A new local invariant of sphere packings and clean-cut solutions of sphere packing problems

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I. Three kinds of sph. packings (of identical size):

1st kind: Packings into a container: $\mathcal{P} \subset \Gamma$

2nd kind: Finite packings without container: e.g. crystals of mono-atomic elements

3rd kind: Infinite packings with the whole space as the container: e.g. f.c.c, h.c.p. etc.

⊙ Central problems on sph. packings are the optimalities of the global densities of three kinds (properly defined for the 2nd & 3rd kinds)

⊙ Density of the 1st kind and its optimality:

$$\rho(\mathcal{P} \subset \Gamma) = \mathrm{vol}\,\mathcal{P} / \mathrm{vol}\,\Gamma$$

$$\hat{\rho}(r, \Gamma) = \mathrm{l.u.b}\,\{\rho(\mathcal{P} \subset \Gamma); \cdots\}$$

$\hat{\rho}(1, k\Gamma)$: $k\Gamma$: the k-time mag. of Γ

$$\hat{\rho}(\Gamma) := \lim \hat{\rho}(1, k\Gamma) \text{ as } k \to \infty$$

II. A new local invariant of sph. packings and the concept of global densities of the 2nd & 3rd kinds

⊙ Basic geom. structures asso. to a given packing $\mathcal{P}$:

(i) Local cell and neighbors of $S_i \in \mathcal{P}$

$$C(S_i, \mathcal{P}) = \bigcap_{j \neq i} H_{ij} = H_{ij_1} \cap \cdots H_{ij_a}$$

$$\mathcal{L}(S_i, \mathcal{P}) = \{ S_i, S_{j_1}, \cdots S_{j_a} \}, \text{ i.e. } S_i \text{ and its nghbrs}$$

(ii) Local cells decomposition of $\mathcal{P}$: $\{ C_i, i \in I \}$

(iii) The dual D-decomposition of $\mathcal{P}$: $\{ \Omega_j, j \in J \}$

⊙ A new local invariant: locally average density: $\bar{\rho}(S_i, \mathcal{P})$

Set: $w_i = \text{vol}\, C_i$, $w^j = \text{vol}\, \Omega_j$, $w_i^j = \text{vol}\, C_i \cap \Omega_j$

$$\rho(\Omega_j) := \text{vol}\, \Omega_j \cap \mathcal{P} / \text{vol}\, \Omega_j$$

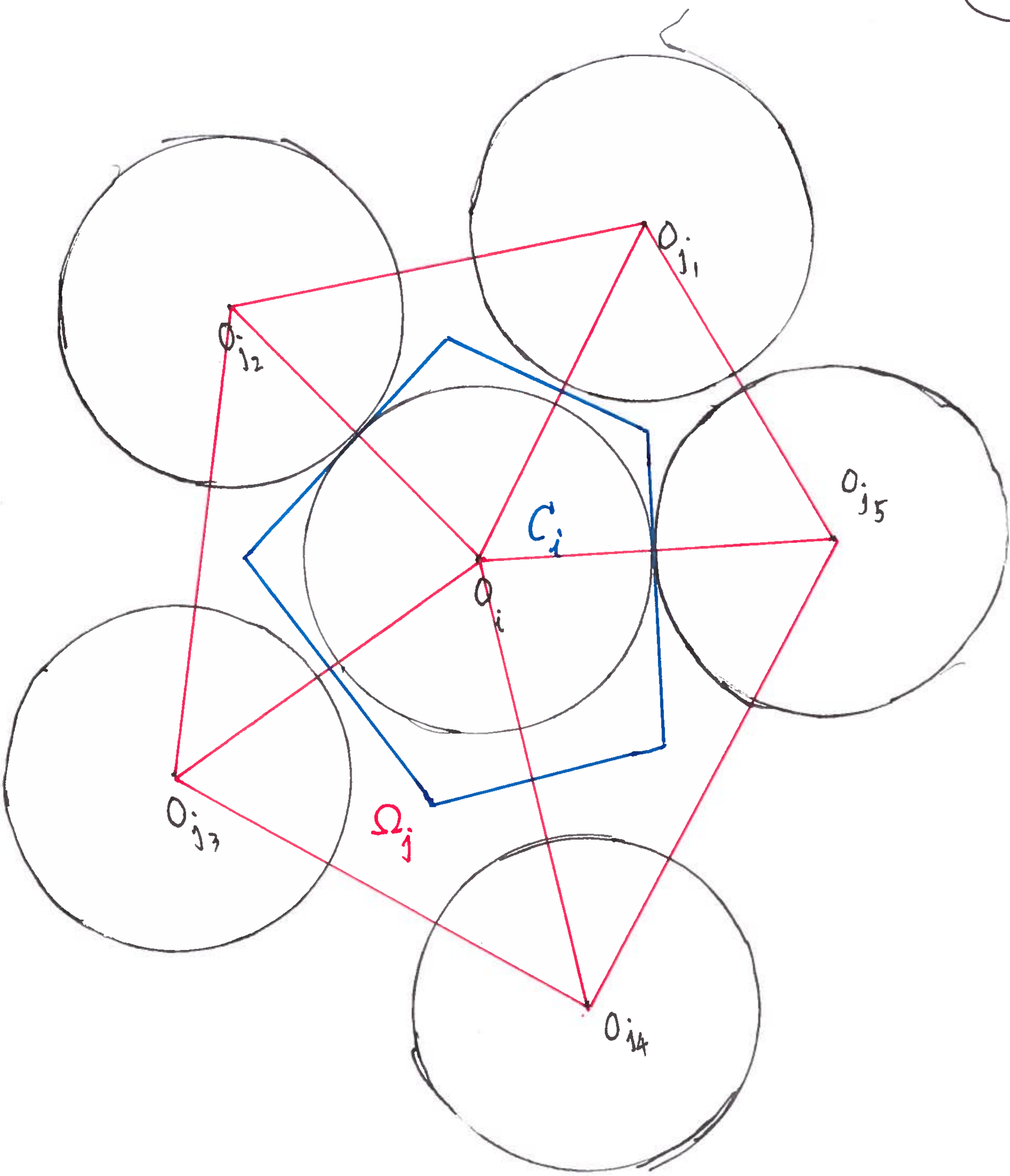
$$\bar{\rho}(S_i, \mathcal{P}) := \sum_{j \in J} w_i^j \cdot \rho(\Omega_j) \Big/ \sum_{j \in J} w_i^j \qquad (*)$$

