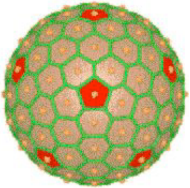

Discretizing compact manifolds with minimum energy:

The attraction of working with the repulsive

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Workshop on Sphere Arrangements
Fields Institute, November 15-18, 2011

A General Problem of Discretization

Given a d-dimensional compact metric space A (with metric m) and a probability density function $\rho(x)$ with respect to d-dimensional Hausdorff measure on A, how can we generate a large number N of points on A that are locally nice (well-separated and without big 'holes') and have (nearly) distribution $\rho(x)$?

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One approach: Use weighted minimal energy points.

Question: How repulsive is repulsive enough?

Riesz Potential and Energy

Fix $x \in A$.

For $0 < s < \infty$, the **Riesz s-potential** at the point y is:

$$k_s(x, y) := \frac{1}{m(x, y)^s}.$$

It is the energy required to place "a unit charge" at the point y in the presence of a charge at the point x.

For most of the talk $A \subset \mathbb{R}^p$ and $m(x, y) = |x - y|$ is the Euclidean metric.

For $s = p - 2$, we get Newton potential.

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

Energy of a Point Set

Notation

Let $\omega_N = \{x_1, x_2, ..., x_N\} \subset A$. For $s > 0$,

$$E_s(\omega_N) := \sum_{i=1}^{N} \sum_{j \neq i} \frac{1}{m(x_i, x_j)^s} = \sum_{i \neq j} k_s(x_i, x_j)$$

is the Riesz s-energy of ω_N.

As $s \to 0$,

$$\frac{k_s(x, y) - 1}{s} \to \log\left(\frac{1}{m(x, y)}\right)$$

so we set

$$k_0(x, y) := \log\left(\frac{1}{m(x, y)}\right), \quad E_0(\omega_N) := \sum_{i \neq j} k_0(x_i, x_j).$$

N-Point Energy of a Set

For given infinite compact metric space (A, m), let

$$\mathcal{E}_s(A, N) := \min\left\{E_s(\omega_N) : \omega_N \subset A, \quad \#\omega_N = N\right\} .$$

Let $\omega_N^* = \omega_N^*(A, s) \subset A$ satisfy

$$E_s(\omega_N^*) = \mathcal{E}_s(A, N) .$$

ω_N^* is called N-point equilibrium configuration for A or a set of minimal s-energy points.

$$E_s(\omega_N^*) \leq E_s(\omega_N) \quad \text{for any} \quad \omega_N \subset A, \quad \#\omega_N = N.$$

In general, ω_N^* is not unique.

Cases $s = 0$ and $s = \infty$

Remark: For $s = 0$, minimal energy points maximize the product

$$\prod_{i \neq j}^{N} m(x_i, x_j) \quad \text{over all} \quad \{x_i\}_1^N \subset A.$$

What about $s = \infty$? For fixed $\omega_N \subset A$, as $s \to \infty$

$$\left(\sum_{i \neq j} \frac{1}{m(x_i, x_j)^s} \right)^{1/s} \to \frac{1}{\min\{m(x_i, x_j),\ i \neq j\}}.$$

So as $s \to \infty$, minimal energy points become **best-packing points**, i.e., they maximize the minimum distance between N points on A.

Road Map

- Overview
- $s < d$: Connections to potential theory
- $s \geq d$: d-rectifiable sets; Poppy Seed Bagel Theorem
- Add weight
- Minimum energy configurations on compact metric spaces
- Zeta functions, $C_{s,d}$, and Sphere-packings in $\mathbb{R}^d$.
  - Connections to analytic number theory
  - Cohn-Elkies sphere-packing bounds. Open problem

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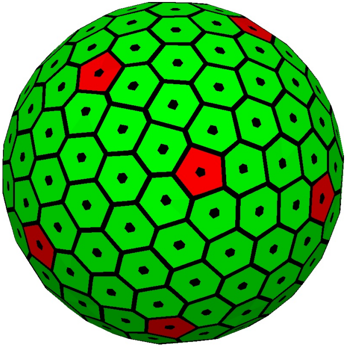
Five points on S^2

Three problems on $A = S^2$

1. Thomson problem: $s = 1$

Determine the minimum energy (ground state) configurations of N electrons restricted to a sphere and interacting through the Coulomb potential.

- $N = 174$ (near) optimal points on S^2 for $s = 1$ energy
- Voronoi cells: pentagons and hexagons.

