ENUMERATION OF IRREDUCIBLE CONTACT GRAPHS ON THE SPHERE

O. R. Musin and A. S. Tarasov UDC 514.17

Abstract. In this article, using the computer, we enumerate all locally-rigid packings by *N* congruent circles (spherical caps) on the unit sphere \mathbb{S}^2 with $N < 12$. This is equivalent to the enumeration of irreducible spherical contact graphs.

1. Introduction

Packings where all spheres are constrained by their neighbors to stay in one location are called *rigid* or *locally-rigid*. So every sphere of this packing is jammed by neighbors and it cannot be shifted to the side in order to increase the minimum distance between the center of the sphere and the other centers of the balls.

Consider N nonoverlapping spheres of the same radius r in \mathbb{R}^3 that are arranged so that they all touch one (central) sphere of unit radius. We denote by $P := \{A_1, \ldots, A_N\}$ the set of points where external spheres touch the central sphere. Join the points A_i and A_j by an edge (minimum arc of a great circle) if the relevant external spheres touch. The resulting graph is called *contact* and denoted $CG(P)$. If this packing on \mathbb{S}^2 is locally rigid, then we say that the graph $CG(P)$ is *irreducible*. Thus, the problem of studying locally rigid packings reduces to the study of irreducible contact graphs.

There are several connections between this geometric problem with other sphere packing problems. The main application outside mathematics is "jammed" (locally rigid) hard-particle packings in materials science (see, for instance, $[12, 17]$). Note that, for most potentials in physics, minimum energy configurations of particles are also locally rigid.

In mathematics, W. Habicht, K. Schütte, B. L. van der Waerden, and L. Danzer applied irreducible contact graphs for the kissing number and Tammes problems [13, 16, 31, 32, 34]. Let us consider briefly these two classical geometric problems.

The *kissing number* k_3 is the highest number of equal nonoverlapping spheres in \mathbb{R}^3 that touch another sphere of the same size. In other words, the kissing number problem asks how many white billiard balls can *kiss* (touch) a black ball.

The most symmetrical configuration, 12 balls around another, is achieved if the 12 balls are placed at positions corresponding to the vertices of a regular icosahedron concentric with the central ball. However, these 12 outer balls do not kiss each other and may all be moved freely. This space between the balls introduces a question: If you moved all of them to one side, would a 13th ball fit?

This problem was the subject of the famous discussion between Isaac Newton and David Gregory in 1694. Most reports say that Newton believed the answer was 12 balls, while Gregory thought that 13 might be possible. That is why it is often called the *thirteen spheres problem*

The problem was finally solved by Schütte and van der Waerden in 1953 [32]. A subsequent two-page sketch of an elegant proof was given by Leech [19] in 1956. Leech's proof was presented in the first edition of the well-known book by Aigner and Ziegler [1]; the authors removed this chapter from the second edition because a complete proof would have to include too much spherical trigonometry.

The thirteen spheres problem continues to be of interest, and new proofs have been published in the last several years by Hsiang [18], Maehara [20, 21] (this proof is based on Leech's proof), Böröczky [5], Anstreicher [2], and Musin [23].

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If N unit spheres kiss the unit sphere in \mathbb{R}^3 , then the set of kissing points is an arrangement on the central sphere such that the (Euclidean) distance between any two points is at least 1. This allows us to state the kissing number problem in another way: How many points can be placed on the surface of \mathbb{S}^2 so that the angular separation between any two points is at least $60°$?

This leads to an important generalization: to find a set X of N points in \mathbb{S}^2 such that the minimum angular distance of distinct points in X is as large as possible. In other words, how are N congruent, nonoverlapping circles distributed on the sphere when the common radius of the circles has to be as large as possible?

The problem was first asked by the Dutch botanist Tammes [33] (see [9, Sec. 1.6, Problem 6]), who was led to this problem by examining the distribution of openings on the pollen grains of different flowers.

