A FORMULATION OF THE KEPLER CONJECTURE

SAMUEL P. FERGUSON, THOMAS C. HALES

The Kepler conjecture asserts that the density of a packing of equal spheres cannot be greater than that of the face-centered cubic packing. There are various optimization problems in finitely many variables that imply the Kepler conjecture. The first was introduced by L. Fejes Tóth [FT]. His formulation was based on the Voronoi decomposition of space. In [H1], a dual formulation based on the Delaunay decomposition was proposed. Later, in [I], the two strategies were combined to partition space by a combination of the Voronoi and Delaunay decompositions.

The Voronoi and Delaunay decompositions can be mixed in infinitely many ways. This gives a large set of optimization problems in finitely many variables that imply the Kepler conjecture. Each of these optimization problems is a formulation of the Kepler conjecture.

The selection of a good formulation of the Kepler conjecture is a central issue in the resolution of the conjecture. Our experience suggests that whenever the technical difficulties become too great it is generally better to rework the formulation of the problem rather than to confront the technical difficulties directly. It is the infinite dimensionality of the problem that gives the flexibility to skirt these technical problems.

In [I], five steps were suggested, which collectively imply the Kepler conjecture. The formulation suggested in [I] was sufficient to see the first two steps to completion. To see the third and fifth steps to completion, it has been necessary to make some adjustments. This paper makes those changes. The proofs of the third and fifth steps, found in [III] and [V], rely essentially on the constructions and results of this paper. We have been careful to modify the constructions in a way that does not affect the proofs of the first two steps of the program. Lemma 3.13, Proposition 3.14, Conjecture 3.15, and Theorem 3.16 are the results needed to bring the results of [I] and [II] into harmony with this paper. Proposition 4.1 is used in [III] and [V]. Proposition 4.7 brings significant simplifications to the calculations of [III].

Our formulation has departed more than ever from the original formulation on the space of Delaunay stars (defined in [H1]). The Delaunay decomposition plays a smaller role here than in any of our previous papers, although many of the concepts it inspired remain (such as the compression of a simplex, quasi-regular tetrahedra, and quarters). To reflect this change in formulation, we now call the stars decomposition stars.

Research supported in part by the NSF

Typeset by \LaTeX
1. Geometric Decomposition

Fix a packing of spheres of radius 1. The centers of the spheres are called vertices. Fix the constant 2.51. It is used throughout this paper and all of our related papers on the subject. A quasi-regular tetrahedron is the simplex formed by four vertices, each at most 2.51 from the others. A quarter is defined as a simplex whose edge lengths $y_1, \ldots, y_6$ can be ordered to satisfy $2.51 \leq y_1 \leq \sqrt{8}$, $2 \leq y_i \leq 2.51$, $i = 2, \ldots, 5$. We call the longest edge of a quarter its diagonal. When the quarter has a distinguished vertex, the quarter is upright if the distinguished vertex is an endpoint of the diagonal, and flat otherwise.

If four quarters fit together along a common diagonal, forming a figure with six vertices, the resulting figure is called an octahedron. The octahedron may have more than one diagonal of length at most $\sqrt{8}$, so its decomposition into four quarters need not be unique. (This definition of octahedron differs from the one given in [I], but we will never return to the earlier definition.)

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

We say that two manifolds with boundary overlap if their interiors intersect. We define the projection of a set $X$ to be the radial projection of $X \setminus 0$ to the unit sphere centered at the origin. We say they cross if their projections to the unit sphere overlap. We label the edges of a simplex $S(y_1, \ldots, y_6)$ as in [I]. In general, let $\text{dih}(S)$ be the dihedral angle of a simplex $S$ along its first edge. When we write a simplex in terms of its vertices $(w_1, \ldots, w_4)$, then $(w_1, w_2)$ is understood to be the first edge. We define a function $E(S(y_1, \ldots, y_6), y'_1, y'_2, y'_3)$ by taking two simplices $S = S(y_1, \ldots, y_6)$ and $S' = S(y'_1, y'_2, y'_3, y_4, y_5, y_6)$, and moving $S'$ until the simplices do not overlap, and the face formed by the fourth, fifth, and sixth edges of $S$ and $S'$ coincide. $E$ is defined only if $S$ and $S'$ exist, and then it is defined as the distance between the origin and the vertex $v'$ of $S'$ opposite the common face (Diagram 1.1).

\[\text{Diagram 1.1}\]

If intervals containing $y_1, \ldots, y_6, y'_1, y'_2, y'_3$ are given, lower bounds on $E$ over that...
domain are generally easy to obtain. For example, if the segment from the vertex \( v' \) of \( S' \) to the origin passes through the face common to \( S \) and \( S' \), then \( \mathcal{E} \) is increasing in the variables \( y_1, y_2, y_3, y_1', y_2', y_3' \) (at least until we deform the simplices sufficiently that the segment no longer passes through the common face). A pivot is the circular motion of a vertex at a fixed distance from two others (see [I]). The axis of the pivot is the line through the two fixed vertices. By using pivots, we observe that \( \mathcal{E} \) is monotonic decreasing in \( y_4, y_5, y_6 \). For example, if we pivot the first vertex away from the third around the axis through the second edge, \( \mathcal{E} \) is unaffected. Because these lower bounds are generally so easily determined, we will state them without proof. We will state that these bounds were obtained by geometric considerations, to indicate that the bounds were obtained by the monotonicity arguments of this paragraph.

**Lemma 1.2.** No vertex of the packing is contained in the interior of a quasi-regular tetrahedron or quarter.

*Proof.* See I.3.5. □

**Corollary.** No vertex of the packing is contained in the interior of an octahedron. □

**Lemma 1.3.** An edge of length 2.51 or less cannot pass through a face whose edges have lengths 2.51, 2.51, and \( \sqrt{8} \) or less.

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

\[
\mathcal{E}(S(2, 2, 2, 2.51, 2.51, \sqrt{8}), 2, 2, 2) > 2.51.
\]

□

**Lemma 1.4.** If the diagonal of a quarter passes through a face of a quasi-regular tetrahedron, then each of the two endpoints of the diagonal edge is at most 2.2 away from each of the vertices of the face (see Diagram I.3.1).