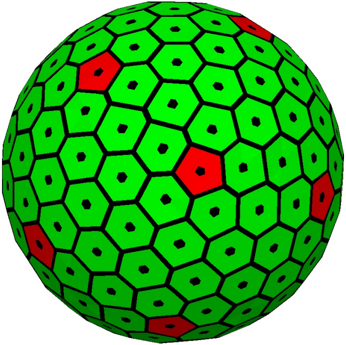


Three problems on $A = S^2$

2. Tammes problem: $s \to \infty$

Determine configurations of N points on S^2 whose minimum pairwise distance is maximal.

- $N = 174$ (near) optimal points on S^2 for $s = 4$ energy
- Voronoi cells: pentagons and hexagons.



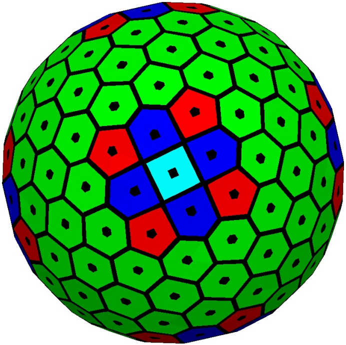
Three problems on $A = S^2$

3. # 7 of Smale's 18 Problems for this Century: $s = 0$

Find $\{x_1, \ldots, x_N\} \subset S^2$ (in polynomial time in N) such that

$$E_0(\{x_1, \ldots, x_N\}) \leq \mathcal{E}_0(S^2, N) + \mathcal{O}(\log N).$$

- $N = 174$ (near) optimal points on S^2 for $s = 0$ energy
- Voronoi cells: quadrilateral, pentagon, hexagon, heptagon.



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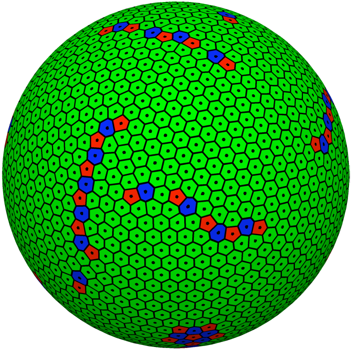

Asymptotics of $\mathcal{E}_0(S^2, N)$

Known:

- Wagner (1989):
  $\mathcal{E}_0(S^2, N) = -(1/2)\log(4/e)N^2 - (1/2)N\log N + \mathcal{O}(N)$

- Rakhmanov, Saff, and Zhou (1994):
  $\mathcal{E}_0(S^2, N) = -(1/2)\log(4/e)N^2 - (1/2)N\log N + C_N(N)$
  where $-0.2255... < C_N < -0.0469...$ for N sufficiently large.

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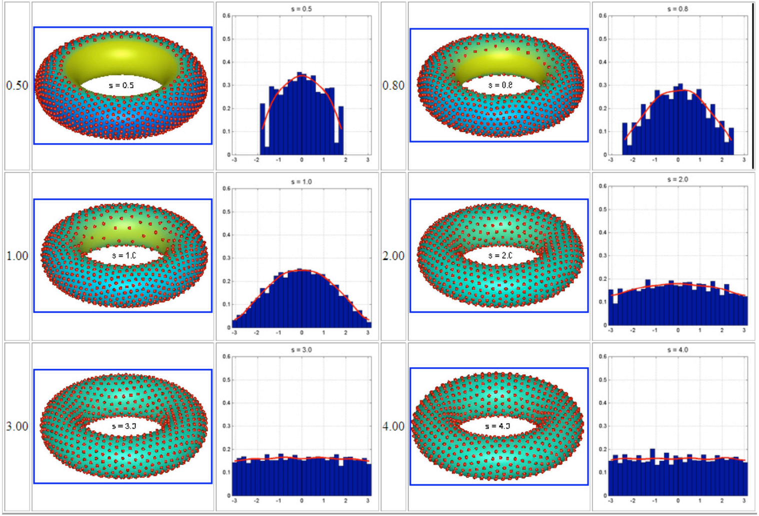
Conjecture:

- Brauchart, H. and Saff (2011):

$$\mathcal{E}_0(S^2 N) = -(1/2)\log(4/e)N^2 - (1/2)N\log N + CN + \mathcal{O}(\log N)$$

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

An Example: Torus (Bagel), $N = 1000$



Classical Potential Theory (cf. books by Landkof or Mattila)

Case: $A \subset \mathbb{R}^p$ compact, $d = \dim_{\mathcal{H}}(A)$, $s < d$, and $m(x, y) = |x - y|$.

