Configuration Spaces and Materials Science

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Texas Geometry and Topology Conference

- Texas Geometry and Topology Conference

- February 19, 2017

- Texas Tech, Lubbock, TX

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Topics Covered

- Part I. Materials Science
- Part II. Configuration Spaces-r=0 case
- Part III. The 12 Spheres Problem: History
- Part IV. The 12 Spheres Problem: Geometry
- Part V. The 12 Spheres Problem: Topology Change Varying r

References

• R. Kusner, W. Kusner, J. C. Lagarias, S. Shlosman,
The Twelve Spheres Problem, eprint. `arXiv:1611.10297`

Part 0. Configuration Spaces

• **Configuration spaces** are topological spaces describing arrangements of a (fixed) number of points on a topological space X, taken to be a manifold, carrying a (global) metric.

• **Constrained configuration spaces** are such spaces with extra geometric constraints imposed on location of the points. The simplest such condition is that they cannot be too close to each other. (It is convenient to have X be a metric space, in order to measure distance beween points.)

• **Packing and tiling problems** can be viewed as special sorts of problems in constrained configuration spaces.

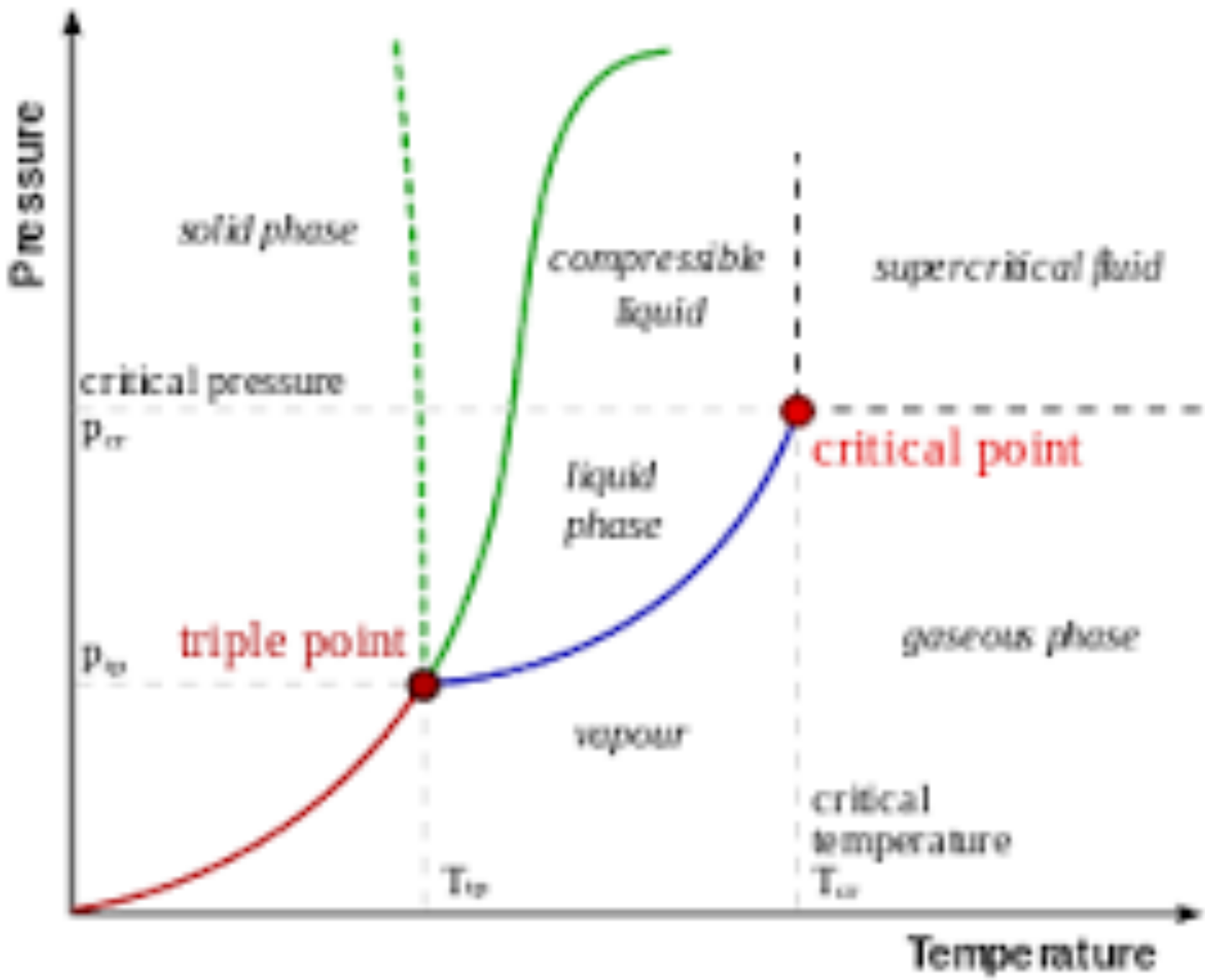
• Talk considers a specific model: constrained configuration spaces of N spheres of radius r touching a central sphere of radius 1.

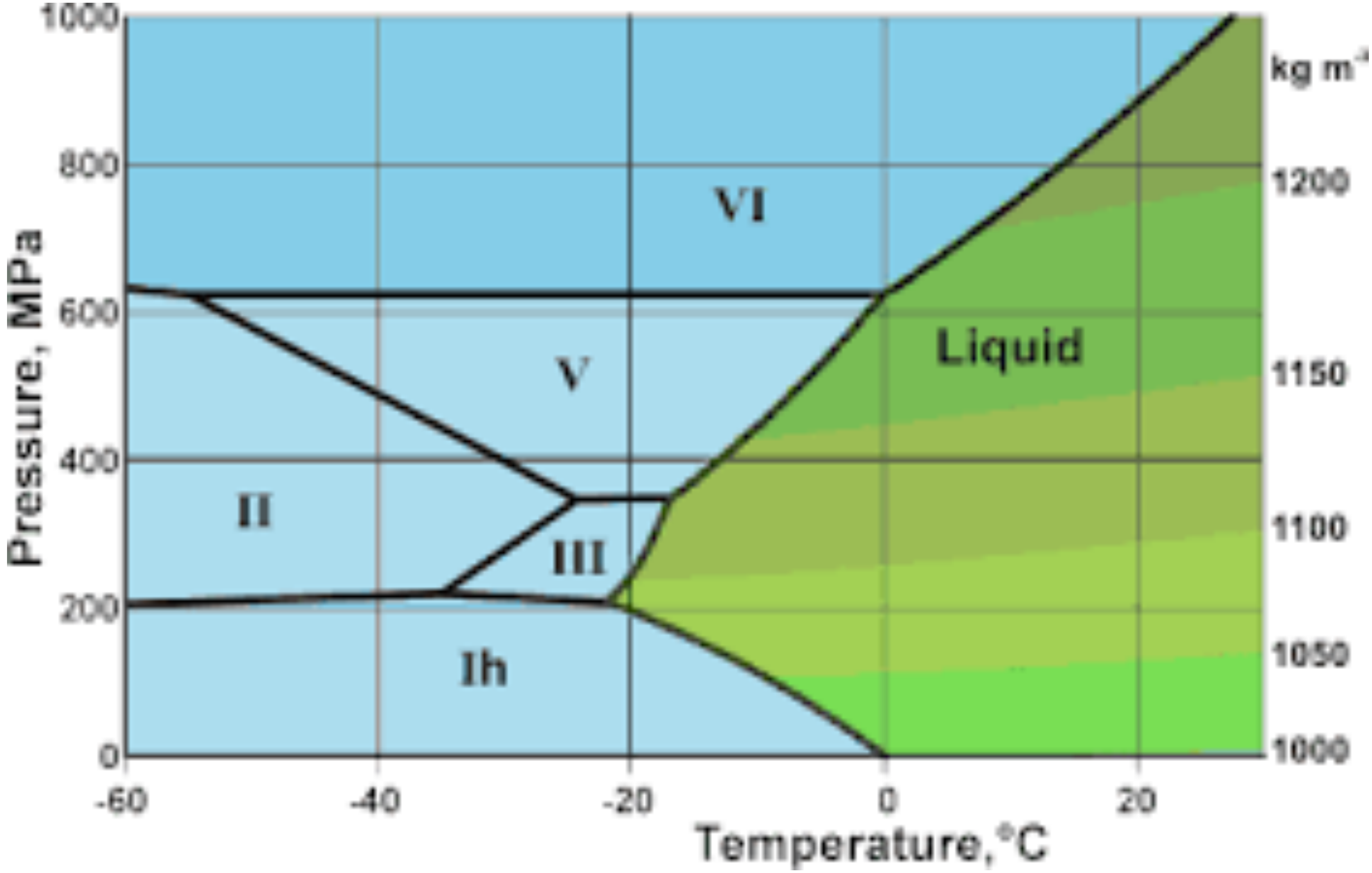
Part I. Materials Science-1

- Problems in materials science can be approached mathematically via “toy model" problems

- A basic question in materials science is to determine the thermodynamic phase diagram of simple materials: gas, liquid, solids in various states.

