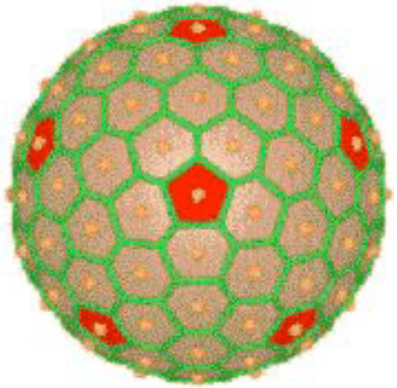

DISCRETE MINIMAL ENERGY PROBLEMS

Lecture II

E. B. Saff
Center for Constructive Approximation
Vanderbilt University

University of Crete, Heraklion May, 2017

Recall Notation

$\omega_N = \{x_1, \ldots, x_N\} \subset A$, A compact, infinite

$K : A \times A \to \mathbb{R} \cup \{+\infty\}$, symmetric and l.s.c.

$$E_K(\omega_N) = \sum_{i \neq j} K(x_i, x_j)$$

$$\mathcal{E}_K(A, N) = \min\{E_K(\omega_N) : \ \omega_N \subset A, \quad \#\omega_N = N\}$$

$$W_K(A) := \min_{\mu \in \mathcal{M}(A)} I_K[A] = \min_{\mu \in \mathcal{M}(A)} \iint_{A \times A} K(x, y)\, d\mu(x) d\mu(y)$$

μ_A equilibrium measure, $I_K[\mu_A] = W_K(A)$

$\nu(\omega_N) = \frac{1}{N} \sum_{x \in \omega_N} \delta_x$, normalized counting measure

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Fundamental Thm: $\lim_{N \to \infty} \mathcal{E}_K(A, N)/N^2 = W_K(A)$. Every weak* limit measure of the sequence $\{\nu(\omega_N^*)\}_{N=2}^{\infty}$ for N-point K-energy minimizing configurations ω_N^* is an equilibrium measure for the continuous problem on A.

Riesz s-Energy in Euclidean Space

Hereafter $A \subset \mathbb{R}^p$ and $|| \cdot || = |x - y|$, Euclidean distance.

The **Riesz s-kernel** is defined by

$$K_s(x, y) := \frac{1}{|x - y|^s}, \ \ s > 0; \qquad K_{\log}(x, y) := \log \frac{1}{|x - y|}, \ \ x, y \in A.$$

We write

$$E_s(\omega) := E_{K_s}(\omega), \ \ \mathcal{E}_s(A, N) = \mathcal{E}_{K_s}(A, N), \ \ s > 0 \text{ or } s = \log .$$

For $p = 3$, $s = 1$, get Coulomb kernel.

For $A \subset \mathbb{R}^p$ and $s = p - 2$, we get Newton kernel.

Some Basic Properties of Riesz Energy

- $A \subset B \;\Rightarrow\; \mathcal{E}_s(A,N) \geq \mathcal{E}_s(B,N)$
- $\mathcal{E}_s(A+x,N) = \mathcal{E}_s(A,N)$
- $\mathcal{E}_s(\alpha A,N) = |\alpha|^{-s}\mathcal{E}_s(A,N)$
- $\mathcal{E}_s(A,N)$ is continuous in s for $s>0$
- $$\lim_{s\to 0^+} \frac{\mathcal{E}_s(A,N) - N(N-1)}{s} = \mathcal{E}_{\log}(A,N)$$

  and for fixed N, every cluster point of minimal s-energy N-point configurations $\omega_N^{(s)}$ as $s \to 0^+$ is an N-point minimal log energy configuration.

Best-Packing and Riesz Energy ($s \to \infty$)

Recall: Separation distance of $\omega_N = \{x_1, \ldots, x_N\} \subset A$

$$\delta(\omega_N) := \min_{1 \le i \ne j \le N} |x_i - x_j|.$$

N-point best-packing distance on A,

$$\delta_N(A) := \sup\{\delta(\omega_N) : \omega_N \subset A,\ \#\omega_N = N\},$$

ω_N^* *is best-packing configuration* if $\delta(\omega_N^*) = \delta_N(A)$.

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Proposition (Prove it)

For each fixed $N \ge 2$,

$$\lim_{s \to \infty} \mathcal{E}_s(A, N)^{1/s} = \frac{1}{\delta_N(A)}.$$

Moreover, every cluster configuration as $s \to \infty$ of s-energy minimizing N-point configurations on A is an N-point best-packing configuration on A.

Amusing Exercise

Let $A = S^1$, the unit circle in the plane $\mathbb{R}^2$.

Prove that for each s, $0 < s < \infty$ or $s = \log$ the N-th roots of unity (or any rotation of them) are minimal s-energy points for S^1. Moreover, they are the only sets of minimal energy points.

More generally: Prove this is true if $K(x, y) = f(|x - y|)$, where f is strictly convex and decreasing on $(0, 2]$.

$S^2 = \{x \in \mathbb{R}^3 \ : \ |x| = 1\}$

What about minimal Riesz energy points on S^2 for

$N = 2$?

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What about minimal Riesz energy points on S^2 for

$N = 2$?

$N = 3$?

$N = 4$?

Optimality of Tetrahedron for $S^2 = \{x \in \mathbb{R}^3 \ : \ |x| = 1\}$

More generally, for the d-dimensional sphere $S^d \subset \mathbb{R}^{d+1}$

Theorem

If $K(x, y) = f(|x - y|^2)$, with f strictly convex and decreasing, then for $2 \leq N \leq d + 2$, the only optimal N-point K-energy configurations on S^d are the vertices of a regular $(N - 1)$-simplex inscribed in S^d centered at 0.