⊙ Relative density and global densities of the 2nd & 3rd kind:

⊙ $\bar{\rho}(\mathcal{P}', \mathcal{P}) := \sum_{i \in I'} w_i \bar{\rho}(S_i, \mathcal{P}) \Big/ \sum_{i \in I'} w_i$, $\mathcal{P}' = \{ S_i, i \in I' \}$

⊙ $\bar{\rho}(\mathcal{P}') := \text{l.u.b.} \{ \bar{\rho}(\mathcal{P}', \mathcal{P}) \} \ \forall \mathcal{P} \supset \mathcal{P}'$

⊙ $\rho(\mathcal{P}) := \text{l.u.b.} \{ \limsup_{n \to \infty} \bar{\rho}(\mathcal{P}_n, \mathcal{P}) \}$



2-dim analog of C-cells & Ω-cells

Figure 1

III. Fundamental problem and fundamental theorem of sphere packings

⊙ Clusters of spheres: A finite packing of r-sphs is called a cluster if any pair of them can always be linked by a chain with consecutive center distance less than $2\sqrt{2}\,r$. A single sph. is, of course, a special kind of cluster.

⊙ Fundamental problem of sph. packings: Set

$$\rho_N := \text{l.u.b.}\,\{\bar{\rho}(\mathscr{C}),\ \#\mathscr{C} = N\}$$

What is ρ_N equal to? and what are the geom. structures of those N-clusters together with their tightest surroundings with $\bar{\rho}(\mathscr{C}, \mathscr{C}^*) = \rho_N$?

Note that "ρ_1" is just the optimal locally averaged density.

⊙ Fundamental theorem of sphere packings

Theorem I: $\rho_1 = \pi/\sqrt{18}$ and $\bar{\rho}(S_0, \mathscr{L}) = \pi/\sqrt{18}$ when and only when $\mathscr{L}(S_0)$ is isometric to that of the f.c.c. or the h.c.p. packings (i.e. that you see in the crystals of dense type).

IV. Major theorems on global optimalities of sph. packings and their clean-cut proofs via Theorem I

Theorem II. (Kepler's conjecture, 1st version)

$$\rho(\mathscr{P}) \le \pi/\sqrt{18} = \rho(\text{hexa. close packings})$$

Theorem III (Least action principle of crystal formation of dense type)

$$\rho_N = \pi/\sqrt{18} \quad \forall N$$

and $\bar{\rho}(\mathscr{C}, \mathscr{C}^*) = \rho_N$ when and only when it is of <u>piecewise hexagonal close packing type</u>, namely, an assemblage of pieces of <u>subclusters</u> of hexagonal close packings.

Theorem IV (Kepler's conjecture, second version)

$$\hat{\rho}(\Gamma) = \pi/\sqrt{18}$$

for all kinds of containers Γ with piecewise smooth boundary $\partial\Gamma$.

Prop. 1: Theorem I $\Rightarrow$ Theorem II

Pf: Theorem I $\Rightarrow \rho(\mathscr{P}_n, \mathscr{P}) \le \pi/\sqrt{18} \quad \forall n$

$$\Rightarrow \limsup_{n\to\infty} \bar{\rho}(\mathscr{P}_n, \mathscr{P}) \le \pi/\sqrt{18} \Rightarrow \rho(\mathscr{P}) \le \pi/\sqrt{18}$$

Prop. 2: Theorem I $\Rightarrow$ Thm III

Pf: First of all, Theorem I implies that $\rho_N = \pi/\sqrt{18}, \forall N$, and moreover $\bar{\rho}(\mathcal{C}, \mathcal{C}^*) = \pi/\sqrt{18}$ when and only when all the local packings $\{\mathcal{L}(s_i, \mathcal{C}^*), s_i \in \mathcal{C}\}$ are either f.c.c. or the h.c.p. Therefore, it is not difficult to show that the uniqueness part of Theorem III follows from the local rigidity geometry of hexagonal close packings.