*Proof.* Let the diagonal edge be \((w_1, w_2)\) and the vertices of the face be \((v_1, v_2, v_3)\). If \(|v_i - w_j| > 2.2\) for some \(i, j\), then geometric considerations give

\[
|w_1 - w_2| \geq \mathcal{E}(S(2, 2, 2, 2.51, 2.51, 2.51), 2, 2, 2) > \sqrt{8}.
\]

□

As in earlier papers, \( \eta(x, y, z) \) denotes the circumradius of a triangle with edge-lengths \( x, y, \) and \( z \). Suppose that \( S \) and \( S' \) are adjacent quasi-regular tetrahedra with a common face \( F \). As in Lemma 1.4, suppose that a diagonal of a quarter runs between the opposite vertices of \( S \) and \( S' \) through the face \( F \). By the lemma, each of the six external faces of the pair of quasi-regular tetrahedra has circumradius at most \( \eta(2.2, 2.2, 2.51) < \sqrt{8} \). A diagonal of a quarter cannot pass through a face of this size [I.3.2]. This pair of quasi-regular tetrahedra is the union of three quarters.
Lemma 1.5. Suppose an edge \((w_1, w_2)\) of length at most \(\sqrt{8}\) passes through the face formed by a diagonal \((0, v_1)\) and one of its anchors. Then \(w_1\) and \(w_2\) are also anchors of \((0, v_1)\).

Proof. \(E(S(2, 2, 2, \sqrt{8}, 2.51, 2.51), 2, 2, 2.51) > \sqrt{8}\). □

The height of a vertex is its distance from the origin. We say that a vertex is enclosed over a figure if it lies in the interior of the cone at the origin generated by the figure.

If we draw a geodesic arc on the unit sphere with endpoints at the projections of \(v_1\) and \(v_2\) for every pair of vertices \(v_1, v_2\) such that \(|v_1|, |v_2|, |v_1 - v_2| \leq 2.51\), we obtain a planar map that breaks the unit sphere into regions called standard regions. (The arcs do not meet except at endpoints \([I.3.10]\).)

By a pair of adjacent quarters, we mean two quarters sharing a face along the diagonal. The common vertex that does not lie on the diagonal is called the base point of the pair of adjacent quarters. The other four vertices are called the corners of the configuration.

Lemma 1.6. Suppose that there exist four vertices \(v_1, \ldots, v_4\) of height at most 2.51 (that is, \(|v_i| \leq 2.51\)) forming a skew quadrilateral. Suppose that the diagonals \((v_1, v_3)\) and \((v_2, v_4)\) have lengths between 2.51 and \(\sqrt{8}\). Suppose the diagonals \((v_1, v_3)\) and \((v_2, v_4)\) cross. Then the four vertices are the corners of a pair of adjacent quarters with base point at the origin.

Proof. Set \(d_1 = |v_1 - v_3|\) and \(d_2 = |v_2 - v_4|\). By hypothesis, \(d_1\) and \(d_2\) are at most \(\sqrt{8}\). If \(|v_1 - v_2| > 2.51\), geometric considerations give the contradiction

\[
\max(d_1, d_2) \geq E(S(2.51, 2, 2.51, \sqrt{8}, 2.51), 2, 2, 2) > \sqrt{8} \geq \max(d_1, d_2).
\]

Thus, \((0, v_1, v_2)\) determines a bounding arc of standard region, as do \((0, v_2, v_3)\), \((0, v_3, v_4)\), and \((0, v_4, v_1)\) by symmetry. □

Lemma 1.7. If, in the context of Lemma 1.6, there is a vertex \(w\) of height at most \(\sqrt{8}\) enclosed over the pair of adjacent quarters, then \((0, v_1, \ldots, v_4, w)\) is an octahedron.

Proof. If the enclosed \(w\) lies over say \((0, v_1, v_2, v_3)\), then \(|w - v_1|, |w - v_3| \leq 2.51\) (Lemma 1.5), where \((v_1, v_3)\) is a diagonal. Similarly, the distance from \(w\) to the other two corners is at most 2.51. □
We will select a nonoverlapping collection of quarters and quasi-regular tetrahedra, called a \( Q \)-system (for quarters and quasi-regulars). For each octahedron, we fix a diagonal of length at most \( \sqrt{8} \) and place the four quarters along that diagonal in the \( Q \)-system, but not the overlapping quarters situated along other diagonals of the octahedron. Place all quasi-regular tetrahedra in the \( Q \)-system. This, of course, prevents us from placing any quarters that overlap these tetrahedra into the \( Q \)-system (as in Lemma 1.4).

Fix the origin at the base point of a pair of adjacent quarters. We investigate the local geometry when another quarter overlaps one of them. This happens, for example, if both diagonals between opposite corners of the pair of quarters have lengths at most \( \sqrt{8} \). We will see that a conflict like this between the diagonals between corners is the only way a pair of adjacent quarters can overlap another quarter. We call these conflicting diagonals. Label the four corners of the pair of quarters \( v_1, v_2, v_3, v_4 \), with \( (v_1, v_3) \) the common diagonal. We say that an edge is short if its length is at most 2.51.

**Case 1.** There is an enclosed vertex \( w \), say over \( (v_1, v_2, v_3) \), where \( (0, w) \) is a diagonal of a quarter. Lemma 1.5 implies that \( v_1 \) and \( v_3 \) are anchors of \( (0, w) \). The only other possible anchors of \( (0, w) \) are \( v_2 \) or \( v_4 \), for otherwise a short edge passes through a face formed by \( (0, w) \) and one of its anchors. If both \( v_2 \) and \( v_4 \) are anchors, then we have an octahedron. Otherwise, \( (0, w) \) has at most 3 anchors: \( v_1, v_3 \), and either \( v_2 \) or \( v_4 \). In fact, it must have exactly three anchors, for otherwise there is no quarter along the edge \( (0, w) \). So there are exactly two quarters along the edge \( (0, w) \). We place the quarters along the diagonal \( (v_1, v_3) \) in the \( Q \)-system. The other two quarters, along the diagonal \( (0, w) \), are not placed in the \( Q \)-system. They form a pair of adjacent quarters (with base point \( v_4 \) or \( v_2 \)) that has conflicting diagonals, \( (0, w) \) and \( (v_1, v_3) \), of length at most \( \sqrt{8} \).

**Case 2.** \( (v_2, v_4) \) is a diagonal of length at most \( \sqrt{8} \) (conflicting with \( (v_1, v_3) \)). By symmetry, we may assume that \( (v_2, v_4) \) passes through the face \( (0, v_1, v_3) \). Assume (for a contradiction) that both diagonals have an anchor other than the corners \( v_i \). Let the anchor of \( (v_2, v_4) \) be denoted \( v_{24} \) and that of \( (v_1, v_3) \) be \( v_{13} \). Assume the figure is not an octahedron, so that \( v_{13} \neq v_{24} \). By Lemma 1.3, it is impossible to draw the edges \( (v_1, v_{13}) \) and \( (v_{13}, v_3) \) between \( v_1 \) and \( v_3 \). In fact, if the edges pass outside the quadrilateral \( (0, v_2, v_{24}, v_4) \), one of the short edges \( (0, v_2), (v_2, v_{24}), (v_{24}, v_4), \) or \( (v_4, 0) \) violates the lemma applied to the face \( (v_1, v_3, v_{13}) \). If they pass inside the quadrilateral, one of the edges \( (v_1, v_{13}), (v_{13}, v_3) \) violates the lemma applied to the face \( (0, v_2, v_4) \) or \( (v_{24}, v_2, v_4) \). We conclude that at most one of the two diagonals has additional anchors.