Minimal Riesz s-Energy for $N = 5$ on $\mathbb{S}^2$

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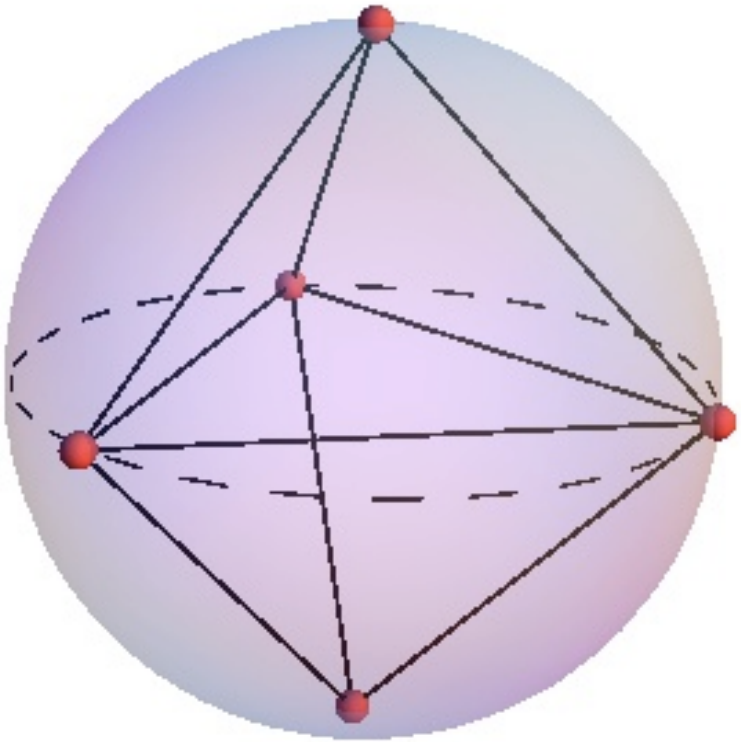
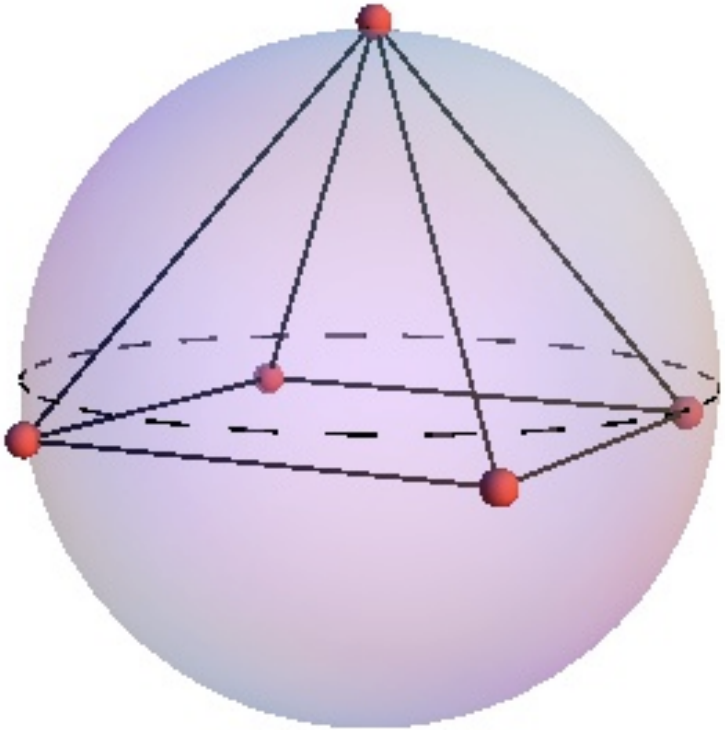
bipyramid

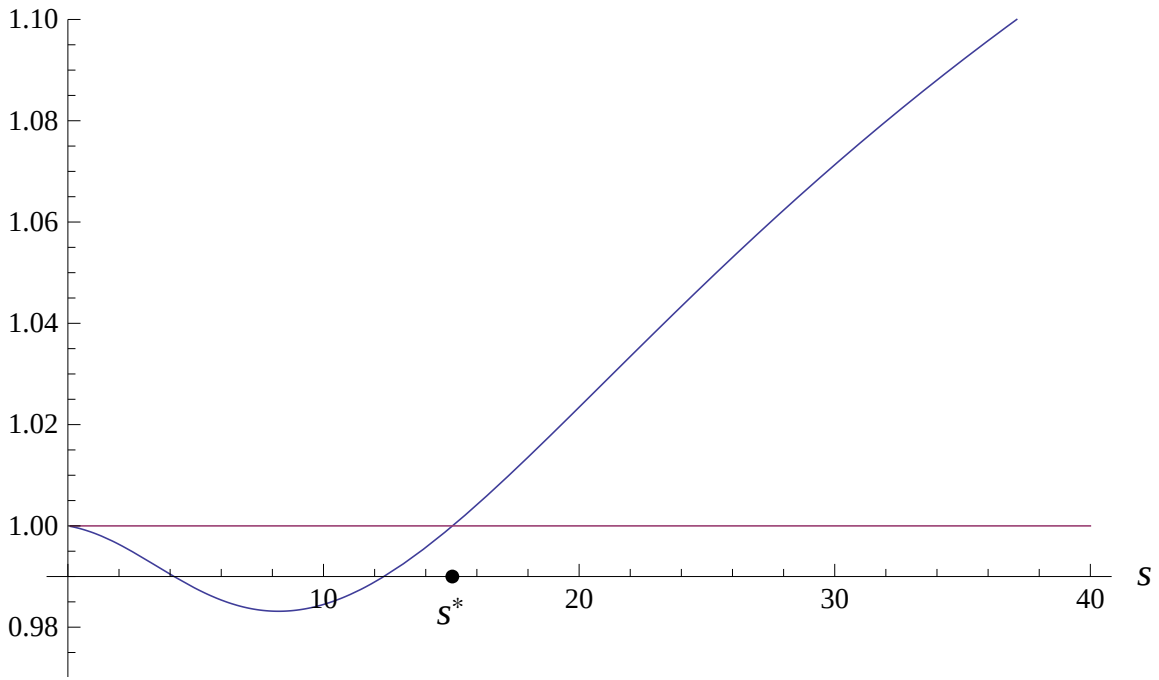


square-base pyramid



Minimal Riesz s-Energy for $N = 5$ on $\mathbb{S}^2$

Ratio of s-energy of **bipyramid** to s-energy of **optimal sq-base pyramid**



Melnyk et al (1977) Bipyramid appears optimal for $0 < s < s^*$ where $s^* \approx 15.04808$.