Prop. 3: Theorem I $\Rightarrow$ Thm IV

Pf: Let $\mathcal{P}$ be a packing into $k\Gamma$ with very large k. The L-decomp. can be defined for $\mathcal{P} \subset k\Gamma$ just the same, while the D-decomp. needs proper modification as follows:

$$\mathcal{P} = \mathcal{P}^{\circ}\text{(interior sphs)} \cup \partial\mathcal{P}\text{(boundary spheres)}$$

Note that the same kind of D-cells construction still applies up until those D-cells containing some faces solely spanned by centers of ∂P. Set R to be the union of all those D-cells and

$$\Omega_0 = k\Gamma \setminus R, \quad \partial\Omega_0 = \partial R + \partial(k\Gamma).$$

$$\rho(\Omega_0) := \mathrm{vol}\, \mathcal{P} \cap \Omega_0 / \mathrm{vol}\, \Omega_0 \sim \pi/\sqrt{27}$$

V. Basic Geom. ideas and brief overview on the proof of Theorem I

⊙ Type-I & non-Type-I local packings:

Local packings containing twelve touching nghrs will be referred as Type-I local packings, while others will be referred as non-Type-I local packings.

⊙ Type-I spherical configurations: Let $\mathcal{L}(\cdot)$ be a Type-I local packing, $\Sigma(\mathcal{L}) \subset S_0$ be the twelve touching points of those touching nghrs of S_0, $I(\Sigma(\mathcal{L}))$ be the inscribing polyhedron (i.e. convex hull) spanned by $\Sigma(\mathcal{L})$. Set $\mathcal{S}(\Sigma)$ to be subdivision of the unit sphere S_0 corresponding that of the total solid angle at O into those central angles spanned by the faces of $I(\Sigma)$, which will be referred as the associated Type-I spherical configuration of $\mathcal{L}(\cdot)$.

Such sph. config. are characterized by the following properties

(i) $\#(\Sigma) = 12$, (ii) edges lengths of at least $\pi/3$ and (iii) "convexity property": each face of $\mathcal{S}(\Sigma)$ is cocircular and the interior of such a circle containing no points of Σ.

⊙ The proof of Theorem I will be divided in two major cases:

Case I: Type-I local packings

Case II: non-Type-I local packings

< As it turns out, the major portion of the proof lies in Case I, while the remaining portion of Case II will be much, much simpler. >

The proof of Theorem I for Case I (a brief overview)

⊙ Let $\mathcal{S}(\Sigma)$ be a given Type-I config. and $\mathcal{L}_\Sigma$ be the local packing consisting of twelve touching nghrs at Σ. If the circumradii of every face of $\mathcal{S}(\Sigma)$ are at most equal to $\pi/4$, then $\mathcal{L}_\Sigma$ is already a saturated local packing. Otherwise, there exists a tightest extension of $\mathcal{L}_\Sigma$ which achieves the highest $\bar{\rho}(\cdot)$ and such a $\bar{\rho}(\cdot)$ will be defined to be the $\bar{\rho}$ of $\mathcal{S}(\Sigma)$.

Let $\mathcal{M}_I$ be the moduli space of congruence classes of Type-I configurations, which is a 21-dim'al semi algebraic variety and the above $\bar{\rho}(\cdot)$ defines

$$\bar{\rho}(\cdot): \mathcal{M}_I \longrightarrow \mathbb{R}^+$$

Thus, the proof of Theorem I for Case I amounts to prove that the above function $\bar{\rho}(\cdot)$ has <u>unique two maximal points</u> at the <u>f.c.c.</u> and the <u>h.c.p.</u> with $\bar{\rho}(\cdot)$ equals to $\pi/\sqrt{18}$.

⊙ For example, in the generic case that $\mathcal{L}_\Sigma$ is already saturated, i.e. $r(\sigma_j) \le \pi/4 \ \forall \sigma_j \in \mathcal{S}(\Sigma)$, the set of D-cells Ω_j with $w_0^j > 0$ consists of the following bouquet of <u>2-isosceles tetrahedra</u>, namely

$$\{ \tau(\sigma_j, 2),\ \sigma_j \in \mathcal{S}'(\Sigma) \}$$

whose densities and weights are given by the following neat formula:

$$\rho(\sigma_j) = \frac{1}{4D(\sigma_j)} \left(\pi + 2|\sigma_j| - 2(d_1 + d_2 + d_3) \right)$$

$$w(\sigma_j) = \frac{1}{6} \sin|\sigma_j| \cdot \left\{ \frac{8}{u(\sigma_j)} - \tan^2 r(\sigma_j) \right\}$$

while the function $\bar{\rho}(\mathcal{S}'(\Sigma))$ is given by their weighted average, namely

$$(*) \qquad \bar{\rho}(\mathcal{S}'(\Sigma)) = \sum_{\sigma_j \in \mathcal{S}'(\Sigma)} w(\sigma_j)\rho(\sigma_j) \Big/ \sum_{\sigma_j \in \mathcal{S}'(\Sigma)} w(\sigma_j)$$

Thus, the remaining task of providing clean-cut solutions to the classical sph. packing problems would be: How to provide a nice proof of such an upper bound estimate of RHS of (✱) together with the strong uniqueness of optimality, namely, in an as simple and as clean-cut as possible way, thus making it easier to understand the geometric insight and also better in paying proper tribute to this wonderful problem of Nature.

