Packing Twelve Spherical Caps to Maximize Tangencies

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Abstract

The maximum number of non-overlapping unit spheres in $\mathbb{R}^3$ that can simultaneously touch another unit sphere is given by the kissing number, $k(3) = 12$. Here, we present a proof that the maximum number of tangencies in any kissing configuration is 24 and that, up to isomorphism, there are only two configurations for which this maximum is achieved. The result is motivated by a three-dimensional crystallization problem.

1 Introduction

The kissing number, $k(n)$, is the maximum number of non-overlapping unit spheres in $\mathbb{R}^n$ that can simultaneously touch a central unit sphere, for $n \in \mathbb{N}$. It is not too difficult to show that $k(1) = 2$ and $k(2) = 6$, and that the associated kissing configurations are unique. The problem for $n = 3$, however, the so-called *kissing problem* or the *problem of the thirteen spheres*, is considerably more involved. The problem dates back to a famous conversation between Isaac Newton and David Gregory in 1694 (see [9] for an interesting account). Most reports agree that Newton favored the answer 12, whilst Gregory thought that a kissing number of 13 was possible. However, Casselman [2] highlights some possible inaccuracies in this story. The first proof that $k(3) = 12$ was given by Schütte and Van der Waerden in 1953 [10].

Unlike the lower-dimensional cases, the kissing configuration in $\mathbb{R}^3$ are highly non-unique and rigidity cannot be guaranteed. In the most symmetrical kissing configuration, for example, the centers of the twelve spheres are placed at the vertices of an icosahedron, so that no two spheres (apart from the central sphere) touch each other.

In this paper, we identify those kissing configurations of unit spheres in $\mathbb{R}^3$, $\{S_i : 1 \leq i \leq 12\}$, for which the number of kissing (or touching) pairs, $\{S_i, S_j\}$, $1 \leq i < j \leq 12$, is maximal. An equivalent viewpoint is to replace each outer sphere with its point of contact with the central sphere to create a spherical code of twelve points on S^2, in which any two distinct points are separated by at least a distance 1 (see, for example, [3] for a discussion of spherical codes). The problem then asks for the maximum number of edges of length 1 in this spherical code. Theorem 4 states that the maximum is 24, which is attained only when the centers of the twelve spheres are placed at the vertices of a *cuboctahedron* or a *twisted cuboctahedron* (see Definition 3). The cuboctahedron is also the convex hull of the set of nearest neighbors of any point in an face centered cubic (fcc) lattice. The twisted cuboctahedron corresponds to the nearest neighborhood of any point in the hexagonally close packed (hcp) lattice.

Closely related to the kissing number is the Kepler conjecture which states that the maximal packing density of non-overlapping spheres with equal radii cannot exceed $\frac{\pi}{\sqrt{18}}$, a value which is achieved by both the fcc lattice and the hcp lattice. A rigorous proof of the Kepler conjecture has been given by T. Hales [5]. The key steps in the proof involve

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a) The reduction to a 150-dimensional optimization problem.
b) A computer based analysis of the optimization problem which shows that the optimizers consist of only two graphs: The kissing arrangement of twelve balls around a central ball in the face-centered cubic packing or the kissing arrangement of twelve balls in the hexagonal-close packing.

Our computer assisted proof of Theorem 4 follows the spirit of Hales' proof. It based on the method of Musin and Tarasov [8] and involves listing all candidate contact graphs (see Definition 5) which satisfy the hypotheses of Theorem 4. In Lemma 6, we identify a set of linear constraints which must be satisfied if a graph is to be realizable as a contact graph. These constraints define a linear program. Using a computer program we show that only for a small number of graphs the linear program has a solution. All the remaining graphs are partially rigid, so that the cartesian coordinates of the vertices of a subgraph can be determined. This calculation shows that none of the remaining subgraphs are contact graphs apart from two. The two remaining graphs are precisely the contact graphs of the cuboctahedron and the twisted cuboctahedron. The programs involved can be downloaded at
`www2.warwick.ac.uk/fac/sci/maths/people/staff/florian_theil/graph-elimination`.