If neither of the two diagonals has more than three anchors, we have nothing more than two overlapping pairs of adjacent quarters along conflicting diagonals. Place the two quarters along the lower edge \( (v_2, v_4) \) into the \( Q \)-system. If there is a diagonal with more than three anchors, place the quarters along the diagonal with more than three anchors in the \( Q \)-system. In both possibilities of case 2, the two quarters left out of the \( Q \)-system correspond to a conflicting diagonal.

By the following lemma, Cases 1, 2, and the octahedron are the only possibilities for a pair of adjacent quarters.
Lemma 1.8. Let $v_1$ and $v_2$ be anchors of $(0, w)$ with $2.51 \leq |w| \leq \sqrt{8}$. If an edge $(v_3, v_4)$ passes through both faces, $(0, w, v_1)$ and $(0, w, v_2)$, then $|v_3 - v_4| > \sqrt{8}$.

Proof. Suppose the figure exists with $|v_3 - v_4| \leq \sqrt{8}$. Label vertices so $v_3$ lies on the same side of the figure as $v_1$. Contract $(v_3, v_4)$ by moving $v_3$ and $v_4$ until $(v_1, u)$ has length 2, for $u = 0, w, v_{i-2}$, and $i = 3, 4$. Pivot $w$ away from $v_3$ and $v_4$ around the axis $(v_1, v_2)$ until $|w| = \sqrt{8}$. Contract $(v_3, v_4)$ again. By stretching $(v_1, v_2)$, we obtain a square of edge two and vertices $(0, v_3, v_4)$. Short calculations based on I.8.3.1 and its partial derivatives give

\begin{align*}
(1.7.1) \quad \text{dih}(S(\sqrt{8}, 2, y_3, 2, y_5, 2)) > 1.075, & \quad y_3, y_5 \in [2, 2.51], \\
(1.7.2) \quad \text{dih}(S(\sqrt{8}, y_2, 2, 2, y_5, y_6)) > 1, & \quad y_2, y_3, y_5, y_6 \in [2, 2.51].
\end{align*}

Then

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

Therefore, the figure does not exist. □

Lemma 1.9. Let $v_1, v_2, v_3$ be anchors of $(0, w)$, where $2.51 \leq |w| \leq \sqrt{8}$, $|v_1 - v_3| \leq \sqrt{8}$, and the edge $(v_1, v_3)$ passes through the face $(0, w, v_2)$. Then $\text{min}(|v_1 - v_2|, |v_2 - v_3|) \leq 2.51$. Furthermore, if the minimum is 2.51, then $|v_1 - v_2| = |v_2 - v_3| = 2.51$.

Proof. Assume $\text{min} \geq 2.51$. As in the proof of Lemma 1.8, we may assume that $(0, v_1, w, v_3)$ is a square. We may also assume, without loss of generality, that $|w - v_2| = |v_2| = 2.51$. This forces $|v_2 - v_i| = 2.51$, for $i = 1, 3$. This is rigid, and is the unique figure that satisfies the constraints. The lemma follows. □

Assume that there are two quarters $Q_1$ and $Q_2$ that overlap. Assume that neither is adjacent to another quarter. Let $(0, u)$ and $(v_1, v_2)$ be the diagonals of $Q_1$ and $Q_2$. Suppose the diagonal $(v_1, v_2)$ passes through a face $(0, u, w)$ of $Q_1$. By Lemma 1.5, $v_1$ and $v_2$ are anchors of $(0, u)$. Again, either the length of $(v_1, w)$ is at most 2.51 or the length of $(v_2, w)$ is at most 2.51, say $(w, v_2)$. It follows that $Q_1 = (0, u, w, v_2)$ and $|v_1 - w| \geq 2.51$. ($Q_1$ is not adjacent to another quarter.) So $w$ is not an anchor of $(v_1, v_2)$.

Let $(v_1, w', v_2)$ be a face of $Q_2$ with $w' \neq 0, u$. If $(v_1, w', v_2)$ does not link $(0, u, w)$, then $(v_1, w')$ or $(v_2, w')$ passes through the face $(0, u, w)$, which is impossible by Lemma 1.3. So $(v_1, v_2, w')$ links $(0, u, w)$ and an edge of $(0, u, w)$ passes through the face $(v_1, v_2, w')$. It is not the edge $(u, w)$ or $(0, w)$, for they are too short by Lemma 1.3. So $(0, u)$ passes through $(w', v_1, v_2)$. The only other anchors of $(v_1, v_2)$ are $u$ and $0$ (by Lemma 1.8). Either $(u, w')$ or $(w', 0)$ has length at most 2.51 by Lemma 1.9, but not both, because this would create a quarter adjacent to $Q_2$. By symmetry, $Q_2 = (v_1, v_2, w', 0)$ and the length of $u, w'$ is greater than 2.51. By symmetry, $(0, u)$ has no other anchors either. This determines the local geometry when there are two quarters that intersect without belonging to a pair of adjacent quarters (see Diagram 1.10).
When there are two isolated but overlapping quarters $Q_1$ and $Q_2$, then we place neither in the $Q$-system. (We call such a configuration an isolated pair.) This completes the specification of the $Q$-system. By construction, if any quarter along a diagonal lies in the $Q$-system, then all quarters along the diagonal lie in the $Q$-system.

**Lemma 1.11.** Two vertices of height at most $\sqrt{8}$ cannot be enclosed over a flat quarter.

**Proof.** Assume the figure exists. The diagonal $(v_1, v_2)$ of the quarter $(0, v_1, v_2, v_3)$ has anchors $(0, v_3, w, w')$. Lemma 1.8 gives $|w'| > \sqrt{8}$. □

## 2. Voronoi Cells

In this section, we show that a mild modification of the Voronoi cells, called $V$-cells, is compatible with the $Q$-system.

Recall from Section I.8.2, that the orientation of the face of a simplex is said to be negative if the plane through that face separates the circumcenter of the simplex from the vertex of the simplex that does not lie on the face. The orientation is positive if the circumcenter and the vertex lie on the same side of the plane.

**Lemma 2.1.** At most one face of a quarter $Q$ has negative orientation.

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

**Lemma 2.2.** Let $Q$ be a quarter with a face $F$ along the diagonal. Let $v$ be any vertex not on $Q$. If the simplex $(F, v)$ has negative orientation along $F$, then it is
a quarter.

A similar result holds for quasi-regular tetrahedra (Part I).