The limiting density is described by the Riesz s-energy equilibrium measure μ_s that minimizes

$$I_s(\mu) := \int \int \frac{1}{|x - y|^s} d\mu(y) d\mu(x)$$

over all probability measures supported on A.

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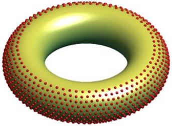
over all probability measures supported on A. That is,

$$\nu_N := \frac{1}{N} \sum_{x \in \omega_N^*} \delta_x \xrightarrow{*} \mu_s \quad \text{as} \quad N \to \infty,$$

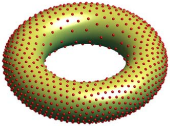
where δ_x is unit point mass at x. Also,

$$\lim_{N \to \infty} \frac{\mathcal{E}_s(A, N)}{N^2} = I_s(\mu_s).$$

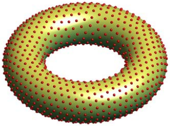
$\mathbf{N} = 1000$ **points**



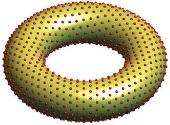
$s = 0.2$



$s = 1.0$

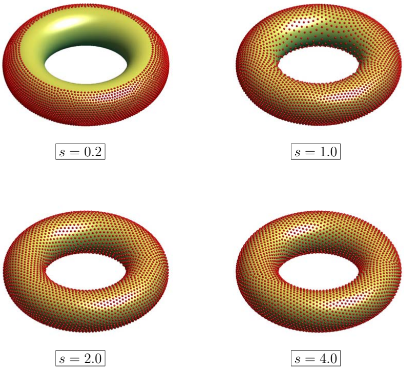


$s = 2.0$



$s = 4.0$

$\mathbf{N} = 4000$ **points**



What is known for $s \geq d = \dim_{\mathcal{H}}(A)$?

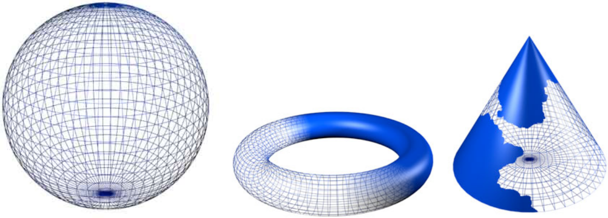
In this case, $I_s(\mu) = +\infty$ for all such μ.

A function $\Phi : T \to \mathbb{R}^p$, $T \subset \mathbb{R}^d$, is a **Lipschitz mapping** if

$$|\Phi(x) - \Phi(y)| \leq L|x - y|, \quad x, y \in T.$$

Definition

$A \subset \mathbb{R}^p$ is a ***d*-rectifiable set** if A is the image of a bounded set in $\mathbb{R}^d$ under a Lipschitz mapping.



"Poppy-Seed Bagel" Theorem (Borodachov, H, Saff 2008)

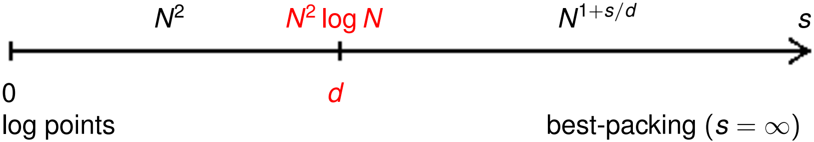
Suppose $s \geq d$ and $A \subset \mathbb{R}^p$ is a d-rectifiable set. When $s = d$ we further assume A is a subset of a d-dimensional C^1 manifold. Then

$$\lim_{N\to\infty} \frac{\mathcal{E}_d(A,N)}{N^2 \log N} = \frac{\mathcal{H}_d(\mathcal{B}^d)}{\mathcal{H}_d(A)}\,,$$

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d(A)]^{s/d}}\,,\ s > d\,. \tag{1}$$

Furthermore, if $\mathcal{H}_d(A) > 0$, then optimal s-energy configurations for $s \geq d$ are asymptotically (as $N \to \infty$) **uniformly distributed** with respect to d-dimensional Hausdorff measure.
(This is not true in general for $s < d$.)