The Tammes problem is presently solved only for several values of N: for $N = 3, 4, 6, 12$ by L. Fejes Tôth [14], for $N = 5, 7, 8, 9$ by Schütte and van der Waerden [31], for $N = 10, 11$ by Danzer [13] (for $N = 11$ see also Böröczky [4]), and for $N = 24$ by Robinson [30]. We recently solved Tammes' problem for the case $N = 13$ [28].

Note that the kissing number problem is currently solved only for dimensions $n = 3, 4, 8$ and 24 (see [8, 22, 24, 25]). Proofs in these papers are based on the Delsarte method and its generalizations (see, for instance, $[3, 11, 26, 27]$.

2. The Irreducible Contact Graphs

2.1. Basic Definitions. Let X be a finite subset of \mathbb{S}^2 . Denote

$$
\psi(X) := \min_{x,y \in X} \{ \text{dist}(x,y) \}, \text{ where } x \neq y.
$$

Denote by d_N the largest angular separation $\psi(X)$ with $|X| = N$ that can be attained in \mathbb{S}^2 , i.e.,

$$
d_N := \max_{X \subset \mathbb{S}^2} \{ \psi(X) \}, \quad \text{where} \quad |X| = N.
$$

Contact graphs. Let X be a finite set in \mathbb{S}^2 . The *contact graph* $CG(X)$ is the graph with vertices in X and edges (x, y) , $x, y \in X$, such that $dist(x, y) = \psi(X)$.

Shift of a single vertex. We say that a vertex $x \in X$ *can be shifted* if in any open neighborhood of x there is a point $x' \in \mathbb{S}^2$ such that

$$
dist(x', X \setminus \{x\}) > dist(x, X \setminus \{x\}).
$$

Irreducible graphs. We say that the graph $CG(X)$ is *irreducible* if there are no shifts of vertices. This terminology was used by Schütte and van der Waerden [31, 32], Fejes Tóth [15], and Danzer [13].

Let us denote by J_N the family of all sets X in \mathbb{S}^2 such that $|X| = N$ and the contact graph CG(X) is irreducible.

D-irreducible graphs. Danzer [13, Sec. 1] defined the following move of a vertex. Let x, y, and z be vertices of CG(X) with dist $(x, y) = \text{dist}(x, z) = \psi(X)$. Denote by x^0 the mirror image of x with respect to the great circle that passes through y and z (see Fig. 1). We call this move a D -flip if dist $(x^0, X \setminus \{x, y, z\}) > \psi(X)$.

Fig. 1. D-flip.

An irreducible contact graph $CG(X)$ is called D-irreducible if it does not admit any D-flip.

Maximal graphs. Suppose that $X \subset \mathbb{S}^2$ with $|X| = N$ and $\psi(X) = d_N$. Then we call this contact graph CG(X) *maximal*.

2.2. Properties of Irreducible Contact Graphs. In this subsection we consider $X \subset \mathbb{S}^2$ such that the graph CG(X) is irreducible, i.e., $X \in J_N$. The following properties of J_N were found in [6,7, 13, 31] (see also [15, Chap. VI]).

Let $a, b, x, y \in X$ with $dist(a, b) = dist(x, y) = \psi(X)$. Then the shortest arcs ab and xy do not intersect. Otherwise, the length of at least one of the arcs ax , ay , bx , or by has to be less than $\psi(X)$. This yields the planarity of $CG(X)$.

Proposition 2.1. *If* X *is a finite subset of* \mathbb{S}^2 , *then* $CG(X)$ *is a planar graph.*

Proposition 2.2. *If* $X \in J_N$ *, then all faces of* CG(X) *are convex polygons in* \mathbb{S}^2 *.*

(Indeed, otherwise, a "concave" vertex of a face P can be shifted to the interior of P.) Let X be a subset of \mathbb{S}^2 with $|X| = N$. We say that X is *maximal* if $\psi(X) = d_N$.

Proposition 2.3. If X is maximal, then for $N > 5$ the graph $CG(X)$ is irreducible.