Proof. The orientation of $F$ is determined by the sign of the function $\chi$ (see Section I.8.2). The face $F$ is an acute triangle, so by the explicit results for $\chi$ in I.8.2, the function $\chi$ is increasing in the lengths of $v$ to the vertices of $F$. We show that $\chi \geq 0$ if any of these lengths is greater than 2.51. We evaluate

$$\chi(2^2, 2^2, 2.51^2, x^2, y^2, z^2), \quad \chi(2^2, 2.51^2, 2^2, x^2, y^2, z^2), \quad \chi(2.51^2, 2^2, 2^2, x^2, y^2, z^2),$$

for $(x, y, z) \in [2, 2.51]^2[2.51, \sqrt{8}]$, and verify that this is so. (The minimum, which must be attained at corner of the domain, is 0.) □

The lemma and the results of [1] imply that if $x \in Q$ lies in the interior of Voronoi cell at a vertex $v$ other than those of $Q$, then $v$ is a vertex of a quarter or quasi-regular tetrahedron adjacent to $Q$. The Voronoi cells at the vertices of simplices in the $Q$-system cover all the simplices in the $Q$-system.

What about regions outside the $Q$-system? A simplex $S$ in the $Q$-system may have negative orientation with respect to a face that does not bound another simplex in the $Q$-system. In this case, the Voronoi cell at the vertex $v_0$ opposite this face protrudes beyond the negatively oriented face. More precisely, we define the tip protruding from a simplex $S$ associated with a vertex $v_0$ of $S$ to be the set of points that are closer to $v_0$ than to any other vertex of $S$ and that are separated from $v_0$ by the plane through the face of $S$ opposite $v_0$. Each point $x$ outside the $Q$-system belongs to finitely many protruding tips from simplices in the $Q$-system, say those associated with the vertices $w_1(x), \ldots, w_k(x)$. (Typically, this collection of vertices is empty.) Deleting the vertices $w_i(x)$ from the packing, we take the Voronoi decomposition of the remaining collection of vertices. The point $x$ lies in the (modified) Voronoi cell at some vertex $w(x) \neq w_i(x)$. The set of points $x$ outside the $Q$-system such that $v = w(x)$ will be called the $V$-cell at $v$. By construction, points in the $Q$-system do not lie in any $V$-cell. Outside the $Q$-system, $V$-cells agree with Voronoi cells except in the treatment of protruding tips. Occasionally, we will refer to the faces of $V$-cells as $V$-faces to distinguish them from other types of faces, such as those of quarters.

This is our decomposition of space: all the simplices in the $Q$-system and all the $V$-cells.

3. Scoring

To each vertex $v$, we attach a decomposition star, which is defined as the union of the $V$-cell at $v$ with all the quasi-regular tetrahedra and quarters in the $Q$-system with a vertex at $v$. Decomposition stars replace the Delaunay stars found in earlier papers. By construction, $V$-cells, the $Q$-system, and decomposition stars are compatible with standard regions. By this, we mean in particular that the intersection of a $V$-cell with the cone over a standard region is entirely determined by the vertices in the cone. (See II.2.2.) Also, each simplex in the $Q$-system lies over a single standard region.
A standard cluster attached to a standard region $P$ is the union of the simplices in the $Q$-system over $P$ with the part of the $V$-cell that lies over $P$. A quad cluster is the standard cluster obtained when the standard region is a quadrilateral.

Recall that the Voronoi function $\text{vor}(S)$ is an analytic continuation, defined initially on simplices $S$ whose faces have positive orientation. Let $\text{sol}(S)$ be the solid angle of $S$ at its distinguished vertex. Set $\delta_{\text{oct}} = (\pi - 4 \arctan(\sqrt{2}/5))/\sqrt{8}$. Set

\begin{equation}
\text{vor}(S) = 4(-\delta_{\text{oct}} \text{vol}(\hat{S}_0) + \text{sol}(S)/3),
\end{equation}

where $\hat{S}_0 \subset S$ is the Voronoi region defined in [I.2]. An explicit formula for $\text{vor}(S)$ is found in [I.8.6.3]. This formula may be analytically continued to simplices $S$ with negatively oriented faces, and $\text{vor}(S)$ is defined in general by this analytic continuation. Let $S_1, \ldots, S_4$ be equal to $S$ as unlabeled simplices, but with different distinguished vertices. Set $4\Gamma(S) = \sum_{i=1}^{4} \text{vor}(S_i)$. $\Gamma$ is called the compression of $S$. The definition here is equivalent to the one in [I].

We define truncated versions $\text{vor}(S, t)$ of the Voronoi function, depending on a truncation parameter $t \leq \sqrt{8}$, and a simplex $S = S(y_1, \ldots, y_6)$. Set $h_i = y_i/2$, $d_i = \text{dih}_i(S)$, the dihedral angle along edge $i = 1, 2, 3$. Let $C(h, t)$ denote the compact cone of height $h$ and circular base of area $\pi(t^2 - h^2)$. Set

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

Then

\begin{equation}
2\pi(1 - h/t)\phi(h, t) = (-\delta_{\text{oct}}\text{vol}(C(h, t)) + \text{sol}(C(h, t))/3),
\end{equation}

represents the score of $C(h, t)$. The solid angle of $C(h, t)$ is $2\pi(1 - h/t)$, so $\phi(h, t)$ is the score per unit area. Also, $\phi(t, t)$ is the score per unit area of a ball of radius $t$. That is, $\phi(t, t) = 4(-\delta_{\text{oct}}\text{vol}/\text{sol} + 1/3)$.

If $R = R(a, b, c)$ is a Rogers simplex (defined in I.8.6), we set

\begin{equation}
6\text{quo}(R) = (a + 2c)(c - a)^2 \arctan(e) + a(b^2 - a^2)e
- 4c^3 \arctan(e(b - a)/(b + c)),
\end{equation}

where $e \geq 0$ is given by $e^2(b^2 - a^2) = (c^2 - b^2)$. The function $\text{quo}(R)$ (the quoin of $R$) is the volume of a wedge-like region situated above the Rogers simplex $R$. It is defined as the region bounded by the four planes through the faces of $R$ and a sphere of radius $c$ at the origin. (See Diagram 3.4.)

**Diagram 3.4**
We set

\[
\text{vor}(S, t) = \text{sol}(S) \phi(t, t) + \sum_{i=1}^{3} d_i (1 - h_i/t) (\phi(h_i, t) - \phi(t, t))
\]

(3.5)

\[
- \sum_{(i,j,k) \in S_3} 4\delta_{\text{oct}} \text{quo}(R(h_i, \eta(y_i, y_j, y_k+3), t)).
\]

In the definition, we adopt the convention that \(\text{quo}(R) = 0\), if \(R = R(a, b, c)\) does not exist (that is, if the condition \(0 < a < b < c\) is violated). In the second sum, \(S_3\) is the set of permutations on three letters. This formula has a simple geometric interpretation when the circumradius of \(S\) is greater than \(t\) and the circumradius of each face is less than \(t\). It represents the score of the part of the Voronoi cell at the origin that lies inside \(S\) and inside a ball of radius \(t\). This can be seen geometrically from Diagram 3.6, which depicts the intersection of \(S\) with the Voronoi cell as three quadrilaterals forming a triangle. The truncation in the second frame is shown as a shaded region. The truncated volume can be decomposed into a solid angle term, three conic terms, and six quoins (with appropriate sign conventions). Hence the formula for \(\text{vor}(S, t)\).