Recently proved by R. Schwartz (over 150 pages + computer assist).
Open problem for $s > s^* + \epsilon$

MORALS

Optimal Riesz s-energy configurations, in general,

depend on s.

Rigorous proofs of computational observations

can be quite difficult.

What do minimal energy points
“look like" for large N ?

What about **asymptotics** of
of the minimal energy as $N \to \infty$?

LET'S TALK FOOTBALL (SOCCER)

The Soccer Ball

Vital Statistics

32 faces $=$ 20 hexagons $+$ 12 pentagons

90 edges

60 vertices

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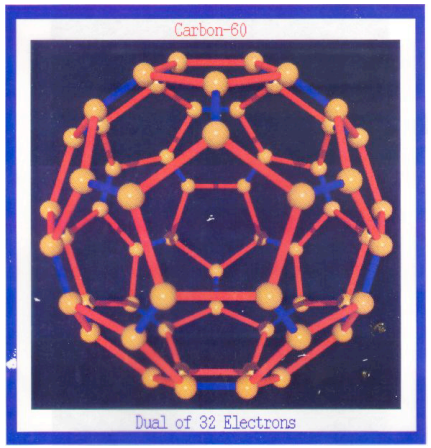

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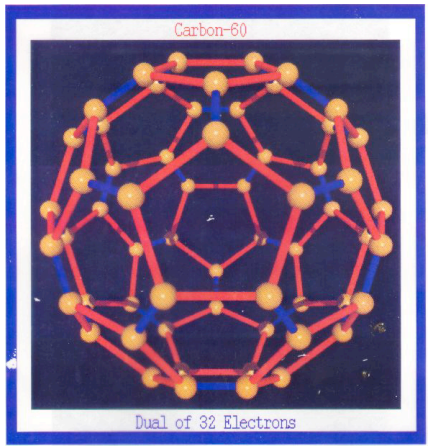
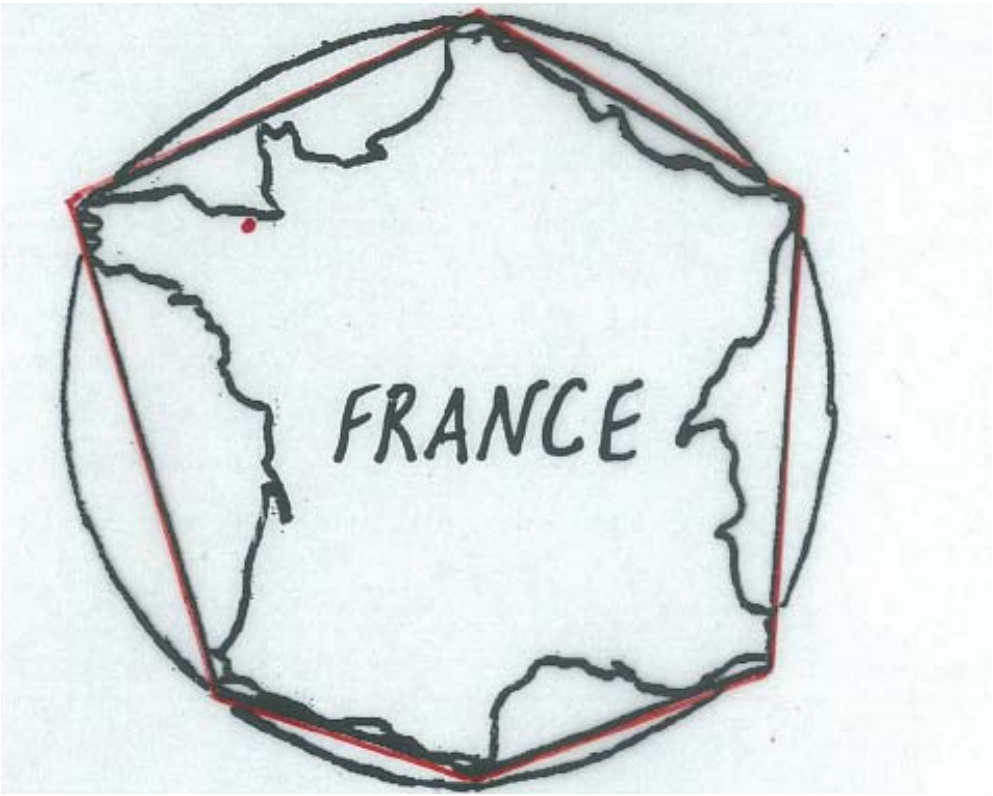


Question (important for France)

Is it possible to cover (tile) a soccer ball (sphere) with only hexagons ?