Proposition 2.4. *If* $X \in J_N$ *, then degrees of its vertices can take only the values* 0 (*isolated vertices*), 3*,* 4*, or* 5*.*

Proposition 2.5. *If* $X \in J_N$ *, then faces of* CG(X) *are polygons with at most* $|2\pi/\psi(X)|$ *vertices.*

The following simple proposition has been proved by Böröczky and Szabó in [6, Lemma 8 and Lemma 9(iii)]. Actually, they considered the case $N = 13$. However, the proof works for all N.

Proposition 2.6. *Let* $X \in J_N$. If $CG(X)$ *contains an isolated vertex, then it lies in the interior of a polygon of* CG(X) *with six or more vertices. Moreover, if it is a hexagon, then it cannot contain two isolated vertices.*

Combining these propositions, we obtain the following combinatorial properties of irreducible contact graphs.

Corollary 2.1. *If* $X \in J_N$ *, then* $G := CG(X)$ *satisfies the following properties:*

- (1) G *is a planar graph*;
- (2) *any vertex of* G *is of degree* 0*,* 3*,* 4*, or* 5;
- (3) *if* G *contains an isolated vertex* v, then v lies in a face with $m \geq 6$ vertices. Moreover, a hexagonal *face of* G *cannot contain two or more isolated vertices.*

3. Danzer's Work on Irreducible Contact Graphs

L. Danzer [13] solved the Tammes problem for $N = 10$ and $N = 11$. His proof is based on the concept of irreducible graphs. (Actually, this paper is a translation of the Habilitationsschrift of Ludwig Danzer *Endliche Punktmengen auf der 2-sphäre mit möglichst großem Minimalabstand*, Universität Göttingen, 1963.) In particular, he added a new idea to shifting a single vertex—a shift that we call here D-flip, i.e., *Danzer's flip*.

In [13], Danzer gives the list of all D-irreducible graphs for $6 \le N \le 10$. Since the contact graph of a maximal set is irreducible (and D-irreducible [13]), this list implies a solution of the Tammes problem for $6 \le N \le 10$. (For the case $N = 11$ Danzer considered only maximal sets.)

Here we give the Danzer list of D-irreducible graphs.

4. Enumeration of Irreducible Contact Graphs

4.1. Geometric Embedding of Irreducible Contact Graphs. Let $X \subset \mathbb{S}^2$ be a finite point set such that its contact graph $CG(X)$ is irreducible. In Corollary 2.1, we collected together combinatorial properties of $CG(X)$. There are several geometric properties.

Recall that all faces of $CG(X)$ are convex (Proposition 2.2). Since all edges of $CG(X)$ have the same lengths $\psi(X)$, all its faces are spherical equilateral convex polygons with at most $|2\pi/\psi(X)|$ vertices.

Any embedding of G in \mathbb{S}^2 is uniquely defined by the following list of parameters (variables):

- (1) the edge length d ;
- (2) the set of all angles u_{ki} , $i = 1, \ldots, m_k$, of faces F_k . Here m_k denotes the number of vertices of F_k .

In our paper [28], where we give a solution of Tammes' problem for $N = 13$, there were considered main relations between these parameters [28, Propositions 3.6–3.11]. Let us give here these results. (We added also a general statement for $m > 4$.)

Proposition 4.1.

- (1) $u_{ki} < \pi$ *for all i and k.*
- (2) $u_{ki} \geq \alpha(d)$ *for all i and k, where*

$$
\alpha(d) := \arccos\left(\frac{\cos d}{1 + \cos d}\right)
$$

is the angle of the equilateral spherical triangle with side length d*.*

- $(3) \sum$ $\tau \in I(v)$ $u_{\tau} = 2\pi$ for all vertices v of G. Here $I(v)$ is the set of all vertices adjacent edges for *a vertex* v*.*
- (4) If $m_k = 3$, then F_k is an equilateral triangle with angles

$$
u_{k1} = u_{k2} = u_{k3} = \alpha(d).
$$

(5) In the case $m_k = 4$, F_k is a spherical rhombus and $u_{k1} = u_{k3}$, $u_{k2} = u_{k4}$. Moreover, we have the *equality:*

