THE TWELVE SPHERES PROBLEM

ROB KUSNER, WÖDEN KUSNER, JEFFREY C. LAGARIAS, AND SENYA SHLOSMAN

ABSTRACT. The problem of 12 spheres is to understand, as a function of r with $0 < r \leq r_{max}(12)$, the configuration space of 12 nonoverlapping equal spheres of radius r touching a central unit sphere. It considers to what extent, and in what fashion, touching spheres can be moved around on the unit sphere, subject to the constraint of always touching the central sphere. Such constrained motion problems are of interest in physics and materials science, and the problem involves topology and geometry. This paper reviews the history of work on this problem, and formulates some conjectures. It also addresses results on configuration spaces of N spheres of radius r touching a central unit sphere, for $3 \leq N \leq 14$. The problem of determining the maximal radius $r_{max}(N)$ is equivalent to the Tammes problem, to which László Fejes-Tóth made significant contributions.

1. INTRODUCTION

The "problem of 13 spheres," so named by Schütte and van der Waerden [100] and Leech [75], concerns deciding whether there exists any configuration of 13 non-overlapping unit spheres that all touch a central unit sphere. It was raised in the time of Newton and eventually resolved mathematically as impossible. Its resolution established that the "kissing number" of equal 3-dimensional spheres is 12.

This paper is concerned with a different problem: *How can 12 spheres of equal radius r touch a given central sphere of radius 1, in what patterns, and how are these patterns related? In other words, what is the topology of the corresponding configuration space of such spheres?* In this paper we present the remarkable history of this problem, survey aspects of what is currently known about it, and present some new results and conjectures.

This problem has come up in physics and materials science. Many atoms and molecules are roughly spherical, and their local interactions are governed by how many of them can get close to a single atom. So the arrangements possible for 13 nearby spheres, and allowable motions between them, are relevant to the nature of local interactions, to measuring the entropy of local configurations, and to phase changes in certain materials. We are particularly motivated by a statement of Frank (1952), made concerning supercooling of fluids, given in Section 2.7. Insisting that exactly 12 equal spheres touch a 13-th central sphere, possibly of a different radius, gives a mathematical toy problem that can be subjected to careful analysis.

As a mathematical problem, the 12 spheres problem has both a metric geometry side and a topology side. László Fejes-Tóth made major contributions to the metric geometry side, which concerns extremal questions, which are packing problems. In connection with the Tammes problem, described in Section 3, he found the largest radius of 12 spheres

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that can touch a central sphere of radius 1, and found other extremal configurations of touching spheres for small N. He posed the Dodecahedral Conjecture concerning the minimal volume Voronoi cell in a unit sphere packing, and posed another conjecture characterizing all configurations that pack space with every sphere having exactly 12 neighboring spheres. Both of these conjectures are now proved. The topological side concerns allowable motions and rearrangements of configurations of spheres, and topological constraints on them. A major part of this paper addresses the topological side of the problem, concerning the topology of configuration spaces, and variation of the topology as the radius r is varied. awk

1.1. Configuration Spaces.

The arrangements of the 12 touching spheres are encoded in the associated *configuration space* of 12-tuples of points on the surface of a unit sphere that remain at a suitable distance from each other. This space has nontrivial topology and geometry. In topology the general subject of configuration spaces started in the 1960s with the consideration of topological spaces whose points denote configurations of a fixed number N of labeled points on a manifold. Here we consider the *constrained* configuration space $\mathrm{Conf}(N)[r]$ of N nonoverlapping spheres of radius r which touch a central sphere $\mathbb{S}^2$ of radius 1, centered at the origin. (Here "non-overlapping" means the spheres have disjoint interiors.) It can also be visualized as the space of 12 spherical caps on the sphere, which are obtained as the radial projection of the external spheres onto the surface of the central sphere, whose *angular diameter* we call θ. (Here $\theta = f(r)$ is a known function of r.) The centers of these caps define a constrained N-configuration on $\mathbb{S}^2$ where no pair of points can approach closer than angular separation θ. For generic ("non-critical") values of r for a range of values $0 < r < r_{max}(N)$ this space is a compact $2N$-dimensional manifold with boundary, not necessarily connected.

The group $SO(3)$ acts as global symmetries of $\mathrm{Conf}(12)[r]$ by rigidly rotating the N-configuration of spheres touching the central sphere. The *reduced constrained configuration space* $\mathrm{BConf}(N)[r] = \mathrm{Conf}(N)[r]/SO(3)$ is obtained by identifying all configurations in an $SO(3)$-orbit. by removing global symmetries of rotations of the central sphere, along with * the touching spheres. For generic values of r it is a compact $(2N-3)$-dimensional manifold with boundary; for the case of 12 spheres this is a 21-dimensional manifold. The subject of constrained configuration spaces has in part been developed for applications to fields such as robotics. For an introduction to the robotics aspect, see Abrams and Ghrist [1] or Farber [37].

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We study both the cases of configuration spaces fixed radius r, and of change in topology in such spaces as the radius r is varied. In the case of varying r the configuration space changes topology at a set of *critical radius values*. Associated to these special values are *critical configurations*, which are extremal in a suitable sense. The change in topology is described by a generalization of Morse theory applicable to the radius function r, which we discuss in Section 4. To determine these changes one studies the occurrence and structure of the critical configurations. The simplest example of such topology change concerns the connectivity of the space of configurations as a function of r, reported by the rank of the 0-th homology group of the configuration space.

The 12-spheres problem includes as its most important special case that of $r = 1$, the case remove - of equal spheres. We discuss the topological space $\mathrm{BConf}(12))[1]$ at length in Sections 5 and 6, and formulate several conjectures related to it. The radius $r = 1$ is a critical radius, and two configurations, FCC configurations and HCP configurations, are critical configurations. The topology of this space appears to be very complicated, and its cohomology groups have not been determined. We describe how it is possible to move in the space $\mathrm{BConf}(12)[1]$ to deform any dodecahedral configuration DOD of 12 labeled spheres to any other such configuration, permuting the 12 spheres arbitrarily. We formulate the (folklore) conjecture that the value $r = 1$ is the largest radius value for which the configuration space $\mathrm{BConf}(12)[r]$ is connected, i.e. it is the largest value for which the 0-th cohomology group of $\mathrm{BConf}(12)[r]$ has rank 1.

We also present results concerning the spaces $\mathrm{Conf}(\mathbb{S}^2, N)[r]$ of N-configurations of spheres with radius r touching a central sphere of radius 1, for small values $3 \le N \le 14$. The simplest question is the metric geometry problem of determining the maximum allowable radius $r_{max}(N)$ for the N spheres; this is a variant of the Tammes problem, which is also treated in the literature under the name *minimal spherical codes*. We survey results on it in Section 3. We completely determine the cohomology of $\mathrm{Conf}(\mathbb{S}^2, 4)[r]$ for allowable r in Section 4.6.

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1.2. Physics and Materials Science.

Configuration spaces are of interest in physics and materials science. Jammed configurations are a granular materials criterion for a stable packing. According to Torquato and Stillinger [108, p. 2634] they are: "particle configurations in which each particle is in contact with its nearest neighbors in such a way that mechanical stability of a specific type is conferred to the packing." Packings of rigid disks and spheres have been studied extensively by simulation (Lubachevsky and Stillinger [79], Donev et al. [30]). It has been empirically discovered that randomly ordered hard spheres achieve in random close packing a density around 66 percent (cf. [102]), and pass through a jamming transition around 64 percent ([76, p. 355]. The appearance of a jamming phase transition, signaled by a change in shear modulus, and the formation of a glass state, is relevant in studying the behavior of colloidal suspensions and granular materials. The large rearrangement of structure required in making a phase transition is relevant in the phenomenon of supercooling of liquids, see Section 2.7. The nature of glass transitions has been called "the deepest and most interesting unsolved problem in solid state theory"(Anderson [3]). For articles and reviews of these topics, see Ediger et al. [31], O'Hern et al. [90], and Liu and Nagel [76]. (For a general survey of hard sphere models, including the idea of a liquid-solid phase transition in packings, see Löwen [77].)

One may make an analogy between the configuration spaces $\mathrm{BConf}(N)[r]$ treated here and a sphere packing model for jamming studied in [90], which treats spheres having repulsive local potential at zero density and zero applied stress, and includes hard spheres for one model parameter value. In the latter model the order parameter is the packing fraction of the spheres. In the configuration space model, a proxy value for the packing fraction is the radius parameter r, which determines the fraction of surface area of $\mathbb{S}^2$ covered by the N spherical caps. An analogue of the jamming transition value in the configuration space model is then the maximal radius $r_{conn}(N)$ at which the constrained configuration space $\mathrm{BConf}(N)[r]$ remains connected; this property is detected by the 0-th cohomology group. Finer topological invariants of this kind are then supplied by the various critical values r_j at which the ranks of the individual cohomology groups $H^k(\mathrm{BConf}(N)[r], \mathbb{Q})$ change. Our configuration model

is simplified in being 2-dimensional, with constrained configurations on the surface of a 2-sphere $\mathbb{S}^2$, a space which however has the new feature of positive curvature, giving a compact configuration space. For the jamming problem itself (constrained) configuration spaces of 3-dimensional hard spheres in a large box seems a more appropriate space. The general direction of inquiry investigating the sizes of critical points of topological invariants (Betti numbers) of configuration spaces could potentially shed new light on the nature of jamming transitions. See section 7 for further remarks on this topic.

1.3. Roadmap.

The sections of the paper have been written to be independently readable. Section 2 gives a brief history of results on the 12 spheres problem and sphere packing. Section 3 surveys results on the maximal radius $r_{\max}(N)$ for configurations of N equal spheres touching a central sphere of radius 1 for small N. This problem is equivalent to the Tammes problem. Section 4 begins with the topology of configuration spaces of N points on $\mathbb{R}^2$ and on the 2-sphere $\mathbb{S}^2$, corresponding to radius $r = 0$. It then considers spaces of configurations of equal spheres of radius r touching a sphere of radius 1 for variable $0 < r \le r_{\max}(N)$. Section 5 discusses the special configuration space of 12 unit spheres touching a 13-th central sphere, i.e. the case of radius $r = 1$. It focuses on properties of the FCC-configuration, the HCP-configuration and the dodecahedral configuration. Section 6 considers the problem of permutability of the spheres of the dodecahedral configuration for $r = 1$, conjecturing that the constrained configuration space at $r = 1$ is connected, and that this is the largest value of r where connectivity holds. It also considers the $r > 1$ case and formulates several conjectures about disconnectness. Section 7 makes some concluding remarks.

2. The Twelve Spheres Problem: History

We begin with some historical vignettes concerning configurations of 12 spheres touching a central sphere, as they have come up in physics, astronomy, biology and materials science.

2.1. Kepler (1611).

Johannes Kepler (1571–1630) studied packings and crystals in his 1611 pamphlet "The Six-cornered snowflake" [71]. In it he asserts that the densest sphere packing of equal spheres is the FCC packing, or "cannonball packing." He states that this packing has 12 unit spheres touching each central sphere:

> In the second mode, not only is every pellet touched by its four neighbors in the same plane, but also by four in the plane above and four below, so throughout one will be touched by twelve, and under pressure spherical pellets will become rhomboid. This arrangement will be more compatible to the octahedron and the pyramid. The packing will be the tightest possible, so that in no other arrangement could more pellets be stuffed into the same container. [1]

[1] "Iam si ad structuram solidorum quam potest fieri arctissimam progredaris, ordinesque ordinibus superponas, in plano prius coaptatos aut ii erunt quadrati A aut trigonici B: si quadrati aut singuli globi ordinis superioris singulis superstabunt ordinis inferioris aut contra singuli ordinis superioris sedebunt inter quaternos ordinis inferioris. Priori modo tangitur quilibit globis a quattuour cirucmstantibus in eodem plano, ab uno supra se, et ab uno infra se: et sic in universum a six aliis, eritque ordo cubicus, et compressione facta fient cubi: sed no erit arctissima coaptatio. Posteriori modo praeterquam quod quileibet globus a quattuor circumstantibus in eodem plano tangitur etiam a quattuor infra se, et a quattuor supra se, et sic in universum a duodecim tangetur; fientque compressione ex globosis rhombica. Ordo hic magis assimilabitur octahedro

He expands on the construction as follows:

> Thus, let B be a group of three balls; set one A, on it as apex; let there be also another group C, of six balls, and another D, of ten, and another E, of fifteen. Regularly superpose the narrower on the wider to produce the shape of a pyramid. Now, although in this construction each one in the upper layer is seated between three in the lower, yet if you turn the figure round so that not the apex but the whole side of the pyramid is uppermost, you will find, whenever you peel off one ball from the top, four lying below it in square pattern. Again as before, one ball will be touched by twelve others, to with, by six neighbors in the same plane, and by three above and three below. Thus in the closest pack in three dimensions, the triangular pattern cannot exist without the square, and vice versa. It is therefore obvious that the loculi of the pomegranate are squeezed into the shape of a solid rhomboid.... [2]

The cannonball packing had been studied earlier by the English mathematician Thomas Hariot [Harriot] (1560–1621). Hariot was mathematics tutor to Sir Walter Raleigh, designed some of his ships, wrote a treatise on navigation, and went on an expedition to Virginia in 1585-1587 as surveyor, reporting on it in 1590 in [60], his only published book. He computed a chart in 1591 on how to most efficiently stack cannonballs using the FCC packing, and computed a table of the number of cannonballs in such stacks (cf. Shirley [103, pp. 242–243]). Hariot supported the atomic theory of matter, in which case macroscopic objects may be packed in arrangements of very tiny spherical objects, i.e. atoms. ([69, Chap. III]). He corresponded with Kepler in 1606-1608 on optics, and mentioned the atomic theory in a December 1606 letter as a possible way of explaining why some light is reflected, and some refracted, at the surface of a liquid. Kepler replied in 1607, not supporting the atomic theory. The known correspondence of Hariot with Kepler does not deal directly with sphere packing.

The statement that the maximal density of a sphere packing in 3-dimensional space equals $\frac{\pi}{\sqrt{18}} \approx 0.74048$, which is attained by the FCC packing, is called the *Kepler Conjecture*. It was settled affirmatively in the period 1998-2004 by ~~T. C.~~ Hales with ~~S.~~ Ferguson, see [74]. A second generation proof, which is a formal proof checked entirely by computer, was recently completed in a project led by ~~T. C.~~ Hales [58].

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2.2. Newton and Gregory (1694). The discussion of Isaac Newton and David Gregory in 1694 was related to preparing a second edition of Newton's *Principia*. It concerned the question

et pyramidi. Coaptatio fiet arctissima, ut nullo praetera ordine plures globuli in idem vas compingi queant." [Translation: Colin Hardie [71, p. 15]]

[2] "Esto enim B copula trium globorum. Ei superpone A unum pro apice; esto et alia copula senum globorum C, et alia denum D et alia quindenum E. Impone semper angustiorem latiori, ut fiat figura pyramidis. Etsi igitur per hanc impositionem singuli superiores sederunt into trinos inferiores: tamen iam versa figura, ut non apex sed integrum latus pyramidis sit loc superiori, quoties unum globulum deglberis e summis, infra stabunt quattuor ordine quadrato. Et rursum tangetur unus globus ut prius, et duodecim aliis, a sex nempe circumstantibus in eodem plano tribus supra et tribus infra. Ita in solida coaptatione arctissima non potest ess ordo triangularis sine quadrangulari, nec vicissim. Patet igitur, acinos punici mali, materiali necessitate concurrente cum rationaibus incrementi acinorum, exprimi in figuri rhombici corporis..." [Translation by Colin Hardie [71, p. 17]]

whether the "fixed stars" are subject to gravitational attraction. What force is "balancing" their apparent fixed positions?

Gregory ([91, Vol III, p. 317]) summarized in a memorandum a conversation with Newton on 4 May 1694 concerning the brightest stars as: [3]

> To discover how many stars there are of a given magnitude, he [Newton] considers how many spheres, nearest, second from them, third etc. surround a sphere in a space of three dimensions, there will be 13 of first magnitude, 4×13 of second, $9 \times 4 \times 13$ of third.

Newton's own star table "A Table of ye fixed Starrs for ye yeare 1671" records 13 first magnitude stars, 43 of the second magnitude, 174 of third magnitude, cf. [91, Vol II, p. 394].

Newton drafted a new Proposition to be included in a second edition of the *Principia*, stating [in translation] ([67, p. 81]):

> Proposition XV. Theorem XV. The fixed stars are at rest in the heavens and are separated by enormous distances from our Sun and from each other.

In a draft proof he wrote [in translation]([67, page 85])

> That the stars are at huge distances from our Sun is clear enough from the absence of parallax; and that they lie at no less distances from each other may be inferred from their differing apparent magnitudes. For there are 13 stars of the first magnitude and roughly the same number of equal spheres can be arranged about a central sphere equal to them.

and:

> For if around some sphere there are arranged more spheres of about the same size, the number of spheres which surround it closely will be 12 or 13; at the second stage about 50; at the third about 110 [roughly 9×12]; at the fourth, 200 [$16 \times 12\frac{1}{2}$], ...

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After further work, through several drafts, Newton abandoned this Proposition, cf. Hoskin [67]. It was not included in the second edition of the *Principia* when it finally came out in 1713.

Gregory considered the geometric problem underlying the spacing of stars. In an (unpublished) notebook[4] he considered the packing problem in 2-dimensional disks in concentric rings and, in 3-dimensions, that of equal spheres, noting that 13 spheres might touch a given equal sphere [91, Vol III, Letter 441, note (10), p. 321]. He continued to consider the 13 sphere question in later years, making the following memorandum in 1704 ([64, p. 21]).

> *Oxon. 23 Nov^r 1704.* Mr. Kyl[5] said that if 13 equal spheres touch an equal inmost sphere, 9×13 must touch one that include these former 14, because there is nine times as much surface to stand on. I told him that we must reckon by the surface passing through their centers.

