Sphere Packings, III. Extremal Cases

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Abstract. 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 was defined, certain points in the domain were conjectured to give the global maxima, and the relation between this conjecture and the Kepler conjecture was 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.

Introduction

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 (fcc) and hexagonal-close packing (hcp) 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.

8. Local Optimality

The first several sections in the previous papers have established the fundamental definitions and constructions of this issue. This section establishes the local optimality of the function $\sigma: DS \rightarrow \mathbb{R}$ in a neighborhood of the decomposition stars of the fcc and hcp.

8.1. Results

Here is a sketch of the proof of local optimality. The fcc and hcp 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 follow 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 fcc configuration, or a bijection with U_{hcp} the twelve tangent unit balls in the hcp 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 $U(D) = U_{\text{fcc}}$ and others exist with $U(D) = U_{\text{hcp}}$.*

Remark 8.2. This theorem is one of the key claims of Section 3.3. This theorem is phrased slightly differently from 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 fcc and hcp, 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 $\sigma(D) = 8\text{pt}$. Moreover, up to Euclidean motion, $U(D)$ is the kissing arrangement of the twelve balls around a central ball in the fcc packing or the kissing arrangement of twelve balls in the hcp.*

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*

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

is monotonically decreasing in each variable.

Proof. This is Rogers’s lemma, as formulated in Lemma 8.6 of [Ha6]. □

Lemma 8.6. *Consider the Rogers simplex $R(a, b, \sqrt{2})$ with vertex at the origin. Assume $1 \leq a \leq b$ and $\eta(2, 2, 2) \leq b \leq \sqrt{2}$. Let A be the volume of the intersection of the simplex with a closed ball of radius 1 at the origin. Then*

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

Fig. 8.1. Some sets of low density.

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 Fig. 8.1. $\square$

Lemma 8.7. *Consider the wedge of a cone*

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

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

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

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

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

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

Proof. This is calculated in Section 4 of [Ha7]. See the second frame of Fig. 8.1. $\square$

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*

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

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

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

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 computer. This full archive appears in [Ha16]. 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 [Ha14] and [Ha6]. 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 [Ha16] 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 $\sigma(S) \leq 1 pt$. 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 Lemma 9.1.1 of [Ha6]). This early proof show by conventional means that $\sigma(S) \leq 1 pt$ 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, $\sigma(Q) \leq 0$. 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 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 inequalities⁴ that hold for all upright quarters Q with distinguished vertex v :

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

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 $\Gamma(Q) \leq 0$, if $\eta^+ \leq \sqrt{2}$ and $s\text{-vor}(Q, v) \leq 0$, if $\eta^+ \geq \sqrt{2}$.

⁴ CALC-522528841 and CALC-892806084.

Consider the case $\eta^+ \leq \sqrt{2}$. If Q is a quarter such that every face has circumradius at most $\sqrt{2}$, then⁵ $\Gamma(Q) \leq 0$. 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 $\eta^+(Q) \leq \sqrt{2}$ 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 $\frac{1}{3}$ the solid angle of Q at v . By the definition of $\text{s-vor}(Q, \sqrt{2})$, it is nonpositive if and only if

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

($\text{VC}(Q, 0)$ 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 8.6–8.8, these three types of solids give inequalities like that of (8.1). Summing the inequalities from these lemmas, we get (8.1).

Consider the case $\eta^+ \geq \sqrt{2}$ and $\sigma = \text{s-vor}$. If the quarter is upright, then⁶ $\text{s-vor}(Q) \leq 0$. The quarters achieving equality are extremal. Thus, we may assume the quarter is flat. If the orientation of a flat quarter is negative along the face containing the origin and the diagonal, then⁷ $\text{s-vor}(Q) \leq 0$. The quarters achieving equality are extremal. In the remaining case, the only possible face along which the orientation is negative is the top face. This means that the analytic continuation defining $\text{s-vor}(Q)$ is the same as

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

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

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

We have $\text{s-vor}(Q, \sqrt{2}) \leq 0$ as in the previous paragraph, by Lemma 8.6–8.8. If equality is attained, the wedges and cones must have zero volume, and each Rogers simplex must

⁵ CALC-346093004.