- Some thermodynamic phases can described by global “order parameters" with phase transitions signaled by sharp change in an order parameter value (as a function of temperature, pressure etc.)


Pressure
solid phase
compressible liquid
supercritical fluid
critical pressure
p_{cr}
critical point
liquid phase
triple point
p_{tp}
gaseous phase
vapour
critical temperature
T_{cr}
T_{tp}
Temperature



1000
800
600
400
200
0
Pressure, MPa
-60
-40
-20
0
20
Temperature,°C
kg m⁻³
1200
1150
1100
1050
1000
VI
V
II
III
Ih
Liquid

Materials Science-4

- One of the mysteries of materials science whether there is some associated phase transition (under rapid cooling or compression) in amorphous glassy materials. Is there a “glass phase transition" between a hard material and a “rubbery" material.

- A simpler question, also unanswered, concerns the possible appearance of a “jamming" phase transition in granular materials.

- Packings of hard particles give simple models for granular materials, glasses, liquids and other random media.

Part I. Materials Science-5

- Materials problems can be approached in complementary ways:

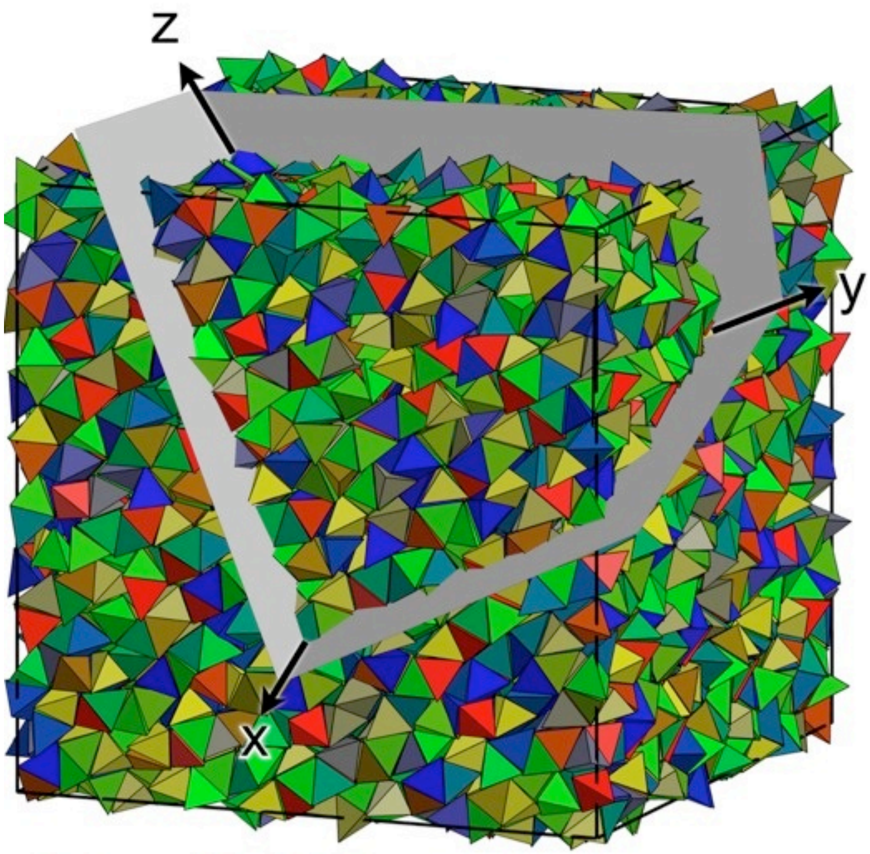
1. empirical, large scale, by Monte Carlo simulations.

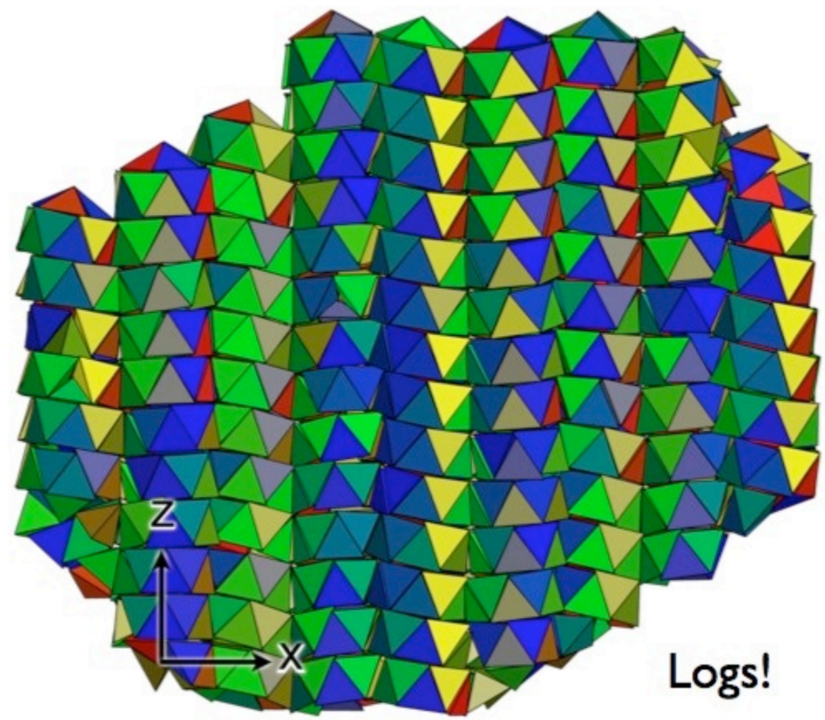
2. statistical mechanics, approximate models. (math + numerical analysis of formula predictions)

3. theoretical, very small scale: “toy models"

- Next slides: some results of simulation: “gas" of hard tetrahedra compressed to given density

A dodecagonal quasicrystal!