The relevance of this result arises from the fact that the nearest neighbors of any point in a face centered cubic lattice (fcc) form a cuboctahedron, and the nearest neighbors in a hexagonally close packed lattice (hcp) form a twisted cuboctahedron. This observation provides a link to the the crystallization problem in 3 dimensions. It is shown in [6, 7] that, given a finite set of identical particles, which are interacting under a suitable pair potential and three-body potential, $V : \mathbb{R}_{>0} \to \mathbb{R}^3$ and $V_3 : \mathbb{R}^3 \to \mathbb{R}^3$ respectively, then the ground state energy per particle converges to the energy per particle of an fcc crystal lattice energy, as the number of particles tends to infinity. Specifically, if $y \in \mathbb{R}^{3\times N}$ encodes the positions of N particles in $\mathbb{R}^3$, then the total energy associated with the configuration y is a sum of the pair and three-body interactions:

$$E_N(y) = \sum_{1\le i<j\le N} V(|y_i - y_j|) + \frac{1}{2} \sum_{\substack{1\le i,j,k\le N \\ i\ne j\ne k}} V_3(y_i, y_j, y_k).$$

The main theorem of [6] then states that

$$\lim_{N\to\infty} \frac{1}{N} \min_{y\in\mathbb{R}^{3\times N}} E_N(y) = E_{\mathcal{L}}, \tag{1}$$

where $E_{\mathcal{L}}$ is the energy per particle in the crystal lattice fcc. The choice of crystal lattice is determined by the third neighbor interactions and the choice of the pair potential, V.

The role of Theorem 4 in the proof of equation (1) is in the analysis of the three-body potential contributions to the total energy. V_3 is chosen to take the following Stillinger-Weber form:

$$V_3(z_1, z_2, z_3) = f(|z_2 - z_1|) f(|z_3 - z_1|) g\left(\angle(z_2, z_1, z_3)\right), \tag{2}$$

where f is a cut-off function, with cut-off distance between 1 and $\sqrt{2}$, and

$$g(\theta) = \begin{cases} \left(\cos(\theta) - \frac{1}{2}\right)^2 & \text{if } \left|\theta - \frac{\pi}{3}\right| \le \alpha, \\ \frac{1}{16} & \text{if } \left|\theta - \frac{\pi}{3}\right| > 2\alpha \end{cases}$$

for a sufficiently small parameter, $\alpha > 0$.

The three-body potential V_3 favors ground states containing a maximum number of angles of $\pi/3$ subtended at z_1 by nearest neighbors to z_1. Equivalently, V_3 favors a maximum number of nearest neighbor edges in the nearest neighborhood of z_1. Theorem 4 states that this maximum is achieved only when the limiting ground state energy per particle of equation (1) is exactly the energy per particle in a close-packed structure (where the nearest neighborhood about each point is a local fcc crystal lattice).

The angular potential V_3 can probably be omitted if the understanding of the rigidity of kissing configurations is improved. To see this we introduce the concept of regular sets.

Definition 1. *A set $X \subset \mathbb{R}^3$ is regular if $|x - y| \ge 1$ for all $x, y \in X$ such that $x \ne y$. For $x \in X$ the set of nearest neighbors be given by*

$$\mathcal{N}(x) := \{y \in X : |x - y| = 1\}.$$

It is plausible that two nearest neighbors in a regular set which have 12 nearest neighbors each share at least 4 nearest neighbors.

Conjecture 2. *Let the set X be regular. If $y \in \mathcal{N}(x)$ and $\#\mathcal{N}(x) = \#\mathcal{N}(y) = 12$ then*

$$\#(\mathcal{N}(x) \cap \mathcal{N}(y)) \geq 4.$$

Thus, if X is regular, $\#\mathcal{N}(x) = 12$ for some $x \in X$, and $\#\mathcal{N}(y) = 12$ for all $y \in \mathcal{N}(x)$, then Conjecture 2 implies that each point $y \in \mathcal{N}(x)$ is the endpoint of not more than four edges with length 1 on the sphere S^2 centered at x. Theorem 4 implies that each point $y \in \mathcal{N}(x)$ is the endpoint of precisely four edges with length 1. It is not hard to see that there are only two sets with this property: The cuboctahedron and the twisted cuboctahedron.