![Diagram 3.6](image)

Similarly, we define \(\text{vor}(P, t)\) for arbitrary standard clusters \(P\). Extending the notation in an obvious way, we have

\[
\text{vor}(P, t) = \text{sol}(P) \phi(t, t) + \sum_{|v_i| \leq 2t} d_i (1 - |v_i|/(2t)) (\phi(|v_i|/2, t) - \phi(t, t))
\]

(3.7)

\[- \sum_{R} 4\delta_{\text{oct}} \text{quo}(R).\]

The first sum runs over vertices in \(P\) of height at most \(2t\). The second sum runs over Rogers simplices \(R(|v_i|/2, \eta(F), t)\) in \(P\), where \(F = (0, v_1, v_2)\) is a face of circumradius \(\eta(F)\) at most \(t\), formed by vertices in \(P\). The constant \(d_i\) is the total dihedral angle along \((0, v_i)\) of the standard cluster. The truncations \(t = t_0 = 1.255 = 2.51/2\) and \(t = \sqrt{2}\) will be of particular importance. Set \(A(h) = (1 - h/t_0)(\phi(h, t_0) - \phi(t_0, t_0)).\)

We are ready to define the scoring of quarters and quasi-regular tetrahedra in the \(Q\)-system. \(\sigma(Q)\) will denote the score of a quarter or a quasi-regular tetrahedron. Let \(S\) be a quasi-regular tetrahedron. We set \(\sigma(S) = \Gamma(S)\) if the circumradius of \(S\) is less than 1.41, and \(\sigma(S) = \text{vor}(S)\) otherwise. This definition agrees with [I].

Fix a quarter \(Q\). Let \(\eta^+(Q)\) be the maximum of the circumradii of the two faces of \(Q\) along the diagonal of \(Q\). Set \(t_0 = 1.255\) and \(\text{vor}_0(Q) = \text{vor}(Q, t_0)\). Set

\[
\mu(Q) = \begin{cases} 
\Gamma(Q), & \text{if } \eta^+(Q) \leq \sqrt{2}, \\
\text{vor}(Q), & \text{otherwise}.
\end{cases}
\]

(3.8)
If $Q$ is a flat quarter, we simply set $\sigma(Q) = \mu(Q)$.

Suppose $Q$ is upright. Let $\hat{Q}$ be the upright quarter, which is the same as $Q$ considered as an unlabeled simplex but whose distinguished vertex lies at the opposite endpoint of the diagonal. We say that the context of $Q$ is $(p, q)$ if there are $p - q$ quarters along the diagonal of $Q$, and if there are $p$ anchors. $q$ is the number of “gaps” between anchors around the diagonal. For example, the context of a quarter in an octahedron is $(4, 0)$. The context of a single quarter is $(2, 1)$. The only possible contexts of upright quarters in a quad cluster are $(4, 0)$, $(3, 1)$, and $(2, 1)$. Of course, $Q$ and $\hat{Q}$ have the same context. The definition of $\sigma(Q)$ depends on the context of $Q$.

context (2, 1): Set $\sigma(Q) = \mu(Q)$.

context (4, 0): Set $2\sigma(Q) = \mu(Q) + \mu(\hat{Q})$.

other contexts: Set $2\sigma(Q) = \mu(Q) + \mu(\hat{Q}) + \text{vor}_0(Q) - \text{vor}_0(\hat{Q})$.

This completes the definition of $\sigma(Q)$. Only the contexts $(2, 1)$, $(3, 1)$, and $(4, 0)$ arise in the third and fifth steps of the Kepler conjecture. (See III.2.2.) When $\eta^+ \leq \sqrt{2}$, we say that the quarter has compression type. Otherwise, we say it has Voronoi type. To say that a quarter has compression type means that $\Gamma(Q)$ is one term of the scoring function. It does not mean that it is the full score.

If $Q_1$, $Q_2$, $Q_3$, and $Q_4$ are the quarter $Q$ with its distinguished vertex placed at the four vertices of $Q$, then it follows directly from our definitions that

$$\sum_{i=1}^{4} \sigma(Q_i) = \sum_{i=1}^{4} \mu(Q_i) = \sum_{i=1}^{4} \Gamma(Q_i) = 4\Gamma(Q).$$

Thus, the new scoring is a local reapportionment of compression, allowing us to relate the score to the densities of packings.

Everything outside of the $Q$-system is scored by $V$-cells. If $P$ is a standard cluster other than a quasi-regular tetrahedron, let $V_P$ be the intersection of the $V$-cell at the origin with the cone over $P$. Set

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

This function is not the same as the analytic Voronoi function, defined on simplices, which is denoted in the same way. Set

$$\sigma(P) = \text{vor}(V_P) + \sum_{Q \subset P} \sigma(Q).$$

The sum runs over quarters of the $Q$-system contained in $P$. If $D^*$ is a decomposition star, set

$$\sigma(D^*) = \sum_{P \subset D^*} \sigma(P).$$

Recall that the constant $pt$, a point, is defined as the score of a regular quasi-regular tetrahedron with edges of length 2. We have $pt = 4 \arctan(\sqrt{2}/5) - \pi/3$. 
Lemma 3.13. A quasi-regular tetrahedron scores at most 1 pt. 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. Other standard clusters have strictly negative scores.

Proof. The statement about quasi-regular tetrahedra is found in [I]. The general context of upright quarters is established by Calculations 3.13.3 and 3.13.4. For the remaining quarters, it is enough to consider μ(Q). We claim that Γ(Q) ≤ 0, on quarters satisfying η(Q) ≤ √2. If the circumradius of every face of the quarter is at most √2, this follows from Section II.4.5.1. Because of this, we may assume that the circumradius of Q is greater than √2. The inequality η(Q) ≤ √2 implies that the faces of Q along the diagonal have nonnegative orientation. The other two faces have positive orientation, by Section I.3.4. Decompose the simplex into Rogers simplices as in [II] (Type IV, etc.). The inequality Γ ≤ 0 now follows from II.4 if η ≤ √2.

Assume that η ≥ √2 and σ = vor. The result follows from [II] if the orientations of the sides are all positive. In fact, we may allow the face opposite the origin to have negative orientation. For the remaining cases we appeal to Calculations 3.13.1 and 3.13.2, listed in the appendix. Calculation 3.13.1 treats flat quarters, and Calculation 3.13.2 treats the upright quarters.