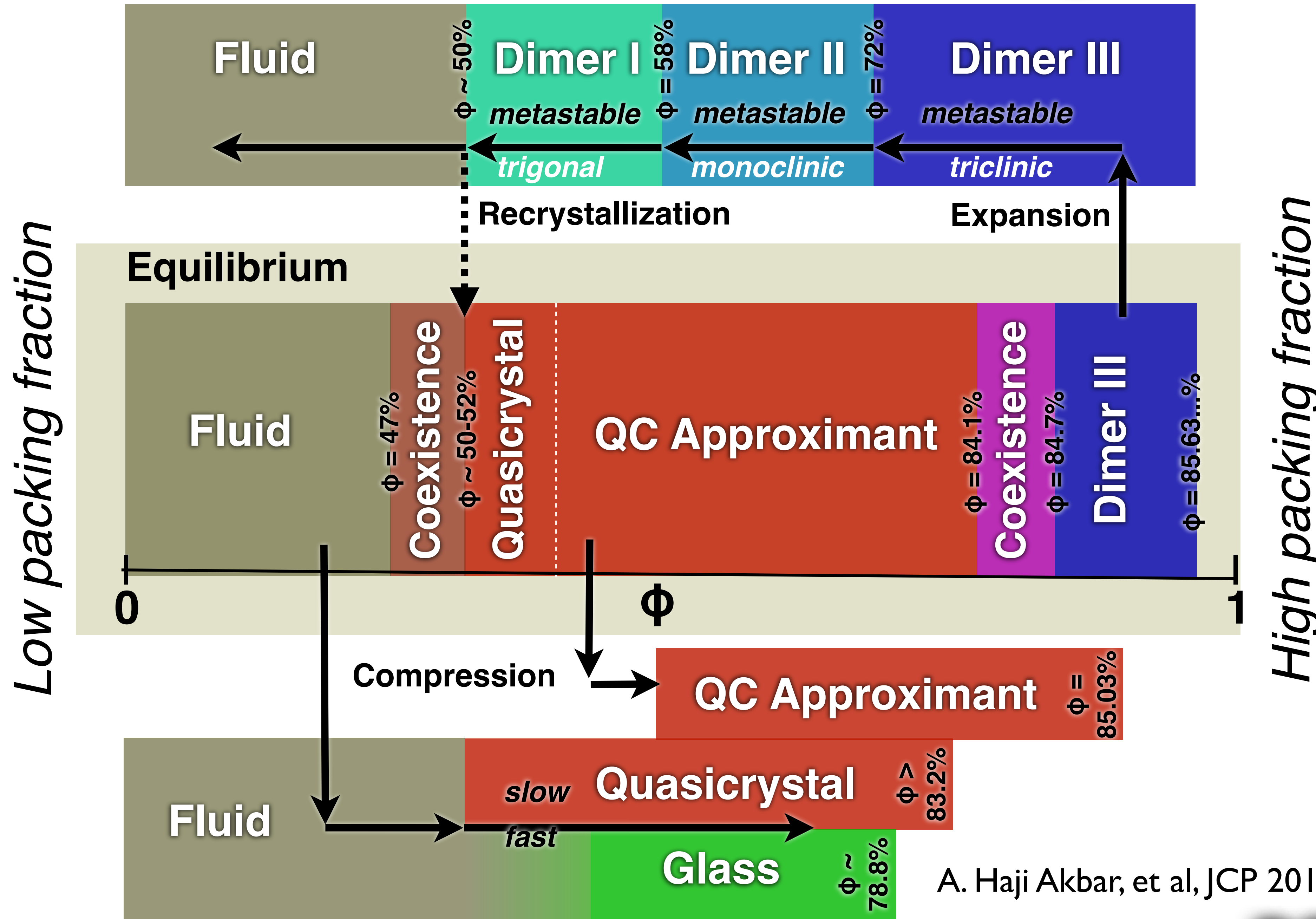




Logs!

N = 13824

Hard Tetrahedron Phase Diagram



A. Haji Akbar, et al, JCP 2011

Materials Science-8

- The problems of materials science involve geometry of interacting objects in three dimensions. They also be described using higher dimensions: the motions of N objects requires 3N coordinates.

- This talk considers simpler and simpler toy problems in which the connection to reality becomes more and more tenuous. But the chance to say something precise increases.

- Talk concentrates on Toy model 2 (coming up)

Materials Science-9

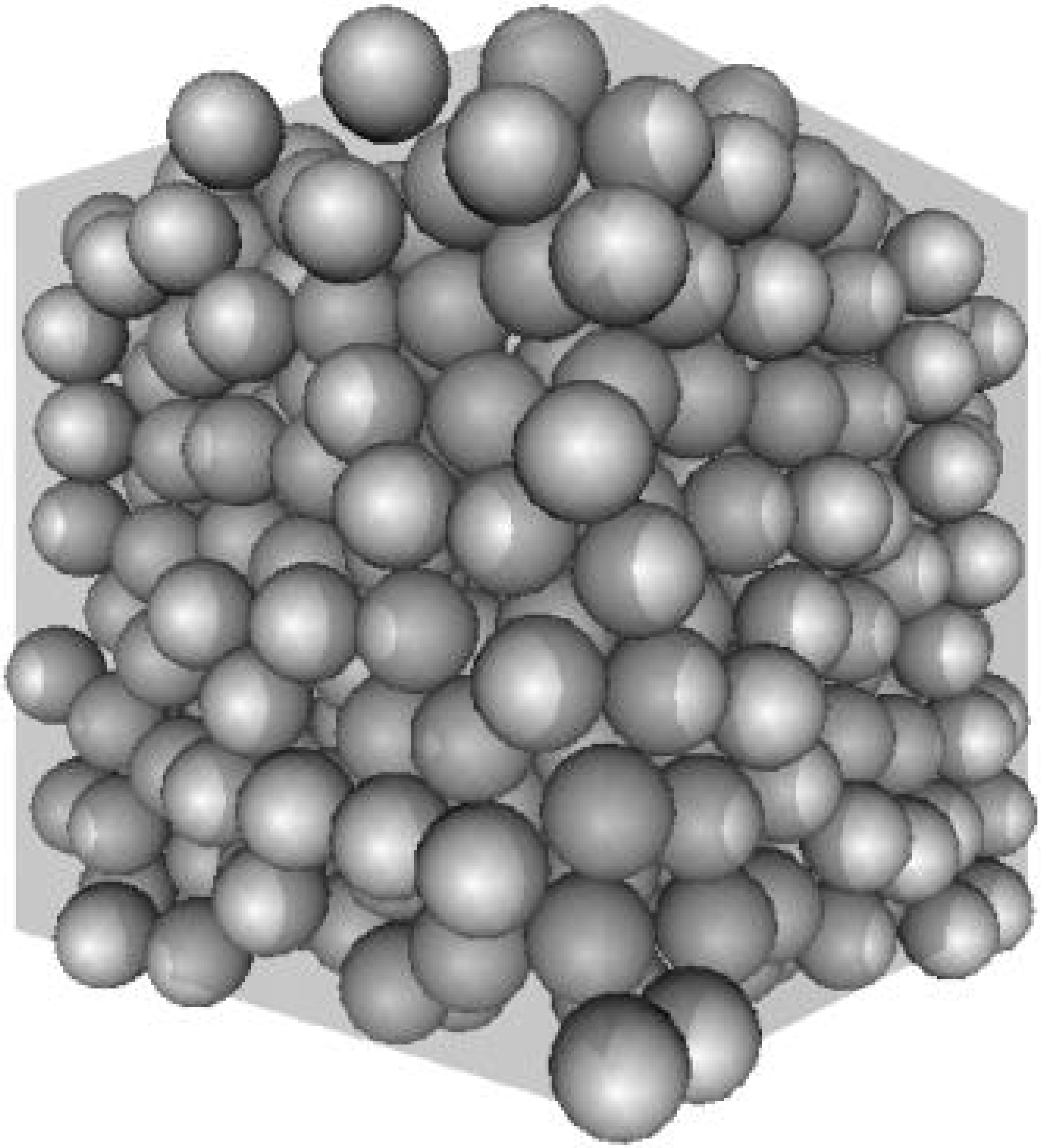
• **Toy model 1:** Assemblies of hard spheres in thermal motion. ("Ball bearings") (J. D. Bernal et al (1967) *Geometry of close-packed hard sphere model.* Structure of liquids.)