2 Main Theorem

Definition 3. *A cuboctahedron is the convex hull of the midpoints of the twelve edges of a cube with sidelength 1. A twisted cuboctahedron is obtained on rotating an upper hemisphere of a cuboctahedron, Q, by an angle of $\pi/3$, about the center of Q and parallel to an equator of Q, where an equator of Q is any regular hexagon of vertices of Q.*

Theorem 4. *Let $X \subset S^2$ be a regular set such that $\#X \leq 12$. Then the maximal number of pairs $\{x, y\} \subset X$ such that $|x - y| = 1$ is equal to 24 i.e.*

$$\sharp\left\{\{x, y\} \subset X : |x - y| = 1\right\} \leq 24. \tag{3}$$

Equality is only attained when $\#X = 12$ and the points of X are placed at the vertices of a cuboctahedron or a twisted cuboctahedron.

3 Contact Graphs

The proof of Theorem 4 takes place on the unit sphere, S^2 and, as such, we reformulate the problem in terms of spherical geometry. To begin, we introduce some notation: For any $x, y \in S^2$, let $e(x, y) \subset S^2$ denote the shortest spherical arc with end-points, x and y. We define $d(x, y) \in [0, \pi]$ to be the spherical length of $e(x, y)$ and $\angle(x, y, z) \in [0, 2\pi]$ to be the spherical angle subtended at y by $e(x, y)$ and $e(y, z)$ in clockwise orientation. Clearly $\angle(x, y, z) \geq \arccos\left(\frac{1}{3}\right)$ and $d(x, y) = \frac{\pi}{3}$ if $|x - y| = 1$. In future we abbreviate $\arccos\left(\frac{1}{3}\right)$ by τ.

Definition 5 (Contact graphs)**.** *If $X \subset S^2$ is a finite collection of vertices on the unit sphere such that $d(x, y) \geq \frac{\pi}{3}$ for $x, y \in X$, $x \neq y$, then the* contact graph*, $CG(X)$, of X is the graph with vertices at points in X and edges, $\mathcal{E}_X$, where*

$$\mathcal{E}_X := \left\{e(x, y) \subset S^2 : x, y \in X \text{ and } d(x, y) = \tfrac{\pi}{3}\right\}.$$

The set of associated faces, $\mathcal{F}_X$, is given by

$$\mathcal{F}_X := \left\{f \subset S^2 : f \text{ is bounded by edges of } \mathcal{E}_X \text{ and } \mathrm{int}(f) \cap \mathcal{E}_X = \emptyset\right\}.$$

For any face, $f \in \mathcal{F}_X$, the set of angles subtended by edges of f is

$$\mathcal{A}(f) := \left\{\angle(x, y, z) : e(x, y), e(y, z) \in \mathcal{E}_X \text{ and } (e(x, y) \cup e(y, z)) \subset \partial f\right\},$$

where ∂f is the boundary of f. The complete set of angles is

$$\mathcal{A}_X := \left\{u \in \mathcal{A}(f) : f \in \mathcal{F}_X\right\}.$$

Lemma 6 lists the linear constraints which much be satisfied by any contact graph. Each constraint is the consequence of geometrical restrictions on the surface of the sphere.

