = 2\sqrt{2}$.

(3) If $|v_2 - v_4| \leq 3.2$, then deform until the cluster has the form

$$(a_1, 2, a_2, 2, a_3, 2, a_4, 2, a_5, 2t_0), \quad a_1, a_3, a_5 \in \{2, 2t_0\}.$$

Then cut along the special simplex to produce a quadrilateral. Disregarding cases already treated by the interval calculations,[159] we can deform it to

$$(a_1, 2, a_2, 2\sqrt{2}, a_4, 2, a_5, 2t_0), \quad a_i \in \{2, 2t_0\},$$

with diagonals at least 3.2. The result now follows from interval calculations.[160]

In summary of (1), (2), (3), we find that by disregarding cases already considered, we may deform the cluster into the form

$$(a_1, 2, a_2, 2, a_3, 2, a_4, 2, a_5, 2t_0), \quad a_i \in \{2, 2t_0\},$$

$|v_1 - v_3| > 2\sqrt{2}$, $|v_3 - v_5| > 2\sqrt{2}$, $|v_2 - v_4| > 3.2$.

(4) Assume $|v_1 - v_3|, |v_3 - v_5| \leq 3.2$. If $\max(a_1, a_3, a_5) = 2t_0$, we invoke interval calculations[161] to prove the inequalities. So we may assume $a_1 = a_3 = a_5 = 2$. The result now follows from interval calculations.[162] This completes the case $|v_1 - v_3|, |v_3 - v_5| \leq 3.2$.

(5) Assume $|v_1 - v_3|, |v_3 - v_5| \geq 3.2$. We deform to

$$(a_1, 2, a_2, 2, a_3, 2, a_4, 2, a_5, 2t_0), \quad a_i \in \{2, 2t_0\}.$$

If $a_2 = 2t_0$ and $a_1 = a_3 = 2$, then the simplex does not exist by Section 13.7. Similarly, $a_4 = 2t_0$, $a_5 = a_3 = 2$ does not exist. The tcc bound gives the result except when $a_2 = a_4 = 2$. The condition $|v_2 - v_4| \geq 3.2$ forces $a_3 = 2$. These remaining cases are treated with interval calculations.[163]

(6) Assume $|v_1 - v_3| \leq 3.2$ and $|v_3 - v_5| \geq 3.2$. This case follows from deformations, interval calculations.[164] This completes the proof of Inequalities 2. □

Proof. *(Inequality 1).* Label the corners of the hexagon $v_1, \ldots, v_6$. The proof to this inequality is similar to the other cases. We deform the cluster by the method

[158] CALC-861511432
[159] CALC-861511432
[160] CALC-746445726
[161] CALC-148776243, CALC-297256991
[162] CALC-897046482
[163] CALC-928952883
[164] CALC-297256991, CALC-673800906

of Section 12 until it breaks into pieces that are small enough to be estimated by interval calculations. If a diagonal between opposite corners has length at most 3.2, then the hexagon breaks into two quadrilaterals and the result follows from Inequality 25.13.2.

If a flat quarter is formed during the course of deformation, then the result follows from Inequality 2 and interval calculations.[165] Deform until the hexagon has the form

$$(a_1, 2, a_2, 2, \ldots, a_6, 2), \quad a_i \in \{2, 2t_0\}.$$

We may also assume that the hexagon is convex (see Section 12.12).

If there are no special simplices, we consider the tcc-bound. The tcc-bound implies Inequality 1, except when $a_i = 2$, for all i. But if this occurs, the perimeter of the convex spherical polygon is $6\,\mathrm{arc}(2,2,2) = 2\pi$. Thus, there is a pair of antipodal points on the hexagon. The hexagon degenerates to a lune with vertices at the antipodal points. This means that some of the angles of the hexagon are π. One of the tccs has the form $C(2, 1.6, \pi)$, in the notation of Section 12.10. With this extra bit of information, the tcc bound implies Inequality 1.

If there is one special simplex, say $|v_5 - v_1| \in [2\sqrt{2}, 3.2]$, we remove it. The score of the special simplex is[166]

$$\begin{array}{ll} \mathrm{vor}_0 & < 0, \quad \tau_0 > 0.05925, \quad \text{if } \max(|v_1|, |v_5|) = 2t_0, \\ \mathrm{vor}_0 & < 0.0461, \quad \tau_0 > 0, \quad \text{if } |v_1| = |v_5| = 2, \end{array}$$

The resulting pentagon can be deformed. If by deformations, we obtain $|v_2 - v_5| = 3.2$ or $|v_1 - v_4| = 3.2$, the result follows from Inequalities 25.13.2 and two interval calculations.[167]

If $|v_5 - v_1| = 2\sqrt{2}$, we use Inequality 2 and interval calculations[168] unless $|v_1| = |v_5| = 2$. If $|v_1| = |v_5| = 2$, we use interval calculations.[169] If a second special simplex forms during the deformations, the result follows from interval calculations.[170]

The final case of Inequality 1 to consider is that of two special simplices. We divide this into two cases. (a) The central vertices of the specials are v_2 and v_6. (b) The central vertices are opposite v_1 and v_4. In case (a), the result follows by deformations and interval calculations.[171] In case (b), the result follows by deformations and interval calculations.[172] This completes the proof of Inequalities 1 and the proof of the Proposition. □

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[165] CALC-148776243
[166] CALC-148776243
[167] CALC-725257062, CALC-977272202
[168] CALC-148776243
[169] CALC-377409251
[170] CALC-586214007
[171] CALC-89384104
[172] CALC-859726639

25.14 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 [Hal05b], which record which branches are followed for any given tame graph. (For most tame graphs, a single linear program suffices.)

This completes the proof of the Kepler conjecture.

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