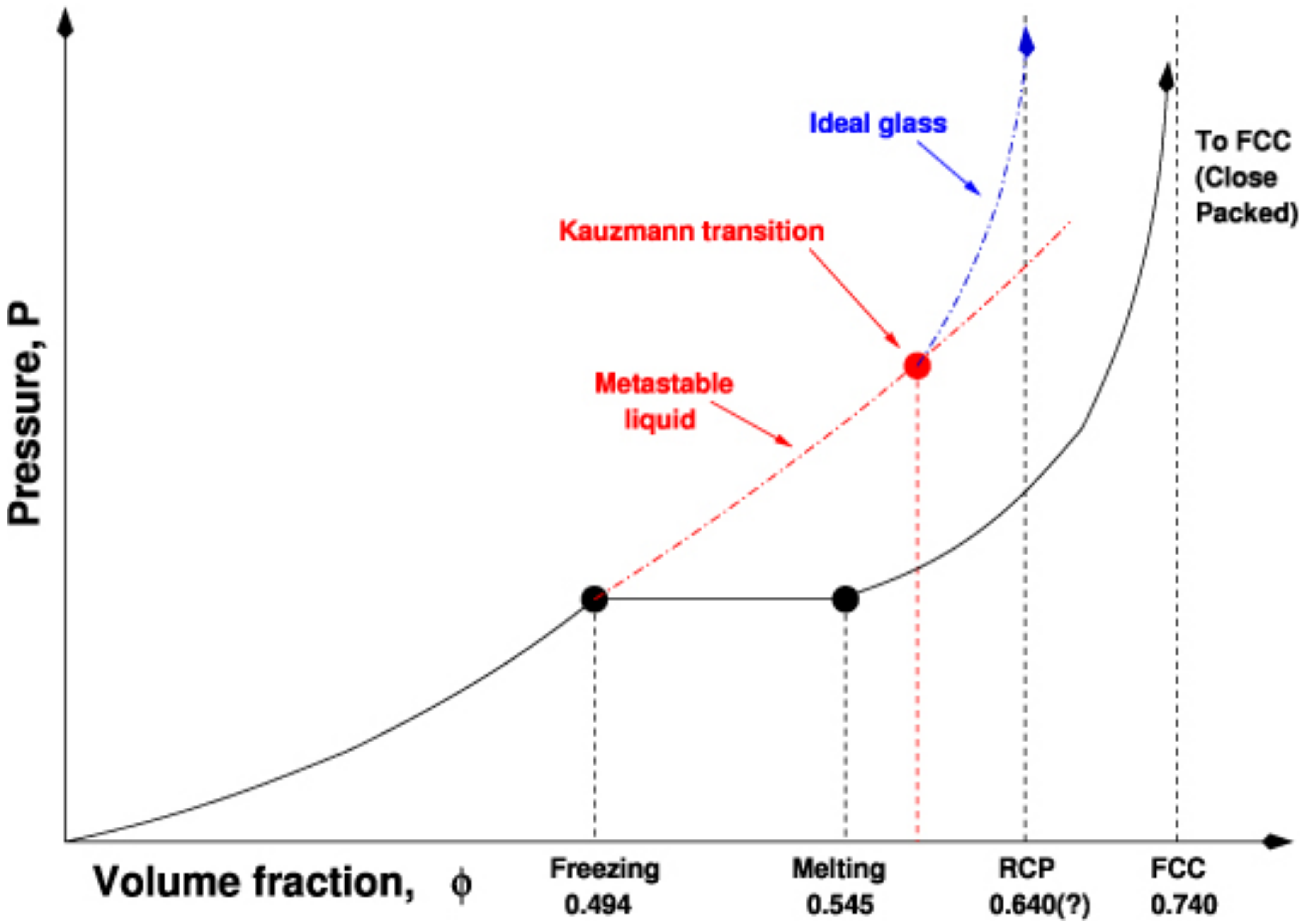
• Parameter to vary: density of packing, and "pressure".

• Maximal density of sphere packing: $\frac{\pi}{\sqrt{18}} \approx 0.74$

• Experimentally a phase change: ("jamming transition") to the "random close packing" (RCP) is observed between density 63% and 64%. There is a change in elastic modulus and in bulk modulus.

• One can study for this model, mainly by simulation, but also by experiment, are: geometry of the final packed states, statistics like average number of contacts among the spheres.




Pressure, P
Ideal glass
To FCC
(Close
Packed)
Kauzmann transition
Metastable
liquid
Volume fraction, ϕ
Freezing
0.494
Melting
0.545
RCP
0.640(?)
FCC
0.740

Materials Science-12

• Toy model 2: Consider spaces consisting of:
(1) N **hard spheres of a fixed radius** r
(2) **each touching a fixed sphere of radius** `1`**.**

Spheres may move, but are restricted to remaining in contact with the central sphere.

• This model has a two-dimensional flavor: One can replace the spheres touching the central spheres with **spherical caps** (“contact lenses") of radius $f(r)$ on the surface of the sphere, which may be moved about, as long as their interiors don’t overlap.

• **Density of a packing** of circular caps is specified the fraction of the total surface area $4\pi^2$ that they cover on the central unit sphere. For fixed radius r it is a linear function of the number of caps N present, they cover a surface areas proportional to Nr.

Disclaimer

• This reductive process of simplification has produced mathematics problems that may be approached. However they only capture limited features of the original problem.

• Work to be described in no way resolves the existence of a “jamming transition " or of a “glass transition".

• Results in quotes: e. g. “**Theorem**" are not yet in preprint form.

Part II. Configuration Spaces-the $r = 0$ case

- *Configuration spaces* of N distinct points on a manifold Z, e.g $\mathbb{R}^2$ or $\mathbb{S}^2$.

$$\text{Conf}(Z, N) := Z^N \setminus \{z_i = z_j : 1 \leq i < j \leq N\}.$$

- Such spaces have been studied by topologists since 1960's. Cohomology and homotopy type of configuration spaces have been extensively studied, with rather complete answers for $\mathbb{R}^n$ and $\mathbb{S}^n$. (Book of Fadell and Husseini (2001).)

Reduced Configuration Spaces-the $r = 0$ case

- *Reduced configuration spaces* mod out by global symmetries. For $\mathbb{S}^2$ the isometries are given by elements of $SO(3)$, a 3-dimensional real Lie group. Set

$$\mathrm{Bconf}(\mathbb{S}^2, N) = \mathrm{Conf}(\mathbb{S}^2, N)/SO(3).$$

- We have

$$\mathrm{Bconf}(\mathbb{S}^2, N) = \mathrm{Conf}(\mathbb{R}^2, N-1)/SO(2),$$

taking the one-point compactification of $\mathbb{R}^2 \simeq \mathbb{C}$.

Betti Numbers of Configuration Spaces $\mathrm{Conf}(\mathbb{R}^2, n)$

$n \setminus k$	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: Betti numbers of $H^k(\mathrm{Conf}(\mathbb{R}^2, n), \mathbb{C})$.

Betti Numbers of Reduced Configuration Spaces $\mathrm{Bconf}(\mathbb{S}^2, n), \mathbb{C})$

$n \setminus k$	0	1	2	3	4	5	6	7
3	1	0	0	0	0	0	0	0
4	1	2	0	0	0	0	0	0
5	1	5	6	0	0	0	0	0
6	1	9	26	24	0	0	0	0
7	1	14	71	154	120	0	0	0
8	1	20	155	580	1044	720	0	0
9	1	27	295	1665	5104	8028	5040	0
10	1	35	511	4025	18424	48860	69264	40320

TABLE: Betti numbers of $H^k(\mathrm{Bconf}(\mathbb{S}^2, n), \mathbb{C})$

Cohomology Calculations

- The cohomology ring of $\mathtt{Bconf}(\mathbb{R}^2, N)$ was computed by Arnol'd(1969), in terms of "colored" braid groups.

- The reduced configuration space $\mathtt{Bconf}(\mathbb{S}^2, N)$ has homotopy type a twisted product of bouquets of circles with $N-3$ factors, with the j-th factor being a bouquet of $j+2$ factors, from $1 \le j \le N-3$. so its cohomology over $\mathbb{Q}$ vanishes above dimension $N-3$.

Constrained Configuration Spaces

- One can *extra constraints* on point locations. In our case, we treat points on $\mathbb{S}^2 = \{(x, y, z) = x^2 + y^2 + z^2 = 1\} \subset \mathbb{R}^3$. and require: minimal distance $d = f(r)$ between points is bounded below.

- *Injectivity radius function* $\rho(\mathbf{U})$ for a collection $\mathbf{U}$ of N points $\mathbf{u}_1, \mathbf{u}_2, \cdots \mathbf{u}_N$ is the minimum distance between any pair of points.

- Can measure distance d as half the spherical angle θ between points. on $\mathbb{S}^2$. Convert θ to radius r via

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

Constrained configuration Spaces -2

- *Constrained configuration space* is

$$Y_N[r] = \mathsf{Conf}(n)[r] = \{(\mathbf{u}_1, .., \mathbf{u}_N) : \rho(\mathbf{U}) \geq \theta(r)\}.$$

- This configuration space has a global symmetry: the group $SO(3)$ of isometries of $\mathbb{S}^2$.