France=Le Hexagon



The Soccer Ball

Euler's Formula for Convex Polyhedra

F = number of faces
V = number of vertices
E = number of edges
Then

$$F + V - E = 2.$$

Examples
Cube: 6+8-12=2
Soccer ball: 32+60-90=2

Tiling with 5,6, and 7-gons

Assume exactly 3 edges from each vertex.
F_5 = number of pentagons
F_6 = number of hexagons
F_7 = number of heptagons
Then

$$3V = 2E$$

$$5F_5 + 6F_6 + 7F_7 = 2E$$

So

$$E = \frac{1}{2}(5F_5 + 6F_6 + 7F_7), \; V = \frac{1}{3}(5F_5 + 6F_6 + 7F_7)$$

Now let's apply Euler Formula:

Tiling with 5,6, and 7-gons

$$F + V - E = 2$$

$$(F_5 + F_6 + F_7) + \frac{1}{3}(5F_5 + 6F_6 + 7F_7) - \frac{1}{2}(5F_5 + 6F_6 + 7F_7) = 2$$

$$\frac{1}{6}F_5 + 0F_6 - \frac{1}{6}F_7 = 2$$

$$F_5 = F_7 + 12$$

Corollary

If tiling has only hexagons and pentagons, there must be exactly 12 pentagons.
You can't tile with hexagons alone!

Why is the regular hexagon so important ?

For the plane, the hexagon (more precisely, the equilateral triangular lattice) solves the best-packing problem and the best covering problem.

Best-Packing Problem in 2 Dimensions

Arrange nonoverlapping disks all of the same radius in the plane so as to cover the maximal percentage of area.

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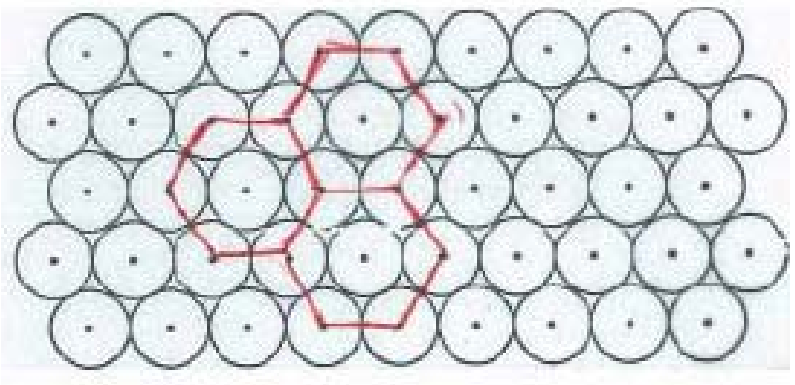
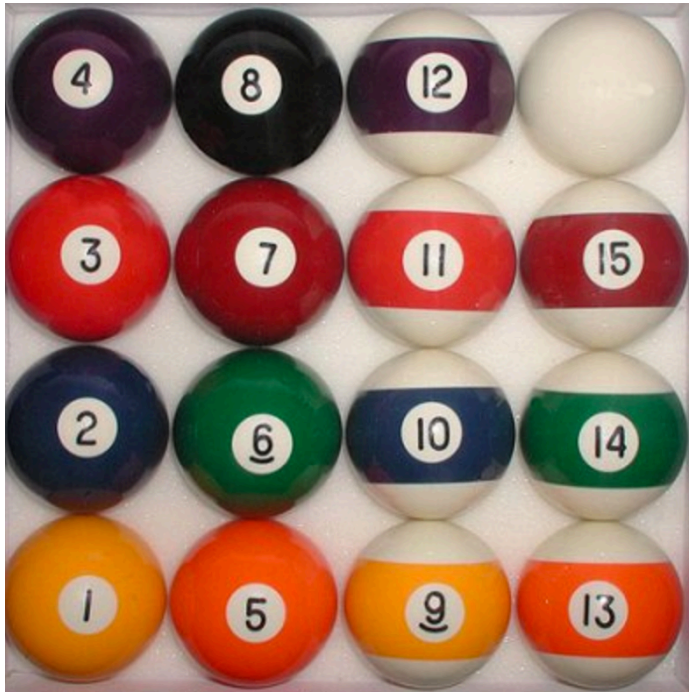
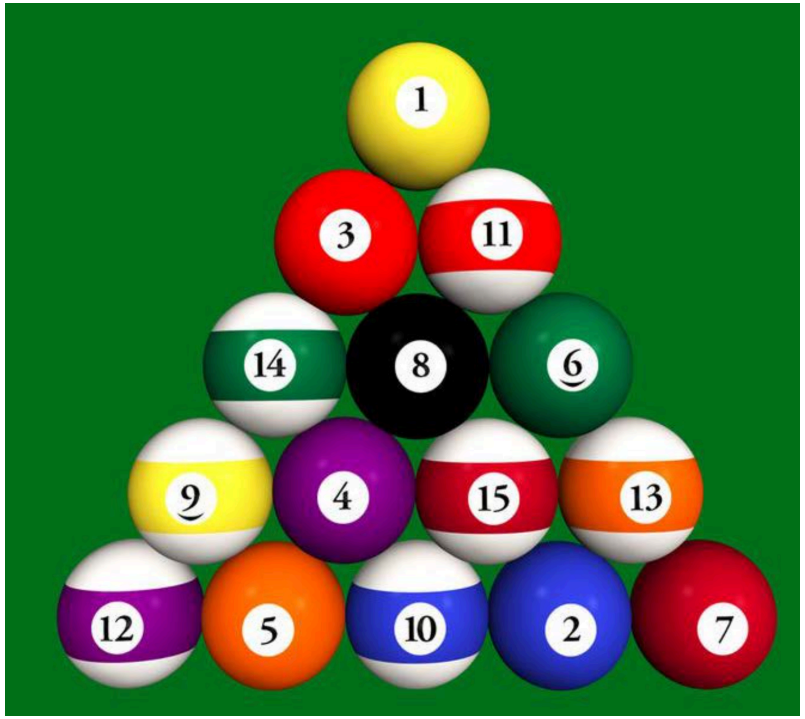


Packing disks in 2 dimensions





proportion of area covered: $\frac{\pi}{4} = .785...$ $\qquad$ $\frac{2}{\sqrt{3}}\frac{\pi}{4} = \frac{\pi}{\sqrt{12}} = .906...$

balls (r=1) per unit area: $\frac{1}{4} = .25$ $\qquad$ $\frac{1}{2\sqrt{3}} = .288...$

Solved by Fejes Toth and also by ...