⁶ CALC-40003553.

⁷ CALC-5901405.

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. $\square$

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 $s\text{-vor}(S) < 0$.*

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, $s\text{-vor}(S) < 0$ if and only if

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

This inequality breaks into six separate inequalities corresponding to the six Rogers's simplices $R(a, b, c)$ constituting $\text{VC}(S, 0)$. Rogers's lemma, 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 have⁸ $s\text{-vor}(S(y_1, y_2, \dots, y_6)) < 0$ for $(y_1, \dots, y_6)$ in any of the following four domains:

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

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 $\mathcal{B}$.*

⁸ CALC-629256313, CALC-917032944, CALC-738318844, and CALC-587618947.

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. $\square$

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 $\mathcal{Q}$ -system, then Lemma 4.34 gives the result. $\square$

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

$$\text{arc}(a, b, c) = \arccos((a^2 + b^2 - c^2)/(2ab)) = \frac{\pi}{2} + \arctan \frac{c^2 - a^2 - b^2}{\sqrt{u(a^2, b^2, c^2)}}$$

with $u(x, y, z) = -x^2 - y^2 - z^2 + 2xy + 2yz + 2zx$.

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

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 $|v| \leq \sqrt{8}$ forces the closest point in C to lie along the edge $\{0, v_2\}$ or $\{0, v_3\}$. Since $|v_2|, |v_3| \leq \sqrt{8}$, 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. $\square$

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 $\mathcal{Q}$ -system if $|v_1 - v_2| \leq 2t_0$ and $|v_1 - v_3| \leq 2t_0$. This is contrary to the 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 $|v_1 - v_2| \leq 2t_0$.

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 $2t_0$. However, these are both equal to $|v_1 - v_2| > 2t_0$, a contradiction. $\square$

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 $\mathcal{Q}$ -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. $\square$

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

Lemma 8.22. For every vertex v of height at most 2.36, we have $C'(v) \subset \text{VC}(0)$.

Proof. Assume for a contradiction that $x \in C'(v) \cap \text{VC}(u)$, 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 $x \in \text{VC}(u)$. 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 $x \in \text{VC}(u)$. The second possibility, together with Lemma 8.18, implies that $\{v, b\}$ is a simplex in the $\mathcal{Q}$ -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 . However, 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 $\arccos(|v|, \sqrt{8}, 2) \geq \arccos(|v|, \sqrt{2}, \sqrt{2})$. 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 $x \in \text{VC}(u)$. The second places x outside the convex hull of $0, b, u$ and gives $|x - u| + |x| > \sqrt{8}$, which is contrary to $|x - u| \leq |x| \leq \sqrt{2}$. The third possibility cannot occur by the observation made at the beginning of the proof that x is unobstructed at 0 . $\square$

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

Lemma 8.23. *Assume $|v| \leq 2.36$. Let $F(v)$ be the intersection of $\Omega(0) \cap \Omega(v)$; that is, the face of the Voronoi cell of $\Omega(0)$ associated with the vertex v . Let $F'(v)$ be the part of $F(v) \cap B(0, 1.18)$ that is not in the cone over any simplex in $\mathcal{Q}_0$. Let $H(v)$ be the closure of the union of segments from the origin to points of $F'(v)$. Let $C''(v)$ be the cone at the origin spanned by $B(0, 1.18) \cap B(v, 1.18)$. Then the closure of $C'(v) \cap C''(v)$ is equal to $H(v)$.*

Proof. We have $F'(v) \subset C''(v)$.