[3] "Ut noscatur quot sunt stellae magnitudinis 1 ae, 2 dae, 3 ae & c. considerando quot spherae proximae, seundae ab his 3 ae & c. spheram in spatio trium dimensionis circumstent: erunt 13 primae, 4×13 2-dae, $9 \times 4 \times 13$ 3 ae."

[4] This notebook is at Christ Church, Oxford, according to J. Leech [75],

[5] John Keill (1671–1721) succeeded Gregory as Savilian Professor.

An argument similar to one of Kepler [[picture]], with roots in the claim of Giordano Bruno, that all stars are suns.

We may infer that Newton left the question of how many spheres might touch unresolved, and that Gregory believed 13 spheres might touch.

2.3. **Bender, Hoppe, Günther (1874).** The issue of whether 13 equal spheres might touch a central equal sphere was discussed in the physics literature in the period 1874–1875, with contributions by Bender [10], Hoppe [66] and Günther [54]. Hoppe noted a mathematical gap in the argument of Bender. Günther offered a physical intuition, but no proof. They all concluded that at most 12 unit spheres could touch a central unit sphere. In 1994 Hales [56] noted a mathematical gap in the argument of Hoppe.

2.4. **Barlow (1883).** In another context the crystallographer William Barlow (1845–1934) noted another optimal sphere packing, the *Hexagonal Close Packing* (HCP). In a paper "Probable nature of the internal symmetry of crystals" ([8, p.186]) he considered five symmetry types for crystal structure. The third kind of symmetry he describes is the FCC packing (Fig. 4 and 4a). He then stated:

> A fourth kind of symmetry, which resembles the third in that each point is equidistant from the twelve nearest points, but which is of a widely different character than the three former kinds, is depicted if layers of spheres in contact arranged in the triangular pattern (plan d) are so placed that the sphere centers of the third layer are over those of the first, those of the fourth layer over those of the second, and so on. The symmetry produced is hexagonal in structure and uniaxial (Figs. 5 and 5a).

Here "plan d" is the two-dimensional hexagonal packing, and Figs. 5 and 5a depict the HCP packing. He suggested that the atoms in a crystal of quartz (SiO_2) occur with the fourth kind of symmetry. See Figure 1.

Barlow also stated later in the paper ([8, p.207], Figure 2) the following about twinned crystal arrays with a connecting layer:

> The peculiarities of *crystal-grouping* displayed in twin crystals can be shown to favour the supposition that we have in crystals symmetrical arrangement rather than symmetrical shape of atoms or small particles. Thus if an octahedron be cut in half by a plane parallel to two opposite faces, and the hexagonal faces of separation, while kept in contact and their centres coincident, are turned one upon the other through 60°, we know that we get a familiar example of a form found in some twin crystals. And a stack can be made of layers of spheres placed triangularly in contact to depict this form as readily as to depict a regular octahedron, the only modification necessary being for the layers above the centre layer to be placed as though turned bodily through 60°, from the position necessary to depict an octahedron (compare Figs. 7 and 8). The modification, as we see, involves *no departure from the condition that each particle is equidistant from the twelve nearest particles.*

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2.5. **Tammes (1930).** The Dutch botanist P. M. L. Tammes made in 1930 a study of the equidistribution of spores on pollen grains [104]. He asked the question: What is the maximum number of circular caps $N(\theta)$ of angular diameter θ that can be placed without overlap on a unit sphere? Here θ is measured from the center of the unit sphere S^2 in

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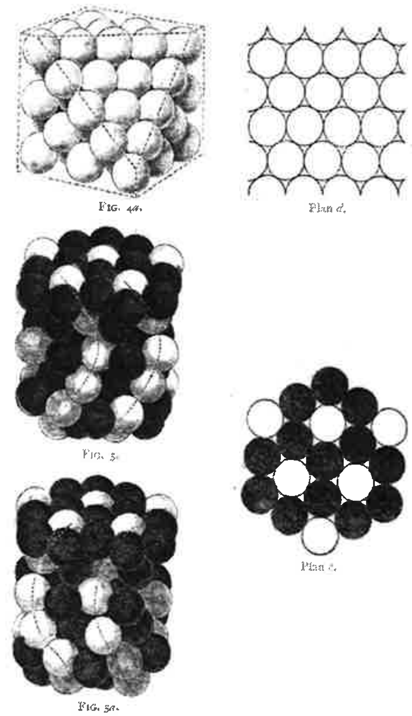

FIGURE 1. Barlow FCC and HCP packings

$\mathbb{R}^3$. Tammes [104, Chap. 3] empirically determined that $N(\frac{\pi}{2}) = 6$, while $N(\theta) \le 4$ for $\theta > \frac{\pi}{2}$. Let $\theta = \theta(N)$ denote the maximal value of θ having $N(\theta) = N$. He concluded that $\theta(5) = \theta(6) = \frac{\pi}{2}$.

The problem of determining various values of $N(\theta)$ is now called the *Tammes problem.* It is related to a dual question of determining the maximal radius $r(N)$ possible for N equal spheres all touching a central sphere of radius 1. Namely, the maximal value of $\theta := \theta(N)$ having $N(\theta) = N$, determines the maximal allowable radius $r(N)$ of N spheres touching a central unit sphere by a formula given in Lemma 3.1 below.

Other allied forms, as allied octahedra or rhombohedra, can be in the same way connected with some one of the five kinds of internal symmetry.

The peculiarities of *crystal-grouping* displayed in twin crystals can be shown to favour the supposition that we have in crystals symmetrical arrangement rather than symmetrical shape of atoms or small particles. Thus if an octahedron be cut in half by a plane parallel to two opposite faces, and the hexagonal faces of separation, while kept in contact and their centres coincident, are turned one upon the other through 60°, we know that we get a familiar example of a form found in some twin crystals. And a stack can be made of layers of spheres placed triangularly in contact to depict this form as readily as to depict a regular octahedron, the only modification necessary being for the layers above the centre layer to be placed as though turned bodily through 60° from the position necessary to depict an octahedron (compare Figs. 7 and 8). The modification, as we see,

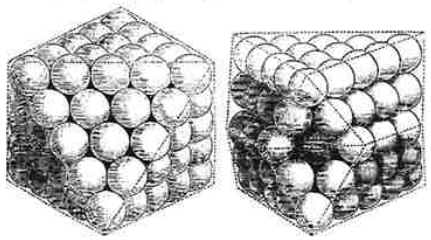

FIG. 7. FIG. 8.

involves *no departure from the condition that each particle is equidistant from the twelve nearest particles.*

FIGURE 2. Barlow Twinned Crystal Packing

2.6. **Fejes-Tóth (1943).** In 1943 László Fejes-Tóth [40] conjectured that the volume of any Voronoi cell of any sphere packing of $\mathbb{R}^3$ by unit spheres is minimized by the dodecahedral configuration of 12 unit spheres touching a central sphere. The Voronoi cell of the central sphere is then a regular dodecahedron circumscribed about the sphere. The packing density of the dodecahedron is approximately 0.7546, which is larger than the density of the known FCC packing of $\mathbb{R}^3$. This conjecture became known as the *Dodecahedral Conjecture* and was settled affirmatively in 2010, see Section 5.4.

2.7. **Frank (1952).** The problem of molecular rearrangement in the liquid-solid phase transition is relevant in materials. The structure of ordinary ice, the H_2O phase labeled ice I_h, has an HCP packing of its oxygen atoms, as observed in 1921 by Dennison [29] (the hydrogen atoms are free to change their orientations to some extent, cf. Pauling [92]). Water exhibits a phenomenon of supercooling at standard pressure down to $-48°C$; under special rapid cooling it can avoid freezing down to $-137°C$, and enter a glassy phase (cf. Angell [5]).

In 1952 Frederick Charles Frank [47] argued that supercooling can occur because the common arrangements of molecules in liquids assume configurations far from what they would assume if frozen. He wrote:

> Consider the question of how many different ways one can put twelve billiard balls in simultaneous contact with another one, counting as different the arrangements which cannot be transformed into each other without breaking contact with the centre ball?' The answer is *three*. Two which come to the mind of any crystallographer occur in the face-centred cubic and hexagonal close packed lattices. The third comes to the mind of any good schoolboy, and it is to put one at the centre of each face of a regular dodecahedron. That body has five-fold axes, which are abhorrent to crystal symmetry: unlike the other two packings, this one cannot be continuously extended in three dimensions. You will find that the outer twelve in this packing do not touch each other. If we have mutually interacting deformable spheres, like atoms, they will be a little closer to the centre in this third kind of packing; and if one assumes they are argon atoms (interacting in pairs with attractive and repulsive potentials proportional to r^{-6} and r^{-12}) one may calculate that the binding energy of the group of thirteen is 8.4% greater than for the other two packings. This is 40% of the lattice energy per atom in the crystal. I infer that this will be a very common grouping in liquids, that most of the groups of twelve atoms around one will be of this form, that freezing involves a substantial rearrangement, and not merely an extension of the same kind of order from short distances to long ones; a rearrangement which is quite costly of energy in small localities, and which only becomes economical when extended over a considerable volume, because unlike the other packing it can be so extended without discontinuities.

The three local arrangements Frank specifies we shall label as FCC (face-centered-cubic), HCP (hexagonal close packing) and DOD (dodecahedral), for convenience. The crystalline arrangements of FCC and HCP are "extremal" (i.e. on the boundary of the configuration space), while the balls in DOD configuration are free to move independently.

Frank's assertion that there are exactly three possible arrangements is *false* if taken literally. There are continuous deformations between any arrangement of types FCC, HCP and DOD and any of the other types, see Section 5.4. There is however an important kernel of truth in Frank's statement, which buttresses his argument made concerning the existence of supercooling: each of the three arrangements above is "remarkable" in some sense (see Section 5). To move from a large arrangement of spheres having many DOD configurations to one frozen in the HCP packing requires substantial motion of the spheres.

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2.8. **Schütte and van der Waerden (1953).** In a paper titled "Das Problem der dreizehn Kugeln" ("The problem of the thirteen spheres") Schütte and van der Waerden [100] gave a rigorous proof that one cannot have 13 unit spheres touching a given central sphere. x full names

There has been much further work on this problem. In his 1956 paper titled "The problem of 13 spheres" John Leech [75] gave a two page proof of the impossibility of 13 unit spheres touching a unit sphere. More accurately he stated: "In the present paper I outline an independent proof of this impossibility, certain details which are tedious rather than difficult have been omitted." Various authors have written to fill in such details, which balloon the length of the proof. These include work of Machara [80] in 2001, who gave in 2007 a simplified proof [81]. Other proofs of the thirteen spheres problem were given by Anstreicher [4] in 2004 and Musin [86] in 2006.

2.9. **Fejes-Tóth (1969).** In 1969 László Fejes-Tóth [45] discussed the problem of characterizing those sphere packings in space that have the property that every sphere in the packing touches exactly 12 neighboring spheres. The FCC and HCP packing both have this property, as already noted by Barlow (1883). There are in addition uncountably many other packings, obtained by stacking plane layers of hexagonally packed spheres ("penny packing"), where there are two choices at each level of how to pack the next level. Fejes-Tóth conjectured that all such packings are obtained in this way.

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This conjecture of Fejes-Tóth's was settled affirmatively by ~~Thomas~~ Hales [57] in 2013.

2.10. **Conway and Sloane (1988).** In their book: *Sphere Packings, Lattices and Groups,* Conway and Sloane considered the question: *What rearrangements of the 12 unit spheres are possible using motions that maintain contact with the central unit sphere at all times?* In [25, Chap. 1, Appendix: Planetary Perturbations] they sketch a result asserting: The configuration space of 12 unit spheres touching a 13-th allows arbitrary permutations of all 12 touching spheres in the configuration. That is, if the spheres are labeled and in the DOD configuration, it is possible, by moving them on the surface of the central sphere, to arbitrarily permute the spheres in a DOD configuration.

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We will describe the motions in detail to obtain such permutations in Section 6.

3. Maximal radius configurations of N spheres: The Tammes Problem

What is the maximal radius $r(N)$ possible for N equal spheres all touching a central sphere of radius 1? This problem is closely related to the *Tammes problem* discussed above, which concerns instead the maximum number of circular caps $N(\theta)$ of angular diameter θ that can be placed without overlap on a sphere. The latter problem is also the problem of constructing good spherical codes, see [25, Chap. 1, Sec. 2.3].

3.1. **Radius versus angular diameter parameterization.** One can convert the angular measure θ into the radius of touching spheres; for a sphere touching a central unit sphere, its associated spherical cap on the central sphere is the radial projection of its points onto the boundary of the central sphere.

Lemma 3.1. *For a fixed value of $N > 2$ the maximal value of $\theta := \theta(N)$ having $N(\theta) = N$ then determines the maximal allowable radius $r_{max}(N)$ of N spheres touching a central unit sphere, using the formula*

$$r_{max}(N) = \frac{\sin\frac{\theta(N)}{2}}{1-\sin\frac{\theta(N)}{2}}.$$

Conversely, given $r = r_{max}(N)$, we obtain

$$\theta(N) = 2\arcsin\left(\frac{r}{1+r}\right),$$

choosing $0 < \theta(N) < \pi$.

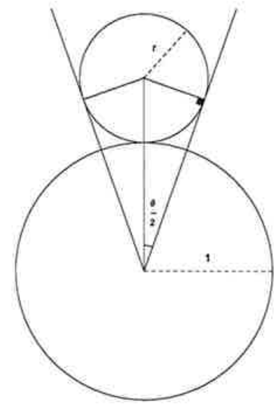

FIGURE 3. Angular measure θ related to radius r

Proof. From the right triangle in Figure 3 we have

$$\sin\frac{\theta}{2} = \frac{r}{1+r}.$$

This relation gives a bijection of the interval $0 \le \theta < \pi$ to the interval $0 \le r < \infty$. □

3.2. **Rigorous results for small N.** The Tammes problem has been solved exactly for only a few values of N, including $3 \le N \le 14$ and $N = 24$.

3.2.1. **Fejes-Tóth:** $N = 3, 4, 6, 12$. The Tammes problem was solved for $N = 3, 4, 6$ and 12 by L. Fejes-Tóth [39] in 1943, where extremal configurations of touching points for $N = 3$ are attained by vertices of an equilateral triangle arranged around the equator, and for $N = 4, 6, 12$ by vertices of regular polyhedra (tetrahedron, octahedron and icosahedron) inscribed in the unit sphere. Fejes-Tóth proved the following inequality: For N points on the surface of the unit sphere, at least two points can always be found with spherical distance

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$$d \le \arccos\left(\frac{(\cot\omega)^2 - 1}{2}\right), \quad \text{with} \quad \omega = \left(\frac{N}{N-2}\right)\frac{\pi}{6}.$$

Note that d is the edge-length of a spherical equilateral triangle with the expected area for an element of an N-vertex triangulation of $\mathbb{S}^2$. The inequality is sharp for $N = 3, 4, 6$ and 12 for the specified configurations above.

In 1949 Fejes-Tóth [41] gave another proof of his inequality. His result was re-proved by Habicht and van der Waerden [55] in 1951. After converting this result to the r-parameter using Lemma 3.1, we may re-state his result for $N = 12$ as follows.

Theorem 3.2. (Fejes-Tóth (1943))

(1) The maximum radius of 12 *equal spheres touching a central sphere of radius* 1 *is:*

$$r_{max}(12) = \frac{1}{\sqrt{\frac{5+\sqrt{5}}{2}} - 1} \approx 1.1085085.$$

Here $r_{max}(12)$ is a real root of the fourth degree equation $x^4 - 6x^3 + x^2 + 4x + 1 = 0$.

(2) An extremal configuration achieving this radius is the 12 *vertices of an inscribed regular icosahedron (equivalently, face-centers of a circumscribed regular dodecahedron).*

3.2.2. **Schütte and van der Waerden:** $N = 5, 7, 8, 9$. The Tammes problem was solved for $N = 5$ in 1950 by van der Waerden, building on work of Habicht and van der Waerden [55]. It was solved for $N = 7$ by Schütte. These solutions, plus those of van der Waerden for $N = 8$ and Schütte for $N = 9$ appear in Schütte and van der Waerden [99]. They give a history of these developments on [99, p. 97].

Their paper used geometric methods, introducing and studying the allowed structure of the graphs describing the touching patterns of arrangements of N equal circles on $\mathbb{S}^2$. These graphs are now called *contact graphs*, and Schütte and van der Waerden credit their introduction to Habicht. Schütte also conjectured candidates for optimal configurations for $N = 10, 13, 14, 15, 16$ and van der Waerden conjectured candidates for $N = 11, 24, 32$, see [99].

L. Fejes-Tóth presented the work of Schütte and van der Waerden of his 1953 book on sphere-packing [42, Chapter VI]. This book uses the terminology of *maximal graph* for the graph of a configuration achieving the maximal radius for N. In 1959 Fejes-Tóth [43] noted that the set of vertices of a square antiprism gave an extremal $N = 8$ configuration on the 2-sphere.

3.2.3. **Danzer:** $N = 6, 7, 8, 9, 10, 11$. In his 1963 Habilitationsschrift [27] (see the 1986 English translation [28]), Ludwig Danzer made a geometric study of the contact graph for a configuration of N circles on the surface of a sphere. This graph has a vertex for each circle and an edge for each pair of touching circles. A contact graph is called *maximal* if it occurs for a set of circles achieving the maximal radius $r_{max}(N)$. It is called *optimal* if it has the minimum number of edges among all maximal contact graphs. A contact graph is called *irreducible* if the radius cannot be improved by altering a single vertex. For each small N, Danzer found a complete list of irreducible contact graphs. He used this analysis to prove the conjectures of Schütte and van der Waerden [99] above for the cases $N = 10, 11$.

Theorem 3.3. (Danzer (1963))

(1) For $7 \le N \le 12$ there is, up to isometry, a unique θ-maximizing unlabeled configuration of spheres with $N(\theta) = N$.

(2) For $N = 12$, the vertices of a regular icosahedron form the unique θ-maximizing configuration. The θ-maximizing configuration for $N = 11$ is a regular icosahedron with one vertex removed.