- *Reduced (constrained) configuration space* is

$$X_N[r] = Y_N[r]/SO(3) := \mathsf{Bconf}(n)[r] = \mathsf{Conf}(N)[r])/SO(3).$$

Part III. The 12 Spheres Problem: History

• We restrict to small N, particularly $N = 12$, which has an extensive history.

• 12 **Spheres Problem:** Describe the topology and geometry of the configuration space of 12 spheres all of radius 1 touching a central sphere of radius 1.

• **Generalized** 12 **Spheres Problem:** Describe the topology and geometry of the configuration spaces of 12 spheres of radius r touching a central sphere of radius 1, and how it changes with varying radius $0 < r \leq r_{max}$.

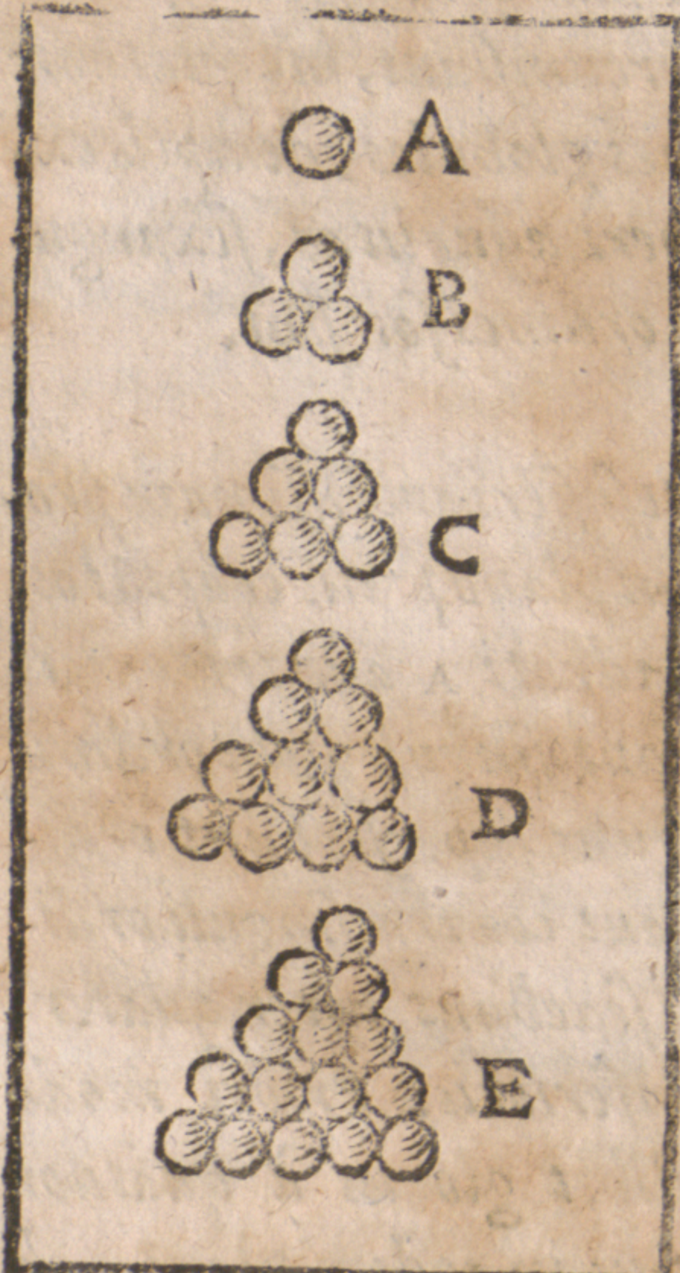
• The history of this problem relates to physics, crystallography, chemistry, biology and architecture.

Kepler (1611): FCC Packing

In “*Strena, Seu de nive Sexangula*" [The Six-Cornered Snowflake]" (Packing of spheres, with woodcut figures)

“*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 in the plane below, so throughout one will be touched by twelve, and under pressure spherical pellets will become rhomboid. [· · ·] The packing will be the tightest possible, so that in no other arrangements could more pellets be stuffed into the same container.*"

[FCC= Face Centered Cubic Lattice Configuration] *quadrilateris. Esto enim B copula trium globorum. Ei superpone A vnum pro apice, esto & alia copula senũ globorum C, & alia demũ D, & alia quindenum E. Impone semper angustiorem latiori, vt fiat figura Pyramidis. Etsi igitur per hanc impositionem singuli superiores sederunt inter trinos inferiores: tamen iam versa figura, vt non apex sed integrum latus pyramidis sit loco superiori, quoties vnum globulum degluberis è summis, infra stabunt quatuor ordine quadrato. Et rursum tangetur vnus globus vt prius, à duodecim alijs, à sex nempe circumstantibus in eadem plano tribus supra & tribus infra. Ita in solida coaptatione arctissima non potest esse ordo triangularis sine quadrangulari, nec vicissim. Patet igitur, acinos Punici mali, materiali*



Gregory (1715): Thirteen spheres can touch

• David Gregory talked with Isaac Newton about locations of stars in the 1690's about the second edition of the Principia. Newton said 12 or 13 could be close to a given star.

• Gregory studied the packing problem. In his lectures on astronomy (published 1715) he said:

"*Now, 'tis certain from Geometry, that thirteen Spheres can touch and surround one in the middle equal to them, (for* Kepler *is wrong in asserting, in* B. I *of the* Epit. *that there may be twelve such, according to the number of Angles of an* Icosaedrum,)"

THE ELEMENTS OF Astronomy, PHYSICAL and GEOMETRICAL.

By DAVID GREGORY M. D. *Savilian* Professor of ASTRONOMY at *Oxford*, and Fellow of the Royal-Society.

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Vol. I.

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to be the cause of their different Magnitude.

And this opinion is very much favoured by the number of the Fix'd Stars of the first and second Magnitude. For if every Fix'd Star did the office of a Sun, to a portion of the Mundane space nearly equal to this that our Sun commands, there will be as many Fix'd Stars of the first Magnitude, as there can be Systems of this sort touching and surrounding ours; that is, as many equal Spheres as can touch an equal one in the middle of them. Now, 'tis certain from Geometry, that thirteen Spheres can touch and surround one in the middle equal to them, (for *Kepler* is wrong in asserting, in *B.* 1 of the *Epit.* that there may be twelve such, according to the number of the Angles of an *Icosaedrum*,) and just so many uncontroverted Stars of the first Magnitude are taken notice of by Observation. For Astronomers are not as yet agreed upon their number: *Hevelius* reckons the *bright Star in the Eagle's Shoulder* of the second magnitude, whereas *Tycho* made it of the first; and on the contrary *Hevelius* makes the *little Dog* and *the right Shoulder of Orion* of the first magnitude, and *Tycho* of the second. And there are others that *Hevelius* himself doubts of.

Again, if it be asked how many Spheres equal to the former can touch the first Order of Spheres, surrounding the Sphere placed in the beginning, (or rather a Sphere comprehending those former thirteen together with a fourteenth in the Center;) the number of these will be

Barlow (1883): Hexagonal Close Packing

"*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)*"

[HCP= Hexagonal Close Packing]

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,

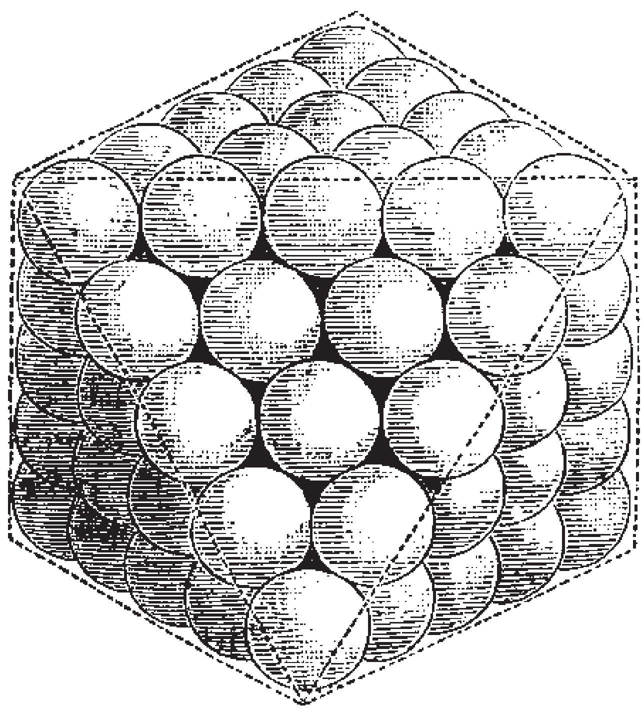


FIG. 7.