First we show that $F'(v)$ lies in the closure of $C'(v)$. For this, we check that points of $F'(v)$ satisfy the (closed counterparts of) Conditions 1–6 defining $C'(v)$ (see Definition 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 $|x - v| \geq t_0$. Since x is equidistant from v and the origin, we find that $|x| \geq t_0$, 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

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

Corollary 8.25. *If $x \in \text{VC}(0)$, with $0 < |x| \leq 1.18$, if the point at distance 1.18 from 0 along the ray $(0, x)$ does not lie in $\text{VC}(0)$, 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 $|v| \leq 2.36$.*

Proof. If $x \in \text{VC}(0) \cap B(0, 1.18)$, 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. $\square$

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. $\square$

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 [Ha7, 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

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

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

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

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

The parts of $\text{VC}(D)$ 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, $\sigma(S) \leq 0$ by Lemma 8.12. The parts of $\text{VC}(D)$ 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 $s\text{-vor}(S)$ on the simplex. Lemma 8.13 shows that $s\text{-vor}(S) < 0$ as desired.

Next we consider the parts of $\text{VC}(D)$ that are not in any $C'(v)$ (with $|v| \leq 2.36$) 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 $\text{VC}(D)$ 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 $w_1, w_2, \dots, w_k$ 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 Fig. 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' .

Fig. 8.2. A planar region.

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

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 $s\text{-vor}(S) < 0$ 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. $\square$

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

Proof of 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. $\square$

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

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

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 $VC(0) \cap C(S) \subset B(t_S) \subset B(t'_S)$, 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 $V^S(t_0)$ 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 $V^S(t_0)$.

In $VC(0)$, there are nonoverlapping sets

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

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

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

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 $v_1, \dots, v_k$ 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 $j \equiv i + 1 \pmod k$, so that $D_0 = \bigcup W_i$.

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 $j \equiv i + 1 \pmod k$. 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 $\{v, v_j, c_j\}$,

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

if the circumradius of $\{0, v_j, v\}$ permits. (An example of this is illustrated in Fig. 9.1.) Let W^e be the 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 $E_\ell = E_{v_\ell}$.

If Condition 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

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

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

Definition 9.3. In both Conditions 1 and 2, set

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

$$\delta(v, W^e) = \Delta(v, W^e) \setminus B(t_0).$$

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 $\varepsilon_v(\Lambda, x) \in \Lambda$ 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 $\varepsilon_0(\Lambda, x) \in \Lambda$.

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

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

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 $\varepsilon'_0(\Lambda, x)$.

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 $\text{rad}(S) < \eta_0(|v|/2)$. 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 $|w - w'| \leq 2t_0$, and $|w' - w| \geq 2.77$.*
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 $\text{rad}(S) < \eta_0(|v|/2)$ 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 $|w - w'| \geq 2.77$, we see that the orientation of each face of $\{0, v, w, w'\}$ is positive. Since $\text{rad}(S) \geq \eta_0$, we have

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

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

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

(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

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

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 $\text{rad}(S) < \eta_0(|v|/2)$. 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, $\text{rad}(S) \geq \eta_0(|v|/2)$.

We now have that the orientation of F is positive and that $\text{rad}(S) \geq \eta_0(|v|/2)$. 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

$$\varepsilon_0(\{0, u_1, u_2, v\}, x) = v.$$

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

$$\varepsilon_0(\{0, u_1, u_2, v\}, y) \in \{u_1, u_2\}.$$

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 $\text{rad}(S) \geq \eta_0(|v|/2)$. Each interior point x of R_w has

$$\varepsilon'_0(\{0, u_1, u_2, v\}, x) = v.$$

However, each point y in F_0 has

$$\varepsilon'_0(\{0, u_1, u_2, v\}, y) \in \{u_1, u_2\}.$$

This proves this case.