In [28, Theorem II] Danzer classified irreducible sets for $72° = \frac{2\pi}{5} < \theta < 90° = \frac{2\pi}{4}$. There are additional N-irreducible graphs for $N = 7, 8, 9, 10$ in these cases. For $N = 6, 7, 8, 9$ he finds one optimal set and one irreducible set with one degree of freedom. He also finds for $N = 8$ an irreducible set with two degrees of freedom. For $N = 10$ he finds one optimal set, two irreducible sets with no degrees of freedom, and five with at least one degree of freedom. Danzer states that the irreducible sets with no degrees of freedom (presumably) give relative optima. An irreducible graph having a degree of freedom fails to be relatively optimal, since deforming along its degree of freedom leads to a boundary graph with an additional edge, where the extrema is reached.

Danzer's work was not published in a journal until the 1980's. In the meantime Böröczky [12] gave another solution for $N = 11$, and Hárs [62] for $N = 10$.

3.2.4. **Musin and Tarasov:** $N = 13, 14$. Very recently the Tammes problem was solved for the cases $N = 13$ and $N = 14$ by Musin and Tarasov [87], [89]. Their proofs were computer-assisted, and made use of an enumeration of all irreducible configuration contact graphs, for which see [88]. For earlier work on configurations of up to 17 points, see Böröczky and Szabó [13], [14]. x names

3.2.5. **Robinson:** $N = 24$. The case $N = 24$ was solved in 1961 by R. M. Robinson [97]. He proved a 1959 conjecture of Fejes Tóth [44], asserting that the extremal $\theta(24) \approx 43° 42'$ and that the extremal configuration of 24 sphere centers are the vertices of a snub cube. Coxeter [26, p. 326] describes the snub cube. x name

3.3. **Tammes Problem: Optimal Contact Graphs and Optimal Parameters.** Table 1 summarizes optimal angular parameters and radius parameters on the Tammes problem for $3 \le N \le 14$ and $N = 24$ (cf. Aste and Weaire [7, Sect. 11.6]). The configuration name given is associated to the vertices in the corresponding polyhedron being inscribed in a sphere, e.g. an icosahedron has $N = 12$ vertices, (see Melnyk et al. [83, Table 2]). In the case $N = 5$ the polyhedron is any from a family of trigonal bipyramids, including the square pyramid as a degenerate case. For $N = 11$ the polyhedron is a singly capped pentagonal antiprism. The cases $N = 7, 9$ and 10 are described in [83, pp. 1747–1749].

Then Figure 4 shows schematically the optimal contact graphs for $3 \le N \le 14$.

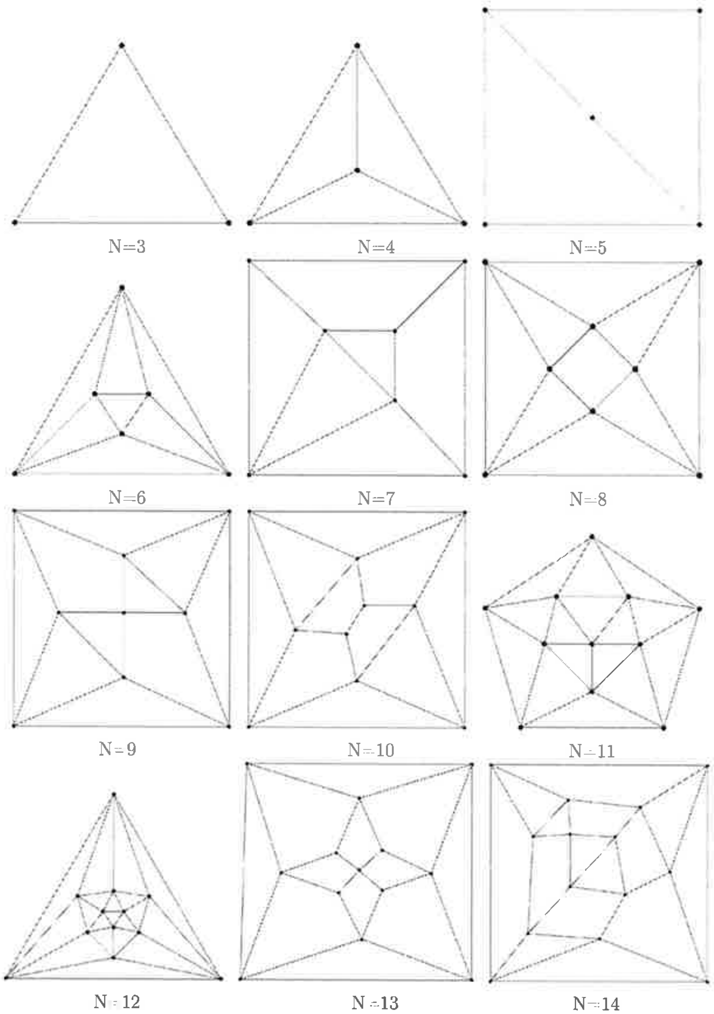

FIGURE 4. Optimal contact graphs associated to the Tammes configurations for $N = 3$ to $N = 14$.

N	$\theta(N)$	$r_{max}(N)$	Configuration	Source
3	$\delta_3 = \frac{2\pi}{3} = 120°$	$3+2\sqrt{3}$ ≈ 6.4641	Equilateral Triangle	Fejes-Tóth (1943)
4	$\delta_4 = \cos^{-1}(-\frac{1}{3})$ $\approx 109.4712°$	$2+\sqrt{6}$ ≈ 4.4495	Regular Tetrahedron	Fejes-Tóth (1943)
5	$\delta_5 = \frac{2\pi}{4} = 90°$	$1+\sqrt{2}$ ≈ 2.4142	Triangular Bipyramid	Fejes-Tóth (1943)
6	$\delta_6 = \frac{2\pi}{4} = 90°$	$1+\sqrt{2}$ ≈ 2.4142	Regular Octahedron	Fejes-Tóth (1943)
7	$\delta_7 \approx 77.8695°$	≈ 1.6913	[No name]	Schutte and van der Waerden (1951)
8	$\delta_8 \approx 74.8585°$	≈ 1.5496	Square Antiprism	Schutte and van der Waerden (1951)
9	$\delta_9 \approx 70.5288°$	$\frac{1+\sqrt{3}}{2}$ ≈ 1.3660	[No name]	Schutte and van der Waerden (1951)
10	$\delta_{10} \approx 66.1468°$	≈ 1.2013	[No name]	Danzer (1963)
11	$\delta_{11} \approx 63.4349°$	$\frac{1}{\sqrt{\frac{5+\sqrt{5}}{2}}-1}$ ≈ 1.1085	Regular Icosahedron minus one vertex	Danzer (1963)
12	$\delta_{12} \approx 63.4349°$	$\frac{1}{\sqrt{\frac{5+\sqrt{5}}{2}}-1}$ ≈ 1.1085	Regular Icosahedron	Fejes-Tóth (1943)
13	$\delta_{13} \approx 57.1367°$	≈ 0.9165	[No name]	Musin and Tarasov (2013)
14	$\delta_{14} \approx 55.6706°$	≈ 0.8759	[No name]	Musin and Tarasov (2015)
24	$\delta_{24} \approx 43.6908°$	≈ 0.5926	Snub Cube	Robinson (1961)

TABLE 1. Tammes Problem for small N.

3.4. **Tammes problem maximal radius: general N.** The most basic question about the maximal radius in the Tammes problem concerns the distinctness of maximal values. The following conjecture was proposed by ~~R. M.~~ Robinson [98, p. 297].

Conjecture 3.4. (Robinson (1969)) *For all $N \geq 4$ the maximal radius satisfies*

$$r_{max}(N) < r_{max}(N-1)$$

except possibly for $N = 6, 12, 24, 48, 60$ and 120.

One has $r_{max}(N) = r_{max}(N-1)$ for $N = 6$ and $N = 12$ by results already given above. In 1991 Tarnai and Gáspár [106] established that $r_{max}(24) < r_{max}(23)$. The remaining cases $N = 48, 60, 120$ are open, but since strict inequality holds for $n = 24$ we expect strict inequality to hold for these values too. Ruling out equality for these three values has so far been computationally difficult to determine $r_{max}(N)$ for large N.

We turn to a potentially easier question. The known exact values of $r_{max}(N)$ are algebraic numbers, i.e. roots of some univariate polynomial having integer coefficients. Table 2 below presents algebraicity data for $3 \le N \le 14$.

N	$r(N)$	Minimal Equation	Figure
3	$r_{max}(3) = 3 + 2\sqrt{3} \approx 6.4641$	$X^2 - 6X - 3$	Equilateral Triangle
4	$r_{max}(4) = 2 + \sqrt{6} \approx 4.4495$	$X^2 - 4X - 2$	Regular Tetrahedron
6	$r_{max}(6) = r_{max}(5) = 1 + \sqrt{2} \approx 2.4142$	$X^2 - 2X - 1$	Regular Octahedron
7	$r_{max}(7) \approx 1.6913$	$X^6 - 6X^5 - 3X^4 + 8X^3 + 12X^2 + 6X + 1$	[No name]
8	$r_{max}(8) \approx 1.5496$	$X^4 - 8X^3 + 4X^2 + 8X + 2$	Square Antiprism
9	$r_{max}(9) \approx 1.3660$	$2X^2 - 2X - 1$	[No name]
10	$r(10) \approx 1.2013$	$4X^6 - 30X^5 + 17X^4 + 24X^3 - 4X^2 - 6X - 1$	[No name]
12	$r_{max}(12) = r_{max}(11) = \frac{1}{\sqrt{\frac{5+\sqrt{5}}{2}} - 1} \approx 1.10851$	$X^4 - 6X^3 + X^2 + 4X + 1$	Regular Icosahedron
24	$r_{max}(24) \approx 0.59262$	$X^6 - 10X^5 + 23X^4 + 20X^3 - 5X^2 - 6X - 1$	Snub Cube

TABLE 2. Tammes Problem radii given as algebraic numbers.

We may ask the question: *Is the optimal radius $r_{max}(N)$ an algebraic number for each $N \ge 3$?* The reason to expect such an algebraicity result to hold is that such a radius should be specified by at least one optimal graph that is *rigid*, i.e. it permits no local deformations preserving optimality. Danzer showed rigidity to be the case for $7 \le N \le 12$. The equal length constraints of the edges of the graph give a system of polynomial equations with integer coefficients that the coordinates of the sphere centers must satisfy. Assuming that the equations cut out an algebraic variety of dimension zero, the solutions for the sphere centers will be algebraic numbers. In addition the distances between two sphere centers will also be an algebraic number, giving the desired result. The system of equations appears overdetermined in the known examples, suggesting it may have no deformations. Even if the rigidity result fails, and deformations always occur, it could still be the case that the optimal radius is algebraic.

4. Configuration Spaces of N Spheres touching a central Sphere

We start with the classical *configuration space* $\mathrm{Conf}(N) := \mathrm{Conf}(\mathbb{S}^2, N)$ of N distinct labeled points on the unit 2-sphere $\mathbb{S}^2$. One may regard these as the points where N surrounding spheres touch a central sphere. Note that $\mathrm{Conf}(N)$ is an open submanifold of the N-fold product $(\mathbb{S}^2)^N$ of unit spheres. We will also consider the *reduced configuration space*

$$\mathrm{BConf}(N) := \mathrm{Conf}(N)/SO(3), \tag{4.1}$$

which divides out the space $\mathrm{Conf}(N)$ by the orientation-preserving isometry group $SO(3)$ of the unit 2-sphere $\mathbb{S}^2$ in $\mathbb{R}^3$. The elements of $SO(3)$ move all configurations to isometric configurations, and these moves are permitted on any configuration. The space $\mathrm{Conf}(N)$ is a non-compact $(2N)$-dimensional manifold and the space $\mathrm{BConf}(N)$ is a non-compact $(2N-3)$-dimensional manifold. We assume $N \ge 3$ to avoid degenerate cases.

We denote a configuration $\mathbf{U} := (\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_N)$, where the $\mathbf{u}_j \in \mathbb{S}^2$ are distinct points. The *angular distance* between points $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{S}^2$ is the angle $\mathbf{u}_1, 0, \mathbf{u}_2$ subtended at the center of the unit sphere that the N spheres all touch; its value is at most π.

Definition 4.1. The *injectivity radius function* $\rho : \mathrm{Conf}(\mathbb{S}^2, N) \to \mathbb{R}^+$ assigns to a configuration $\mathbf{U} := (\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N) \in (\mathbb{S}^2)^N$ the value

$$\rho(\mathbf{U}) := \frac{1}{2}\big(\min_{i \ne j} \theta(\mathbf{u}_i, \mathbf{u}_j)\big),$$

where $\theta(\mathbf{u}_i, \mathbf{u}_j)$ denotes the angular distance between $\mathbf{u}_i$ and $\mathbf{u}_j$. In particular $0 < \rho(\mathbf{U}) \le \frac{\pi}{2}$. Since the function ρ is invariant under the action of $SO(3)$, it yields a well-defined function on $\mathrm{BConf}(N;\theta)$, which we also denote ρ.

Our main topic in this section is the study of spaces which are *superlevel sets* for the injectivity radius function ρ, and how these change at configurations which are critical for maximizing ρ.

Definition 4.2. We define the *(constrained) angular configuration spaces*

$$\mathrm{Conf}(N;\theta) = \mathrm{Conf}(\mathbb{S}^2, N;\theta) := \{\mathbf{U} = (\mathbf{u}_1, ..., \mathbf{u}_N);\ \theta(\mathbf{u}_i, \mathbf{u}_j) \ge \theta \text{ for } 1 \le i < j \le N\}$$

for angles $0 < \theta \le \pi$, whose points label configurations of N distinct marked labeled points $\mathbf{u}_i$ which are pairwise at *angular distance* at least θ from each other. Equivalently

$$\mathrm{Conf}(N;\theta) := \{\mathbf{U} = (\mathbf{u}_1, ..., \mathbf{u}_N);\ \rho(\mathbf{U}) \ge \frac{\theta}{2}\}.$$

The *reduced (constrained) angular configuration spaces* $\mathrm{BConf}(N;\theta)$ are

$$\mathrm{BConf}(N;\theta) := \mathrm{Conf}(N;\theta)/SO(3).$$

This space is well-defined since rotations preserve angular distance.

The spaces $\mathrm{Conf}(N;\theta)$ and $\mathrm{BConf}(N;\theta)$ are compact topological spaces. Away from critical values θ the spaces $\mathrm{Conf}(N;\theta)$ are closed manifolds with boundary; at critical points they need not be manifolds. The descriptions as superlevel sets show that the spaces $\mathrm{Conf}(N;\theta)$ are ordered by set inclusion as decreasing functions of θ. If $\theta_1 > \theta_2$ then we have

$$\mathrm{Conf}(N;\theta_1) \subset \mathrm{Conf}(N;\theta_2) \subset \mathrm{Conf}(N).$$

We have similar inclusions for $\mathrm{BConf}(N;\theta)$. The interiors of these spaces are

$$\mathrm{Conf}^-(N;\theta) := \{\mathbf{U} = (\mathbf{u}_1, ..., \mathbf{u}_N);\ \rho(\mathbf{U}) > \frac{\theta}{2}\}$$

and

$$\mathrm{BConf}^-(N;\theta) := \mathrm{Conf}^-(N;\theta)/SO(3),$$

respectively. They are open manifolds for all values of the parameter θ.

The (constrained) angular configuration space $\mathrm{Conf}(N;\theta)$ can be reparametrized as the *(constrained) radial configuration space*

$$\mathrm{Conf}(N)[r] := \mathrm{Conf}(\mathbb{S}^2, N)[r]$$

which consists of N marked labeled spheres of equal radius $r = r(\theta)$ in $\mathbb{R}^3$ which all touch a given unit radius central sphere $\mathbb{S}^2$, with the N touching points being the labeled points of the configuration. The radius $r(\theta)$ is determined by the condition that the spherical cap on the central sphere $\mathbb{S}^2$ obtained by radial projection of all the points of the given touching sphere has angular diameter exactly θ. A configuration belongs to $\mathrm{Conf}(N;\theta)$ exactly when the N spheres of radius $r(\theta)$ have disjoint interiors. There is a maximal angle $\theta_{max} := \theta_{max}(N)$ for which N spherical caps of that angular measure can fit on the surface of $\mathbb{S}^2$ without overlap of their interiors.

Recall from the proof of Lemma 3.1 that the value $r = r(\theta)$ is implicitly given by the equation

$$\sin\frac{\theta}{2} = \frac{r}{1+r}.$$

For $N \geq 3$ the function $r(\theta)$ is monotone increasing in θ up to a maximal value $r_{max}(\theta)$, so we may use either r or θ to parametrize the family of all spaces $\mathrm{Conf}(N;\theta)$ or $\mathrm{Conf}(N)[r]$. Note that we can identify the configuration spaces $\mathrm{Conf}(N)$ with $\mathrm{Conf}(N,0)$, as well as with $\cup_{\theta>0}\mathrm{Conf}(N,\theta)$ and $\cup_{r>0}\mathrm{Conf}(N)[r]$.

In the following subsections we review the topology and geometry of the spaces $\mathrm{Conf}(N;\theta)$ and $\mathrm{BConf}(N;\theta)$.