<u>Some basic geom ideas and fundamental techniques of areawise estimation of geom. invariants</u>

(1) Conceptually, $\bar{P}(\cdot)$ provides a wonderful local invariant of sph. packings which, as indicated in the above brief discussion, enables us to achieve a clean-cut <u>localization</u> of <u>global optimalities</u> of <u>the three kinds of sph. packings</u>; In particular, for the most important one of the 2nd kind, that the <u>global optimality</u> is actually the <u>consequence</u> of <u>local optimality everywhere</u>!! Note that, the spherical geom. is exactly

the localized geometric invariant theory of the physical space (often referred as the Euclidean 3-space), while the explicit formula of (*) should be regarded as the basic geometric invariant theory on the key local invariant $\bar{P}(\cdot)$

(2) One of the most fundamental theorem in local solid geometry is that the total solid angle at every point is equal to 4π (Archimedes Theorem), while the associated spherical config. $\mathcal{S}(\Sigma)$ is, geometrically, the proper subdivision of the total solid angle at the center of S_0 associated to the local packing $\mathcal{L}_{\Sigma_j}$ and moreover, the formula (*) expresses the contribution of each sub-solid-angle (i.e. $\sigma_j \in \mathcal{S}(\Sigma)$) toward $\bar{P}(\mathcal{S}'(\Sigma))$. Therefore, it is quite natural to find a way of suitable areawise estimates to achieve such a proof.

(3) Area preserving deformations and techniques of areawise estimation of geometric invariant:

In the setting of local solid geometry, area is the most important, basic invariant of spherical geometry and techniques of areawise estimates of various geom. invariants such as $\rho(\cdot)$, $w(\cdot)$ etc. are often the most useful ones in the study of solid geometry.

(i) A triple of area formula of sph. Δ's

(A) A.A.A-type: $|\sigma| = A+B+C-\pi$ (localization of Archimedes Theorem)

(B) S.S.S-type: $\tan\frac{1}{2}|\sigma| = \frac{D}{u}$, $u = 1+\cos a+\cos b+\cos c$

(sph. version of Heron formula)

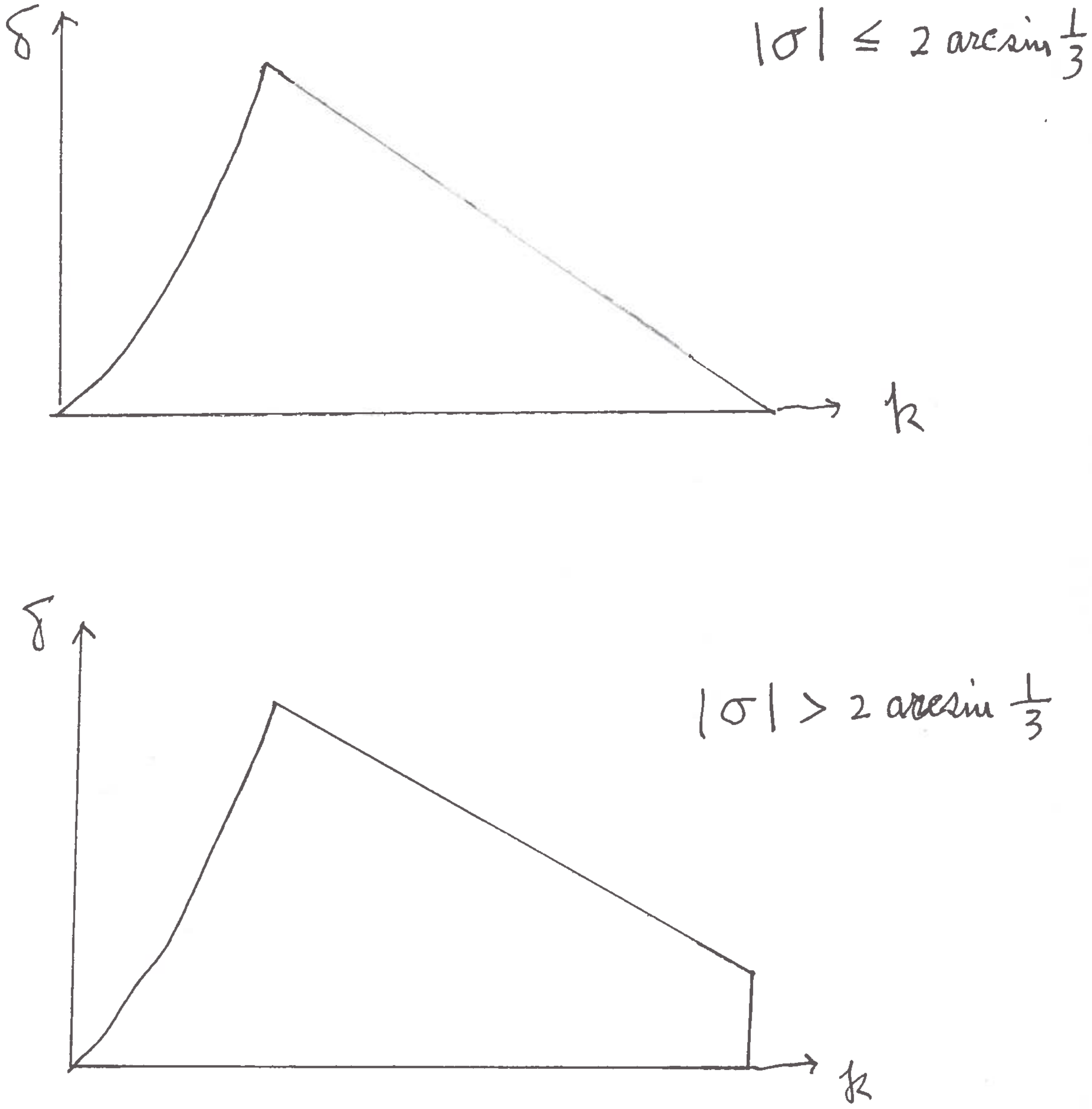
(C) S.A.S. Type: $\tan\frac{1}{2}|\sigma| = \dfrac{\sin C}{\cot\frac{a}{2}\cot\frac{b}{2}+\cos C}$

(sph. version of $|\Delta| = \frac{1}{2}a\cdot b\sin C$)

(ii) A triple of simple, basic area preserving deformations and the (h,δ)-parametrization of the $|\sigma|$-level surface in the moduli sphere of sph. Δ's:

(A) The well-known Lexell's Theorem and Lexell's deformation that fixes a base edge, say c, and $|\sigma|$

(B) The dual of Lexell's deformation that fixes $|\sigma|$ and an angle, say C. (As a corollary of the S.A.S. area formula.)