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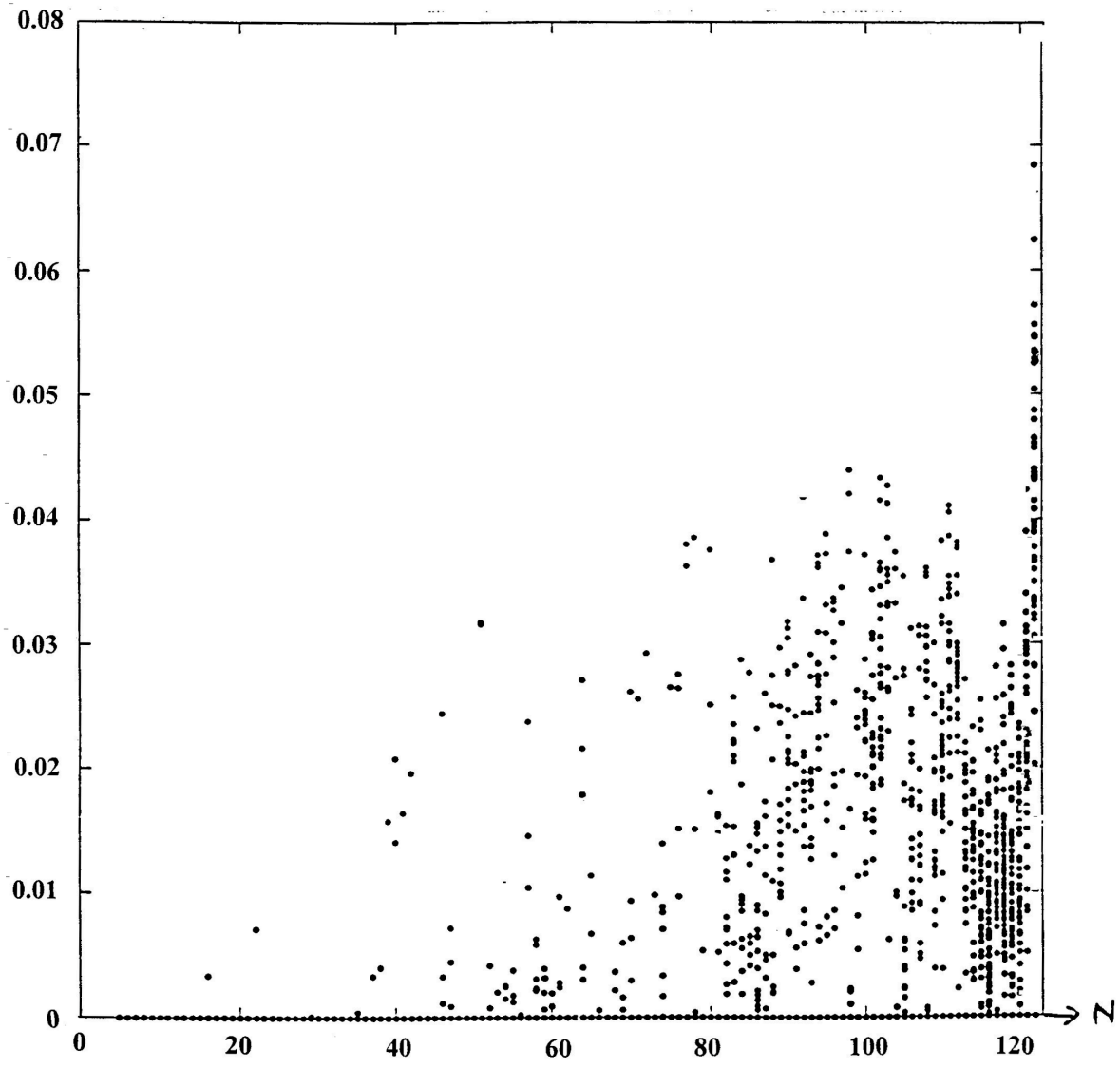
What do minimum energy points for the sphere S^2 look like ?

Massive high precision experiments were conducted to determine $\mathcal{E}_s(S^2, N)$ for $s = \log$, $s = 1$ and $N = 2, 3, \ldots, 200$.

Bad News: There are many local minima of energy that are not global minima. Moreover, the local minima have energies very close to $\mathcal{E}_s(S^2, N)$.

Good News: Equilibrium points try to distribute themselves over a nearly spherical hexagonal net.