Until the end of the proof, we may assume that $w \notin \{u_1, u_2\}$. If the value of $\varepsilon_0(\{0, u_1, u_2, w\}, \cdot)$ 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 $\text{rad}(S') < \eta_0(|v|/2)$, then each point of R_w is obstructed from u_1 (by Lemma 9.7). However, no point of F_0 is obstructed from u_1 . Thus, R_w and F_0 are disjoint in this case. Assume that $\text{rad}(S') \geq \eta_0(|v|/2)$. 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 $\varepsilon_0(S', x) = w$ 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 $\varepsilon = u_1$ are obstructed from u_1 by $\{0, v, w\}$. However, none of the points of F_0 with $\varepsilon = u_1$ are obstructed from u_1 . $\square$

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. $\square$

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 $\text{rad}(S) < \eta_0(|v|/2)$. 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 $\text{rad}(S) \geq \eta_0(|v|/2)$. 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

$$\varepsilon_0(\{0, u_1, u_2, v\}, x) = v.$$

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

$$\varepsilon_0(\{0, u_1, u_2, v\}, y) \in \{u_1, u_2\}.$$

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 $\text{rad}(S) \geq \eta_0(|v|/2)$. Each interior point x of R_w has

$$\varepsilon'_0(\{0, u_1, u_2, v\}, x) = v.$$

However, each point y in F_0 has

$$\varepsilon'_0(\{0, u_1, u_2, v\}, y) \in \{u_1, u_2\}.$$

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 $\varepsilon_0(\{0, u_1, u_2, w\}, \cdot)$ 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. $\square$

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 $\text{rad}(S)$ 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 $\text{rad}(S) \geq \eta_0(|v|/2)$. 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 $\varepsilon_0 = w$ at $x \in F_0$, let $S'' = \{0, u_1, w, u_2\}$. We have that $\varepsilon_0 = w$ 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 $\varepsilon_0 = u_2$. This case is excluded in the same manner as the parallel case in the earlier Lemmas 9.8 and 9.10. $\square$

Lemma 9.12. *Let $\{0, v\}$ be an upright diagonal of a quarter in the $\mathcal{Q}$ -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. However, 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. $\square$

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 $\text{VC}(0)$.*

Proof. We begin by showing that $\Delta^-(v, W^e) \subset \text{VC}(0)$. Suppose to the contrary, that a point x in the interior of Δ^- lies in $\text{VC}(w)$, 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 $\text{VC}(u)$, 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 $\text{rad}(S) < \eta_0(|v|/2)$, then u and w are anchors. In this case the result follows from Lemma 9.7.

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

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

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

Thus, $\varepsilon_0(S, \cdot)$ 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

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

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 $\varepsilon_0(\{0, w, w'\}, \cdot)$ separates the sets, we are done. Otherwise, we may assume say that $\varepsilon_0(\{0, w, w'\}, x) = w'$ from some $x \in R_w^{(u)}$. Let $S = \{0, u, w, w'\}$.

If w' is not an anchor of u , then $\text{rad}(S) \geq \eta_0(|u|/2)$ and the orientation of S along $\{0, w, u\}$ is positive. In this case we have $\varepsilon_0 = w$ on $R_w^{(u)}$, which is contrary to the 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 $\text{rad}(\{0, u, w, w'\}) < \eta_0(|u|/2)$, then Lemma 9.7 implies that each point of R_w is obstructed from w' . However, 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, and 9.11.) So $\text{rad}(\{0, u, w, w'\}) \geq \eta_0(|u|/2)$. This is contrary to $\varepsilon_0(\{0, w, w'\}, x) = w'$ from some $x \in R_w^{(u)}$. $\square$

9.4. The $\mathcal{S}$ -System Defined

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

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

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

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

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

Type C . This family consists of certain simplices $S(y_1, \dots, y_6)$ 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 $\mathcal{Q}$ -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 $\mathcal{Q}$ -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 $\mathcal{Q}$ -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 $\mathcal{Q}$ -system place the quarters around this diagonal in the $\mathcal{Q}$ -system. So neither $\{0, w, v_1, v_3\}$ nor $\{0, w, v_2, v_3\}$ is in the $\mathcal{Q}$ -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 $\mathcal{Q}$ -system. $\square$