γ
$|\sigma| \leq 2 \arcsin \frac{1}{3}$
k
γ
$|\sigma| > 2 \arcsin \frac{1}{3}$
k

Figure 2

(C) Set C to be the largest angle and assuming σ containing its own circumcenter, $a \leq b$. Then

$$k = \cot\frac{a}{2}\cot\frac{b}{2} \text{ and } \delta = \cot\frac{a}{2} - \cot\frac{b}{2} \geq 0$$

Consists an advantageous "coordinate - parameters" for the $|\sigma|$-level surface, while fixing δ but varying k also provides a simple area-preserving deformations

(iii) (k, δ) - analysis of triangular geometric invariant restricted to a given $|\sigma|$-level surface

The restriction of a given triangular geometric invariant such as $\rho(\sigma)$, $w(\sigma)$ etc to a $|\sigma|$-level surface can be expressed as a function of the (k, δ)-parameter, which often exhibit remarkabley simple properties such as monotonicity, thus providing a set of powerful tools for study areawise estimates not only for a single triangle, but also for the collective estimate of specific kind of weighted average over clusters of triangles such star clusters or pair of triangles of a buckled quadrilaterals

(4) Some pertinent geometric insight on the geometry of Type - I configurations

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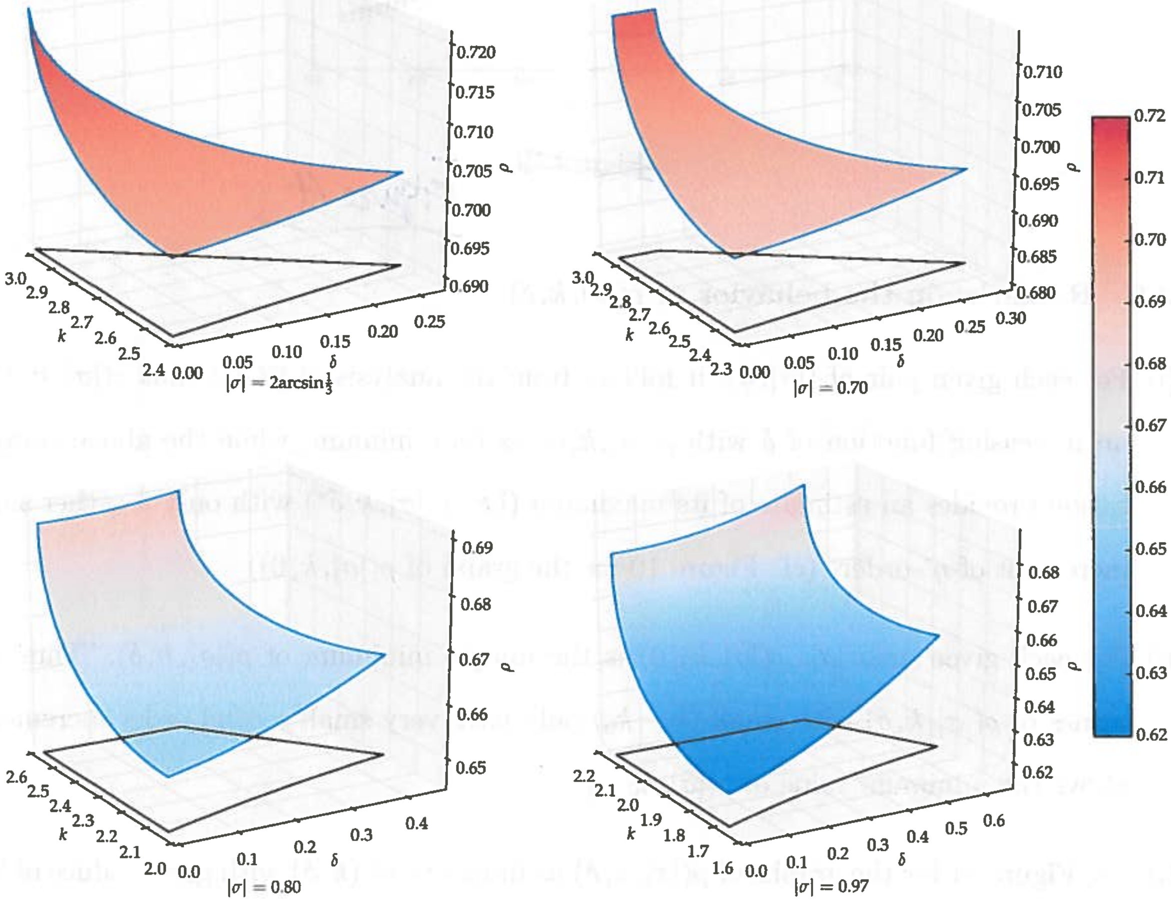