For regions outside the Q-system we proceed as in Part II. We show that the score of the V-cell under any Voronoi face is negative. We adapt the fan of Part II by adding a face to the fan if it belongs to a simplex in the Q-system, or if the circumradius of the face is at most √2. Lemma II.4.4 is still valid, but its proof must be adapted. In the notation of [II], consider the simplex formed by F_1 and F_2. If its circumradius is at most √2, the argument for small simplices in Part II applies. Otherwise, if the point p (constructed in the Lemma) is at most √2 from the vertices of F_1, the face F_2 of the simplex has negative orientation, giving it a circumradius greater than √2. By Lemma 2.2, this means that the simplex is a quarter. If it is a quarter, since F_2 was included in the fan, there is a quarter in the Q-system along the diagonal. So every quarter along the diagonal lies in the Q-system. But we have assumed that we are outside the Q-system. The proof is complete. □

Thus, we recover the main results of [I] and [II] under this new scoring scheme. Set δ_{ot}(s) = 16πδ_{oct}/(16π − 3s). The following proposition is a minor adaptation of Lemma I.2.1.

Proposition 3.14. If every decomposition star in a saturated packing scores at most s < 16π/3, then the density of the packing is at most δ_{ot}(s). If the score of every decomposition star is at most 8 pt, then the density of the packing is at most π/√18.

Proof. Let D^*(v) be the decomposition star around a vertex v. Let Λ_N be the set of sphere centers inside a large ball B_N of radius N. Set

\[ \text{vor}(D^*(v)) = 4(-δ_{oct}\text{vol}(V(v)) + 4π/3), \]
where $V(v)$ is the Voronoi cell around $v$. We have
\[
\sum_{\Lambda N} \sigma(D^*(v)) = \sum_{\Lambda N} \text{vor}(D^*(v)) + O(N^2) = 4(-\delta_{\text{oct}}\text{vol}(B_N) + |\Lambda_N|\frac{4\pi}{3}) + O(N^2).
\]

This identity holds because the score of a decomposition star $\sigma(D^*(v))$ is a local reapportionment of vor. In fact, $\Gamma$ is obtained by averaging the Voronoi volumes, and $V$-cells are obtained from Voronoi cells by reapportioning protruding tips among neighboring Voronoi cells. These modifications of the Voronoi cells make no difference except at the boundary of $B_N$, when we sum over $\Lambda_N$. The term $O(N^2)$ accounts for the boundary effects from decomposition stars that lie partially outside $B_N$.

The inequality $\sigma(D^*(v)) \leq s$ gives
\[
4(-\delta_{\text{oct}}\text{vol}(B_N) + |\Lambda_N|\frac{4\pi}{3}) \leq s|\Lambda_N| + O(N^2).
\]

Rearranging this inequality as in the proof of Lemma I.2.1, and taking the limit as $N$ tends to infinity, we obtain the result. The second statement of the Lemma is the special case $s = 8$ pt. □

Proposition 3.14 suggests the following conjecture.

**Conjecture 3.15.** The score of a decomposition star is at most $8$ pt.

**Theorem 3.16.** If a decomposition star is made entirely of quasi-regular tetrahedra, its score is less than $8$ pt.

*Proof.* Nothing has changed for quasi-regular tetrahedra. See [I] for a proof. □

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 compression or the Voronoi function is used on each. (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 an 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 an 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 $P$ is $\text{vor}(P, \sqrt{2})$. 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.

### 4. Bounds on the Score

**Proposition 4.1.** The score of a mixed quad cluster is less than $-1.04$ pt.

*Proof.* Any enclosed vertex in a quad cluster has length at least 2.51 by Section III.2.2. In particular, the anchors of an enclosed vertex are corners of the the quad cluster. There are no flat quarters.
We generally truncate the V-cell at $\sqrt{2}$. This increases the score, and yet by [II] and Lemma 3.13, it breaks into pieces whose score is nonpositive. Thus, if we identify certain pieces that score less than $-1.04\text{ pt}$, the result follows. Nevertheless, a few simplices will be left untruncated in the following argument. We will leave a simplex untruncated only if we are certain that each of its faces has positive orientation and that the simplices sharing a face $F$ with $S$ either lie in the $Q$-system or have positive orientation along $F$. If these conditions hold, we may use the Voronoi function on $S$ rather than truncation. (See Calculations 4.1.1 and 4.1.3.)

By enclosed vertex, we now mean one of height at most $\sqrt{2}$. Let $v$ be an enclosed vertex with the fewest anchors. Consider the part of the V-cell under the V-face determined by $v$. If there are no anchors, under this face lies the right-circular cone $C(h, \eta_0(h))$, where $\eta_0(h) := \eta(2h, 2, 2.51)$ and $|v| = 2h$. In fact, any neighboring face corresponds to a corner of the quad cluster or to an enclosed vertex of height at least $2.51$. In either case, the set of points in the face’s plane, at distance at most $\eta_0(h)$ from the origin, belongs to the face. By Formula 3.2, the score of this cone is $2\pi(1 - h/\eta_0(h))\phi(h, \eta_0(h))$. An optimization in one variable gives an upper bound of $-4.52\text{ pt}$, for $1.255 \leq h \leq \sqrt{2}$. This gives the bound of $-1.04\text{ pt}$ in this case.

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

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

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

where

$$K_0(y_1, y_2, y_6) = \text{vor}(R(y_1/2, \eta(y_1, y_2, y_6), \sqrt{2})) + \text{vor}(R(y_2/2, \eta(y_1, y_2, y_6), \sqrt{2}))$$

$$- \text{dih}(R(y_1/2, \eta(y_1, y_2, y_6), \sqrt{2}))(1 - y_1/\sqrt{8})\phi(y_1/2, \sqrt{2}).$$

(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 $y_1$ (Diagram 4.3).
Fix an enclosed vertex \( v \) and draw its anchors. 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 4.1.1 or 4.1.2 gives the bound \(-1.04 \, \text{pt}\), 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 \( 0.52 \, \text{pt}\). This occurs if the circumradius of the face \((0, v, v_2)\) is less than \( \sqrt{2} \) by Calculation 4.1.3, or if the circumradius of the face is greater than \( \sqrt{2} \) by Calculation 4.1.4, provided that the length of \((v, v_1)\) is at most \( 2.2 \). The second alternative 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 \( 0.52 \, \text{pt} \) (see Calculations 4.1.5 and 4.1.6). In fact, if there are two such simplices \( S \) and \( S' \) along \( Q \), then the three simplices \( Q, S, \) and \( S' \) pull the score below \(-1.04 \, \text{pt} \) (see Calculation 4.1.7). 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 \(-0.31 \, \text{pt} \). In each case, \( S \) and the adjacent simplex through \((0, v, v_1)\) score less than \(-0.52 \, \text{pt} \). Since \( v \) has at least two anchors, the quad cluster scores less than \( 2(-0.52) \, \text{pt} = -1.04 \, \text{pt} \). □

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

\[
crown(h) = 2\pi(1-h/\eta_0(h))(\phi(h, \eta_0(h)) - \phi_0).
\]