Lemma 6. *Let $X \subset S^2$ be a discrete set of vertices such that $|X| = 12$ and $|x - y| \geq 1$ for all $x, y \in X$, $x \neq y$. Then the associated contact graph, $CG(X)$, satisfies the following properties:*

1. *$u \geq \tau$ for every $u \in \mathcal{A}_X$, where τ is the angle of a spherical equilateral triangle with sides of length $\frac{\pi}{3}$;*
2. *$\sum_{u \in I(x)} u = 2\pi$ for all $x \in X$, where $I(x) \subset \mathcal{A}_X$ is the set of angles that are adjacent to x.*
3. *Any vertex of $CG(X)$ has order at most 5, that is $\#I(x) \leq 5$ for all $x \in X$.*
4. *If $f \in \mathcal{F}_X$ is a quadrilateral face, then $u = v$, for any two opposite angles, $u, v \in \mathcal{A}(f)$ of f.*
5. *If u, v are adjacent angles in a quadrilateral face, then $u + v \leq 2(\pi - \tau)$, where $\pi - \tau$ is the angle of a spherical square with sides of length $\frac{\pi}{3}$.*
6. *If $f \in \mathcal{F}_X$ is a triangular face, then $u = \tau$ for all $u \in \mathcal{A}(f)$.*
7. *If $f \in \mathcal{F}_X$ is a quadrilateral face, then $u \leq 2\tau$ for all $u \in \mathcal{A}(f)$.*
8. *If $f \in \mathcal{F}_X$ is a pentagonal face, then $u \leq 3\tau$ for all $u \in \mathcal{A}(f)$.*

Proof. Statements 1, 2 and 6 are clear from simple spherical geometry and an application of the spherical cosine rule. Statement 3 follows directly from statement 1 since $5\tau < 2\pi < 6\tau$.

To prove statement 4 we first define x_1, x_2, x_3, x_4 to be the vertices of the quadrilateral face enumerate in clockwise orientation. Let $u = \angle(x_1, x_2, x_3)$, $v = \angle(x_2, x_3, x_4)$. The spherical cosine rule gives

$$\cos(\angle(x_3, x_2, x_1)) = \cos(\angle(x_2, x_1, x_4)) = \frac{1}{3}(4\cos(d(x_2, x_4)) - 1).$$

The solution $\angle(x_3, x_2, x_1) = -\angle(x_2, x_1, x_4)$ corresponds to the situation where the points in S^2 associated with the vertices x_1 and x_3 are identical. But this is impossible since $d(x_1, x_3) \geq \frac{\pi}{3}$ and we conclude that

$$\angle(x_3, x_2, x_1) = \angle(x_2, x_1, x_4)$$

is the only possible solution. This implies statement 4.

To prove statement 5 we observe that the spherical cosine rule implies that

$$\cos(\angle(x_3, x_2, x_4)) = g(\cos(v)), \tag{4}$$

$$\tag{5}$$

where, for every $z \in [-1, 1]$,

$$g(z) = \sqrt{\frac{1 - z}{5 + 3z}}. \tag{6}$$

This implies that

$$u + v \geq h(v) = v + 2\arccos(g(\cos(v))),$$

Differentiation with respect to v yields that

$$h'(v) = 1 - \frac{4}{5 + 3\cos(v)} = \frac{1 + 3\cos(v)}{5 + 3\cos(v)}$$

and we obtain that $h'(v) \geq 0$ if $v \in [\tau, \pi - \tau]$ and $h'(v) \leq 0$ if $v \in [\pi - \tau, 2\tau]$. Since $h(\tau) = h(2\tau) = 3\tau$ and $h(\pi - \tau) = 2(\pi - \tau)$ this shows $u + v \geq 3\tau$ and statement 5 has been established.

To prove statement 7, we first show that

$$\cos(\angle(x,y,z)) \geq \frac{1}{3} \tag{7}$$

for any three points $x, y, z \in X$ such that $d(x,z) = \frac{\pi}{3}$, $d(x,y), d(z,y) \leq \frac{2\pi}{3}$. Indeed, we obtain the bounds $\cos(d(x,y))\cos(d(z,y)) \leq \frac{1}{4}$ and $\sin(d(x,y))\sin(d(z,y)) \geq \frac{3}{4}$. The spherical cosine theorem implies that

$$\cos(\angle(x,y,z)) = \frac{1 - 2\cos(d(x,y))\cos(d(y,z))}{2\sin(d(x,y))\sin(d(y,z))} \geq \frac{1-\frac{1}{2}}{2\frac{3}{4}} = \frac{1}{3},$$

and thus equation (7).