Asymptotics for $\mathcal{E}_s(A, N)$ for d-rectifiable A



critical index $= d = \dim_{\mathcal{H}}(A)$

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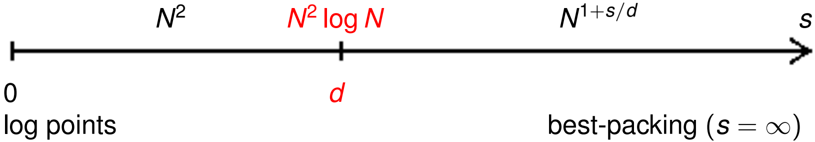

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$$\mu_{s,A} \xrightarrow{*}$$

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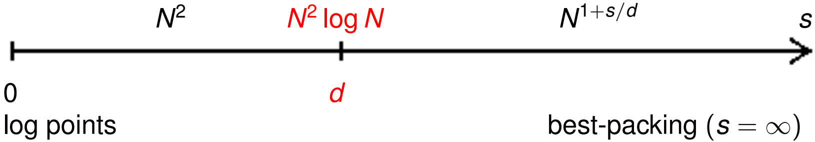


critical index $= d = \dim_{\mathcal{H}}(A)$

$$\mu_{s,A} \xrightarrow{*} \mathcal{H}_{d,A} := \mathcal{H}_d(\cdot \cap A)/\mathcal{H}_d(A)$$

strongly d-rectifiable case: H and Calef, 2009;
self-similar fractal case: Calef, 2009

Add Weight

Notation

- SLP weight: $w : A \times A \to [0, \infty)$ is Symmetric and Lower semi-continuous on $A \times A$ and Positive on the diag$(A \times A) := \{(a, a) \colon a \in A\}$.
- CPD weight: SLP weight Continuous at every point in diag$(A \times A)$.
- For $s > 0$ and $\omega_N = \{x_1, \ldots, x_N\} \subset A$,

$$E_{s,w}(\omega_N) := \sum_{i \neq j} \frac{w(x_i, x_j)}{m(x_i, x_j)^s}.$$

Weighted Riesz Energy

Theorem (BHS, 2008)

If $s > d$ and w is a CPD-weight on A, then

$$\lim_{N\to\infty} \frac{\mathcal{E}_s^w(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{\left[\mathcal{H}_d^{s,w}(A)\right]^{s/d}},$$

where $\mathcal{H}_d^{s,w}$ is weighted Hausdorff measure on Borel sets $\mathcal{B}$,

$$\mathcal{H}_d^{s,w}(B) = \int_B \frac{1}{w(x,x)^{d/s}} d\mathcal{H}_d(x).$$

Moreover, if $\mathcal{H}_d(A) > 0$, then any sequence of (w,s)-energy minimizing points has limit distribution

$$\mathcal{H}_d^{s,w}(\cdot)\big|_A .$$

Weighted Riesz Energy

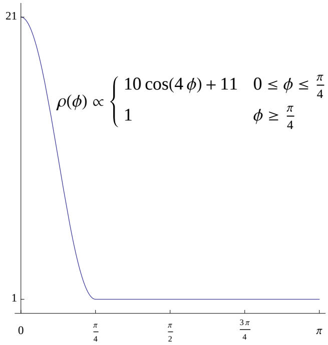
Corollary

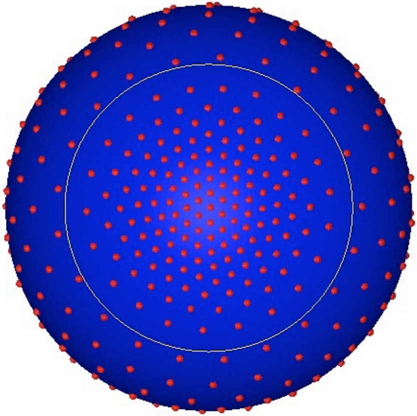
To distribute points on A according to a positive and continuous density $\rho(x)$ on a d-rectifiable set A, choose

$$w(x, y) := (\rho(x)\rho(y))^{-s/2d}$$

and compute minimal weighted s-energy points for any $s > d$.

Example[1]: $A = S^2$; $N = 400$; $s = 3$; nonuniform weight





[1] Computations and graphics by R. Womersley (UNSW)

Separation and Mesh Norm

Now let A be a compact metric space with metric m.