(1) In Section 4.1 we describe results on the homotopy type and cohomology of the configuration spaces $\mathrm{Conf}(N)$ and reduced configuration spaces $\mathrm{BConf}(N)$, which are well studied.
(2) In Section 4.2 we use ideas from Morse theory, applied to the injectivity radius function ρ, to study general features of the change in topology for fixed N as the angular parameter θ (or radius parameter r) is increased. The topology changes at certain *critical values* of θ. Since the injectivity radius function ρ is semi-algebraic, for each N we expect there to be a finite set of critical values of ρ on $\mathrm{BConf}(N)$. We give a criterion for a configuration in $\mathrm{BConf}(N)$ to be critical.
(3) In Section 4.3 we show that for small enough θ, the angular configuration space $\mathrm{Conf}(N;\theta)$ has the same homotopy type as $\mathrm{Conf}(N)$ and hence the same cohomology.
(4) In Section 4.4 we treat large θ near θ_{max}, in terms of the radius parameter r. For larger angular diameter θ, the topology of $\mathrm{Conf}(N;\theta)$ may differ drastically from that of $\mathrm{Conf}(N)$. For example, in Table 1 for the Tammes problem many of the maximal configurations are isolated, and the associated labeled spheres cannot be continuously interchanged for large θ near $\theta_{max}(N)$. In such situations, the space $\mathrm{Conf}(N;\theta)$ is disconnected for large θ, while the space $\mathrm{Conf}(N)$ is connected. We conjecture that near θ_{max} the cohomology of $\mathrm{BConf}(N)[r]$ is concentrated in dimension 0 and discuss the associated Betti number.
(5) In Section 4.5 we show by examples that the set of critical configurations at a critical value can have many connected components and can have variable dimension.
(6) In Section 4.6 we treat the case of topology change as θ varies for the simplest case $N = 4$. We determine all the critical values for the injectivity radius function ρ on $\mathrm{BConf}(N)$.
(7) In Section 4.7 we briefly discuss topology change in cases $N \geq 5$. We study properties of the $N = 12$ case in Sections 5 and 6.

4.1. Topology of Configuration Spaces. Configuration spaces $\mathrm{Conf}(\mathbf{X}, N)$ of N distinct, labeled points on a d-dimensional manifold $\mathbf{X}$ have been studied as fundamental spaces in topology. Recall that the *configuration space* of labeled N-tuples on a manifold $\mathbf{X}$ is

$$\mathrm{Conf}(\mathbf{X}, N) := \{(x_1, x_2, ..., x_N) \in \mathbf{X}^N :\ x_i \neq x_j \text{ if } i \neq j\}.$$

The symmetric group Σ_N acts freely on the space $\mathrm{Conf}(\mathbf{X}, N)$ to permute the points, and

$$B(\mathbf{X}, N) := \mathrm{Conf}(\mathbf{X}, N)/\Sigma_N$$

is the configuration space of unlabeled (i.e. *unordered*) N-tuples of points on $\mathbf{X}$. Configuration spaces of this type were first considered in the 1960's by Fadell and Neuwirth [35], [33]. The state of the art for $\mathbf{X} = \mathbb{R}^d$ and $\mathbb{S}^d$ as of 2000 is given in Fadell and Husseini [34]. Other useful references are Totaro [109] and Cohen [19].

We begin with the most well-known of these spaces, the configuration space $\mathrm{Conf}(\mathbb{R}^2, N)$ of labeled N-tuples of points on $\mathbf{X} = \mathbb{R}^2$, the plane. Fadell and Neuwirth [35] showed that the unlabeled configuration space $B(\mathbb{R}^2, N)$ is a classifying space (Eilenberg-Maclane space $K(\pi, 1)$), with fundamental group π_1 isomorphic to Artin's *braid group* B_N on N strings. Thus the cohomology of $B(\mathbb{R}^2, N)$ is just the cohomology of B_N; it was computed by Fuks [48] and Cohen [18].

The labeled configuration space $\mathrm{Conf}(\mathbb{R}^2, N)$ is by definition the complement of a finite set of complex hyperplanes given by $x_i = x_j$ for $i \neq j$ in $\mathbb{C}^N \cong (\mathbb{R}^2)^N$. This arrangement is sometimes called the (complexified) A_{N-1}-arrangement of hyperplanes, cf. Postnikov and Stanley [96], where A_{N-1} refers to a Coxeter group. The space $\mathrm{Conf}(\mathbb{R}^2, N)$ is also a classifying space with fundamental group equal to the *pure braid group* PB_N, the subgroup of B_N consisting of all N-strand braids which induce the identity permutation. It sits in a short exact sequence $0 \to PB_N \to B_N \to \Sigma_N \to 0$. The rational cohomology of $\mathrm{Conf}(\mathbb{R}^2, N)$ is then the cohomology of the pure braid group; the cohomology ring structure of PB_N was determined by Arnold [6] in 1969.

The *Betti numbers* of a topological space are the ranks of its homology groups (which equal the ranks of its cohomology groups, for fixed coefficients, here $\mathbb{Q}$ or $\mathbb{C}$.) The generating function for this sequence of ranks is called the *Poincaré polynomial*. Arnold [6, Corollary 2] determined the Poincaré polynomial for the pure braid group PB_N on N strands to be

$$P_N(t) = (1+t)(1+2t)\cdots(1+(N-1)t). \tag{4.2}$$

Table 3 gives these Betti numbers for small N. They are of combinatorial interest, being unsigned Stirling numbers of the first kind,

$$\dim H^k(PB_N, \mathbb{Q}) = \left[{N \atop N-k} \right], \quad \text{for} \quad 0 \le k \le N-1,$$

see [53, Sect. 6.1].

x \vspace

$N \backslash k$	0	1	2	3	4	5	6	7	8
1	1	0	0	0	0	0	0	0	0
2	1	1	0	0	0	0	0	0	0
3	1	3	2	0	0	0	0	0	0
4	1	6	11	6	0	0	0	0	0
5	1	10	35	50	24	0	0	0	0
6	1	15	85	225	274	120	0	0	0
7	1	21	175	735	1624	1764	720	0	0
8	1	28	322	1960	6769	13132	13068	5040	0
9	1	36	546	4536	22449	67284	118124	109584	40320

TABLE 3. Betti numbers of pure braid group cohomology $H^k(PB_N, \mathbb{Q}) \cong H^k(\mathrm{BConf}(\mathbb{R}^2, N), \mathbb{Q})$.

Our interest here is configuration spaces on

$$\mathbf{X} = \mathbb{S}^2 = \{(x, y, z) : x^2 + y^2 + z^2 = 1\},$$

the unit 2-sphere embedded in $\mathbb{R}^3$. The configuration spaces of $\mathbb{S}^2$ have a close relationship to those of $\mathbb{R}^2$, since $\mathbb{S}^2$ is the one-point compactification of $\mathbb{R}^2$. Note also that $\mathbb{S}^2$ is homeomorphic to $\mathbb{C}P^1$, the complex projective line. Tautologically the configuration space $\mathrm{Conf}(\mathbb{S}^2, 1) \cong \mathbb{S}^2$; and the space $\mathrm{Conf}(\mathbb{S}^2, 2)$ is homeomorphic to an $\mathbb{R}^2$-bundle over $\mathbb{S}^2$, hence homotopy equivalent to $\mathbb{S}^2$, see [19, Example 2.4]. For $N \ge 3$ points we have a well-known result, given in Feichtner and Ziegler [38, Theorem 1].

Theorem 4.3. *For $N \ge 3$ the configuration space $\mathrm{Conf}(\mathbb{S}^2, N)$ of N distinct labeled points on the 2-sphere is the total space of a trivial $PSL(2, \mathbb{C})$-bundle over $\mathcal{M}_{0,N}$, the moduli space of conformal structures on the N-punctured complex projective line, modulo conformal automorphisms. Hence there is a homeomorphism*

$$\mathrm{Conf}(\mathbb{S}^2, N) \cong PSL(2, \mathbb{C}) \times \mathcal{M}_{0,N}$$

Note that $PSL(2, \mathbb{C})$ is homotopy equivalent to its maximal compact subgroup $SO(3)$, the group of orientation preserving isometries of $\mathbb{S}^2$.

The $SO(3)$-action on $\mathrm{Conf}(\mathbb{S}^2, N)$ permits us to rotate the first point to the north pole, from which we stereographically project the rest of the unit sphere to the plane $\mathbb{R}^2$. Since we are still free to rotate about the north pole, which corresponds to $SO(2)$ rotations in the plane, we can identify $\mathrm{BConf}(N)$ with $\mathrm{Conf}(\mathbb{R}^2, N-1)/SO(2)$. The action of $SO(2)$ on $\mathrm{Conf}(\mathbb{R}^2, N-1)$ is free when $N \ge 3$, so we can regard $\mathrm{Conf}(\mathbb{R}^2, N-1)$ as a principal $SO(2)$-bundle over $\mathrm{BConf}(N)$. Thus the reduced $\mathbb{S}^2$-configuration space $\mathrm{BConf}(N)$ is homotopy equivalent to the $\mathbb{R}^2$-configuration space $\mathrm{Conf}(\mathbb{R}^2, N-1)/SO(2)$.

The principal bundle $\mathrm{Conf}(\mathbb{R}^2, N-1) \to \mathrm{Conf}(\mathbb{R}^2, N-1)/SO(2)$ has a section, so the Poincaré polynomial $\tilde{P}_N(t)$ may be computed as the quotient of the well-known Poincaré polynomials $P_N(t) = (1+t)(1+2t)\cdots(1+(N-2)t)$ for $\mathrm{Conf}(\mathbb{R}^2, N-1)$ (from (4.2))and $p(t) = (1+t)$ for $SO(2)$. It follows that $\mathrm{BConf}(N)$ and $\mathcal{M}_{0,N}$ both have Poincaré polynomial

$$\tilde{P}_N(t) = P(t)/p(t) = (1+2t)\cdots(1+(N-2)t). \tag{4.3}$$

We give the first few Betti numbers in the following table:

$N \backslash k$	0	1	2	3	4	5	6	7	8	9
3	1	0	0	0	0	0	0	0	0	0
4	1	2	0	0	0	0	0	0	0	0
5	1	5	6	0	0	0	0	0	0	0
6	1	9	26	24	0	0	0	0	0	0
7	1	14	71	154	120	0	0	0	0	0
8	1	20	155	580	1044	720	0	0	0	0
9	1	27	295	1665	5104	8028	5040	0	0	0
10	1	35	511	4025	18424	48860	69264	40320	0	0
11	1	44	826	8624	54649	214676	509004	663696	362880	0
12	1	54	1266	16884	140889	761166	2655764	5753736	6999840	3628800

TABLE 4. Betti numbers for reduced configuration space cohomology $H^k(\mathrm{BConf}(\mathbb{S}^2, N); \mathbb{Q})$

By taking the alternating sum of each row, or more directly by evaluating $P_N(-1)$, we can compute the Euler characteristic

$$\chi(\mathrm{BConf}(N)) = (-1)^{N-3}(N-3)!$$

of $\mathrm{BConf}(N)$ for $N \ge 3$.

We also have ([38, Proposition 2.3]):

Theorem 4.4. (Feichtner-Ziegler (2000)) *For $N \ge 3$ the moduli space $\mathcal{M}_{0,N}$ is homotopy equivalent to the complement of the affine complex braid arrangement of hyperplanes $\mathcal{M}({}^{\mathit{aff}}\mathcal{A}^{\mathbb{C}}_{N-2})$ of rank $N-2$, since*

$$\mathcal{M}_{0,N} \times \mathbb{C} \simeq \mathcal{M}({}^{\mathit{aff}}\mathcal{A}^{\mathbb{C}}_{N-2}).$$

Its integer cohomology algebra is torsion-free. It is generated by 1-dimensional classes $e_{i,j}$ with $1 \le i < j \le N-1$ with $(i,j) \ne (1,2)$ and has a presentation as an exterior algebra

$$H^*(\mathcal{M}({}^{\mathit{aff}}\mathcal{A}^{\mathbb{C}}_{N-2})) \cong \Lambda^* \mathbb{Z}^{\binom{N-1}{2}-1}/\mathcal{I},$$

where the ideal $\mathcal{I}$ is generated by elements

$$e_{1,i} \wedge e_{2,i}, \quad 2 < i \le N-1$$

and

$$e_{i,\ell} \wedge e_{j,\ell} - e_{i,j} \wedge e_{j,\ell} + e_{i,j} \wedge e_{i,\ell} \quad 1 \le i < j < \ell \le N-1, \ (i,j) \ne (1,2).$$

Here the complexified A_{N-2}-arrangement of hyperplanes $\mathcal{A}_{N-2}^{\mathbb{C}}$ of rank $N-2$ is cut out by the hyperplanes

$$z_i - z_j = 0 \quad 1 \le i < j \le N-1.$$

Its complement $\mathcal{M}(\mathcal{A}_{N-2}^{\mathbb{C}}) := \mathbb{C}^{N-1} \setminus \bigcup \mathcal{A}_{N-2}^{\mathbb{C}}$ is homeomorphic to $\mathrm{Conf}(\mathbb{C}, N-1)$. The associated affine arrangement is:

$$^{aff}\mathcal{A}_{N-2}^{\mathbb{C}} := \{(z_1, z_2, \cdots, z_{N-1} \in \mathcal{A}_N^{\mathbb{C}} : z_2 - z_1 = 1\}.$$

Treating $\mathbb{C}^{N-2} \cong \{(z_1, z_2, \cdots, z_{N-1}) : z_2 - z_1 = 1\}$, we set

$$\mathcal{M}(^{aff}\mathcal{A}_{N-2}^{\mathbb{C}}) := \mathbb{C}^{N-2} \setminus {}^{aff}\mathcal{A}_{N-2}^{\mathbb{C}}.$$

A more refined result determines the integral cohomology ring for the configuration spaces of spheres, which includes torsion elements. It was determined by Feichtner and Ziegler, who obtained in the special case of $\mathrm{Conf}(\mathbb{S}^2, N)$ the following result ([38, Theorem 2.4]).

Theorem 4.5. (Feichtner-Ziegler (2000)) *For $N \ge 3$, the integer cohomology ring $H^*(\mathrm{Conf}(\mathbb{S}^2, N), \mathbb{Z})$ has only 2-torsion. It is given as*

$$H^*(\mathrm{Conf}(\mathbb{S}^2, N), \mathbb{Z}) \cong (\mathbb{Z}(0) \oplus \mathbb{Z}/2\mathbb{Z}(2) \oplus \mathbb{Z}(3))) \otimes \Lambda^*(\oplus_{i=1}^{\binom{N-1}{2}-1} \mathbb{Z}(1))/\mathcal{I},$$

in which $\mathcal{I}$ is the ideal of relations given in Theorem 4.4.

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In this result the expression $G(i)$ denotes a direct summand of G in cohomology of degree i, e.g. there is a $\mathbb{Z}/2\mathbb{Z}$ direct summand in $H^2(\mathrm{Conf}(\mathbb{S}^2, N), \mathbb{Z})$.

4.2. **Generalized Morse theory and topology change.** Morse theory, as treated in Milnor [84], concerns how topology changes for the *sublevel sets*

$$\mathbf{X}^u := \{x \in \mathbf{X} : f(x) \le u\}$$

of a given nice-enough real-valued function f on a manifold $\mathbf{X}$, as the level set parameter u varies. At the *critical values* of the function, where its gradient vanishes, the topology changes. This change can be described by adding up the contributions of individual *critical points* of the function that occur at the critical values. More precisely, a *Morse function* is a smooth enough function that has only isolated *critical points*, each of which is non-degenerate, and arranged so that only one critical point occurs at each critical level $f(x) = u$. Here *non-degenerate* means that the function is twice-differentiable and its Hessian matrix $[\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}]$ is nonsingular at the critical point. The topology of a sublevel set $\mathbf{X}^u$ is changed as one passes a critical level, up to homotopy, by the addition of a cell of dimension equal to the *index* of the critical point: the number of negative eigenvalues of the Hessian.

Our interest here will be in *superlevel sets*

$$\mathbf{X}_v := \{x \in \mathbf{X} : f(x) \ge v\},$$

whose topology changes as we pass a critical level by adding a cell of dimension equal to the *co-index* of the critical point: the number of positive eigenvalues of the Hessian.

In the 1980's Goresky and MacPherson [52] developed Morse theory on more general topological spaces than manifolds, namely *stratified spaces* in the sense of Whitney, and applicable to a wider class of real-valued functions. The configuration spaces such as $\mathrm{Conf}(N;\theta)$ studied here are in general stratified spaces in Whitney's sense.

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For the case at hand of $\mathbb{S}^2$ and the injectivity radius function ρ, we have a further problem that ρ is not a Morse function. Its critical points are degenerate and non-isolated, and even the notion of "critical" needs care in defining, since ρ is a min-function of a finite number of smooth functions (cf. Definition 4.1). Technically, the angular distance function from $\mathbf{u}$ is not smooth at the antipodal point $-\mathbf{u}$, with angular distance π on $\mathbb{S}^2$; however we can treat these functions as if they were smooth using the following trick, valid for the nontrivial cases $N \ge 3$ where $\rho_{\max} \le \frac{\pi}{3}$: simply include the constant function $\frac{\pi}{3}$ among those functions over which we take the min, and smoothly cut off the other pairwise angular distance functions $\theta(\mathbf{u}_i, \mathbf{u}_j)$ if they exceed $\frac{2\pi}{3}$.

An appropriate version of Morse theory that applies in this context, called *min-type Morse theory*, has only recently been sketched by Gershkovich and Rubinstein [51], see also Baryshnikov et al. [9]. Related work includes Carlsson et al [17] and Alpert [2]. The treatment of [9] studies a notion of topologically critical value.

In what follows we develop an alternative max-min approach to criticality and a Morse theory for the injectivity radius function ρ on configurations that is in the spirit of the criticality theory for maximizing *thickness* or normal injectivity radius (also known as *reach*) on configurations of curves subject to a length constraint (or in a compact domain of $\mathbb{R}^3$, or in $\mathbb{S}^3$) studied earlier in optimal ropelength and rope-packing problems by Cantarella et al. [16]. This approach provides a notion of critical configuration, refining the notion of a critical value. The Farkas Lemma (and its infinite-dimensional generalizations in the case of the ropelength problem) is a key tool used in these works that relates criticality to the existence of a balanced system of forces on the configuration. A more detailed treatment is planned in [73].