$$
\cot \frac{u_{k1}}{2} \cot \frac{u_{k2}}{2} = \cos d.
$$

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- (6) In the case $m_k > 3$, $F_k = A_1 A_2, \ldots, A_{m_k}$ is a convex equilateral spherical polygon with angles u_{k1}, \ldots, u_{m_k} . The polygon F_k is uniquely defined (*up to isometry*) by its $s := m_k - 3$ angles *and* d. Then there are uniquely defined functions g_i and ζ_{ij} such that $u_{ki} = g_i(u_{k1}, \ldots, u_{ks}, d)$ and $dist(A_i, A_j) = \zeta_{i,j}(u_{k1}, \ldots, u_{ks}, d)$ *. From this it follows that*
	- (a) $u_{ki} = g_i(u_{k1}, \ldots, u_{ks}, d)$ *for* $i = m_k 2, m_k 1, m_k$;
	- (b) $\zeta_{i,j}(u_{k1},\ldots,u_{ks},d) \geq d$ *for* $i \neq j$.
- (7) *Now consider the case where inside* $F_k = A_1 A_2, \ldots, A_{m_k}$ *there is an isolated vertex* (*this is possible only if* $m_k > 5$ *). Define*

$$
\lambda(u_{k1},\ldots,u_{ks},d):=\max_{p\in F_k}\min_i\{\text{dist}(p,A_i)\}.
$$

Then $\lambda(u_{k1},\ldots,u_{ks},d) > d$.

4.2. Algorithm's Description. In this section, we briefly consider our algorithm for enumeration of irreducible contact graphs with N vertices. More details can be found in $http://dcs.isa.ru/taras/$ irreducible/.

The algorithm consists of two steps.

- (I) First, we create the list L_N consisting of all graphs with N vertices that satisfy Corollary 2.1.
- (II) Using linear approximation of relations from Proposition 4.1 we remove from L_N all graphs that cannot be embedded in the sphere.

(I) For the list L_N we applied the program *plantri* (the authors of this program are Gunnar Brinkmann and Brendan McKay; see [29]). This program generates nonisomorphic planar graphs, including triangulations. (In [10], main methods and algorithms of plantri are given.)

(II) Consider a graph G from L_N . We start from the level of approximation $\ell = 1$. Proposition 4.1 gives the possibility to write linear equalities and inequalities for parameters (angles) $\{u_i\}$ of G.

For $\ell = 1$ we use the following relations:

(i) N linear equations:

$$
\sum_{k \in I(v)} u_k = 2\pi
$$

 $(Proposition 4.1(3));$

- (ii) for $2\pi/N \leq d$, we obtain $2\pi/N \leq \alpha$;
- (iii) Proposition 4.1(5) for a quadrilateral implies the equalities $u_3 = u_1$, $u_4 = u_2$, and the inequalities $\alpha \leq u_i \leq 2\alpha, i = 1, 2;$
- (iv) from the equality $u_2 = \rho(u_1, d)$, using the fact that ρ is monotonic in both parameters, we obtain maximum and minimum bounds for u_2 :

$$
\rho(u_{1,\max}, d_{\min}) \le u_2 \le \rho(u_{1,\min}, d_{\max}).
$$

So from these linear equalities and inequalities we can obtain maximum and minimum values for each variable. This gives us a domain D_1 that contains all solutions of this system if they exist there. If D_1 is empty, then we can remove G from the list L_N .

This step "kills" almost all graphs.

Next we consider $\ell = 2$. In this step, D_1 is divided into two domains and for both we can add the same linear constraints as for $\ell = 1$. Moreover, for this step we add new linear constraints for polygons with five or more vertices. Some details of this process are given below as well as in our paper [28, Sec. 4] and in http://dcs.isa.ru/taras/irreducible/.

In this level, we obtain the parameters domain D_2 . If this domain is empty, then G cannot be embedded to \mathbb{S}^2 and it can be removed from L_N .