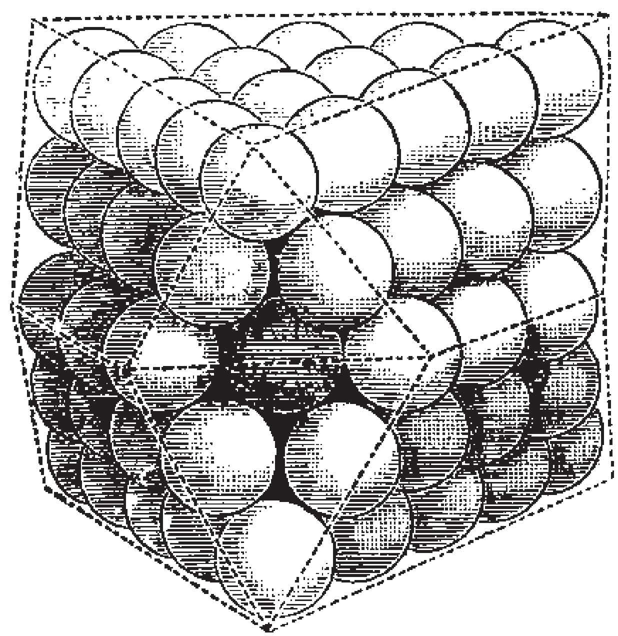


FIG. 8.

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

Tammes (1930) Maximal Radius $r_{max}(N)$

- The *Tammes problem* (1930) concerns the maximum angular separation θ achievable for N points on a sphere.

- Problem studied by P.M. L. Tammes concerned distribution of pores on pollen grains in plants.

- **Radial Tammes Problem.** What is the maximum radius $r = r_{max}(N)$ achievable for N equal spheres of radius r touching a radius 1 central sphere?

  Equivalence of the problems: $\sin \frac{\theta}{2} = \frac{r}{r+1}$.

N	$r(N)$	Minimal Equation for $r(N)$
4	$r_{max}(4) = 2 + \sqrt{6}$ ≈ 4.4495	$X^2 - 4X - 2$ Regular Tetrahedron
5- 6	$r_{max}(5) = r_{max}(6) =$ $1 + \sqrt{2} \approx 2.4142$	$X^2 - 2X - 1$ Regular Octahedron (N=6)
7	$r_{max}(7) \approx 1.6913$	$X^6 - 6X^5 - 3X^4$ $+8X^3 + 12X^2 + 6X + 1$
8	$r_{max}(8) \approx 1.5496$	$X^4 - 8X^3 + 4X^2 + 8X + 2$ Square Antiprism
9	$r_{max}(9) \approx 1.3660$	$2X^2 - 2X - 1$
10	$r_{max}(10) \approx 1.2013$	$4X^6 - 30X^5 + 17X^4$ $+24X^3 - 4X^2 - 6X - 1$
11-12	$r_{max}(11) = r_{max}(12) =$ $\frac{1}{\sqrt{\frac{5+\sqrt{5}}{2}-1}} \approx 1.10851$	$X^4 - 6X^3 + X^2 + 4X + 1$ Regular Icosahedron (N=12)
23-24	$r_{max}(23) = r_{max}(24) =$ ≈ 0.59262	$X^6 - 10X^5 + 23X^4$ $+20X^3 - 5X^2 - 6X - 1$ Snub Cube (N=24)

Frederick Charles Frank (1952)

In “Supercooling of liquids" he says:

“*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 that cannot be transformed into each other without breaking contact with the centre ball. The answer is* **three.** *Two which come to mind of any crystallographer occur in the face-centred cubic and hexagonal close packed lattce. The third [· · ·] is to put one at the centre of each face of a regular dodecahedron. This body has five-fold axes, which are abhorrent to crystal symmetry.*"

[DOD= dodecahedral configuration]

Frederick Charles Frank (1952)

In “Supercooling of liquids" he also says:

“*one may calculate that the binding energy of [the dodecahedral cluster of* 13 *atoms] is* 8.4% *greater than the other two packings. This is* 40 *percent 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 will be of this form."*

Main Physics Idea. The phase transition of freezing (liquid to solid) involves a substantial rearrangement of atoms into a new order, there is a local energy barrier to making the rearrangement.

Note. Ice Ih (standard ice) has its oxygen atoms in the HCP packing, forms/melts at $0^\circ C$. However under some conditions pure water can be supercooled to $-45^\circ C$ at standard pressure and remain liquid.

Motivating Question

• Frank singles out three configuations: Call them FCC, HCP and DOD.

• **Question.** Is Frank's assertion about the space of configurations of unit distance spheres (mathematically) accurate?

• Frank asserts that the configuration space $X_{12}[1]$ of 12 unit spheres on a central unit sphere is *disconnected*. Furthermore, he states there are **three** types of connected components.

[Two variant questions: Considering *unlabeled* spheres, versus considering *labeled* spheres, numbered 1 to 12. For labeled spheres, the number might not be **three**.]

Motivating Question-Answers: Yes and No

Mathematical Answer 1. No.
There are explicit deformations showing that DOD, FCC and HCP are in same connected component of the configuration space $X_{12}[1]$.

Conjecture: The configuration space $X_{12}[1]$ is *connected,* i.e. its 0-th cohomology group $H^0(X_{12}[1], \mathbb{C}) = \mathbb{C}$.

Physics Answer 2. Yes. It is “almost true" in various senses.

[FCC and HCP configurations are points on the boundary of the 24-dimensional space $X_{12}[1]$.]

Conjecture. The configuration space $X_{12}[r] := \mathtt{Conf}(12)[r]$ of 12 spheres of any fixed radius $r > 1$ touching a central unit sphere is *disconnected*.

Part IV. The 12 Spheres Problem: Geometry

• We consider the 21-dimensional space $\mathtt{Bconf}(12)[r]$ for $0 < r \le r_{max}$. The first question concerns: **value of** r_{max}. It corresponds to the *Tammes problem* for $N = 12$.

• **Theorem** (László 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, the face-centers of a circumscribed regular dodecahedron). [It is unique, up to isometry.]*

Local Maxima for the Generalized 12 Spheres Problem

• **Question.** *Are there additional local maxima of the radius function for some value* $0 < r < r_{max}$*?*

• If so, it must have $r > 1$. Such values would give connected components of $\texttt{Bconf}(12)[r]$ that do not contain any DOD configurations.

Permutation Problem for 12 Spheres

Permutation Problem. Considering labeled spheres, we have the following questions:

• **Question 1.** What is the largest radius r_p at which all 12 spheres can be arbitrarily *permuted*?

• **Theorem.** Conway and Sloane (1998) *All spheres in* DOD *can be arbitrarily permuted at* $r = 1$*. Thus* $r_p \geq 1$*.*

• **Question 2.** What is the largest radius r_c for which the configuration space is *connected*? [One has $r_c \leq r_p$.]

• **Conjecture.** *The equality* $r_c = r_p = 1$ *holds. The maximal radius is equal spheres case.* (Requires to show the inequality $r_c \geq 1$.)

Deformation from DOD to FCC/HCP-1

(0) Put unit sphere center at $(0, 0, 0)$.

(1) Put (rescaled) DOD configuration with three spheres at $z = h$, three at $z = -h$, where $h = \frac{\phi^2}{\sqrt{3\phi^2+3}} \approx 0.79569$, forming a non-touching triangle of spheres. Put the remaining 6 spheres near equator, three above it and three below it, in the DOD configuration.

(2) Phase one. Let the three spheres with $z = h$ move radially towards north pole at same speed, till they meet on a plane $z = \alpha$. Same for three spheres $z = -h$, till they meet at plane $z = -\alpha$.