To understand criticality for the injectivity radius function ρ on $\mathrm{Conf}(N) = \mathrm{Conf}(\mathbb{S}^2; N)$, we first need to make sense of varying a configuration $\mathbf{U} = (\mathbf{u}_1, ..., \mathbf{u}_N) \in \mathrm{Conf}(N) \subset (\mathbb{S}^2)^N$ along a tangent vector $\mathbf{V} = (\mathbf{v}_1, ..., \mathbf{v}_N)$ to $\mathrm{Conf}(N)$ at $\mathbf{U}$; here $\mathbf{v}_i$ is a tangent vector to $\mathbb{S}^2$ at $\mathbf{u}_i$, for $i = 1, 2, ..., N$. For sufficiently small t we can define a nearby configuration

$$\mathbf{U}\#t\mathbf{V} = (\frac{\mathbf{u}_1 + t\mathbf{v}_1}{|\mathbf{u}_1 + t\mathbf{v}_1|}, ..., \frac{\mathbf{u}_N + t\mathbf{v}_N}{|\mathbf{u}_N + t\mathbf{v}_N|}) \in \mathrm{Conf}(N) \subset (\mathbb{S}^2)^N$$

by translating and projecting each factor back to $\mathbb{S}^2$. (This approximates the exponential map.) The operation taking $\mathbf{U}$ to $\mathbf{U}\#t\mathbf{V}$ can be thought of as the spherical analog of translating $\mathbf{U}$ by $t\mathbf{V}$ via vector addition in the linear case (hence the suggestive sum notation). In particular, the $\mathbf{V}$-directional derivative f' of a smooth function f on $\mathrm{Conf}(N)$ at $\mathbf{U}$ is simply $f' = \frac{d}{dt}|_{t=0} f(\mathbf{U}\#t\mathbf{V})$, so $\mathbf{U}$ is a critical point for smooth f provided all its $\mathbf{V}$-directional derivatives vanish at $\mathbf{U}$; this means that the increment $f(\mathbf{U}\#t\mathbf{V}) - f(\mathbf{U}) = o(t)$, where $o(t)$ is a function which tends to 0 faster than linearly.

Definition 4.6. A configuration $\mathbf{U} = (\mathbf{u}_1, ..., \mathbf{u}_N) \in \mathrm{Conf}(N)$ is *critical for maximizing ρ* provided for every $\mathbf{V} = (\mathbf{v}_1, ..., \mathbf{v}_N)$ and sufficiently small t, we have

$$[\rho(\mathbf{U}\#t\mathbf{V}) - \rho(\mathbf{U})]_+ = o(t),$$

where $[f]_+ = \max\{f, 0\}$. That is, a configuration $\mathbf{U}$ is critical if no variation $\mathbf{V}$ can increase ρ to first order.

Otherwise, a configuration $\mathbf{U}$ is *regular*, that is, there exists a variation $\mathbf{V}$ which *does* increase ρ to first order, and so, by the definition of ρ as a min-function, this means that for all pairs $(\mathbf{u}_i, \mathbf{u}_j)$ realizing the minimal angular distance $\theta(\mathbf{u}_i, \mathbf{u}_j) = \theta_o$, their distances increase to first order under the variation $\mathbf{V}$ as well. Note that the set of regular configurations is open. If each configuration in this $\rho = \frac{\theta_o}{2}$-level set is regular, then this level is *topologically regular:* that is, there a deformation retraction from $\mathrm{Conf}(N; \frac{\theta_o}{2} - \varepsilon)$ to $\mathrm{Conf}(N; \frac{\theta_o}{2} + \varepsilon)$ for some $\varepsilon > 0$ (see [9, Lemmas 3.2, 3.3 and Corollary 3.4]).

Definition 4.7. For $\mathbf{U} \in \mathrm{Conf}(N; \theta)$, the *contact graph* of $\mathbf{U}$ is the graph embedded in $\mathbb{S}^2$ with vertices given by points $\mathbf{u}_i$ in $\mathbf{U}$ and edges given by the geodesic segments $[\mathbf{u}_i, \mathbf{u}_j]$ when $\theta(\mathbf{u}_i, \mathbf{u}_j) = \theta$.

Examples of contact graphs for extremal values of the Tammes problem were given in Figure 4 in Section 3.

Definition 4.8. A *stress graph* for $\mathbf{U} \in \mathrm{Conf}(N; \theta)$ is a contact graph with nonnegative weights w_e on each geodesic edge $e = [\mathbf{u}_i, \mathbf{u}_j]$.

A stress graph gives rise to a system of *tangential forces* associated to each geodesic edge $e = [\mathbf{u}_i, \mathbf{u}_j]$ of the contact graph. These forces have magnitude w_e, are tangent to $\mathbb{S}^2$ at each point $\mathbf{u}_i$ of $\mathbf{U}$, and are directed along the outward unit tangent vectors $\{T_e|_{\mathbf{u}_i}, T_e|_{\mathbf{u}_j}\}$ to the edge e at its endpoints $\{\mathbf{u}_i, \mathbf{u}_j\}$.

Definition 4.9. A stress graph is *balanced* if the vector sum of the forces in the tangent space of $\mathbb{S}^2$ at $\mathbf{u}_i$ is zero for all points of $\mathbf{U}$. A configuration $\mathbf{U}$ is *balanced* if its underlying contact graph has a balanced stress graph for some choice of non-negative, not everywhere zero weights on its edges.

Theorem 4.10. *To each critical value $\frac{\theta}{2}$ for the injectivity radius ρ, there exists a balanced configuration $\mathbf{U}$ with $\rho(\mathbf{U}) = \frac{\theta}{2}$. The vertices of the contact graph are a subset of the points in $\mathbf{U}$ and the geodesic edges of the contact graph all have length θ.*

Proof. Following [9, Corollary 3.4 and Equation 2], since ρ is a min-function on $\mathrm{Conf}(N) \subset (\mathbb{S}^2)^N$, if $\frac{\theta}{2}$ is not a topologically regular value of ρ, then some configuration $\mathbf{U} \in \rho^{-1}(\frac{\theta}{2})$ is balanced. Because $\rho(\mathbf{U}) = \frac{\theta}{2}$, the conditions on the vertices and edge lengths are clearly met. □

We now prove a converse result.

Theorem 4.11. *If a configuration $\mathbf{U}$ on $\mathbb{S}^2$ is balanced, then $\mathbf{U}$ is critical for maximizing the injectivity radius ρ.*

We will need a preliminary lemma. Consider a planar graph G embedded on the unit sphere $\mathbb{S}^2$ via a map $\mathbf{u} : G \to \mathbb{S}^2$ which is C^2 on the edges of G. (By slight abuse of notation, a point on its image in $\mathbb{S}^2$ may also be denoted by $\mathbf{u}$.) Suppose each edge e of G is assigned a *nonzero* weight $w_e \in \mathbb{R}$. Let $L_e(\mathbf{u})$ denote the length of edge $\mathbf{u}(e)$ induced by the map $\mathbf{u}$ and let $\mathbb{L}(\mathbf{u}) = \sum w_e L_e(\mathbf{u})$ be the total *weighted length* of the embedded graph $\mathbf{u}(G)$. We can vary the map $\mathbf{u}$ using a C^2 vector field $\mathbf{v}$, just as we varied a configuration: for sufficiently small t, each point $\mathbf{u} \in \mathbb{S}^2$ on the image of the graph is moved to $\mathbf{u}\#t\mathbf{v} = \frac{\mathbf{u}+t\mathbf{v}}{|\mathbf{u}+t\mathbf{v}|}$. Let $\mathbb{L}'(\mathbf{v})$ denote the first derivative at $t = 0$ of weighted length for this varied graph, i.e. the *first variation* of $\mathbb{L}(\mathbf{u})$ along $\mathbf{v}$.

Lemma 4.12. *The first variation $\mathbb{L}'(\mathbf{v})$ of the weighted lengh $\mathbb{L}(\mathbf{u})$ for the embedded graph $\mathbf{u}(G)$ vanishes for every vector field $\mathbf{v}$ on $\mathbb{S}^2$ if and only if the following two conditions hold:*

(1) each edge e joining a pair of vertices e^-, e^+ of G maps to a geodesic arc $\mathbf{u}(e) = [\mathbf{u}(e^-), \mathbf{u}(e^+)] = [\mathbf{u}^-, \mathbf{u}^+]$ in the embedded graph $\mathbf{u}(G)$;

(2) at any vertex $\mathbf{u}$ of the embedded graph $\mathbf{u}(G)$, the weighted sum $\sum w_{e^*} T_{e^*}|_{\mathbf{u}} = 0$, where the sum is taken over the subset of edges $\mathbf{u}(e^*)$ incident to $\mathbf{u}$, and where $T_{e^*}|_{\mathbf{u}}$ is the outer unit tangent vector of $\mathbf{u}(e^*)$ at $\mathbf{u}$.

Proof. This lemma is a direct consequence of the first variation of length formula

$$L_e'(\mathbf{v}) = \mathbf{v} \cdot T|_{\mathbf{u}(e^-)}^{\mathbf{u}(e^+)} - \int_{\mathbf{u}(e)} \mathbf{v} \cdot \mathbf{k}$$

(see, for example, Hicks [63, Chapter 10, Theorem 7, page 148]). Here T is the unit tangent vector field of the edge $\mathbf{u}(e)$, and $\mathbf{k}$ is the geodesic curvature vector of $\mathbf{u}(e)$; with respect to any local arclength parameter on $\mathbf{u}(e)$, the geodesic curvature vector is the projection to $\mathbb{S}^2$ of the acceleration: $\mathbf{k} = \ddot{\mathbf{u}} + \mathbf{u}$, which is tangent to $\mathbb{S}^2$ and normal to $\mathbf{u}(e)$, and which vanishes iff $\mathbf{u}(e)$ is a geodesic arc.

Now express $\mathbb{L}'(\mathbf{v}) = \sum w_e L_e'(\mathbf{v})$ as a sum of edge terms and vertex terms. The geodesic arc condition (1) - that $\mathbf{k} = 0$ along every edge - implies the edge terms in $\mathbb{L}'(\mathbf{v})$ all vanish for any variation $\mathbf{v}$ of the map $\mathbf{u}$; and the force balancing condition (2) implies all vertex terms vanish for any variation $\mathbf{v}$.

Conversely, given any interior image point $\mathbf{u}$ of an edge, take a variation $\mathbf{v}$ supported in an arbitrarily small neighborhood of $\mathbf{u}$, and orthogonal to $\mathbf{u}(e)$ at $\mathbf{u}$: the vanishing of $\mathbb{L}'(\mathbf{v})$ implies condition (1) that $\mathbf{k} = 0$; similarly, at any given vertex $\mathbf{u}$, consider a pair of variations $\mathbf{v}_1, \mathbf{v}_2$ supported in an arbitrarily small neighborhood of $\mathbf{u}$ which approximate an orthogonal pair of translations of the tangent space to $\mathbb{S}^2$ at $\mathbf{u}$: the vanishing of $\mathbb{L}'(\mathbf{v})$ for both of these $\mathbf{v}_1, \mathbf{v}_2$ implies the forces balance (2). □

Remark. In case $w_e = 0$, vanishing for the first variation of $\mathbb{L}$ does not imply $\mathbf{u}(e)$ is a geodesic arc: instead, the edges with nonzero weights form a balanced geodesic subgraph of the original embedded graph $\mathbf{u}(G)$.

Lemma 4.12 suggests the following definition.

Definition 4.13. An embedded graph satisfying properties (1) and (2) is called a *balanced geodesic graph.* (Note that there is no requirement here that the geodesic edge lengths are integer multiples of some basic length, as would be the case for a contact graph.)

Lemma 4.12 shows that a balanced geodesic graph has vanishing first variation of weighted length $\mathbb{L}$, even if some of its edge weights w_e are zero.

Proof of Theorem 4.11. By hypothesis, there are non-negative edge weights (not all zero) so that the resulting stress graph $\mathbf{u}(G)$ for the configuration $\mathbf{U}$ is balanced. By Lemma 4.12 the first variation $\mathbb{L}'(\mathbf{v})$ of weighted length for $\mathbf{u}(G)$ vanishes for all variation vector fields $\mathbf{v}$ on $\mathbb{S}^2$.

Suppose (to the contrary) that $\mathbf{U}$ were *not* critical for maximizing the injectivity radius ρ. Then there would be a variation $\mathbf{V}$ of $\mathbf{U}$ so that every geodesic edge of the stress graph has length increasing at least linearly in $\mathbf{V}$. Extend $\mathbf{V}$ to an ambient C^2 variation vector field $\mathbf{v}$ on $\mathbb{S}^2$. Since the edge weights are *nonnegative*, and not all zero, that implies the weighted length of the stress graph also increases at least linearly in $\mathbf{v}$, a contradiction. $\square$

4.3. **Small Radius Case.** For small radii, it is convenient to state results for $r = r(\theta)$ in terms of the angle parameter θ. For sufficiently small angles, the superlevel sets $\mathrm{Conf}(N;\theta)$ will have the same homotopy type as the full configuration space $\mathrm{Conf}(N)$. In terms of the radius function, the conclusion of this result applies for $0 \le r < r_1(N)$, where $r_1(N) = \sin\left(\frac{\pi}{N}\right) / \left(1 - \sin\left(\frac{\pi}{N}\right)\right)$ is the smallest critical value for $\mathrm{Conf}(N)[r]$.

Theorem 4.14. *Suppose $N \ge 3$. The smallest critical value for maximizing ρ on $\mathrm{BConf}(N)$ is $\frac{\pi}{N}$, achieved uniquely by the N-ring configuration of equally spaced points along a great circle. Then for angular diameter $0 \le \theta < \frac{2\pi}{N}$ the following hold.*

(i) The space $\mathrm{Conf}(N;\theta)$ is a strong deformation retract of the full configuration space $\mathrm{Conf}(N) = \mathrm{Conf}(N;0)$.

(ii) The reduced space $\mathrm{BConf}(N;\theta) = \mathrm{Conf}(N;\theta)/SO(3)$ is a strong deformation retract of the full reduced configuration space $\mathrm{BConf}(N)$.

Consequently each has, respectively, the same homotopy type and cohomology groups as the corresponding full configuration space.

Proof. This result corresponds to [9, Theorem 5.1]. First note that the N-ring is balanced (using equal weights on each of its edges) and hence a critical configuration by Theorem 4.11. The balanced contact graph on $\mathbb{S}^2$ of a $\frac{\theta}{2}$-critical N-configuration has geodesic edges with angular length θ. In order to balance, its total angular length must be at least 2π, the length of a complete great circle. Thus if $\theta < \frac{2\pi}{N}$, then the total length $N\theta < 2\pi$ and there is no balanced N-configuration in $\mathrm{Conf}(N;\theta)$ and $\frac{\theta}{2}$ is not a critical value for ρ. In this case, a weighted ρ-gradient-flow provides the strong deformation retraction of $\mathrm{Conf}(N)$ to $\mathrm{Conf}(N;\theta)$. $\square$

Corollary 4.15. *For $\theta < \frac{2\pi}{N}$ and $N \ge 4$ the configuration spaces $\mathrm{Conf}(N;\theta)$ and $\mathrm{BConf}(N;\theta)$ are path-connected, but not simply-connected.*

Proof. These spaces have the same homotopy type as $\mathrm{Conf}(N)$ (resp. $\mathrm{BConf}(N)$), which is connected since $H^0(\mathrm{Conf}(N),\mathbb{Q}) = \mathbb{Q}$ (resp. $H^0(\mathrm{BConf}(N),\mathbb{Q}) = \mathbb{Q}$). They each are closures of open manifolds and are connected, so are path-connected. We have $H^1(\mathrm{BConf}(n),\mathbb{Q}) = \mathbb{Q}^k$ for some $k = k(N) \ge 2$, using the formula (4.3) applied for $N \ge 4$ so $\mathrm{BConf}(N)$ is not simply-connected. Finally $\mathrm{Conf}(N)$ is not simply connected via the product decomposition in Theorem 4.3. $\square$

4.4. **Large Radius Case.** We consider reduced configuration spaces $\mathrm{BConf}(N)[r]$ having radius parameter r sufficiently close to $r_{max}(N)$, depending on N. Using the finiteness of set of critical values, there is an $\epsilon(N) > 0$ such that the upward "gradient flow" of the injectivity radius function ρ (or of the corresponding sphere-touching radius function r) defines a deformation retraction from $\mathrm{BConf}(N)[r]$ to $\mathrm{BConf}(N)[r_{max}(N)]$ for $r_{\max}(N) - \epsilon(N) < r < r_{max}(N)$.

The simplest topology that may occur at r_{max} is where $\mathrm{BConf}(N)[r_{\max}(N)]$ has all its connected components contractible; the property holds for most small N, all $N \le 14$ except $N = 5$. When it holds, the cohomology groups for $\mathrm{BConf}(N)[r]$ in this range of r will have the following very simple form:

Purity Property. *There is some $\epsilon = \epsilon(N) > 0$ such that for*

$$r_{\max}(N) - \epsilon(N) < r < r_{max}(N)$$

there is an integer $s = s(N) \ge 1$ such that the cohomology groups of the reduced configuration space are

$$H^k(\mathrm{BConf}(N)[r],\mathbb{Q}) = \begin{cases} \mathbb{Z}^{s(N)} & \text{if } k = 0 \\ 0 & \text{if } k \ge 1. \end{cases}$$

For $N = 5$ the cohomology does *not* have the Purity Property. The reduced configuration space $\mathrm{BConf}(5)[r]$ is 7-dimensional for $r < r_{max}(5)$ but becomes 2-dimensional at $r = r_{max}(5)$. The optimal maximum radius configuration at $r_{max}(5) = 1+\sqrt{2}$ has room for an extra sphere (giving $N = 6$), and since the sphere centers form five vertices of an octahedron, either of the antipodal pairs can freely and independently move towards the sixth (unoccupied) vertex of the octahedron. The resulting reduced configuration space $\mathrm{BConf}(5)[1+\sqrt{2}] = \mathrm{BConf}(5;\frac{\pi}{2})$ is a simplicial 2-complex which is not contractible; it is pictured schematically in Figure 5. It has a single connected component having Euler characteristic $\chi(\mathrm{BConf}(5;\frac{\pi}{2})) = -10$. See Section 4.5 for further discussion of this space as a critical stratum.