Remark 9.16. The proof of this lemma does not make use of all the hypotheses on C . The conclusion holds for any simplex $S(y_1, \dots, y_6)$, 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 $|v_4|, |v_5| \leq 2t_0$ cannot cross two of the edges $\{v_i, v_j\}$ of S . In fact, it cannot cross any edge $\{v_i, v_j\}$ with $|v_i|, |v_j| \leq 2t_0$ by Lemma 4.30. The only possibility is that the edge $\{v_4, v_5\}$ crosses the two edges with endpoint v_1 , with $|v_1| \geq 2t_0$ in case C . However, 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 $|v_4| \leq 2t_0$, $|v_5| \leq 2\sqrt{2}$. 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 $2.77 \geq \mathcal{E} > 2.77$. $\square$

9.6. Separation of Simplices of Type A

Let $V_S = \text{VC}(0) \cap C(S)$, 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 a 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, $\text{VC}(0) \cap C(S)$ 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 $S(y_1, \dots, y_6)$ 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. However, 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

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

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 i th edge. We establish that the solids representing the conic and Rogers terms of formula (7.12) lie over $C(S)$ by showing⁹ that $\beta_\psi(\text{arc}(y_1, y_3, y_5)) < \text{dih}_3(S(y_1, \dots, y_6))$, 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 $S(y_1, \dots, y_6)$ 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 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.

⁹ CALC-193836552.

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 a 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'),
- $V^S(t_0)$, 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 9.6–9.8, $\sigma(D)$ can be broken into a corresponding sum,

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

By dropping the final term, $4\delta_{\text{oct}} \text{vol}(\delta'_P)$, we obtain an upper bound on $\sigma(V_P)$. Because of the separation results of Sections 9.6–9.7, we may score $V_P^S(t_0)$ 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 star 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 Fig. 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 [Ha6, 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, $\tau = 0$.) $\square$

10. Bounds on the Score in Triangular and Quadrilateral Regions

10.1. The Function τ

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

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

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 $\text{sol}(R) > 0$, so that the result is immediate. If R is a quasi-regular tetrahedron, the result appears in the archive of inequalities CALC-53415898. $\square$

Lemma 10.2.

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

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

$$\sigma(D) = \sum_R \sigma_{R_i}(D) + \left(4\pi - \sum_R \text{sol}(R_i)\right) \zeta pt = 4\pi \zeta pt - \sum_R \tau_{R_i}(D). \quad \square$$

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 $4\pi\zeta pt \approx 22.8pt$. To say that a decomposition star does not contravene is to say that at least $(4\pi\zeta - 8)pt \approx 14.8pt$ 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 [Ha1], the score $s_0 = 4\pi\zeta pt$ corresponds to the *effective density* $16\pi\delta_{\text{oct}}/(16\pi - 3s_0) = \sqrt{2}/\zeta \approx 0.7796$, 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 [Ha6, 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 $\tau_{\text{LP}}(p, q)/pt$ by Table 10.1. The entries marked with an asterisk will not be needed.

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

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

Table 10.1. $\tau_{\text{LP}}(p, q)/pt$

	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	*	*	*	*	*

Proof. Set

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

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 $\tau_{LP}(p, q)$ was chosen to be slightly smaller than the actual minimum of this linear programming problem.

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

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

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

and

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

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

The proof of the first inequalities relies on seven calculations.¹⁰ Throughout the proof, we refer to these inequalities simply as inequality i , for $i = 1, \dots, 7$.

We claim (Claim 1) that if $S_1, \dots, S_5$ are quasi-regular tetrahedra around an edge $\{0, v\}$ and if $S_1 = S(y_1, \dots, y_6)$, where $y_5 \geq \xi$ 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 $\sum_1^5 \text{dih}(S_i) = 2\pi$ and inequalities 3 and 4.

Now let $S_1, \dots, S_8$ 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 calculations¹¹ rather than the seven given above. Claims analogous to Claims 1 and 2 hold for the σ bound by this new group of seven inequalities.

¹⁰ CALC-636208429.

¹¹ CALC-129662166.