It is equal to \(-4\delta_{\text{act}} \) 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 \( 2h \in [2.51, \sqrt{8}] \), such that every other vertex \( v' \) of the standard cluster satisfies

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

then the volume 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,

\[
\text{vor}(V_P) < \text{vor}_0(V_P) + \text{crown}(|v|/2).
\]

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. Diagram 4.4 illustrates the terms in the definition of \( \text{anc}() \).
Set
\[
\text{anc}(y_1, y_2, y_0) = -\text{dih}(R_1) \text{ crown}(y_1/2)/(2\pi) - \text{sol}(R_1) \phi_0 + \text{vor}(R_1)
- \text{dih}(R_2)(1 - y_2/2.51)(\phi(y_2/2, t_0) - \phi_0) - \text{sol}(R_2) \phi_0 + \text{vor}(R_2),
\]
where \( R_i = R(y_i/2, \eta(y_1, y_2, y_0), \eta_0(y_1/2)) \), 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
\[
\text{vor}(V_P) < \text{vor}_0(V_P) + \text{crown}(|v|/2) + 2 \text{anc}(|v|, |v'|, |v - v'|).
\]
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
\[
\text{vor}(V_P) < \text{vor}_0(V_P) + (1 - \text{dih}(Q)/(2\pi)) \text{ crown}(|v|/2)
+ \text{anc}(|v|, |v'|, |v - v'|) + \text{anc}(|v|, |v''|, |v - v''|).
\]
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 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 \( P \) is a mixed quad cluster, let \( P_0 \) be the new quad cluster obtained by removing all the enclosed vertices. We define a \( V \)-cell \( V_{P_0} \) of \( P_0 \) and the truncation of \( V_{P_0} \) at \( t_0 \). We take its score \( \text{vor}_0(P_0) \) as we do for standard clusters. \( P_0 \) does not contain any quarters.

**Proposition 4.7.** If \( P \) is a mixed quad cluster, \( \sigma(P) < \text{vor}_0(P_0) \).

**Proof.** Suppose there exists an enclosed vertex that has context \((2, 1)\); that is, there is a single upright quarter \( Q = S(y_1, y_2, \ldots, y_6) \) and no additional anchors. In this context \( \sigma(Q) = \mu(Q) \). Let \( v \) be the enclosed vertex. To compare \( \sigma(P) \) and \( \text{vor}_0(P_0) \), 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 \( V_{P_0} \) be the truncation at height \( t_0 \) of \( V_P \) under the \( V \)-face determined by \( v \) and under the four Rogers simplices stemming from the two anchors. (Diagram 4.6 shades the truncated parts of the quad cluster.) As a consequence

\[
\text{vor}(V_P) < (1 - \frac{\text{dih}(Q)}{2\pi}) \text{crown}(y_1/2) + \text{anc}(y_1, y_2, y_6) + \text{anc}(y_1, y_3, y_5) + \text{vor}(V_{P_0}).
\]

Combining this inequality with Calculations 4.7.2, 4.7.3, and 4.7.4, we find

\[
\text{vor}(V_P) + \mu(Q) < \text{vor}(V_{P_0}) + \text{vor}_0(Q).
\]

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 \( \text{rad}(0, v, v_1, v_3) > \eta(|v|, 2, 2.51) \). In this case, the use of correction terms to the crown are legitimate (in relation to the note of caution about the possible overlap of Rogers simplices). Proceeding as in context \((2, 1)\), we find that

\[
\text{vor}(V_P) < (1 - (\text{dih}(Q_1) + \text{dih}(Q_2))/(2\pi)) \text{crown}(|v|/2) + \text{anc}(F_1) + \text{anc}(F_2) + \text{vor}(V_{P_0}).
\]

Here \( V_{P_0} \) 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 \( \text{anc} \). 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 Calculation 4.7.1 applied to both \( Q_1 \) and \( Q_2 \), we have

\[
\text{vor}(V_P) + \sum_{i=1}^{2} \sigma(Q_i) < \text{vor}(V_{P_0}) + \sum_{i=1}^{2} \text{vor}_0(Q_i).
\]

That is, by truncating near \( v \), and changing the scoring of the quarters to \( \text{vor}_0 \), 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

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

and this implies \(|v| \geq 2.696\). We have

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

by Calculation 4.7.5. Inequality 4.11 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 4.9 or 4.11. 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 \( V_P^Z = \cap_{v \in Z} V_P^v \), and \( V_P^{Z, Z} = V_P^Z \cap V_P^v \). Coherence means that we obtain valid inequalities by adding the superscript \( Z \) to \( V_P \) and \( V_P^v \) in Inequalities 4.9 and 4.11, if \( v \notin Z \). In sum, \( \sigma(P) < \text{vor}_0(P_0) \). \( \square \)
The following inequalities have been proved by computer using interval methods. The standard methods described in [I] have been used, together with various improvements in method that will be described elsewhere. Let \( S = S(y) = S(y_1, \ldots, y_6) \). Set \( \eta_{234} \equiv \eta(y_2, y_3, y_4) \) and \( \eta_{126} \equiv \eta(y_1, y_2, y_6) \). The function \( K(S) \) is introduced in Section 4.1.

**Calculation 3.13.1.** \( \text{vor}(S) \leq 0 \), for \( y \in [2, 2.51]^3 \mathbb{R} \mathbb{S} [2, 2.51]^2 \) if the orientation is negative for the face containing the origin and the long edge.

**Calculation 3.13.2.** \( \text{vor}(S) \leq 0 \), for \( y \in [2.51, \sqrt{2}] [2, 2.51]^5 \).

**Calculation 3.13.3.** \( 2\Gamma(S) + \text{vor}_0(S) - \text{vor}_0(\hat{S}) \leq 0 \), for all upright quarters \( S \).

**Calculation 3.13.4.** \( \text{vor}(S) + \text{vor}(\hat{S}) + \text{vor}_0(S) - \text{vor}_0(\hat{S}) \leq 0 \), for all upright quarters \( S \).

**Calculation 4.1.1.** \( \text{vor}(S) < -1.04 \text{pt} \), provided \( \eta_{234} \leq \sqrt{2} \) and

\[
y \in [2, 2.51][2.51, 2.7]^2[2, 2.32][2, 2.51]^2,
\]

or provided \( \eta_{234}, \eta_{126} \leq \sqrt{2} \) and

\[
y \in [2, 2.51][2.51, 2.7]^2[2, 2.32][2, 2.51][2.51, 2.7].
\]

(We have \( y_4 \leq 2.32 \) because otherwise \( \eta_{234} > \eta(2.51, 2.51, 2.32) > \sqrt{2} \). Similarly, \( y_2, y_3 \leq 2.7 \); otherwise \( \eta_{234} > \eta(2.51, 2.7, 2) > \sqrt{2} \). Similarly, \( y_6 \leq 2.7 \) if \( \eta_{126} \leq \sqrt{2} \).)