(Local – Global) Energies $4 \leq N \leq 122$



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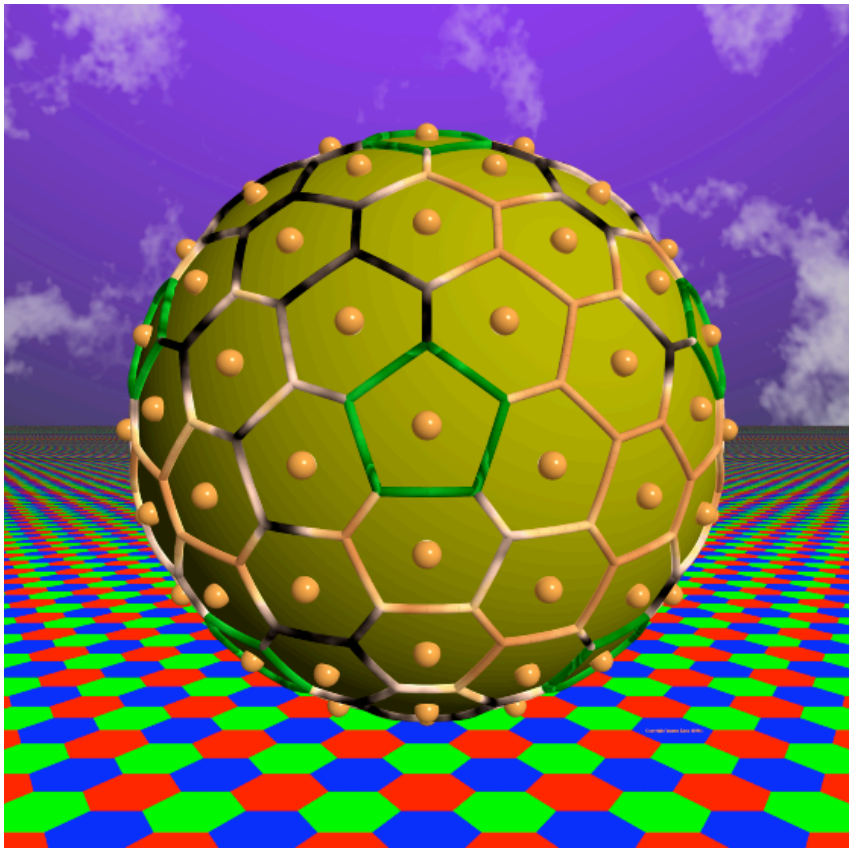
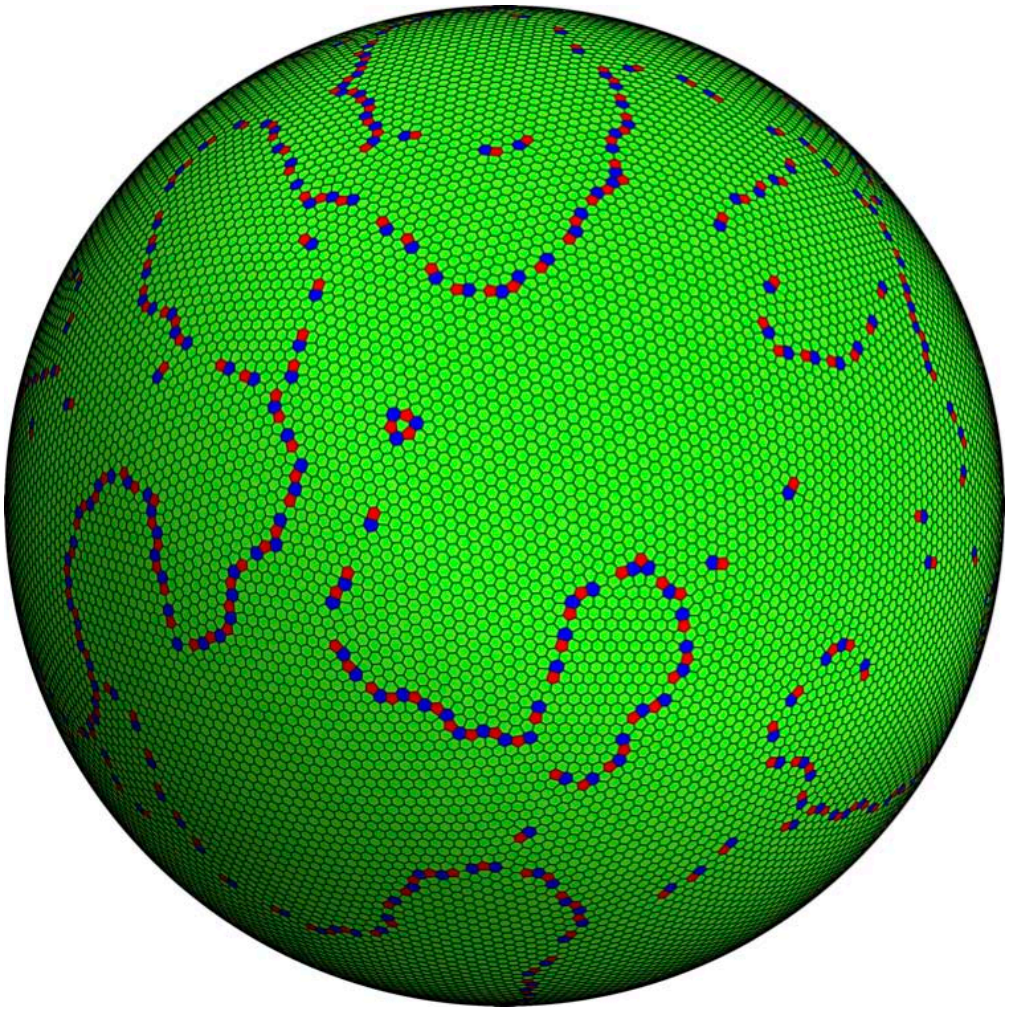


$N = 122$ electrons in equilibrium ($s = 1$)