Let now f be a quadrilateral face and $\{x_1, x_2, x_3, x_4\} \subset X$ be a clockwise labeling of the vertices of f such that $u = \angle(x_1, x_2, x_3)$. Then we split the angle u into two parts:

$$u \leq u_1 + u_2$$

where $u_1 = \angle(x_1, x_2, x_4)$, $u_2 = \angle(x_4, x_2, x_3)$. Equality holds if and only if each of both triangles are oriented clockwise. Equation (7) implies that $0 \leq u_1, u_2 \leq \tau$, and thus statement 7 holds true. The proof of statement 8 is analogous. □

4 Proof of Theorem 4

For each regular set X we consider the associated contact graph $CG(X)$.

Definition 7. *A graph is 2-connected if it is connected and remains connected when any one vertex is removed.*

It can be assumed wlog that $CG(X)$ is 2-connected, since otherwise, edges of $\mathcal{E}_X$ can be rotated without decreasing the number of edges so that every vertex is of degree at least 2.

4.1 Generating the Graphs

Let A_0 be the set of all 2-connected planar graphs with 12 vertices, at least 24 edges and at most 5 edges adjacent to any given vertex. We eliminate all graphs in A_0 which cannot be a contact graph. This is done in several stages. After stage k, we call the set of remaining graphs A_k. A_2 consists of only the two graphs stated in the theorem.

The set A_0 contains 1,430,651 graphs. The graphs in A_0 can be listed using the program plantri [1][1]. All computer codes used in this section can be downloaded at
`www2.warwick.ac.uk/fac/sci/maths/people/staff/florian_theil/graph-elimination`.

[1]The program plantri can be downloaded at `http://cs.anu.edu.au/~bdm/plantri`

4.2 First Stage of Elimination

By Lemma 6, the angles associated the contact graph, $CG(X)$, must satisfy the following linear inequalities:

$$-u \leq -\tau \text{ for all } u \in \mathcal{A}_X; \tag{8}$$

$$\sum_{u \in I(x)} u \leq 2\pi \text{ for all } x \in X, \text{ where } I(x) \subset \mathcal{A}_X \text{ is the set of angles that are adjacent to } x; \tag{9}$$

$$-\sum_{u \in I(x)} u \leq -2\pi \text{ for all } x \in X; \tag{10}$$

$$u - v \leq 0 \text{ whenever } u, v \in \mathcal{A}(f) \text{ are opposite angles in a quadrilateral face, } f \in \mathcal{F}; \tag{11}$$

$$u - v \geq 0 \text{ whenever } u, v \in \mathcal{A}(f) \text{ are opposite angles in a quadrilateral face, } f \in \mathcal{F}; \tag{12}$$

$$u + v \leq 2(\pi - \tau) \text{ whenever } u, v \in \mathcal{A}(f) \text{ are adjacent angles in a quadrilateral face, } f \in \mathcal{F}; \tag{13}$$

$$u \leq \tau \text{ for all } u \in \mathcal{A}(f), \text{ whenever } f \in \mathcal{F} \text{ is a triangular face;} \tag{14}$$

$$u \leq 2\tau \text{ for all } u \in \mathcal{A}(f), \text{ whenever } f \in \mathcal{F} \text{ is a quadrilateral face;} \tag{15}$$

$$u \leq 3\tau \text{ for all } u \in \mathcal{A}(f), \text{ whenever } f \in \mathcal{F} \text{ is a pentagonal face;.} \tag{16}$$

We eliminate all graphs in A_0 which do not satisfy the constraints, (8)-(16), to obtain a new set of contact graphs, $A_1 \subset A_0$.