~~Figure 11~~ Figure 3

p. 11 2/3 the otherside

(4) 6$\square$-Type-I and 6⧄-Type I configurations

⊙ The f.c.c. and the h.c.p. are the only two Type-I configs containing sextuple of $\square$'s

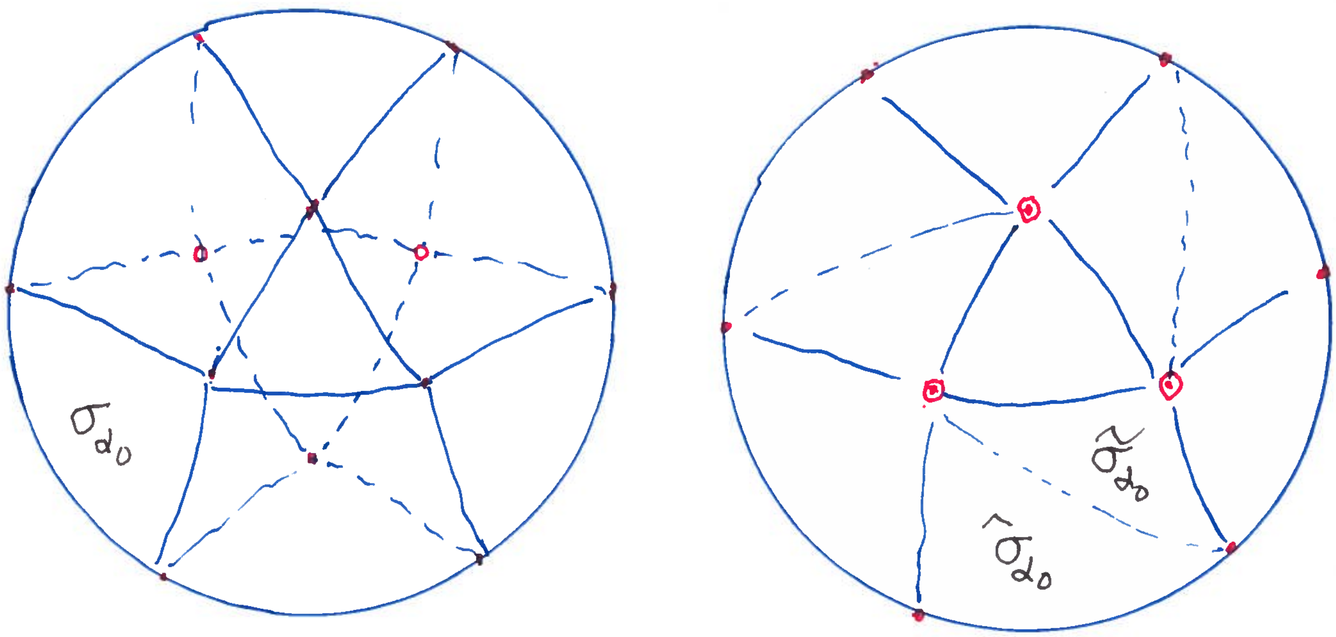
⊙ The h.c.p. is an isolated point in $\mathcal{M}_I$, while the f.c.c is a cusp singularity with tangent cone of dim. 1, thus having a rather extensive neighborhood consisting of 6⧄-Type-I, i.e. having sextuple of buckled quadrilaterals

⊙ All the twelve stars of the f.c.c. are $\{\triangle, \square, \triangle, \square\}$, while the h.c.p. has sextuple of $\{\triangle, \square, \triangle, \square\}$ and another sextuple of $\{\triangle, \triangle, \square, \square\}$.

⊙ Both the f.c.c. and the h.c.p. has triangulations of icosahedron type (i.e all its stars are of 5$\triangle$-type), in which, the f.c.c. has twelve stars of $\{\triangle$, ⧄, $\triangle, \nabla\}$ while the h.c.p. has sextuple of them and another sextuple of $\{\triangle, \triangle$, ⧄, $\nabla\}$. Anyhow, all of them have total area of π and averaged ~~dens~~ density of $\pi/\sqrt{18}$

⊙ <u>Lemma 1</u>: A Type-I ~~config.~~ icosahedron containing a star of $\{\triangle$, ⧄ $\triangle, \nabla\}$ must be just such a triangulation of the f.c.c. or the h.c.p

(i) 6 $\square$ - Type - I's and 6 $\boxtimes$ - Type - I's :



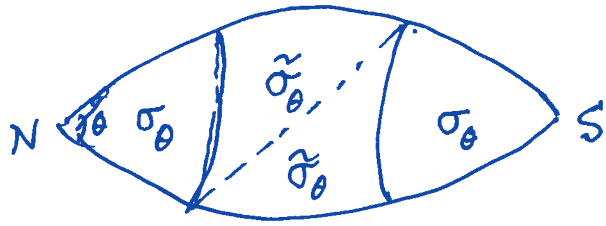
$$\{8\,\sigma_{\alpha_0} + 12\,\tilde{\sigma}_{\alpha_0}\}$$

$$8\,\Delta_{\pi/3} + 6\,\square_{\pi/3} = 4\pi$$

Figure 3

(ii) 5□-Type-I and 5☒-Type-I configurations

Lune-clusters: $L(\theta)$, $\alpha_0 \leq \theta \leq \gamma$, $\alpha_0 = \arccos\frac{1}{3}$, $\gamma = 2\pi - 4\alpha$