FIGURE 5. The r-maximal stratum for $N = 5$.

Does the purity property hold for all or most large N? We do not know. One might expect that extremal configurations in high dimensions N at $r = r_{max}(N)$ will have most spheres held in a rigid structure, and for r near it all individual spheres will only be able to move in a tiny area around them, each contributing a connected component to the reduced configuration space. Against this expectation, computer experiments packing N two-dimensional equal disks confined to a circle suggest the possibility for some N that extremal configurations could have *rattlers*, which are loose disks that have motion permitted even at $r = r_{max}$

(Lubachevsky and Graham [78]). However even with rattlers one could still have contractibility of individual connected components. The hypothesis of extremal configurations being rigid (and unique) is known to hold for $6 \le N \le 12$.

When the purity property holds one can (in principle) determine the number of connected components for the set of near-maximal configurations; call it $s = s(N)$. This value depends on the symmetries of each maximal configuration under the $SO(3)$ action. Denoting the isomorphism types of the connected components of maximal rigid (labeled) configurations of N points at $r = r_{max}(N)$ by $C_{i,N}$ for $1 \le i \le e(N)$, one would have

$$s(N) = \sum_i \frac{N!}{|Aut(C_{i,N})|}.$$

For $3 \le N \le 12$, excluding $N \neq 5$, the extremal configurations for the Tammes problem are known to be unique up to isometry; call them $C_{1,N}$. The analysis of Danzer given in Theorem 3.3 covers the cases $7 \le N \le 10$. For the case $N = 12$ the unique extremal configuration DOD of vertices of an icosahedron has $Aut(C_{1,12}) = A_5$, the alternating group, of order 60, whence $s(12) = \frac{12!}{60} = 7983360$.

4.5. **Structure of Critical Strata.** Connected components of critical strata necessarily have dimension at least three from the $SO(3)$-action. In what follows we consider reduced critical strata that quotient out by this action. At a critical value ρ there can be several disconnected reduced critical strata, and such strata can have positive dimension. We give examples of each.

For $N = 5$ a positive dimensional reduced critical stratum occurs at the maximal radius value $r_{max}(5) = 1 + \sqrt{2}$. The set of (reduced) critical configurations forms a family, which is two-dimensional. A generic contact graph at the maximal injectivity radius $\rho = \frac{\pi}{4}$ is a Θ-graph having 2 polar vertices and 3 equatorial vertices. This contact graph has 3 faces and 6 edges and is optimal. The three angles between equatorial vertices can range between $\frac{\pi}{2}$ and π, with the condition that their sum is 2π, defining a 2-simplex. As long as none of the equatorial angles is π, criticality is achieved using weights that are non-zero on all the edges. When an equatorial angle is π, corresponding to a corner of the 2-simplex, these equatorial vertices may be regarded as a new pair of polar vertices. In this configuration, as the angles between equatorial angles go to π, some weights of the stress graph can go to 0 and the support of the weights degenerates to a 4-ring. The limit contact graph consists of the edges of a square pyramid whose base is that 4-ring.This gives a non-optimal contact graph pictured for $N = 5$ in Figure 4; it has 5 faces and 8 edges.

For $N = 12$ there are at least two distinct reduced critical strata at the critical value $\rho = 1$, those corresponding to the FCC-configuration and HCP-configurations, singled out in Frank's discussion in Section 2.7. These configurations are defined in Section 5.2 below, and their criticality is shown in Theorem 5.3.

4.6. **Topology change for variable radius:** $N = 4$. For very small N it is possible to completely work out all the critical points and the changes in topology. We illustrate such an analysis on the simplest nontrivial example $N = 4$ (see Figure 6, explained below).

We consider the reduced superlevel sets $\mathrm{BConf}(4)[r]$. Since $\mathrm{Conf}(4)$ is 8-dimensional, away from the critical values these spaces are 5-dimensional manifolds with boundary.

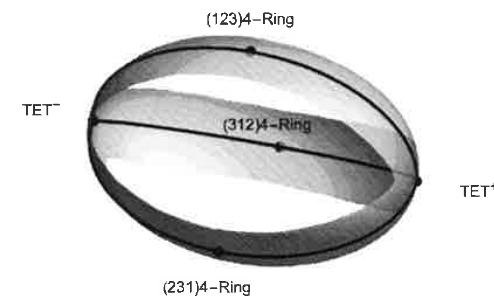


FIGURE 6. Part of the configuration space for $N = 4$.

If we ignore the labelling of points and classify the contact graphs for four vertices, there are exactly two geometrically distinct ρ-critical 4-configurations in $\mathrm{BConf}(4)$:

(1) The 4-Ring of four equally spaced points around a great circle on $\mathbb{S}^2$ with $\theta = \frac{\pi}{2}$ which is asaddle configuration for ρ. There is a 1-dimensional subspace of the tangent space to $\mathrm{BConf}(4)$ at the 4-Ring along which ρ increases to second order, i.e. the co-index is $k = 1$. The critical value for r for the 4-ring is $r_1 = 1 + 2\sqrt{2} \approx 3.8284$.
(2) The vertices of the regular tetrahedron TET with $\theta = \cos^{-1}(-\frac{1}{3})$, which is the maximizing configuration for ρ on $\mathrm{BConf}(4)$, i.e the co-index $k = 0$. The critical value for r for TET is $r_2 = r_{max}(4) = 2 + \sqrt{6} \approx 4.4495$.

There are two open intervals $(0, r_1)$ and $(r_1, r_2]$ on which the topology of $\mathrm{BConf}(4)[r]$ remains constant. From Theorem 4.3, it can be seen that on the interval $(0, r_1)$, $\mathrm{BConf}(4)[r]$ is homeomorphic to $\mathrm{BConf}(4)$, and from Theorem 4.14, $\mathrm{BConf}(4)[r_1]$ is a strong deformation retract of $\mathrm{BConf}(4)$. This has the homotopy type of $\mathbb{R}^2$ punctured at two points, hence

$$H^0(\mathrm{BConf}(4)[r], \mathbb{Z}) = \mathbb{Z}, \quad H^1(\mathrm{BConf}(4)[r], \mathbb{Z}) = \mathbb{Z}^2, \quad H^k(\mathrm{BConf}(4)[r], \mathbb{Z}) = 0, \text{ for } k \ge 2.$$

On the open interval (r_1, r_2), the manifold $\mathrm{BConf}(4)[r]$ has two connected components, each diffeomorphic to a 5-ball, which can be seen from the strong deformation retract to $\mathrm{BConf}(4)[r_2]$ consisting of the two points associated to the orientated labelings of TET configurations, TET^+ and TET^-. Hence

$$H^0(\mathrm{BConf}(4)[r], \mathbb{Z}) = \mathbb{Z}^2, \quad H^k(\mathrm{BConf}(4)[r], \mathbb{Z}) = 0, \text{ for } k \ge 1.$$

Figure 6 above is only a schematic picture, since we cannot draw a 5-dimensional manifold. It compresses four of the dimensions. The visible points take r-values with $r_1 \le r \le r_2$. The value $r = r_1$ is a circular vertical ring in the middle, and the values of r increase as one moves to the left or right, reaching a maximum at TET^+ and at TET^-.

From Table 4, we can easily compute the Euler characteristic $\chi(\mathrm{BConf}(4)) = -1$. The indexed sum of critical points of the function $\rho : \mathrm{BConf}(4) \to \mathbb{R}$ gives an alternative computation of the Euler characteristic as

$$\chi(\mathrm{BConf}(4)) = \sum_k (-1)^k \#(\text{ critical points of co-index} = k).$$

We count the *labeled* configurations in BConf(4): since the 4-Ring has symmetry group D_4 of order 8 in $SO(3)$, there are $3 = |S_4/D_4|$ critical points of this type with co-index 1; and since TET has symmetry group A_4 of order 12 in $SO(3)$, there are really $2 = |S_4/A_4|$ critical points of this type with co-index 0; and so we obtain

$$\chi(\mathrm{BConf}(4)) = 2 - 3 = -1,$$

as predicted. In fact, the Morse complex for ρ captures the fact that BConf(4) itself has the homotopy type of the Θ-graph: there are 2 vertices (0-cells) in the complex corresponding to the maxima (co-index 0) TET^+ and TET^- configurations; there are 3 edges (1-cells) corresponding to the 3 saddle (co-index 1) 4-Ring configurations.

4.7. **Topology change for variable radius: $N \ge 5$.** The complexity of the changes in topology of the configuration space grows rapidly with N. For larger values of N there are many ρ-critical configurations which are not maximal.

The value $N = 12$ is large enough to be extremely challenging to obtain a complete analysis of the critical configurations of the configuration space, analyze the variation of the topology as a function of the radius r. The Betti numbers for $N = 12$ for radius $r = 0$ given in Table 4 differ greatly from those at $r = r_{max}$ where the cohomology of $\mathrm{BConf}(12)[r_{max}]$ is entirely in dimension 0, according to the Purity Property in Section 4.4, which holds for $N = 12$ by results in Section 3. This topology change appears to require millions of critical points. It remains a task for the future.

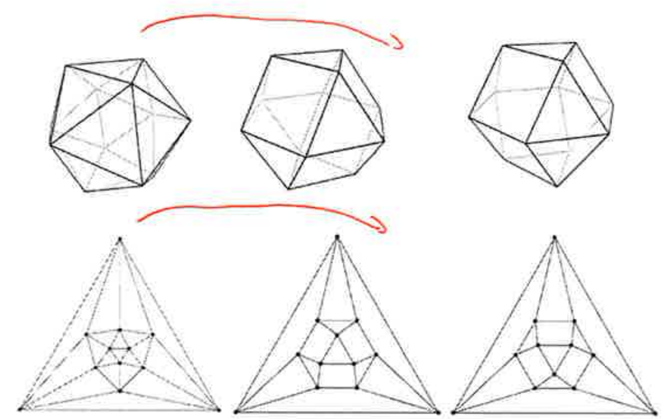
5. Unit Radius Configuration Space for 12 Spheres

In this section, we discuss Conf(12)[1] and BConf(12)[1], the configuration spaces of 12 unit spheres touching a central unit sphere $\mathbb{S}^2$. These configuration spaces are remarkable and have some uniquely special properties. The value 1 for the radius function is a critical value and has at least two geometrically distinct critical points, the FCC and HCP configurations. We believe 1 is also the maximal radius r for which all the spheres in a configuration of 12 equal radius r spheres touching a unit radius sphere $\mathbb{S}^2$ are arbitrarily permutable with motions remaining on $\mathbb{S}^2$, see Section 6.5.

5.1. **Generalities.** The case in which all spheres are unit spheres, has been extensively studied in connection with sphere packing. The value $r = 1$ turns out to be a critical value of the radius function r , and we will see that the associated configuration spaces Conf(12)[1] and BConf(12)[1] are certainly not manifolds. To better understand their topology, it is

useful to consider the spaces $\mathrm{Conf}(12)[r]$ and $\mathrm{BConf}(12)[r]$ for r in a neighborhood of 1. These are stratified spaces naturally embedded in $(\mathbb{S}^2)^{12}$ and filtered by r. For noncritical values of r, the spaces $\mathrm{Conf}(12)[r]$ and $\mathrm{BConf}(12)[r]$ are submanifolds with boundary. For all $r < r_{max}$, the space $\mathrm{Conf}(12)[r]$ has top dimension 24. After factoring out the ambient $SO(3)$-action the space $\mathrm{BConf}(12)[r]$ has top dimension 21.

5.2. **Three remarkable configurations of unit spheres: rigidity properties.** We now consider the three configurations of 12 kissing spheres singled out by Frank (1952) [47]. In Figure 7 we picture polyhedra whose vertices are located at the 12 kissing sphere centers of these three configurations, and whose centroids are located at the center of the central sphere. The edges of these polyhedra specify the contact graphs of these configurations, also pictured schematically in Figure 7. The DOD configuration gives the optimal contact graph for $N = 12$ given in Figure 4 in Section 3.3.



x
move DOD to middle
and scale

FIGURE 7. DOD, FCC, HCP Configurations, and their corresponding contact graphs

- The DOD configuration is obtained by placing 12 spheres touching a central 13-th sphere at the vertices of an inscribed icosahedron; such touching points are also the centers of the faces of a circumscribed dodecahedron. It has oriented symmetry group the icosahedral group A_5 of order 60 and in BConf(12)[1] there are $\frac{|S_{12}|}{|A_5|} = \frac{12!}{60} = 7983360$ of these.
- The FCC configuration is obtained by stacking three layers of the hexagonal lattice, with the third layer not lying over the first layer. The inscribed polyhedron formed by the convex hull of the 12 points of the DOD configuration where the spheres touch the central sphere is a cuboctahedron. The circumscribed polyhedron which

has the 12 points as the center of its faces is a rhombic dodecahedron. It has oriented symmetry group the octahedral group S_4 of order 24 and in BConf(12)[1] there are $\frac{|S_{12}|}{|S_4|} = \frac{12!}{24} = 19958400$ of these.

- The HCP configuration is obtained by stacking three layers of the hexagonal lattice, with the third layer lying directly over the first layer. The inscribed polyhedron formed by the convex hull of the 12 points of HCP where the spheres touch the central sphere is a triangular orthobicupola. This polyhedron is the Johnson solid J_{27}. The circumscribed dual polyhedron which has the 12 points as the center of its faces is a trapezoidal rhombic dodecahedron. It has oriented symmetry group D_3 the dihedral group of order 6 and in BConf(12)[1] there are $\frac{|S_{12}|}{|D_3|} = \frac{12!}{6} = 79833600$ of these.

The FCC and HCP configurations are elements of ∂BConf(12)[1], while the DOD configuration is an interior point of BConf(12)[1].

We first consider rigidity properties of these packings. In the following definition we identify a sphere tangent to the 2-sphere with the circular disk on $\mathbb{S}^2$ that it produces by radial projection.

Definition 5.1. (Connelly [24, p. 1863]) A packing of spherical caps ("disks") on $\mathbb{S}^2$ is *locally jammed* if each disk is held fixed by its neighbors. That is, no disk in the packing can be moved if all the other disks are held fixed.

We say a configuration of disks is *jammed* if it can only be moved by rigid motions. We call it *completely unjammed* if each disk can be moved slightly holding all the other disks fixed.

Theorem 5.2. *The* DOD *configuration in* Conf(12)[1] *is completely unjammed. Its space of (infinitesimal) deformations has dimension* 24. *The deformation space is* 21 *dimensional if viewed in* BConf(12)[1].

Proof. The maximal radius for 12 spheres is $r_{\max}(12) > 1$ and is achieved in the DOD configuration. Therefore the deformation space at DOD is full dimensional. $\square$

In contrast, both the FCC and HCP configurations are *locally jammed*, i. e. they are rigid against motion of any one point holding all the other points fixed; their deformation spaces are each of codimension at least 2.

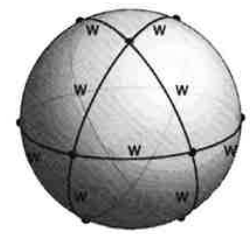
In Section 5.4 we describe a deformation of the DOD packing to the FCC packing. This deformation, properly adjusted, has 6 moving balls during its final phase arriving at FCC. (The 6 fixed balls form a pair of opposite (horizontal, centrally symmetric) "triangles".) We believe this value 6 to be the smallest number of moving balls needed to unjam the FCC configuration. See the Appendix (Section 8) below for a manual on how to unlock FCC.

A deformation of the DOD configuration to the HCP configuration, also described in section 5.4, requires 9 moving balls at the instant of arrival at HCP. We believe this value 9 to be the smallest number of moving balls needed to unjam the HCP configuration. See the Appendix for the unlocking of HCP. A possible reason for the larger number of moving balls needed to unjam the HCP configuration compared with that of the FCC configuration is that the HCP configuration has fewer local symmetries.

5.3. Three remarkable configurations of unit spheres: criticality properties. The FCC and HCP configurations are critical configurations for $r = 1$. According to Theorem 4.11 it suffices to show that these configurations carry balanced contact graph structures.

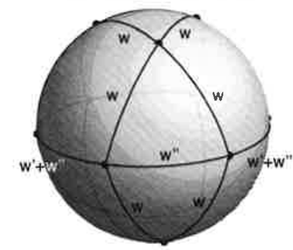
Theorem 5.3. *The* FCC *configuration and* HCP *configuration for* $r = 1$ *carry balanced contact graph structures. In consequence* $r = 1$ *is a critical value of the radius function for* BConf(12)[r].

Proof. By Theorem 4.11, a sufficient condition for the criticality of a configuration for maximizing injectivity radius is that its contact graph can be balanced: that is, a set of positive weights may be assigned to the edges of the contact graph so that the outward weighted vector sum, defined by the incident edges force, balance in $\mathbb{S}^2$ at each vertex.



x
these could be side by side

(a) FCC Configuration



(b) HCP Configuration

FIGURE 8. Stress Graphs for FCC and HCP configurations

We now indicate weight values for the FCC and HCP configurations; see Figure 8.

(1) At radius $r = 1$ the contact graph for the FCC configuration, the stress graph is balanced when all the weights are equal. This can be seen from the cubic or S_4-symmetry of the contact graph.

(2) At radius $r = 1$ for the HCP configuration, consider a weight w_1 on edges between triangular faces and square faces, a weight w_2 on edges between pairs of square faces, and a

weight w_3 on edges between pairs of triangular faces. From the symmetries of the contact graph, it is possible to choose a constant $w_1 > 0$ and find a weight $w_2 = w' > 0$ which balances the associated stress graph. This suffices to balance this configuration with some zero weights. However, it is also possible to add a uniform constant weight $w'' = w_3 > 0$ to the equatorial great circle, giving a balanced stress graph with positive weights on all edges of $w_1, w_2 := w' + w'', w_3 := w''$. □

The DOD configuration is not a critical configuration for $r = 1$; instead it is a critical configuration at the maximal radius $r = r_{max}(12) \approxeq 1.10851$. As noted in Section 2 Fejes-Tóth [40] conjectured that this configuration does have a certain extremality property for local packing by equal spheres, that it gives a minimizer for a single Voronoi cell of a unit sphere packing. This statement, the Dodecahedral Conjecture, was proved in 2010 by Hales and McLaughlin [59].