Example: 30K ‘minimal’ $s = 3.5$-energy points on $\mathbb{S}^2$



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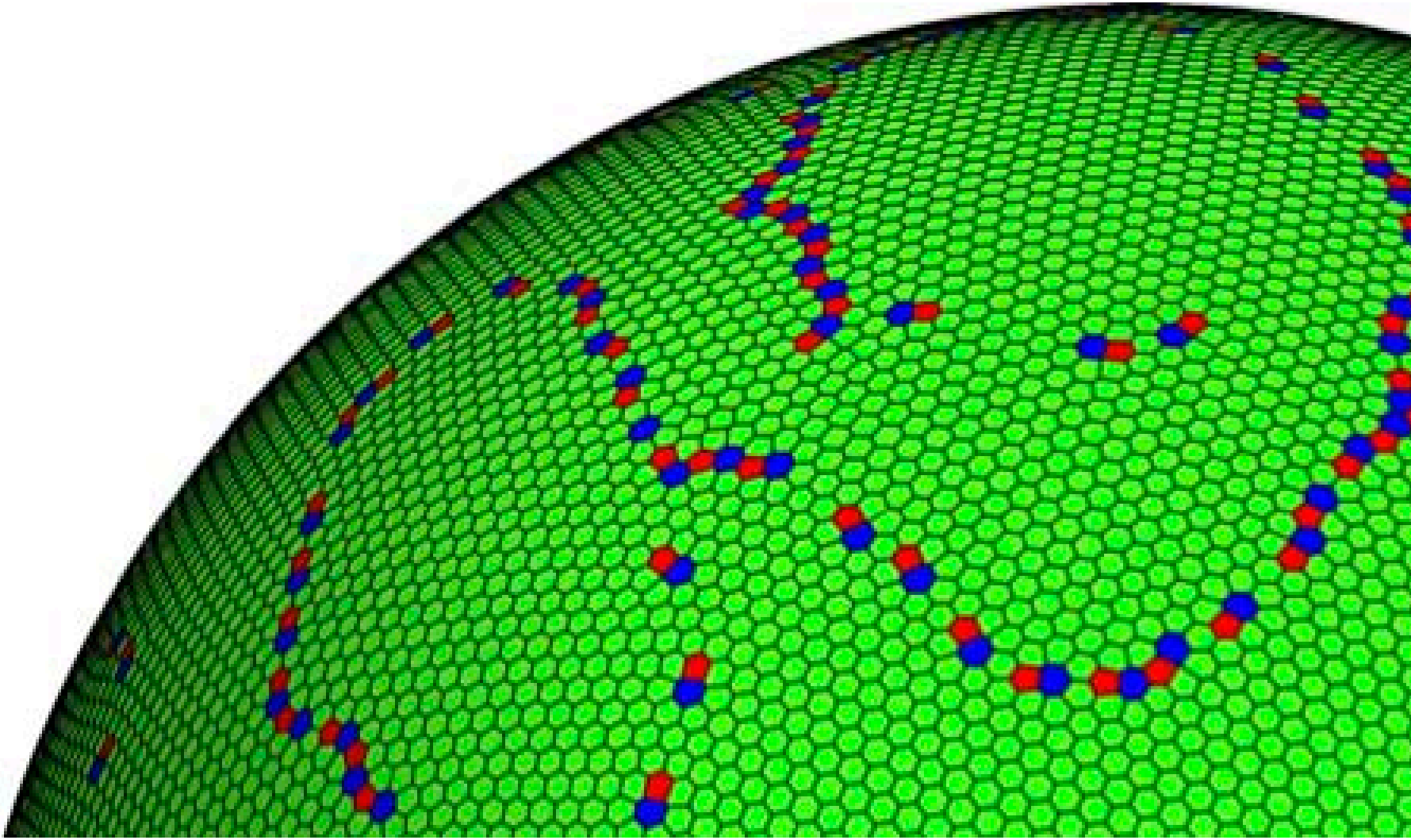
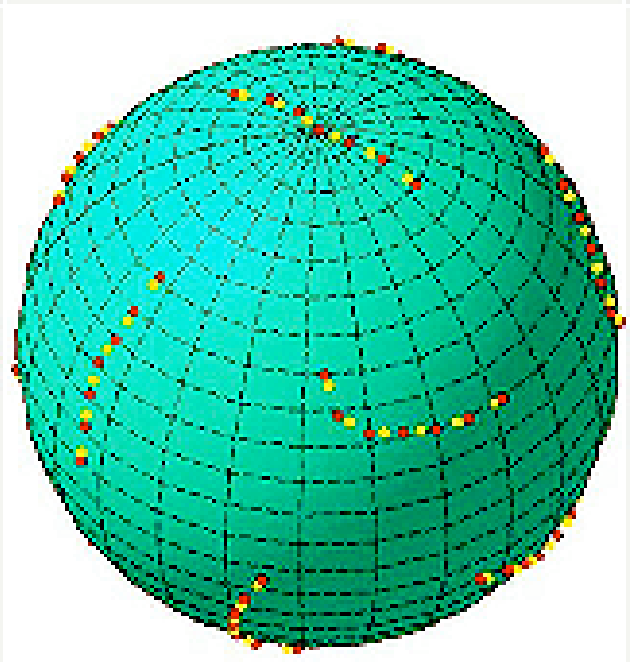


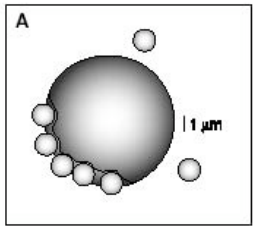
Bausch, Bowick, et al

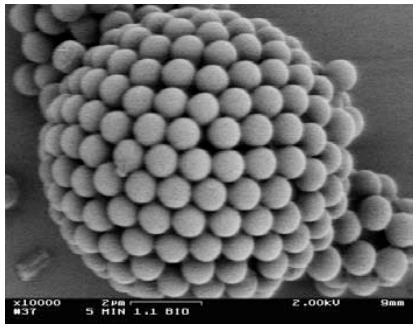
Grain Boundary Scars and Spherical Crystallography
Science, March 2003



Model grain boundaries

Spherical crystallography of “colloidosomes”



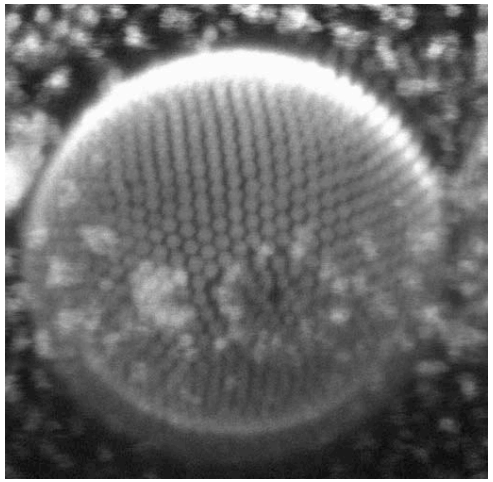


“Colloidosome” = colloids of radius ***a*** coating water droplet (radius ***R***) -- Weitz Laboratory

- ✱ Adsorb, say, latex spheres onto lipid bilayer vesicles or water droplets
- ✱ Useful for encapsulation of flavors and fragrances, drug delivery

  [H. Aranda-Espinoza e.t al. Science **285**, 394 (1999)]

- ✱Strength of colloidal ‘armor plating’ influenced by defects in shell….
- ✱ For water droplets, surface tension prevents buckling….