σ_θ: $\pi/3$-isosceles of top angle θ

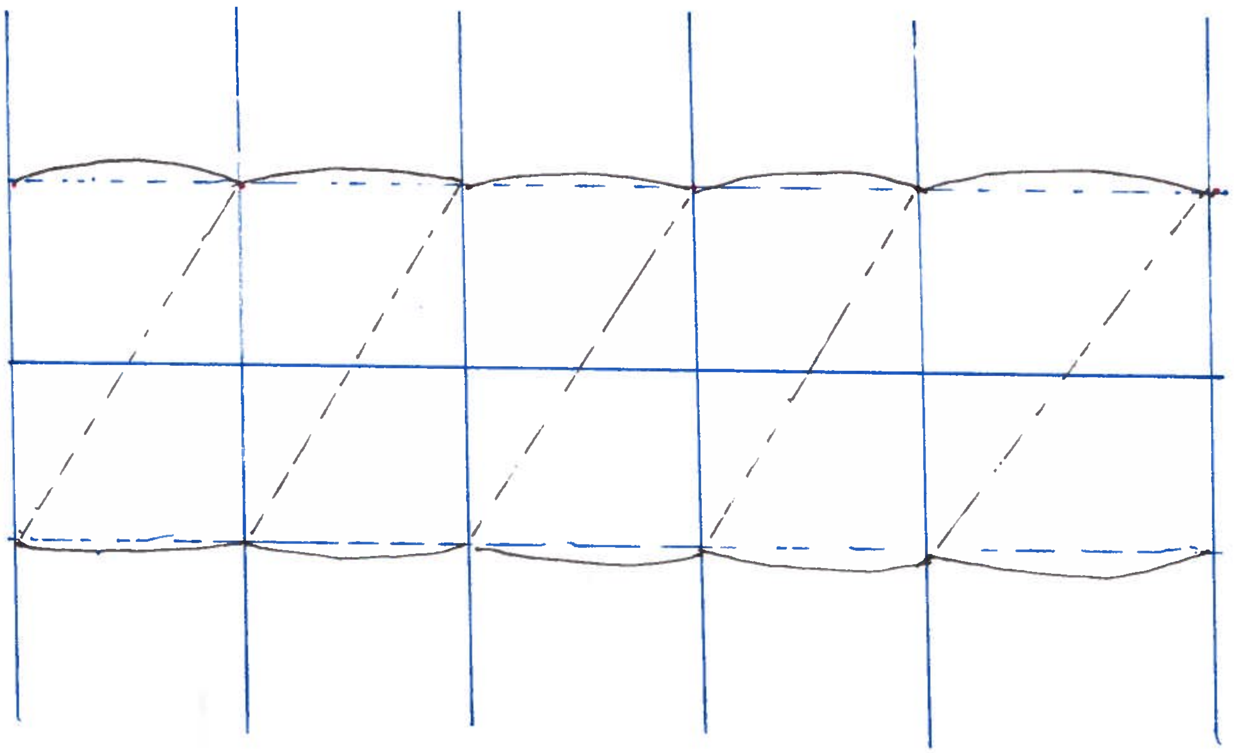
To a given angular distribution $\{\theta_i \geq \alpha_0, \sum\theta_i = 2\pi\}$ there is a 5□-Type-I consists of the assemblage of quintuple of Lune-clusters $\{L_{\theta_i}\}$

⊙ Such a 5□-Type-I has a pair of small stars with uniform $\pi/3$-radial edges together with ten stars of the kind of {△, △, □, □}.

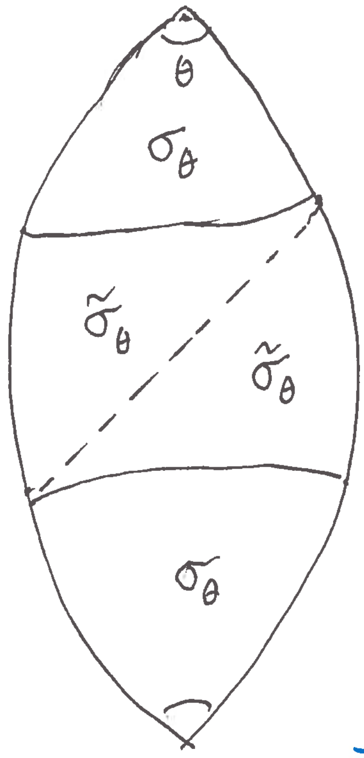
⊙ Every 5□-Type-I has both icosahedron as well as non-icosahedron triangulations, while the former has ten 5△-star of the kind of {△, △, ☒, ◸}.

⊙ The totality of 5□-Type-I's constitutes a singular subvariety of dim. 4 which has an extensive neighborhood consisting 5□-Type-I's

5 □-Type-I's and 5 ⊠-Type-I's



$L(\theta)$



$$\underbrace{\arccos\frac{1}{3}}_{=\alpha_0} \leq \theta < (2\pi - 4\alpha_0)$$

Figure 4

Lemma 2: Let $S'(\Sigma)$ be a non-icosahedron Type-I. Then it is either just such a trigngulation of the f.c.c. or the h.c.p, or $S'(\Sigma)$ is a $5\boxtimes$-Type-I.