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 . 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 $0.55pt$ 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, and 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, and 7. $\square$

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 $S_1, \dots, S_5$ be quasi-regular tetrahedra around the edge $\{0, v\}$. Then*

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

Proof. If any of the top edges has length greater than ξ , we use a slightly improved calculation¹² that yields this constant. Otherwise, the same calculation¹³ that was used in the previous lemma gives the desired estimate

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

¹² CALC-241241504-1.

¹³ CALC-82950290.

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 $0.1317 \approx 2.37838774 \text{ pt}$.

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

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

Proof. A calculation¹⁴ asserts precisely this. $\square$

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. Calculations¹⁵ 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 . $\square$

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 $\tau_{LP}(p, q) > (4\pi\zeta - 8)pt$, 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. $\square$

Remark 10.11. In summary of the preceding two lemmas, we find that we may restrict our attention to the following types of vertices:

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

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

¹⁴ CALC-996268658.

¹⁵ CALC-657406669, CALC-208809199, CALC-984463800, and CALC-277330628.

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 $\text{vor}_P(D, \sqrt{2})$. 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 $v_1, \dots, v_4, v$ subject to the constraints*

$$\begin{aligned} 2 &\leq |v_i| \leq 2t_0, \\ 2 &\leq |v_i - v_{i+1}| \leq 2t_0, \\ 2 &\leq |v_i - v_{i+2}|, \\ h_i &\leq |v - v_i|, \\ 2 &\leq |v| \leq 2t_0, \quad \text{for } i = 1, \dots, 4 \pmod{4}, \end{aligned}$$

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 $v_1, \dots, v_4$ and v subject to the constraints above together with the additional constraints

$$\begin{aligned} |v_i - v_{i+1}| &= 2t_0, \\ |v_i| &= 2, \quad \text{for } i = 1, \dots, 4, \\ |v| &= 2t_0. \end{aligned}$$

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

Proof. This lemma in pure geometry is a special case of Lemma 4.3 of [Ha6]. □

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

Proof. Let $v_1, \dots, v_4$ be the corners of the quad cluster, and let v be an enclosed vertex of height at most $2t_0$. We cannot have $|v_i - v| \leq 2t_0$ 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 $i = 1, \dots, 4$. Reindexing and perturbing v as necessary, we may assume that $2 \leq |v_1 - v| \leq 2t_0$ and $|v_i - v| \geq 2t_0$, 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. $\square$

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

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 $-1.04pt$, 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 use¹⁶ the function $s\text{-vor}$ on S rather than truncation $s\text{-vor}_0$.

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 $u \neq v$, 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 formula (7.11), the score of this cone is $2\pi(1 - h/\eta_0(h))\varphi(h, \eta_0(h))$. An optimization in one variable gives an upper bound of $-4.52pt$, for $t_0 \leq h \leq \sqrt{2}$. This gives the bound of $-1.04pt$ 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 $-4.52pt/2 < -1.04pt$.

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

$$K(S) = K_0(y_1, y_2, y_6) + K_0(y_1, y_3, y_5) + \text{dih}(S)(1 - y_1/\sqrt{8})\varphi(y_1/2, \sqrt{2}), \quad (10.1)$$

¹⁶ CALC-185703487, CALC-69785808, and CALC-104677697.

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

where

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

(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 (Fig. 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 $\sqrt{2}$.

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 calculations¹⁷ 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 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 . Calculations¹⁸ 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 alternative¹⁹ 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 score²⁰ below

¹⁷ CALC-104677697, CALC-69785808, CALC-586706757, and CALC-87690094.

¹⁸ CALC-185703487 and CALC-441195992.

¹⁹ CALC-848147403, CALC-969320489, and CALC-975496332.

²⁰ CALC-766771911.