Ordering on a sphere ➔ a minimum of 12 5-fold disclinations, as in soccer balls and fullerenes -- what happens for $R/a >> 1$?

$S^d := \{x \in \mathbb{R}^{d+1} : |x| = 1\}$

Uniformly distributed spherical configurations

A sequence of N-point configurations $\omega_N = \{x_{1,N}, x_{2,N}, \ldots, x_{N,N}\}$, $N = 1, 2, \ldots$ is said to be **uniformly distributed** on the sphere S^d if

$$\nu(\omega_N) \xrightarrow{*} \sigma_d, \quad N \to \infty,$$

where σ_d denotes **normalized surface area measure** on S^d.

Equivalently, for all $f \in C(S^d)$,

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(x_{i,N}) = \int_{S^d} f(x)\, \mathrm{d}\sigma_d(x).$$

Simple Examples

If $\omega_N = \{e^{2k\pi i/N}\}_{k=0}^{N-1}$, the N**-th roots of unity**, then these configurations are **uniformly distributed on the unit circle** S^1. The normalized counting measures converge weak* to $d\theta/2\pi$, normalized arclength on the unit circle.

Verify that the same is true for the sequence $\{e^{\lambda k\pi i}\}_{k=1}^{\infty}$, whenever λ is an irrational real number.

Distributing Points Uniformly on the Sphere

Applications:

- best-packing on sphere
- viral morphology
- crystallography
- electrostatics
- stable molecules (fullerenes)
- data sampling (numerical integration, spherical designs)
- finite normalized tight frames
- testing radar for aircraft
- “soccer” ball designs

Minimizing Riesz energy is one method for generating uniformly distributed points.

3 Classical Problems on S^2

- For $s = 1$, get **Thomson's Problem** for Coulomb potential.

  Answers known for $N = 2, ..., 6$ and 12.

- For $s \to \infty$ with N fixed we get the **Tammes' Problem**; that is, the **best-packing problem**.
  Answers known for $N = 2, ..., 14$ and $N = 24$.

- For $s = 0$, related to

  Smale's Problem # 7 for 21st century:

  Design polynomial-time algorithm for constructing $\omega_N \subset S^2$ such that

$$E_{\log}(\omega_N) - \mathcal{E}_{\log}\left(S^2, N\right) \leq C \log N, \quad N \geq 2.$$

Asymptotics of $\mathcal{E}_{\log}(S^2, N)$

Known:

- Wagner (1989):
  $\mathcal{E}_{\log}(S^2, N) = -(1/2)\log(4/e)N^2 - (1/2)N\log N + \mathcal{O}(N)$

- Rakhmanov, Saff, and Zhou (1994):
  $\mathcal{E}_{\log}(S^2, N) = -(1/2)\log(4/e)N^2 - (1/2)N\log N + C_N N$,
  where $-0.2255... < C_N < -0.0469...$ for N sufficiently large.
- Bétermin, Sandier (2016) and Sandier, Serfaty (2015) establish that $C_{\log} := \lim_{N\to\infty} C_N$ exists.

Conjecture:

- Brauchart, Hardin, and Saff (2011):

$$C_{\log} = (1/2)\log(4/e) + \zeta'_{\Lambda_2}(0) = \log\frac{2}{\sqrt{3}} + 3\log\frac{\sqrt{2\pi}}{\Gamma(1/3)} = -0.0556...$$

Unit Sphere $S^d := \{x \in \mathbb{R}^{d+1} : |x| = 1\}$

WHAT'S KNOWN ABOUT LARGE N ASYMPTOTICS ?

For $0 < s < d$.

- The Riesz s-potential of normalized surface area σ_d satisfies

$$U_s^{\sigma_d}(x) = I_s[\sigma_d] = \frac{\Gamma(\frac{d+1}{2})\Gamma(d-s)}{\Gamma(\frac{d-s+1}{2})\Gamma(d-s/2)}, \quad x \in S^d.$$

- $K_s(x,y) = \frac{1}{|x-y|^s}$ is strictly positive definite on S^d.
- σ_d is the unique Riesz s-equilibrium measure.
- $$\lim_{N\to\infty} \frac{\mathcal{E}_s(S^d, N)}{N^2} = W_s(S^d) = I_s[\sigma_d] < \infty\,,$$

  and any sequence of optimal N-point s-energy configurations is asymptotically uniformly distributed on S^d.

What About $s \geq d$?

Not difficult to show

$W_s(S^d) = \infty$ for $s \geq d$.

Moreover, for $s > d$, there exist C_1 , $C_2 > 0$ such that

$$C_1 N^{1+s/d} \leq \mathcal{E}_s(S^d, N) \leq C_2 N^{1+s/d}, \text{for all } N \geq 2\,.$$

Questions: Does

$$\lim_{N\to\infty} \mathcal{E}_s(S^d, N)/N^{1+s/d} \text{ exist?}$$

What about the limiting distribution of N-point minimal s-energy configurations?