Lemma 3: Let $S'(\Sigma)$ be a Type-I icosahedron. If it contain a star of the kind of $\{\Delta, \Delta, \boxdot, \triangleright\}$ or a small deformation of that, then $S'(\Sigma)$ must be a $5\boxtimes$-Type-I

(iii) Simple proofs of Theorem I for $6\boxtimes$-Type-I's ~~and~~ (resp. $5\boxtimes$-Type-I's) via areawise estimates of $\boxtimes$-clusters (resp. lune-clusters)

It is very simple to provide the following areawise estimates for $\boxtimes$-clusters (resp. lune-clusters), namely

$$\odot \begin{cases} \tilde{\rho}(\boxtimes) \leq \tilde{\rho}(\square) \text{ with } |\square| = |\boxtimes| \text{ if } |\boxtimes| \geq \square_{\pi/3} \\ \tilde{\rho}(\boxtimes) < \tilde{\rho}(\square_{\pi/3}) \text{ if } |\boxtimes| < \square_{\pi/3} \end{cases}$$

$$\odot \begin{cases} \tilde{\rho}(\tilde{L}) \leq \tilde{\rho}(L_\theta) \text{ with } |L_\theta| = |\tilde{L}| \text{ if } |\tilde{L}| \geq L_{\alpha_0} \\ \tilde{\rho}(\tilde{L}) \leq \tilde{\rho}(L_{\alpha_0}) \text{ if } |\tilde{L}| < L_{\alpha_0} \end{cases}$$

and moreover, the proof for $6\boxtimes$-Type-I's (resp. $5\boxtimes$-Type-I's follows directly from the above estimate

(5) Areawise estimates of star clusters and the proof of Theorem I for Type-I icosahedra

Let $\mathcal{S}'(\Sigma)$ be a Type-I icosahedron, i.e. all $St(A_i)$ are of 5Δ-type. Then $\bar{\rho}(\cdot)$ can also be expressed as the weighted averge of the twelve intermediate average densities of star clusters, namely

$$\tilde{\rho}(St(A_i)) = \sum_{\sigma_j \in St(A_i)} w(\sigma_j)\,\rho(\sigma_j) \Big/ \sum_{\sigma_j \in St(A_i)} w(\sigma_j)$$

while

$$\bar{\rho}(\cdot) = \sum_{A_i \in \Sigma} \tilde{w}(St(A_i))\,\tilde{\rho}(St(A_i)) \Big/ \sum_{A_i \in \Sigma} \tilde{w}(St(A_i))$$

Therefore, areawise upper bound estimates of $\tilde{\rho}(\cdot)$ may provide an advantageous route to prove Theorem I for such a case. Anyhow, this naturally leads to the discovery of the following pair of key lemmas.

⊙ Let us begin with the following families of Examples

Example 1 As indicated in Fig. 5

$$St_1(\theta) = \{2\sigma_{\alpha_0},\, 2\sigma_\theta,\, \sigma_{\tilde{\theta}}\}$$

$$\cancel{\alpha_0 = \arccos\tfrac{1}{3},\ \alpha_0 \le \theta \le \arccos(-\tfrac{1}{3}),\ \tilde{\theta} = \pi - \alpha_0}$$

Extremal stars for $|St(\cdot)| \leq \pi$

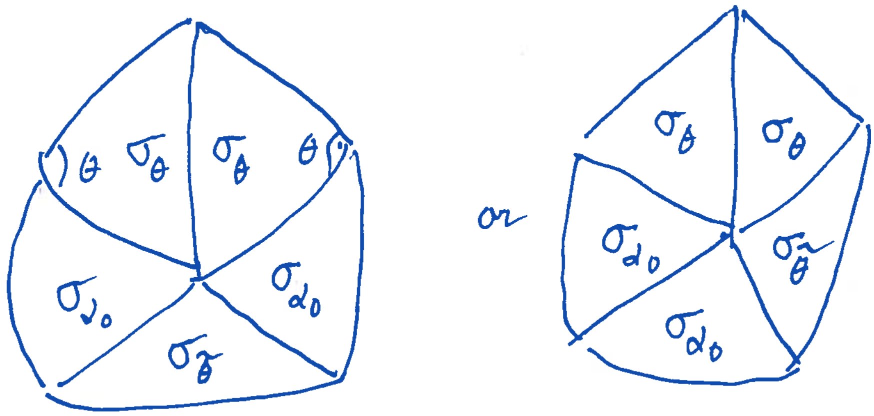
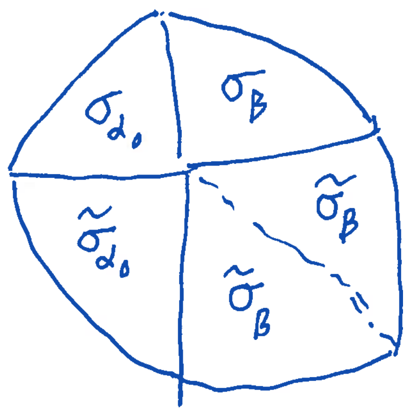


Figure 5

Extremal stars for $\pi \leq |St(\cdot)| < \pi + 0.21672$



$\alpha_0 \leq \beta \leq \gamma = 2\pi - 4\alpha_0$

Figure 6

Lemma 4: For $|St(\cdot)| < \pi$, the extremal stars (i.e. the ones achieving the highest $\hat{\rho}(\cdot)$ with given area) are as indicated in Figure 5.
For $|St(\cdot)| \in [\pi, \pi + 0.21672)$, the extremal stars are as indicated in Figure 6

Lemma 4' For $|St(\cdot)| \in [\pi + 0.21672, \pi + 0.62]$ the extremal stars or stars with almost optimal areawise density only occur in spherical config's with a pair of opposite small stars.

The proof of Theorem I for the case of Type-I icosahedra follows easily from Lemmas 4 and 4'.