(The FCC and HCP moves are the same for this part.)

Deformation from DOD to FCC/HCP-2

(3) Phase two. The six equatorial balls move radially towards equator, all at same speed. At the same time the balls on $z = \alpha$ rotate clockwise at a (variable) radial speed, aiming to move 60 degrees. The radial speed function is not unique, it must be adjusted to avoid the equatorial spheres. The south pole three balls do exactly the same motion, either moving clockwise for HCP or counterclockwise for FCC.

• Physical model: Buckminster Fuller (1948+) found a jointed framework (“*jitterbug*" configuration) permitting a (rescaled) deformation moving from FCC (cuboctahedron) to DOD (icosahedron) with no unscaled spheres touching till the final moment. In this model the distance between sphere centers remains constant while the radius of central sphere decreases.

Deformation from DOD to FCC/HCP-Locking at Final Point

• The FCC configuration is **jammed** in the sense that one cannot move one sphere, while still touching the central sphere, while the other 11 spheres remain in their current positions. In fact the minimal known deformation to “unlock" the FCC configuration requires 6 balls to move simultaneously with respect to holding the other 6 fixed.

• The HCP configuration is **jammed** in the same sense. The minimal known deformation to “unlock" the HCP configuration requires 9 balls to move simultaneously with respect to holding the other 3 balls fixed.

FCC and HCP are on the boundary of space $X_{12}[1]$

It appears that both FCC and HCP are “pinch points" on the boundary of $X_{12}[1]$. They appear to be accessible from the interior $X_{12}[1]$ with a single normal direction.

- **“Theorem"** (1) Take an ϵ-neighborhood $U_\epsilon(\mathrm{FCC})$ of a (labeled) FCC configuration. Then $U_\epsilon(\mathrm{FCC}) \setminus \{\mathrm{FCC}\}$ is disconnected, with 2 *connected components.*

  (2) Take an ϵ-neighborhood $U_\epsilon(\mathrm{HCP})$ of a (labeled) HCP configuration. Then $U_\epsilon(\mathrm{HCP}) \setminus \{\mathrm{HCP}\}$ is disconnected, with 2 *connected components.*

FCC and HCP are on the boundary of space $X_{12}[1]$

It is plausible that both FCC and HCP are “unavoidable" configurations in $X_{12}(1)$ in the permutability problem.

• **Conjecture.** *To continuously deform a labeled* DOD *configuration to another* DOD *configuration at the same sphere centers in* $X_{12}[1]$*, which is an odd permutation of the* 12 *spheres, at some point in the deformation the configuration is either an* FCC *configuration or an* HCP *configuration.*

• That is, one must traverse through one of the “pinch points" on the boundary of $X_{12}(1)$ to get from one configuration to the other.

Part V. Topology change with varying r: Min-Max Morse theory

• **Problem.** *Determine how the topology of the constrained configuration spaces vary as a function of* r*.*

[These spaces are *super-level sets* of the radius function r.]

• **Problem.** *Determine all the* **critical values** *where the topology changes, and compute the changes.*

• **Approach.** Use a suitable generalization of Morse theory.

• **Eventual Objective.** Carry this program out for small values of N. [Already $N = 12$ is a huge computational problem, out of reach.]

Topology change with r for $N = 12$: Betti number changes

r /k	0	1	2	3	4
$r = 0$	1	54	1266	16884	140889
	5	6	7	8	9
$r = 0$	761166	2655764	5753736	6999840	3628800
r/ k	0	1	2	3	4
$r = r_{max}$	7983360	0	0	0	0
	5	6	7	8	9
$r = r_{max}$	0	0	0	0	0

• Betti numbers for $r = 0$ are those of $\mathrm{Bconf}(\mathbb{S}^2, 12)$. Millions of critical points seem necessary to achieve the large change in Betti numbers occurring as r varies from 0 to r_{max}.

Morse Theory

- Compute topological invariants of manifold using (lower)-level sets of a nice enough real-valued function $f : M \to \mathbb{R}$ (“Morse function")

- A *Morse function* is C^2, finite number of isolated critical points, non-degenerate Hessian at critical points, defines signature at point.

- Change in topology (up to homotopy equivalence) found by attaching cells of dimension related to to the indexes of the critical points.

Extensions of Morse Theory

• Morse theory extended to stratified spaces (Goresky and MacPherson (1988)).

• The injectivity radius function is not a Morse function. It is a minimum of several functions, each of which separately is (almost) a Morse function.

• Its critical manifolds can be higher dimensional. This happens for $N = 5$.

• Morse theory for min functions for hard spheres only recently initiated (Baryshnikov et al, IMRN (2014)).

• Related approach: balanced stress functions.

Balanced Configurations: Stress Graphs

- Start with the contact graph of a configuration.

- Put a set of nonnegative real weights on the edges, called *stresses*

- *Balanced stress condition* requires the tangent vector sum of the stresses along edges at a vertex add up to 0.

- **Theorem.** *If a configuration is* **critical** *for its injectivity radius value then its contact graph must have a set of* **balanced stress weights.**

Balanced Configurations-2

- Balancing conditions are a testable, computable condition.

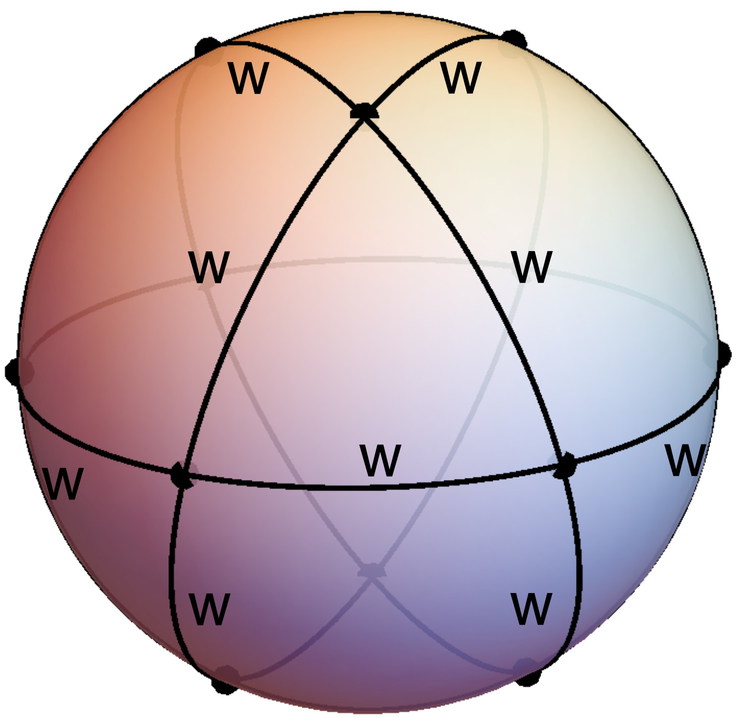
- The problem is one of computational real algebraic geometry.

- **“Theorem".** For $X_N[r]$ constrained configuration space.