Lemma 8. *If a graph in A_1 has fewer than 13 vertices and admits face angles satisfying the inequalities (8)-(16), then the graph has 12 vertices. The number of such graphs is 67.*

Proof. For each graph the inequalities (8)–(16) constitute a linear programming problem for which the existence of solutions can be decided with the simplex algorithm (e.g. [4]), using the face angles of the graph as variables. The inequalities take the form $\sum_i \alpha_{i,j} u_i \leq b_j$ for suitably chosen coefficients $\alpha_{i,j}$, b_j which depend on the graph. After introducing slack variables one obtains the linear equations

$$\sum_i \alpha_{i,j} u_i + z_j = b_j, \tag{17}$$

together with the constraints u_i, $z_j \geq 0$.

To transform the system into standard form we introduce an artificial variable y_j, giving the system of equalities:

$$\sum_i \alpha_{i,j} u_i + z_j - \varepsilon_j y_j = b_j \tag{18}$$

with $\varepsilon_j = 1$ if $b_j < 0$ and $\varepsilon_j = 0$ if $b_j \geq 0$.

The equalities (18) have a solution $u_i = 0$ for all i, $z_j = 0, y_j = -b_j > 0$ for each j such that $b_j < 0$ and $z_j = b_j$ for each j such that $b_j \geq 0$. The equalities (17) then have a solution if and only if there exists values of $u_i, z_j, y_k \geq 0$ satisfying the equalities (18) such that all of the y_k are equal to zero. We therefore use a simplex algorithm to minimize the objective function $\sum_j \varepsilon_j y_j$ subject to the constraints given in the equalities (18) and $u_i, z_j, y_j \geq 0$ for all i, j.

For a given graph in A_1, if the optimal value of the objective function is 0, then we have a feasible solution to the inequalities. If the optimal value is however not equal to zero, there is no feasible solution to the inequalities and we eliminate the graph.

Running this procedure on all of the graphs in A_1, the algorithm terminates after a finite number of iterations in each case, and there are 67 graphs with 12 vertices for which the absolute value of the optimal value is less than $\frac{1}{1000}$. □

4.3 Eliminating Rigid Graphs

Definition 9. *A graph in A_2 is rigid if it contains subgraph only one set of feasible angles satisfying the inequalities (8) – (16).*

By inspecting each of the 67 graphs in A_2 we see that all of them are at least partially rigid in the sense that several angles are determined by the inequalities.

For each of these 67 graphs, we take the set of feasible angles and calculate the Euclidean coordinates of the points in S^2. For each of the graphs we find that either the Euclidean distance between two of the points is less than 1, or the Euclidean distance between two points joined by an edge is greater than 1. In either case it is clear that the graph cannot be a contact graph of a solution to Theorem 4 and so can be eliminated, leaving the set A_3 containing only the graphs of the cuboctahedron and twisted cuboctahedron. This completes the proof of the theorem.

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References

[1] G. Brinkmann and B. D. McKay. Fast generation of planar graphs, *MATCH Commun. Math. Comput. Chem.* **58** (2007), no. 2, 323-357.

[2] B. Casselman. The Difficulties of Kissing in Three Dimensions, *Notices of the AMS*, **51(8)**, (2004), 884-885

[3] J. H. Conway and N. J. A. Sloane. *Sphere Packings, Lattices and Groups*, Springer-Verlag, New York, 1988.

[4] G. B. Dantzig. *Linear Programming and Extensions*, Princeton University Press, 1998.

[5] T. Hales. A Proof of the Kepler Conjecture. *Ann. Math.* **162**, (2005), 1065-1185.

[6] L. C. Harris. Face-centred cubic structures in energy-minimizing atomistic configurations, *PhD Thesis*, Warwick University (2011).

[7] L. C. Harris & F. Theil. Face-centered cubic crystallization of atomistic configurations. *In preparation* (2012).

[8] O. R. Musin and A. L. Tarasov, *The strong thirteen spheres problem*, http://arxiv.org/pdf/1002.1439v2.

[9] F. Pfender and G. M. Ziegler. Kissing Numbers, Sphere Packings, and Some Unexpected Proofs, *Notices of the AMS*, **51(8)**, (2004), 873-883

[10] K. Schütte and B. L. van der Waerden, Das Problem der dreizehn Kugeln, *Math. Ann.*, **125**, (1953), 325-334.