For $\ell = 3$ we can repeat the previous step, divide D_2 into two domains and obtain additional constraints as for $\ell = 2$ for both parts independently.

We can repeat this procedure more and more times. In fact, increasing ℓ we increase the number of subcases. However, for practically every step some subcases vanish.

We repeat this process for $\ell = 1, 2, \ldots, m$ and obtain a chain of embedded domains:

$$
D_m \subset \cdots \subset D_2 \subset D_1.
$$

If this chain ends with the empty set, then G can be removed from L_N .

In the case where a graph G after certain m steps still "survives," i.e., $D_m \neq \emptyset$, then it is checked by numerical methods, namely by the so-called nonlinear "solvers." (We used, in particular, ipopt.) If a solution there exists, then G is declared as a graph that can be embedded, and if not, then G is removed from L_n .

Below we give some details of this algorithm.

4.3. Linear Approximations and the Spherical Law of Cosines. In Proposition 4.1, for polygons with four and more vertices we defined functions $g_i(u_{k1},...,u_{ks}, d)$ and $\zeta_{i,j}(u_{k1},...,u_{ks}, d)$. These functions can be calculated by the spherical law of cosines.

Let M be a polygon with $m > 3$ sides. Let us triangulate M by diagonals and enumerate the angles of triangles. For instance, in the case of a pentagon (see Fig. 2), we have nine angles (variables) that with angles of this pentagon (our variables) are connected by obvious equations.

Fig. 2. Pentagons' angles.

Actually, if d is fixed, then we have $m-3$ independent variables. To find relations between angles we need just one fact from the spherical trigonometry—the law of cosines:

$$
\cos \phi = \cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos \varphi,
$$

where for a spherical triangle ABC the lengths of its sides are denoted as $dist(A, B) = \theta_1$, $dist(A, C) = \theta_2$, $dist(B, C) = \phi$, and $\angle BAC = \varphi$.

For every triangle from a triangulation we can apply the law of cosines. Then by interval analysis all nonlinear inequalities can be approximated by linear inequalities. Let us consider some details.

4.3.1. Linear inequalities for the functions sin *and* cos*.* Now we are going to find linear estimations of f, where $f(x) = \cos(x)$ or $f(x) = \sin(x)$. If x lies inside a given interval $[x_0 - \delta, x_0 + \delta]$, then $C \leq kx - f(x) \leq D.$

Consider the Taylor series of f at x_0 :

$$
f(x) = f(x_0) + f'(x_0)(x - x_0) + \cdots + \frac{f^{(n)}(x_0)(x - x_0)^n}{n!} + \cdots
$$

It is easy to see that the sum of even terms is bounded by $f''(x_0)(x - x_0)^2/2$, and the sum of odd terms starting with the third is bounded by $f'''(x_0)/(x-x_0)^3/6$. Therefore, we have $k = f'(x_0)$ and

$$
C = -f(x_0) + kx_0 + \min\left(0, \frac{f''(x_0)\delta^2}{2}\right) - \frac{|f'''(x_0)|\delta^3}{6},
$$

$$
D = -f(x_0) + kx_0 + \max\left(0, \frac{f''(x_0)\delta^2}{2}\right) + \frac{|f'''(x_0)|\delta^3}{6}.
$$

We can replace by these inequalities all sin and cos functions in equalities and inequalities.

4.3.2. Linear inequalities for a product ab. If we have two variables a and b, $a \in [a_0 - \delta_a, a_0 + \delta_a]$ and $b \in [b_0 - \delta_b, b_0 + \delta_b]$, then we have the following linear inequalities:

$$
C \le k_a a + k_b b - ab \le D,
$$

where $k_a = b_0$, $k_b = a_0$, $C = a_0b_0 - \delta_a\delta_b$, and $D = a_0b_0 + \delta_a\delta_b$.