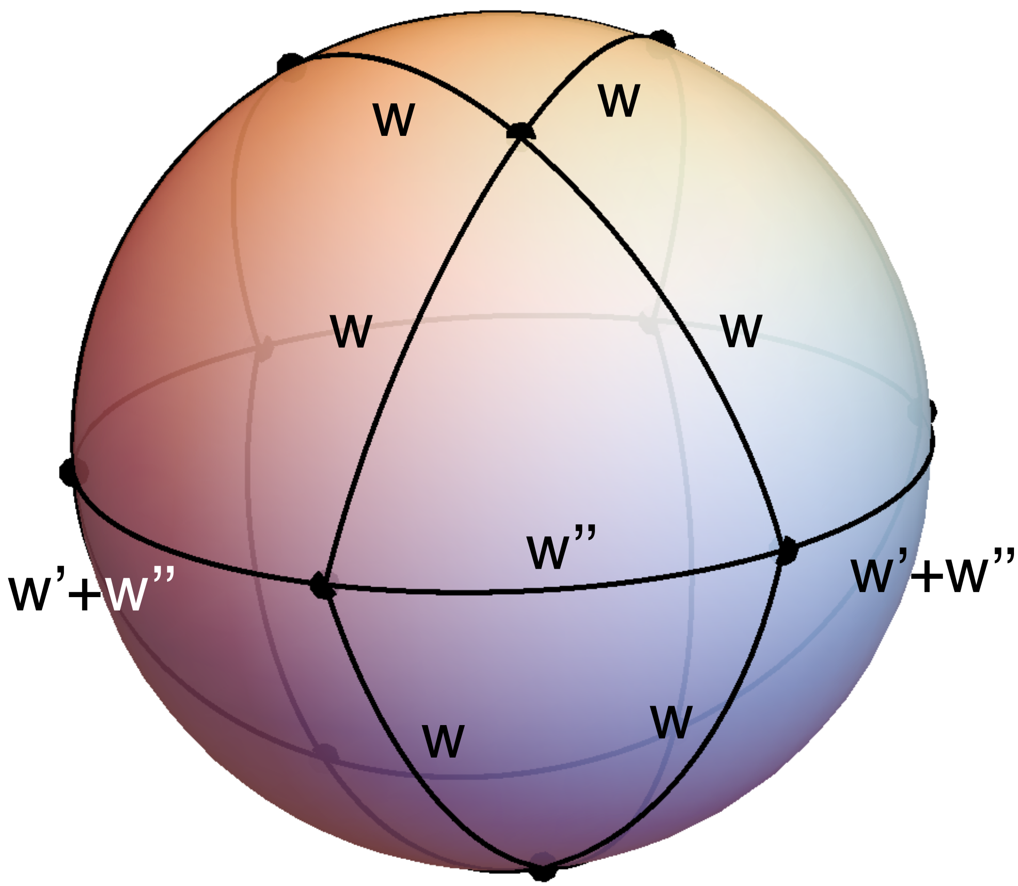
  (1) There are only finitely many radii values r' which have a balanced stress configuration.

  (2) Any such radius values r' are algebraic numbers.

FCC Configuration Balanced Stress Graph



HCP Configuration Balanced Stress Graph



Minimal Balanced Configuration.

• The minimal balanced configuration is a ring of 12 spheres around the equator. It occurs at raidus corresponding to $\theta = \frac{2\pi}{12}$. Set

$$r_0 = \frac{\sin\frac{2\pi}{24}}{1 - \sin\frac{2\pi}{24}} \approx 0.0908.$$

• **Theorem.** *For $r < r_0$ the space $X[r]$ has a strong deformation retract onto the reduced configuration space* $\mathrm{Bconf}(12)$. *In particular its cohomology ring is constant for* $0 < r < r_0$.

Connectedness Conjecture for $X_{12}[r]$-1

For $X_{12}[r] = \mathsf{Bconf}(12)[r]$ we have:

- For $0 < r \leq 1$,

$$H^0(X_{12}[r], \mathbb{Q}) = \mathbb{Q}$$

- For $1 \leq r < r_1^*$,

$$H^0(X_{12}[r], \mathbb{Q}) = \mathbb{Q}^2$$

- For $r_2^* \leq r < r_{max}(12) = \frac{1}{\sqrt{\frac{5+\sqrt{5}}{2}-1}} \approx 1.10851$,

$$H^0(X_{12}[r], \mathbb{Q}) = \mathbb{Q}^{7983360}$$

Connectedness Conjecture for $X_{12}[r]$-2

For $X_{12}[r] = \mathtt{Bconf}(12)[r]$ we have:

- For $r_1^* < r < r_2^*$ complicated things might happen. ("phase transition"?)

- There might be interior maximal of the radius function, giving connected components of $X_{12}(r)$ that do not contain any DOD configuration.

- This leaves open the possiblity of values of r with $r_1^* < r < r_2^*$ having

$$H^0(X_{12}[r], \mathbb{Q}) = \mathbb{Q}^{b_0}$$

with $b_0 > 7983360$.

Conclusions

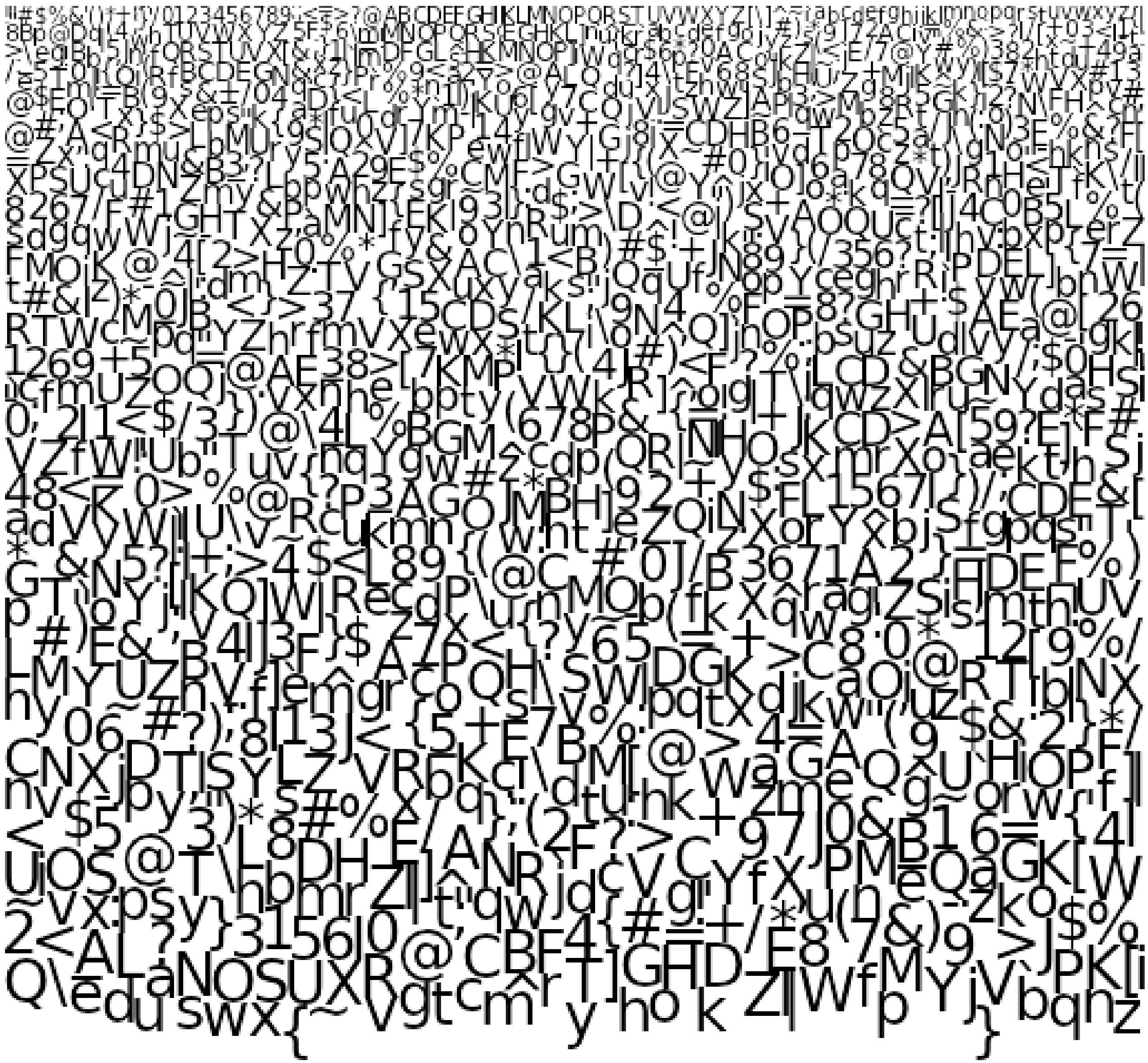
It seems computationally challenging to prove things rigorously in this area for $N = 12$*.*

Future objectives include:

- Carry out research problem for small N up to $N = 12$. (The latter has an (unquantified) enormous number of critical configurations.)
- Determine connections between topological information and properties of materials. (Critical configurations are analogous to jammed configurations in granular materials..)

Conclusion

- There is still some mystery...



Thank you for your attention!