Theorem 5.4. (Hales and McLaughlin (2010)) *A* DOD *configuration of unit spheres minimizes the volume of a Voronoi cell of a unit sphere with center at the origin of* $\mathbb{R}^3$ *over all sphere packing configurations of unit spheres containing that sphere.*

The volume of this Voronoi cell gives a local sphere packing density of approximately 0.7546, which exceeds the 3-dimensional sphere packing density $\frac{\pi}{18} \approxeq 0.74048$.

5.4. **Three remarkable configurations of unit spheres: deformation properties.** We now show that the DOD configuration can be continuously deformed inside BConf(12)[1] to the FCC configuration and to the HCP configuration.

Theorem 5.5. *(1) On the space* Conf(12)[1] *there is a continuous deformation of the* DOD *configuration to the* FCC *configuration, that remains in the interior* $\mathrm{Conf}^{-}(12)[1]$ *of* Conf(12)[1] *till the final instant.*

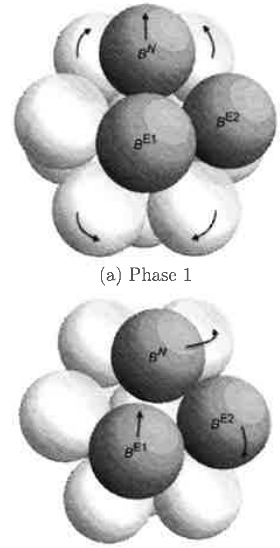
(2) There is also a continuous deformation of the DOD *configuration to the* HCP *configuration that remains in the interior* $\mathrm{Conf}^{-}(12)[1]$ *of* Conf(12)[1] *till the final instant.*

The motions of the two deformations, measured from the touching points of the 12 spheres to the central sphere, can be given by piecewise analytic functions on the 2-sphere. The proof is given in Sections 5.4.1 - 5.4.6. An unlocking manual for doing it is given in the Appendix (Section 8).

5.4.1. *Coordinates for the icosahedral configuration* DOD. To describe the deformations we will need coordinates. In Sections 5.4.1 - 5.4.5 we suppose a ball with radius 1 centered at 0 touches all the 12 balls of the same given radius r. We initially allow all values $0 < r \leq r_{max}(12)$, but in the move M_6 described in later subsections we will (necessarily) restrict to $r \leq 1$.

We take DOD to consist of 12 equal balls (of radius r, say), positioned at 12 vertices of the icosahedron I inscribed inside the unit sphere. We view this icosahedron I as embedded in $\mathbb{R}^3$ so that we have:

- its centroid is at the center, $(0, 0, 0)$ of the unit sphere.
- it has two opposite faces parallel to the plane xy; in other words, for some $z = h$ the intersections $I \cap \{z = \pm h\}$ are triangular faces of I. Here $h = \frac{\phi^2}{\sqrt{3\phi^2+3}} \approx 0.79659$, where $\phi = \frac{1+\sqrt{5}}{2}$ is the golden ratio.



(a) Phase 1

(b) Phase 2

x
these could be side by side

FIGURE 9. M_6 configurations

The *top three balls* are those which have their centers in the plane $\{z = h\}$. The *bottom three balls* are those which have their centers in the plane $\{z = -h\}$.

The top three balls form a *Northern triangle* triple which is centrally symmetric to the bottom *Southern triangle* triple, as in FCC.

Together with *Northern triangle* and *Southern triangle*, we have 6 remaining balls, which will be called *equatorial*, even though in the initial configuration they do not have their centers on the equator. The equator lies in the plane $z = 0$.

To fix their positions, let the *Greenwich meridian* be defined as $S \cap \{x \geq 0, y = 0\}$, and the longitude $\varphi \in [0, 2\pi)$ be measured from it in the clockwise direction. We require:

- The center of one of the Northern triangle balls is in the half-plane of the Greenwich meridian, i.e. this ball touches the Greenwich meridian. Let us call this ball B^N.
- The center of one of the equatorial balls is in the half-plane of the Greenwich meridian. Let us call it B^{E1}. It will necessarily be in the Southern hemisphere.

This fixes the location of all 12 balls. With this orientation of the icosahedron, the meridians of the Northern triangle are spaced by $\frac{2\pi}{3}$. Furthermore the meridians of the other three balls in the upper hemisphere are also spaced by $\frac{2\pi}{3}$ and the meridians combined are spaced by $\frac{2\pi}{3}$ as in FCC. The same holds for the six balls in the lower hemisphere.

5.4.2. *The M_6-move: two variants.* We now define a deformation M_6 ("the 6-move"), which has two variants, one leading from DOD to the FCC configuration, and the other leading to the HCP configuration. This move proceeds in two phases.

The first phase is the same for both variants. It moves the 6 balls that are not equatorial at constant speed along meridians towards the poles, until they form Northern and Southern triangles of three mutually touching balls. The 6 "equatorial" balls do not move.

In the second phase all 12 balls are moving. In both variants the 6 "equatorial" balls, initially not on the equator, move towards the equator along their meridians at constant speed, to arrive on the equator at the end of the move, forming a ring of six balls on the equator. This ring is an allowed configuration only if $r \leq 1$. They do not touch during this move, until the last moment, and then all touch if $r = 1$. At the same time the Northern and Southern triangle balls will rotate at a variable speed, the same for all six balls, in such a way as to avoid the equatorial balls. They will rotate by $\frac{\pi}{3}$ to their final position. For the FCC move the Northern triangle balls and Southern triangle balls rotate in the same direction, while for the HCP move they rotate in opposite directions. A key issue is to suitably specify the variable speed of rotation.

5.4.3. *The first phase of M_6-move: two triangles move away from the equator.* Denote by P the parallel $z = z_1$ where the three centers of the Northern triangle stop. Let $-P$ be the parallel $z = -z_1$ where the South triangle stops.

5.4.4. *The second phase of M_6-move: rotating the two triangles.* Each of the six centers of the equatorial balls, initially not on the equator, will move at constant speed along their respective meridians towards their final position on the equator. Parametrize this motion so that at $t = 0$, the 6 balls are at their initial positions, while at $t = 1$, the 6 balls are at their final positions on the equator.

The centers of the Northern triangle are on P at $t = 0$ and will remain on P throughout the move. Similarly, the centers of the Southern triangle are on $-P$ at $t = 0$ and will remain on $-P$ throughout the move. The triangles simply rotate.

It now suffices to specify functions $\varphi^N(t)$, which describe the *increment* of the longitude of the *top three balls* during the time $[0, t]$ and $\varphi^S(t)$, the *increment* of the longitude of the *bottom three balls* during the time $[0, t]$. We will take $\varphi^N(t)$ to be a continuous, non-decreasing, with $\varphi^N(0) = 0$, $\varphi^N(1) = \frac{\pi}{6}$.

We get two different moves to FCC and HCP depending on which direction the bottom three balls rotate. The motion $\varphi^S = \varphi^N$ will take us to FCC, and choosing the opposite rotation $\varphi^S = -\varphi^N$ will take us to HCP.

5.4.5. *The choice of φ^N.* The function φ^N, defined so that no ball from the two triangles hits any equatorial one, is certainly not unique.

Here is a minimal definition of φ^N, beginning at the second phase. Recall that

- the center of one of the Northern triangle balls, B^N, is on the half-plane of the Greenwich meridian.

- the center of one of the equatorial balls, B^{E1}, is also on the half-plane of the Greenwich meridian.
- there is an equatorial ball with the longitude $\frac{\pi}{3}$. Call it B^{E2}.

Note that the center of B^{E1} is below the plane $z = 0$, while that of B^{E2} is above the plane $z = 0$.

Throughout the second phase of M_6 the ball B^{E1} will move up while B^{E2} moves down. Let $B^{E1}(t)$, $B^{E2}(t)$ denote their positions, $t \in [0, 1]$. Then for every $\varphi \in [0, 2\pi)$ define $B^N(\varphi)$ to be the ball with the center at P and with the longitude φ. For example, $B^N(0) = B^N$.

Now let us define the function φ^N as follows:

$$\varphi^N(t) = \inf\left\{\varphi \geq 0 : B^N(\varphi) \cap B^{E1}(t) = \varnothing\right\}. \tag{5.1}$$

Clearly, $\varphi^N(t) = 0$ for all t small enough. The only thing one needs to check is that

$$B^N\left(\varphi^N(t)\right) \cap B^{E2}(t) = \varnothing \tag{5.2}$$

holds for all $t \in [0, 1]$.

Lemma 5.6. *An increment function $\varphi^N(\cdot)$ exists: $\varphi^N(t)$ as defined by* (5.1) *satisfies* (5.2).

Proof. We use Euler coordinates on the sphere. The altitude ϑ of the parallel P is $\pi - \theta$, where θ satisfies

$$\sin(\theta) = \frac{1}{\sqrt{3}}, \cos(\theta) = \sqrt{\frac{2}{3}}, \tan(\theta) = \frac{1}{\sqrt{2}}.$$

By symmetry, it is enough to consider the movement of three balls:

- B^N on the parallel P. Its initial angle $\varphi(t = 0) = 0$. The altitude ϑ of B^N is constant.
- B^{E1} on the Greenwich meridian $\varphi = 0$. Its initial altitude is $\vartheta(t = 0) = \frac{2\pi}{3} - \theta < 0$ and final altitude is $\vartheta(t = 1) = 0$. On the interval, its altitude is given by $\vartheta(t) = \left(\frac{2\pi}{3} - \theta\right) t$.
- B^{E2} on the meridian $\varphi = \frac{\pi}{3}$. Its initial altitude is $\vartheta(t = 0) = -\left(\frac{2\pi}{3} - \theta\right) > 0$ and final altitude is $\vartheta(t = 1) = 0$. On the interval, its altitude is given by $\vartheta(t) = \left(\theta - \frac{2\pi}{3}\right) t$.

The function $\varphi^N(t)$ is uniquely defined by

- $\varphi^N(t) \geq 0$,
- At every time $t < 1$ (after initial contact), the ball $B^N(t)$ kisses the ball $B^{E1}(t)$.

To complete the proof of Lemma 5.6 it remains to check that the balls $B^N(t)$ and $B^{E2}(t)$ of radius $r \leq 1$ are disjoint for $0 < t < 1$. This fact will follow from the next lemma. □

Lemma 5.7. *Let $0 < t < 1$. Consider the isosceles spherical triangle ABO, where A has $\varphi = 0$, $\vartheta(t) = \left(\frac{2\pi}{3} - \theta\right) t$, B has $\varphi = \frac{\pi}{3}$, $\vartheta(t) = -\left(\frac{2\pi}{3} - \theta\right) t$, and $O = O(t)$ is defined by $\vartheta(O) = \pi - \theta$ and the kissing condition. Then $|AO| = |BO| > \frac{\pi}{3}$.*

Proof. Let D be the middle point of the arc AB. It does not depend on t and is given by $\vartheta(D) = 0$, $\varphi(D) = \frac{\pi}{6}$. Let $\varkappa(t)$ be the arc perpendicular to the arc AB at D. Then $O(t)$ is nothing else as the intersection of $\varkappa(t)$ and the parallel P.

The triangle $O(t)\,DA(t)$ is a right triangle. Evidently, the legs $O(t)\,D$ and $A(t)\,D$ become shorter as t increases. Hence the hypotenuse $O(t)\,A(t)$ becomes shorter as well. Since $O(1)\,A(1) = \frac{\pi}{3}$, the proof follows. □

5.4.6. *Completion of proof of Theorem 5.5.*

Proof of Theorem 5.5. Lemmas 5.6 and 5.7 complete a proof that there exists a deformation path from the DOD configuration to a FCC configuration, resp. a HCP configuration. However the deformation path obtained does not satisfy one required condition of the theorem: that of remaining in the interior of the configuration space. It exits from the interior of Conf(12)[1] at the end of the first phase and remains on the boundary during the second phase: the three north pole balls are touching and the three south pole balls are touching.

We can modify the construction above so that no balls touch throughout the deformation until the final instant. To do this we halt the first phase just short of the three balls touching, at $z = 1 - \epsilon_1$, say. Then in the second phase, we allow z to increase monotonically in the northern triangle at some variable speed $\psi(t)$ as the rotation proceeds, in such a way as to avoid contact with the equatorial balls. The southern triangle z variable is to decrease monotonically in the reflected motion of $-z$ at the same time. Lemma 5.7 implies that if z approaches 1 rapidly enough in the motion we can avoid contact. (This is an open set condition at each point t so by compactness of the motion interval we have a finite subcover to attain it.) □

Remark. (1) This motion process can be continued by concatenation with an inverse M_6 using $-\varphi(1-t)$, in such a way as to arrive back at a DOD configuration, differently labeled. This is possible because there are two exit directions (tangent vectors) from the FCC configuration (in BConf(12)[1]) , and two exit directions from the HCP configuration. Section 6.1 studies the group of permutations obtainable by such deformations.

(2) Starting from the FCC or HCP configurations, there is a reference frame in which the Northern triangle remains fixed. The inverse of the second phase of M_6 describes a move which unlocks the FCC configuration with 6 moving balls and 6 fixed balls and unlocks the HCP configuration with 9 moving balls and 3 fixed balls, see the Appendix (Section 8).

5.5. **Buckminister Fuller "jitterbug" framework moving FCC configuration to DOD configuration.** According to his recollection, in 25 April 1948 Buckminster Fuller found a "jitterbug" construction given by a jointed framework motion that, among other things, permits an FCC configuration (given as the vertices of a cuboctahedron) to be continuously deformed into a DOD configuration (given as the vertices of an icosahedron), cf. [101, p. 273].

In Buckminster Fuller's construction, the joint distances remain constant during the motion, so that they can be rigid bars, while the radii of the associated touching spheres continuously contract during the deformation. At each instant during the motion the central sphere and the 12 touching spheres all have equal radii, and this radius varies monotonically in time.

In retrospect one may see that it is possible to rescale space during the motion via homotheties varying in time such that all spheres retain the fixed radius 1 throughout the deformation. In this case the joint lengths will change continuously in the motion. The rescaled motion no longer corresponds to a physical object with rigid bars, but it does give a continuous motion in the configuration space of 12 equal spheres touching a 13-th central sphere that continuously deforms the FCC configuration to the DOD configuration.

The work of Buckminster Fuller on the "jitterbug" movable jointed framework is described in Schwabe [101]. Fuller described it in his book Synergetics [49, Sec. 460.00-463.00]. The construction is also described in Edmondson [32, Chap. 11], with a detailed analysis in Verheyen [110].

Remark. The "jitterbug" motion immediately enters the interior $\mathrm{BConf}^-(12)[1]$ after the initial instant (in contrast to the "unlockings" described in Appendix 8, which adhere to its boundary).

6. Permutability of unit spheres in DOD configuration: Connectedness Conjectures

The number of connected components of the configuration space Conf(12)[r] is related to the ability to permute labeled spheres by deformations on it. The possible permutability of the (labeled) spheres in the DOD configuration in Conf(12)[r], depends on the radius r of the touching spheres.

6.1. **Permutations of DOD configurations for radius $r = 1$.** Conway and Sloane [25, Chap. 1, Appendix, pp. 29–30] give a terse proof that for radius 1 the labels on labeled spheres in DOD configurations can be arbitrarily permuted using continuous deformations inside the space Conf(12)[1].

Theorem 6.1. (Permutability at radius $r = 1$) *For the radius parameter $r = 1$ each labeled* DOD *configuration can be continuously deformed in the configuration space* BConf(12)[1] *to a* DOD *configuration at the same* 12 *tangency points with any permutation of the labeling.*

We follow the outline in Conway and Sloane [25, Chap. 1, Appendix, pp. 29–30]. A main ingredient is an additional set of permutation moves which we call M_5-moves, detailed next.

6.2. **The M_5-move.** Beginning from the DOD configuration centered at the origin, we rotate it so that two opposite balls have their centers on the z axis. Call these balls the N-ball and S-ball. Note that the centers of 5 of the 10 remaining balls are in the upper half-space, while the remaining 5 centers are in the lower half-space.

First phase. Move the upper 5 balls towards the N-ball, in such a way that their centers remain on their corresponding meridians, until each of them touches the N-ball. Note that the 5 balls do not touch each other, only the N-ball. Indeed, their centers are located at the

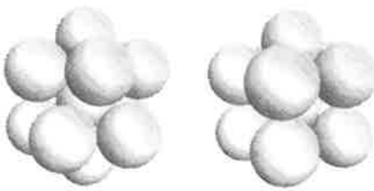


FIGURE 10. The 5-move M_5

altitude $\vartheta = \frac{\pi}{6}$, the longitude differences between the neighboring ball centers is $\frac{2\pi}{5}$, while the angle at which each of the 5 balls is seen from the z-axis, is $\arccos\left(\frac{1}{3}\right)$ and

$$\zeta = \frac{2\pi}{5} - \arccos\left(\frac{1}{3}\right) \approx 0.025 > 0.$$

The remaining 5 balls may be moved into the southern hemisphere in the same manner.

Second phase. Note that for $r = 1$, the 6 upper balls fit into the northern hemisphere, while the 6 lower balls fit into the southern hemisphere. The union of all the 6 balls in the northern hemisphere may be rotate as a solid body, by $\frac{2\pi}{5}$, keeping the remaining balls fixed.

Third phase. Reverse the first phase.

The net result of an M_5-move is a cyclic permutation p_2 of DOD of length 5, which is an even permutation.