4.3.3. Linear inequalities for abc. Let $a \in [a_0 - \delta_a, a_0 + \delta_a], b \in [b_0 - \delta_b, b_0 + \delta_b],$ and $c \in [c_0 - \delta_c, c_0 + \delta_c].$ Then we have

$$
C \le k_a a + k_b + k_c c - abc \le D,
$$

where $k_a = b_0c_0$, $k_b = a_0c_0$, $k_c = a_0b_0$,

$$
C = 2a_0b_0c_0 - |a_0\delta_b\delta_c| - |\delta_a b_0\delta_c| - |\delta_a \delta_b c_0| - |\delta_a \delta_b \delta_c|,
$$

$$
D = 2a_0b_0c_0 + |a_0\delta_b\delta_c| + |\delta_a b_0\delta_c| + |\delta_a \delta_b c_0| + |\delta_a \delta_b \delta_c|.
$$

4.3.4. Linear inequalities for triangles. For the law of cosines

 $\cos c = \cos a \cos b + \sin a \sin b \cos \gamma$.

Using intervals for cos and sin we already have linear inequalities. For each triangle we write six pairs of linear inequalities for all sides and angles.

4.4. On Optimization of the Algorithm. It is very important to reduce the time complexity of the algorithm. We use several ideas for this.

(1) For every step ℓ , using branch-and-bound algorithm, we choose a variable that is divided in two parts. For each graph, there is defined the minimum set of variables that uniquely defines other variables. Then we divide only these variables and $a = \alpha(d)$, which is equal to the angle of an equilateral triangle with side length d (see Proposition 4.1). This increases the speed substantially, in some cases up to 1000 times.

(2) For variable bounds we have used the following heuristic algorithm. If for some variable we decreased its interval successfully, then we consider its "neighbors," i.e., variables that appear together in formulas.

4.5. On Complexity of Computations. We have already noted that there are two steps for enumerating irreducible contact graphs. In the first step, where the table L_N is created, the number of graphs grows very fast. For instance, for $N = 6, 7, 8$ we have $|L_N| = 7, 34, 257$. However, for $N = 13$ we have $|L_N| = 94\,754\,965.$

In the second step, most graphs are removed from L_N for $\ell = 1$. However, when N increases, the number of "bad" graphs (i.e., graphs that cannot be embedded in the sphere but survived after many iterations) essentially increases. For these graphs we must use nonlinear solvers, and so the computations increase substantially. This is the main reason why we have tables only up to $N = 11$.

5. Results

We applied the method discussed above and obtained the following theorem.

Theorem. The list of all irreducible contact graphs for $N = 7, 8, 9, 10, 11$ on the sphere \mathbb{S}^2 is given in *tables in Secs.* 5.1–5.5*. Here* ∗ *means that this graph is found by Danzer and therefore is D-irreducible, and* $**$ *means that this graph is maximal. The tables also show bounds for d,* $d_{\min} \leq d \leq d_{\max}$. (*However, note that here values of* d_{min} *and* d_{max} *are found numerically and so can be a little different from the actual values.*)

5.1. Irreducible Graphs with 7 Vertices.

5.2. Irreducible Graphs with 8 Vertices.

 N $\hspace{1cm}d_{\min}$ $\hspace{1cm}d_{\max}$ 1 1.17711 1.18349 ∗ 1.28619 1.30653 $1.23096\,$ ∗∗ 1.30653 1.30653

5.3. Irreducible Graphs with 9 Vertices.

5.4. Irreducible Graphs with 10 Vertices.

 \searrow 2

 $\begin{array}{ccc} & & A & \ & \searrow & \end{array}$

> g)\$

 \mathscr{A} \longrightarrow \uparrow

5.5. Irreducible Graphs with 11 Vertices.

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Oleg R. Musin Institute for Information Transmission Problems, Russian Academy of Sciences, Moscow, Russia, University of Texas at Brownsville, Brownsville, Texas, USA E-mail: oleg.musin@utb.edu

Alexey S. Tarasov

Institute for Information Transmission Problems, Russian Academy of Sciences, Moscow, Russia E-mail: tarasov.alexey@gmail.com