'Quality' metrics for $\omega_N = \{x_1, \ldots, x_N\} \subset A$

- separation distance of ω_N:

$$\delta(\omega_N) := \min_{1 \le i \ne j \le N} m(x_i, x_j),$$

- mesh norm (or fill radius) *of ω_N with respect to A*:

$$\rho(\omega_N, A) := \max_{y \in A} \min_{1 \le i \le N} m(y, x_i).$$

- mesh ratio of ω_N in A

$$\gamma(\omega_N, A) := \rho(\omega_N, A)/\delta(\omega_N).$$

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$\{\omega_N\}_{N=2}^{\infty}$ is quasi-uniform on A if $\gamma(\omega_N, A) < C$ for $N \ge 2$.

α-Regular metric spaces

- A Borel regular measure μ on A is (Ahlfors) α-regular, if

$$C^{-1} r^{\alpha} \leq \mu(B(x,r)) \leq C\, r^{\alpha} \qquad (x \in A,\ 0 < r \leq \operatorname{diam}(A)).$$

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- A metric space A is α-regular if $\exists$ α-regular measure μ on A.
- If A is α-regular then $\exists$ c such that for any sequence $\{\omega_N\}$ of N-point configurations in A

$$\delta(\omega_N) \leq c\, N^{-1/\alpha} \text{ and } c^{-1}\, N^{-1/\alpha} \leq \rho(\omega_N, A), \qquad (N \geq 2).$$

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- If A is α-regular and $\{\omega_N\}_{N=2}^{\infty}$ is quasi-uniform on A, then

$$\delta(\omega_N) \asymp N^{-1/\alpha} \text{ and } \rho(\omega_N, A) \asymp N^{-1/\alpha}.$$

Mesh-norm and quasi-uniformity

Theorem (H, Saff, Whitehouse (2011))

Suppose

- $\tilde{A}$ *is compact* α*-regular metric space with* α*-reg measure* μ*,*
- $A \subseteq \tilde{A}$ *is compact set of positive* μ*-measure,*
- w *is bounded SLP weight on* A*,*
- $s > \alpha$*.*

For $N \geq 2$*, let* ω_N^* *be an* N*-point* (s, w)*-energy minimizing configuration on* A*. Then* $\{\omega_N^*\}_{N=2}^{\infty}$ *is quasi-uniform on* A*.*

Remark: The set A need not inherit the lower α-regularity of $\tilde{A}$.
Previous results: Separation (Kuijlaars, Saff, Borodachov, H, 1998-2008...); Mesh norm (Damelin, Maymeskul (2005))

Mesh-norm and quasi-uniformity

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Quasi-uniformity and radial basis approximation: Narcowich and Ward 2002, ...
Recent paper by Fuselier and Wright used minimum energy points we provided.
Contact us if you have an interesting problem requiring good nodes.

Open Problem

What is the constant $C_{s,d}$ for $s \geq d$?

For some values of d (e.g., $d = 1, 2, 8, 24$), it appears that $C_{s,d}$ is a zeta function $\zeta_\Lambda(s)$ for a d-dimensional lattice $\Lambda \subset \mathbb{R}^d$ where

$$\zeta_\Lambda(s) := \sum_{0 \neq v \in \Lambda} |v|^{-s}.$$

In fact, $d = 1$: Since N-th roots of unity are optimal on unit circle (also see MMRS),

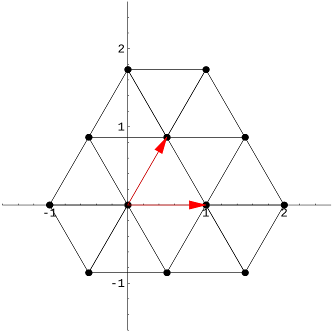
$$C_{s,1} = 2\zeta(s) = \zeta_{\mathbb{Z}}(s) \quad \text{for} \quad s > 1.$$

The Constant $C_{s,2}$

Conjecture: $C_{s,2} = \left(\sqrt{3}/2\right)^{s/2} \zeta_{\mathcal{L}}(s)$, $s > 2$,

where $\zeta_{\mathcal{L}} := \sum_{0 \neq \mathbf{v} \in \mathcal{L}} |\mathbf{v}|^{-s}$,

$\mathcal{L} = \{k_1 \mathbf{v}_1 + k_2 \mathbf{v}_2 : \ k_1, k_2 \in \mathbb{Z}\}$.



Equivalent to an (unproved) assumption common in 2D solid state physics that the hexagonal lattice describes the ground state for particles in the plane interacting through a Riesz potential r^{-s}.

Connections to Analytic Number Theory

$$C_{s,d} \leq \zeta_d^{\min}(s) := \min_{\Lambda} |\Lambda|^{s/d} \zeta_\Lambda(s), \quad s > d.$$

Determining $\zeta_d^{\min}(s)$ for different values of s and d is of interest in analytic number theory.