6.3. Proof of permutability theorem at radius $r = 1$.

Proof of Theorem 6.1. The first step is to show that there is a continuous deformation of DOD to itself, which permutes the labels by an odd permutation. To exhibit it, we use the move M_6, defined before, and deform DOD into an FCC configuration (note that we can do it for all $r \leq 1$, but not for $r > 1$). Note that the FCC configuration has three axes of 4-fold symmetry passing through the opposite squares of four balls. By rotating $\frac{\pi}{2}$ around any such an axis and then deforming our configuration back to DOD via M_6^{-1}, we induce a a permutation p_1 of 12 balls, which is a product of three (disjoint) cyclic permutations, each of length 4. Every such cycle is an odd permutation, hence their product p_1 is also odd.

The second step uses M_5-moves. Each such move gives a cyclic permutation of order 5. Since there are 12 options for choosing the N-ball, we get 12 such 5-cycles $p_2^{(i)}$. It is shown in Conway and Sloane [25, pp. 29–30] (using a very elegant argument about the Mathieu group M_{12}, see [25, pp. 328–330]) that all such $p_2^{(i)}$ generate the alternating group A_{12}, the subgroup of even permutations of S_{12}.

Combined with any odd permutation p_1, the full permutation group S_{12} is generated. □

6.4. Persistence of M_5-moves for some $r > 1$. The move M_5 can be modified in such a way that it continues to work for all values $r \leq r_1$, for some r_1 slightly bigger than 1. We first explain the modification and then propose the value of r_1. The modification deals only with the second phase of M_5. In order to explain it, it is enough to follow the 10 points of tangency of our balls with the equator. For $r = 1$, the upper 5 balls U_j touch the equator at the points u_j, $j = 1, ..., 5$, and we can suppose that at the initial moment these points are $u_j(t = 0) = (j-1)\frac{2\pi}{5}$. The points v_j are defined similarly as the tangency points of the lower balls V_j, and $v_j(t = 0) = (j-1)\frac{2\pi}{5} + \frac{\pi}{5}$. Our initial move looks now as follows:

$$u_j(t) = (j - 1 + t)\frac{2\pi}{5},\ v_j(t) = v_j(0).$$

Of course there is no need for all the points u_j move with the same speed; the only constraint is that the distance between consecutive u_j should equal or exceed $\arccos\left(\frac{1}{3}\right)$ at all times. In particular, we can modify the speeds in such a way that at any time t, $u_j(t) = v_j(t)$ for at most one value of j.

Let now the radius r be slightly bigger than 1. Then at the moment t when $u_j(t) = v_j(t)$ the corresponding balls U_j, V_j will intersect.

This, however, can be avoided by the making the following small deformation of our 12 ball configuration:

- the ball U_j moves up along its meridian, by the distance $r - 1$.
- the ball N moves along the same meridian in the same direction by the distance $2(r-1)$.
- the ball V_j moves down along its meridian, by the distance $r - 1$.
- the ball S moves along the same meridian in the same direction by the distance $2(r-1)$.
- other balls may be rearranged in such a way that they do not intersect.

The non-intersection condition can be satisfied when $r - 1 > 0$ is small enough, since there were no other collisions.

Below we will show there will be 5 *bottleneck configurations* that one encounters on the way to perform the modified M_5 move. Each one defines a value $r_1^{(j)} > 1$, for $1 \leq j \leq 5$ which is the maximal radius for which this configuration is allowed. We set $r_1 := \min_{j=1,...,5} r_1^{(j)} > 1$.

Theorem 6.2. *For every $r \leq r_1$ the move M_5 can be modified in such a way that one can reach from an initial labeled* DOD *configuration any labeled* DOD *configuration whose labels are an even permutation of the initial labels. That is, the alternating group A_{12} is generated by the compositions of different M_5 moves.*

Proof. There will occur 5 bottleneck configurations of the 12 r-balls touching the unit central ball, described by certain kissing patterns of the balls, that correspond to the configurations appearing during the move M_5 at the moment when the ball U_j passes over the ball V_j.

Each of the 5 configurations has one common pattern. It consists of 4 kissing balls centered on the same meridian, two of them in the upper half-space, and the remaining two – in the lower half-space. We denote them by N, U_j, V_j, S. This set of 4 balls is symmetric with respect to the plane $z = 0$. (As r is slightly bigger than 1, the balls N and S, being the northern and the southern balls slightly inflated and moved, are centered, strictly speaking, not on the meridian containing U_j and V_j, but on the opposite one, obtained from it by adding a rotation by π. The eight other balls are the remaining ones from $U_1, ..., U_5; V_1, ..., V_5$. Each of the balls U_j, $j = 1, ..., 5$ (resp. V_j, $j = 1, ..., 5$) kisses the ball N (resp., S). The 5 bottleneck configurations differ by the order in which the remaining balls U_j, V_j are kissing, as one goes along the equator. The following are 5 such kissing patterns.

1. U_1, U_2, V_2, U_3, V_3, and U_4, V_4, U_5, V_5, V_1,
2. U_2, U_3, V_3, U_4, V_4, and U_5, V_5, V_1, U_1, V_2,
3. U_3, U_4, V_4, U_5, V_5, and V_1, U_1, V_2, U_2, V_3,
4. U_4, U_5, V_5, V_1, U_1, and V_2, U_2, V_3, U_3, V_4,
5. U_5, V_1, U_1, V_2, U_2, and V_3, U_3, V_4, U_4, V_5.

No other pairs of balls are kissing. A moment's thought shows that for any $r > 1$ and for any of the 5 kissing patterns such a configuration is unique, if it exists, and that it does exist if $r - 1 > 0$ is small enough. We define the values $r_1^{(j)} > 1$ as maximal ones, for which the above configurations do exist. These numbers are algebraic, so the value r_1 is algebraic as well. □

We are not asserting that the value $r_1 > 1$ defined above is the true critical value, above which the (small perturbation) of the move M_5 cannot be performed. Indeed, we imposed some a priori constraints in making our construction of the modified M_5, and did not rule out the possibility of a more 'optimal' modification of M_5.

Definition 6.3. *Let R_1 be the maximal value of the radius r for which there exists some modified move M_5. We call it the upper critical radius..*

From the previous theorem we know that $R_1 \geq r_1 > 1$. We expect R_1 to be a critical point of the radius function.

6.5. **Connectedness Conjectures for** Conf(12)[1]. Based on Theorem 5.5 and Theorem 6.1 about deformation and permutability of labeled DOD configurations, it is natural to propose the following statement.

Conjecture 6.4. (Connectedness Conjecture) *The configuration space* Conf(12)[1] *is connected. That is, every set of* 12 *distinct labeled points on the* 2*-sphere pairwise separated by spherical angle at least $\delta_{12} = \frac{\pi}{3}$ can be deformed into* 12 *other distinct labeled points, with all points remaining at least at spherical angle at least δ_{12} apart during the deformation.*

This problem appears to be approachable but difficult to prove, despite the supporting evidence of permutability in Theorem 6.1. One may approach it by cutting the space BConf(12)$[r_0]$ into many small path-connected "convex" pieces and gluing them together in some fashion. The computational size of the problem, since the dimension of the space is 21, and has a complicated boundary, is daunting.

We also propose a stronger statement.

Conjecture 6.5. (Strong Connectedness Conjecture) *The radius $r = 1$ is the largest radius value at which configuration space* Conf(12)$[r]$ *is connected.*

In support of Conjecture 6.5, the M_6-move appears to be possible only when $r \leq 1$. At one time instant it has 6 spheres fitting in a ring around the equator, a condition which is allowed only for $r \leq 1$. We also know that the $r = 1$ satisfies the necessary condition of being a "critical value" for the r-parameter.

We formulate one further conjecture concerning the connectivity structure of BConf(12)[1] A further analysis (not included here, see [73]) indicates that BConf(12)[1] has "pinch points" at each of the $\frac{12!}{24}$ FCC-configuration points and each of the $\frac{12!}{6}$ HCP-configurations. A *pinch point* **p** of a metric space is a point which when removed, disconnects a small open neighborhood of the point. That is, these configurations are points at which the space BConf(12)$[r]$ locally disconnects as r increases past 1. The following conjecture asserts that these "pinch points" form unavoidable bottlenecks in making certain rearrangements of spheres in the configuration space.

Conjecture 6.6. (FCC and HCP bottlenecks) *Any piecewise smooth continuous curve in the reduced configuration space* BConf(12)[1] *which starts at a labeled* DOD *configuration and ends at another labeled* DOD *configuration with the labels permuted by an odd permutation must necessarily pass through either an* FCC *configuration or a* HCP *configuration.*

This conjecture asserts that FCC and HCP configurations play a remarkable role in rearrangements of configurations, illuminating the analysis of Frank (1952) given in Section 2.7.

6.6. **Disconnectedness conjectures for** $r > 1$. For the region $1 < r \leq R_1$ we propose the following conjecture.

Conjecture 6.7. (Two connected components case) *Let R_1 be the upper critical radius defined after Theorem 6.2. Then the space* Conf(12)$[r]$ *for $1 < r < R_1$ has exactly two connected components. Two labeled configurations,* DOD *and w*(DOD)*, where $w \in S_{12}$ is a permutation of twelve labels, belong to different connected components if and only if the permutation w is odd.*

In view of the existence of the M_5-move, the argument in Theorem 6.1 indicates that there can be at most 2 connected components containing DOD configurations in this region. Conjecture 6.6 and Conjecture 6.7 are closely related.

We next note that the five "bottlenecks" in the 5-move lead to the possibility of connected components not containing any DOD configuration for certain ranges of r. During the M_5 move joining two DOD configurations, there are 5 bottlenecks all open at least up to a radius $r_1 > 1$. There is however room for configurations of spheres of larger radius occurring between the bottlenecks. If we increase the radius above the smallest two of the bottleneck radii we expect there is room for a sphere to get stuck in the middle one of these regions, so it can neither go backwards nor forwards to a DOD configuration. Assuming that "trapped" configurations (from blocking of the M_5 move) exist containing no DOD configuration, eventually as we increase r the "trapped" configuration must become a critical configuration. It must then be a local maximum in the configuration space, an isolated point. It would be a new type of "locally jammed" configuration. The critical value at which this occurs would be strictly smaller than r_{max}, using the result of Danzer (Theorem 3.3) showing that the extremal configuration for $N = 12$ is unique. This would therefore be a connected component not containing a DOD configuration. Therefore we propose for definiteness the following conjecture.

Conjecture 6.8. (Non-DOD components case) *There is a nonempty interval of values of $r > 1$ such that the reduced configuration space* BConf(12)$[r]$ *has connected components that do not contain any copy of a* DOD *configuration.*

The argument in favor of Conjecture 6.8 remains heuristic because we have not ruled out other types of deformation "moves" besides the M_5-move, permitting escape from such "trapped" configurations. Conjecture 6.8 leads to the possibility that there is a value of r such that the number of connected components of $\mathrm{BConf}(12)[r]$ could exceed the number of labeled DOD configurations, which is $\frac{12!}{12\times 5} = 7983360$ (see Conjecture 6.9 below).

Conjecture 6.7 requires that below the threshold value R_1 there are no connected components not containing a DOD configuration. We now define R_2 be the largest critical value below r_{max}, but above or equal to R_1, at which a local maximum critical point occurs, and if no local maximum occurs (so Conjecture 6.8 is false) then we set $R_2 = R_1$. , we set $R_2 = R_1$. For the remaining region $R_2 < r < r_{max}(12)$ our belief is the following:

Conjecture 6.9. (Many connected components case) *There is a radius $R_2 < r_{max}$ such that for $r > R_2$ the spaces $\mathrm{Conf}(12)[r]$ and $\mathrm{BConf}(12)[r]$ each have exactly $\frac{12!}{12\times 5} = 7983360$ connected components, with each component containing a DOD configuration.*

The number 7983360 needs an explanation. Let us take the DOD configuration and label its 12 balls. There are 12! such labelings. Two labeled configurations are equivalent (i.e. the same in $\mathrm{BConf}(12)[r]$) iff one can be obtained from the other by the $SO(3)$ rotation action. Clearly, there are 12×5 labelings in every equivalence class. For $r > r_2$, we believe that in every connected component of $\mathrm{Conf}(12)[r]$ there is exactly one such equivalence class of DOD configurations.

7. Concluding remarks

This paper treated configuration spaces of touching spheres for very small values of N. We have shown that configuration space of 12 equal spheres touching a central 13-th sphere is already large enough to exhibit interesting behavior in its critical points. The special case of $N = 12$ in the equal radius case $r = 1$ has some unique properties, some conjectural.

- We clarified an assertion of Frank (1952) given in Section 2.7 showing that in the space $\mathrm{BConf}(12)[1]$ there are deformations interconnecting all FCC, HCP and DOD configurations.
- We gave evidence suggesting that $\mathrm{BConf}(12)[1]$ is a connected space. We conjectured that $r = 1$ is the largest parameter value where $\mathrm{BConf}(12)[r]$ is connected.
- We showed that all elements of the the finite set of FCC and HCP configurations all lie on the boundary of the topological space $\mathrm{BConf}(12)[1]$ and are critical points for maximizing the radius parameter.
- x We conjectured that the (finite set of) FCC and HCP configurations in $\mathrm{BConf}(12)[1]$
  " are "unavoidable points" in making deformations of 12 spheres making an odd permutation of elements in a DOD configuration.

There remain many challenging and computationally difficult problems to better understanding the constrained configuration space $\mathrm{BConf}(12)[1]$.

As mentioned in the introduction, configuration spaces are of interest in physics and materials science, particularly in connection with jamming in materials. Hard sphere models for jamming have been extensively studied, which view spheres packed inside a box. Materials scientists have studied configuration spaces of small numbers of hard spheres by simulation (x name) in connection with nanomaterials. Recently, ~~Miranda~~ Holmes-Cerfon [65] developed an algorithm that enumerates rigid sphere clusters and has determined those with up to 16 spheres. The cases of small numbers of spheres (but larger than the N treated here) were studied in

Phillips et al. [94] and ~~Sharon C.~~ Glotzer et al. [95], giving estimates for extremal config- x name urations at values of N larger than can be currently treated mathematically. We note that simulations of phase space can sample only a small part of it. In the simulation experiments reported in [94] for $N = 12$ equal spheres the experimenters were unable to detect that the radii at which the M_5-move and the M_6-move permutation cease being feasible are in fact different (as discussed in Section 6.4).

Study of the jamming problem leads to the sub-problem of what is a good notion of x rigidity for such configurations. There is a notion of "locally jammed configuration" in which " no particle can move if its neighbors are fixed. The Tammes problem or (extremal) spherical codes problem, of determining $r_{max}(N)$ is analogous to determining maximally dense jammed configurations of spheres in a box. Various notions of rigidity for spherical codes were formulated in Tarnai and Gáspár [105]. More recently Cohn et al. [23] give a mathematical treatment of rigidity of extremal n-dimensional spherical codes. In configuration theory models like $\mathrm{BConf}(N)[r]$ of this paper, certain critical configurations at critical values of the radius parameter might serve as a proxy for jammed configurations, with the balancing condition in Theorem 4.11 capturing the locally jammed condition. Perhaps only a subclass x of critical configurations should be interpreted as "jammed", for example those that are local " maxima of the radius function.

8. Appendix: Unlocking manual for the FCC and HCP configurations

8.1. The FCC configuration. To unlock the FCC configuration, a good way is to do it with the help of a friend, hereafter called Charles[6]. Please follow these steps:

(1) Ask Charles to hold the 3 north triangle balls and the 3 south triangle balls firmly in their positions. These 6 polar balls remain fixed during the whole process. As a result, the 13-th central ball stays fixed as well.
(2) Roll the remaining 6 equatorial balls in a direction roughly parallel to the equator. If properly lubricated, this does not require a big effort.
(3) The equatorial balls can all be pushed either to the east or to the west, in a coordinated way.
(4) At all times you must ensure the 6 rolling balls touch the central ball. This requires some practice, but it is possible and not terribly hard.
(5) Observe that the 6 balls roll around the central ball along the equatorial "valley" between the north and south triangle balls kept fixed by Charles. These rolling balls cannot always move horizontally, but instead ascend or descend slightly, in an alternating manner, as you roll them.
(6) Because the 6 rolling balls ascend and descend, some of them do not touch each other any more: free space may appear between them. Also, some space can be created between them and the 6 balls kept fixed by Charles. This is normal.
(7) As you proceed by $\frac{\pi}{3}$, the 6 rolling balls realign in the horizontal plane, touching each other and the top-bottom balls. Note that at this moment the configuration is locked back into FCC. Each of the 6 rolled balls is touching two of its horizontal neighbors: one ball above and one ball below.

[6]Après Charles Radin

(8) Note finally that the equatorial balls underwent a cyclic permutation of length 6, which is an odd permutation.

8.2. **The** HCP **configuration.** Unlocking the HCP configuration is similar to the FCC configuration, except that Charles has somewhat more to do. Please follow these steps:

(1) Ask Charles to hold firmly the three north triangle balls and the three south triangle balls. The three south triangle balls will remain fixed during the whole process. But the north triangle has to be rotated as a whole in its horizontal plane, at some constant speed, which can be either eastward or westward, there are two choices. It will move through an angle $\frac{2\pi}{3}$. The central – 13-th – ball stays fixed as before.
(2) Roll all the remaining 6 balls in the (roughly, same) equatorial direction, as the northern triangle is rotating. This movement direction is forced on all six equatorial balls by the motion of the northern triangle.
(3) The rest of the process goes basically in the same way as for the FCC configuration.
(4) As Charles proceeds to rotate the north triangle by $\frac{2\pi}{3}$, you proceed by $\frac{\pi}{3}$, the six middle balls align back into the equatorial plane, touching each other and the six north-south triangle balls. Note that at this moment the configuration is locked back into the HCP configuration. Each of the 6 rolled balls is touching two of its horizontal neighbors, one ball above and one ball below.
(5) Note that the 6 equatorial balls underwent a cyclic permutation of length 6 while the north triangle underwent a cyclic permutation of length 3. The overall permutation is thus odd again.

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