$-1.04 pt$. 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 $\varphi_0 = \varphi(t_0, t_0) \approx -0.5666$. We define

$$\text{crown}(h) = 2\pi(1 - h/\eta_0(h))(\varphi(h, \eta_0(h)) - \varphi_0). \quad (10.2)$$

It is equal to $-4\delta_{\text{oct}}$ 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 $\text{crown}(|v|/2)$ lies outside the truncated V -cell, but inside the V -cell, so that if P is a quad cluster,

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

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 $\text{anc}(|v'|, |v|, |v - v'|)$ to account for this. Figure 10.2 illustrates the terms in the definition of $\text{anc}()$.

Set

$$\begin{aligned} \text{anc}(y_1, y_2, y_6) = & -\text{dih}(R_1) \text{crown}(y_1/2)/(2\pi) - \text{sol}(R_1)\varphi_0 + \text{r-vor}(R_1) \\ & - \text{dih}(R_2)(1 - y_2/2t_0)(\varphi(y_2/2, t_0) - \varphi_0) \\ & - \text{sol}(R_2)\varphi_0 + \text{r-vor}(R_2), \end{aligned} \quad (10.3)$$

Fig. 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

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

In general, when there are multiple anchors around the same enclosed vertex v , we add a term $(2 - k) \text{anc}$ 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 $\text{anc}()$ at v' and v'' overlap. When this occurs, the geometric decomposition on which the correction terms $\text{anc}()$ are based is no longer valid. In this case, other methods must be used.

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 $\text{vor}_{0,P}(D')$ as we do for standard clusters. (P, D') does not contain any quarters.

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

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 $Q = S(y_1, y_2, \dots, y_6)$ and no additional anchors. In this context $\sigma(Q) = \mu(Q)$. Let v be the enclosed vertex. To compare $\sigma_P(D)$ with $\text{vor}_{0,P}(D')$, consider the V -cell near Q . The quarter Q cuts a wedge of angle $\text{dih}(Q)$ 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

$$\begin{aligned} \text{c-vor}(V_P) &< (1 - \text{dih}(Q)/(2\pi)) \text{crown}(y_1/2) + \text{anc}(y_1, y_2, y_6) \\ &+ \text{anc}(y_1, y_3, y_5) + \text{c-vor}(V_P^v). \end{aligned} \tag{10.4}$$

Fig. 10.3. The terms anc near an upright quarter.

Combining this inequality with calculations,²¹ we find

$$\text{c-vor}(V_P) + \mu(Q) < \text{c-vor}(V_P^v) + \text{s-vor}_0(Q). \quad (10.5)$$

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: $\text{dih}(Q_1) + \text{dih}(Q_2) < \pi$ or $\text{rad}(0, v, v_1, v_3) \geq \eta(|v|, 2, 2t_0)$. 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

$$\begin{aligned} \text{c-vor}(V_P) &< (1 - (\text{dih}(Q_1) + \text{dih}(Q_2))/(2\pi)) \text{crown}(|v|/2) \\ &+ \text{anc}(F_1) + \text{anc}(F_2) + \text{c-vor}(V_P^v). \end{aligned} \quad (10.6)$$

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, $\text{anc}(F_i) = \text{anc}(y_i, y_j, y_k)$ for a face F_i with edges y_i along an upright quarter. By a calculation²² applied to both Q_1 and Q_2 , we have

$$\text{c-vor}(V_P) + \sum_{i=1}^2 \sigma(Q_i) < \text{c-vor}(V_P^v) + \sum_{i=1}^2 \text{s-vor}_0(Q_i). \quad (10.7)$$

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.

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

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

²¹ CALC-906566422, CALC-703457064, and CALC-175514843.

²² CALC-554253147.

and this implies $|v| \geq 2.696$. We have²³

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

Inequality (10.7) 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 (10.5) or (10.7). 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 $\text{anc}()$ overlap. More precisely, if Z is a set of enclosed vertices, set $V_P^Z = \bigcap_{v \in Z} V_P^v$, 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 (10.5) and (10.7), if $v \notin Z$. In sum, $\sigma_P(D) < \text{vor}_{0,P}(D)$. $\square$

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²³ CALC-855677395.