- $\zeta_2^{\min}(s) = \zeta_{\mathcal{L}}(s)$ (Rankins 1951, Cassels 1959, Montgomery 1986).
- In dimensions 8 and 24, Sarnak and Strömbergsson (2006) show E_8 and Leech lattice are local minima of $f(\Lambda) = |\Lambda|^{s/d}\zeta_{\Lambda(s)}$.
- Cohn, Kumar (2007) conjecture these lattices ($d = 2, 8, 24$) minimize a periodized energy with potentials of the form $f(|x - y|^2)$ for completely monotone f with sufficient decay. If true, then

$$C_{s,d} = |\Lambda_d|^{s/d} \zeta_{\Lambda_d}(s)$$

in these dimensions.

Connection to Best-Packing

Theorem (BHS)

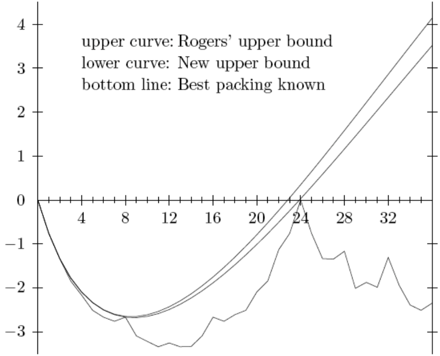
$$(C_{s,d})^{1/s} \to (1/2)(\beta_d/\triangle_d)^{1/d} \text{ as } s \to \infty,$$

where $\triangle_d$ is largest sphere packing density in $\mathbb{R}^d$ and $\beta_d = \mathrm{Vol}(\mathcal{B}^d)$.

$\Delta_1 = 1$,
$\Delta_2 = \pi/\sqrt{12}$ (Thue and Fejes Tóth),
$\Delta_3 = \pi/\sqrt{18}$ (Hales).

The exact value of Δ_d for $d > 3$ is unknown.

Cohn & Elkies (2003) provide extremely precise upper bounds for Δ_d in dimensions 2, 8, and 24.



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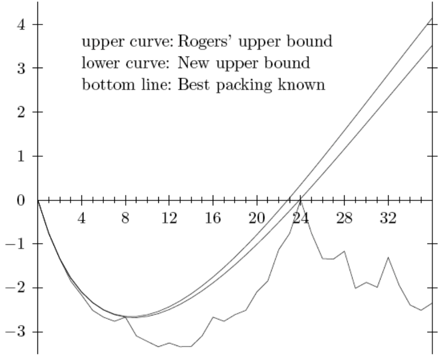

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Best packing in dimensions $d = 2, 8,$ and 24

Theorem (Cohn, Elkies (2003))

Suppose $f : \mathbb{R}^d \to \mathbb{R}$ *is an admissible function satisfying :*

(1) $f(0) = \hat{f}(0) > 0$,

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Then $\Delta_d \leq \dfrac{\pi^{n/2}}{(n/2)!}(r/2)^d$.

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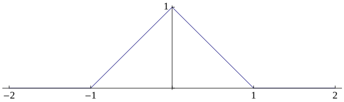

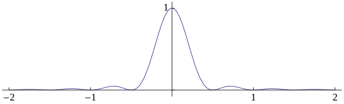

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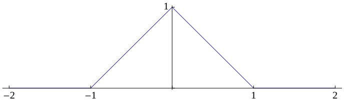

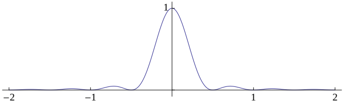

shows $\quad \Delta_1 = \dfrac{\sqrt{\pi}}{(1/2)!}(1/2) = 1.$

Open Problem: Find f for $d = 2$, 8, and 24.

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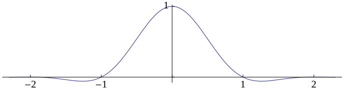

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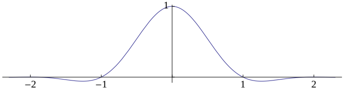
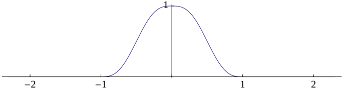


$$\hat{f}(t) = \left(1 - |t| + \frac{\sin 2\pi |t|}{2\pi}\right) \chi_{[-1,1]}(t)$$



THANKS!