**Calculation 4.1.2.** \( K(S) < -1.04 \text{pt} \), provided \( \eta_{234} \geq \sqrt{2} \) and

\[
y \in [2, 2.51][2.51, \sqrt{2}]^2[2, 2.51]^3,
\]

or provided \( \eta_{234} \geq \sqrt{2} \geq \eta_{126} \) and

\[
y \in [2, 2.51][2.51, \sqrt{2}]^2[2, 2.51]^2[2.51, 2.7].
\]

**Calculation 4.1.3.** \( \text{vor}(S) < -0.52 \text{pt} \), provided \( \eta_{234} \leq \sqrt{2} \) and

\[
y \in [2, 2.51]^2[2.51, 2.7]^2[2, 2.51]^2.
\]

(We have \( y_4 \geq 2.51 \), because \( S \) is assumed not to be a quarter.)

**Calculation 4.1.4.** \( K(S) < -0.52 \text{pt} \), provided \( \eta_{234} \geq \sqrt{2} \) and

\[
y \in [2, 2.51]^2[2.51, \sqrt{2}]^2[2, 2.2][2, 2.51].
\]

**Calculation 4.1.5.** \( K(S) < -0.31 \text{pt} \), provided \( \eta_{234} \geq \sqrt{2} \) and

\[
y \in [2, 2.51]^2[2.51, \sqrt{2}]^2[2, 2.51]^2.
\]
Calculation 4.1.6. \( \sigma(Q) < -0.21 \) pt in the contexts (2, 1) and (3, 1) for 
\[ y \in [2.51, \sqrt{8}][2, 2.51]^4[2.2, 2.51]. \]

Calculation 4.1.7. \( \sigma(Q) < -0.42 \) pt in the context (2, 1) for 
\[ y \in [2.51, \sqrt{8}][2, 2.51]^3[2.2, 2.51]^2. \]

Calculation 4.7.1. For all upright quarters \( Q \),
\[
\mu(Q) + \mu(\hat{Q}) + (1 - \text{dih}(Q)/\pi) \text{crown}(y_1/2) + 2 \text{anc}(y_1, y_2, y_6) < \text{vor}_0(Q) + \text{vor}_0(\hat{Q}).
\]

Calculation 4.7.2. \( \text{crown}(h) < -0.1378 \), for \( h \in [1.255, \sqrt{2}] \).

Calculation 4.7.3. \( \text{anc}(y_1, y_2, y_6) < 0.0263 \), for 
\[ (y_1, y_2, y_6) \in [2.51, \sqrt{8}][2, 2.51]^2. \]

Calculation 4.7.4. \( \mu(Q) + (1 - \text{dih}(Q)/2\pi)(-0.1378) + 2(0.0263) < \text{vor}_0(Q) \), for all upright quarters \( Q \).

Calculation 4.7.5. \( \mu(Q) + \mu(\hat{Q}) < \text{vor}_0(Q) + \text{vor}_0(\hat{Q}) + 0.02(\pi/2 - \text{dih}(Q)) \), for 
\[ y \in [2.69, \sqrt{8}][2, 2.51]^5. \]
Appendix 2. Compatibility Notes

It has been useful to make various changes in the program that was published in *Sphere Packings I*. This appendix makes a few comments about the global compatibility of the results and terminology from various papers.

The definition of *quasi-regular octahedron* in *Sphere Packings I* is obsolete. The definition that is used appears in Section I of this paper. Also, there is an old definition of *standard cluster* for Delaunay stars that should be replaced with the standard cluster in a decomposition star in [F].

The Sections I.8.6.4, I.8.6.5, I.8.6.6, I.8.6.7 are no longer needed because of improvements in the numerical methods used to calculate the Voronoi function. Also, Lemma I.9.1.1 can now be verified quickly by computer, so the technical proof that is given is no longer needed. Lemmas I.9.17 and I.9.18 are proved by a long argument that is no longer necessary because of improvements in numerical methods.

Many of the papers rely on the arctan formula for the dihedral angle, rather than the arccos formula that appears in I.8.

\[
\text{dih}(S) = \frac{\pi}{2} + \arctan\left(-\frac{\Delta_4}{\sqrt{4x_1\Delta}}\right).
\]

This leads to simple formulas for the derivatives of the dihedral angles that have been used extensively throughout the collection without explicit mention

\[
\partial_2 \text{dih} = -\frac{y_1\Delta_3}{(u_{126}\sqrt{\Delta})},
\]

etc.

In *Sphere Packings II* the notion of a *small* simplex is made obsolete by the constructions of [F]. Delaunay stars are replaced by decomposition stars. *Restricted cells* are replaced with V-cells in [F]. Simplices of *compression type* undergo a small change in meaning when the scoring functions are adjusted in [F]. In [II], in constructing the standard regions, we remove all arcs that do not bound a region, but in the classification of standard regions in a later paper these arcs will not be removed.

Lemma II.2.2 can be proved by simpler means. After the first paragraph of the proof, we observe that \(S = (v_0, v_1, v_2, w)\) has negative orientation along \(F = (v_0, v_1, v_2)\). Hence \(S\) is a quasi-regular tetrahedron by I.3.4. Various lemmas are revised in [F] to account for the change in decomposition. (Lemma II.2.4, Section II.3.1, Lemma II.3.2, Theorem II.4.1.b). Several of the cases in II.4.5.2 are unnecessary in light of the revisions in [F]. The technical results in the appendix can now be obtained quickly by computer.

When we say that a simplex has compression type, it means the the scoring rule for \(\eta^+(Q) \leq \sqrt{2}\) is used. Here \(\eta^+\) is the function of Section 3. To say that a simplex has compression type implies that the compression function is one term of the scoring function. But there will often be various correction terms, so that the scoring
function need not be identical with the compression function. Similar comments apply to simplices of Voronoi type, which means precisely that $\eta^+(Q) > 2\sqrt{2}$. It means loosely that the Voronoi function appears as part of the scoring function. In general, the terms Voronoi, Voronoi scoring, Voronoi function, and so forth are used loosely for objects related to the $V$-cells in the decomposition star.
References.

[FT] L. Fejes Tóth, Lagerungen in der Ebene auf der Kugel und im Raum, Berlin, Springer-Verlag, 1953.

[V] S.P. Ferguson, Sphere Packings, V, thesis, University of Michigan, 1997.

[H1] T.C. Hales, Remarks on the density of sphere packings in three dimensions, Combinatorica, 13(2), 1993, 181-197.

[H2] T.C. Hales, the Sphere Packing Problem, J. Comp. App. Math. 44, 1992, 41-76.

[I] T.C. Hales, Sphere Packings I, Disc. Comp. Geom. 1997, 17:1-51. [II] Sphere Packings II, DCG. 1997, 18:135-149. [III] Sphere Packings III, preprint.