

Energy minimization problems on the sphere

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Discrete and continuous energy

Let $F : [-1, 1] \rightarrow \mathbb{R}$.

Discrete energy: $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$

$$E_F(Z) = \frac{1}{N^2} \sum_{i,j=1}^N F(z_i \cdot z_j)$$

Energy integral: μ – Borel probability measure on \mathbb{S}^d

$$I_F(\mu) = \int \int_{\mathbb{S}^d \mathbb{S}^d} F(x \cdot y) d\mu(x) d\mu(y),$$

i.e. $E_F(Z) = I_F\left(\frac{1}{N} \sum \delta_{z_i}\right)$

Questions:

- Which configurations minimize E_F for a given N ?
- Which probability measures minimize I_F ?
- Is σ a minimizer? Is it unique?
- Difference between discrete and continuous energies?

Thomson problem (1904)

Find the minimal energy configuration of N electrons interacting according to Coulomb's Law and constrained to the sphere \mathbb{S}^2 , i.e. minimize the energy

$$\sum_{i \neq j} \frac{1}{\|z_i - z_j\|}$$

- Answer is known for $N = 2, 3, 4, 5, 6$ and $N = 12$
- 5 points on \mathbb{S}^2 , $s = 1$: triangular bi-pyramid (R.E. Schwartz, 2013, computer-assisted proof)



Riesz s -energies

Find the minimal energy configuration of N points on the sphere \mathbb{S}^d for the energies

$$E_s(Z) = \sum_{i \neq j} \frac{1}{\|z_i - z_j\|^s} \quad (s > 0)$$

and, if $s = 0$,

$$E_{\log}(Z) = \sum_{i \neq j} \log \frac{1}{\|z_i - z_j\|}$$

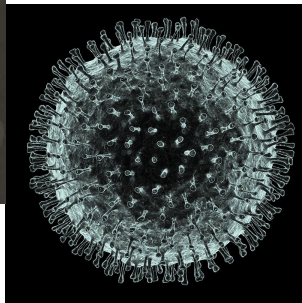
- $s = d - 1$: Thompson's problem (Coulomb/Newtonian potential)
- $s = \log$ ($s = 0$): Smale problem, logarithmic/Fekete points
(on \mathbb{S}^2 the answer is known for $N = 2, 3, 4, 5, 6$ and $N = 12$)
- $s < 0$: maximize!
- $s = -1$: sum of distances (Fejes-Tóth Problem)
(on \mathbb{S}^2 the answer is known for $N = 2, 3, 4, 5, 6$ and $N = 12$)

$s = \infty$: Tammes Problem (optimal packing)

Tammes Problem (1930)

When $s = \infty$, the problem becomes the following: find the configuration of N points on the sphere \mathbb{S}^d which maximizes the minimal distance between points (optimal codes). The problem is named after a Dutch botanist who posed the problem in 1930 while studying the distribution of pores on pollen grains.

- On \mathbb{S}^2 the answer is known for $N = 2, \dots, 14$ and $N = 24$.



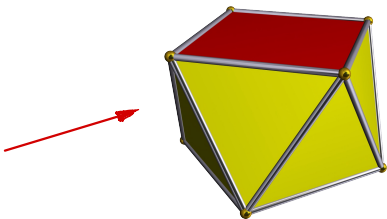
$s = \infty$: Tammes Problem (optimal packing)

Tammes Problem (1930)

When $s = \infty$, the problem becomes the following: find the configuration of N points on the sphere \mathbb{S}^d which **maximizes the minimal distance** between points (optimal codes).

The problem is named after a Dutch botanist who posed the problem in 1930 while studying the distribution of pores on pollen grains.

- On \mathbb{S}^2 the answer is known for $N = 2, \dots, 14$ and $N = 24$.
- $N = 4$ simplex
- $N = 6$ octahedron
- $N = 12$ icosahedron
- $N = 8$ square antiprism
NOT cube



(L. Fejes Tóth)

Fejes Tóth Problem on the sum of distances (1959)

Find the configurations of N points on the sphere \mathbb{S}^d which maximize the sum of distances

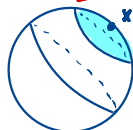
$$E_{-1}(Z) = \sum_{i \neq j} \|z_i - z_j\|.$$

- on \mathbb{S}^2 the answer is known for $N = 2, 3, 4, 5, 6$ and $N = 12$
- Closely related to the spherical cap discrepancy (Stolarsky)

Spherical cap discrepancy

Spherical caps: $x \in \mathbb{S}^d$, $t \in [-1, 1]$

$$C(x, t) = \{y \in \mathbb{S}^d : \langle x, y \rangle \geq t\}.$$



Spherical cap L^2 discrepancy: $Z = \{z_1, z_2, \dots, z_N\} \subset \mathbb{S}^d$
define

$$D_{L^2, \text{cap}}^2(Z) = \int_{\mathbb{S}^d} \int_{-1}^1 \left| \frac{\#(Z \cap C(x, t))}{N} - \sigma(C(x, t)) \right|^2 dt d\sigma(x).$$

Theorem (Beck, '84)

There exists constants $c_d, C_d > 0$ such that

$$c_d N^{-\frac{1}{2} - \frac{1}{2d}} \leq \inf_{\#Z=N} D_{L^2, \text{cap}}(Z) \leq C_d N^{-\frac{1}{2} - \frac{1}{2d}}.$$

Theorem (Stolarsky invariance principle)

For any finite set $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$

$$\begin{aligned} \frac{1}{N^2} \sum_{i,j=1}^N \|z_i - z_j\| + c_d \left[D_{L^2, cap} \right]^2 &= \text{const} \\ &= \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\| d\sigma(x) d\sigma(y). \end{aligned}$$

Discrepancy and sum of distances: Stolarsky Principle

Theorem (Stolarsky invariance principle)

For any finite set $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$

$$\begin{aligned} c_d \left[D_{L^2, \text{cap}}(Z) \right]^2 &= \\ &= \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\| d\sigma(x) d\sigma(y) - \frac{1}{N^2} \sum_{i,j=1}^N \|z_i - z_j\|. \end{aligned}$$

Theorem (Stolarsky invariance principle)

For any finite set $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$

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Proofs:

- K. Stolarsky (1973),
- J. Brauchart, J. Dick (2012) ,
- DB, F. Dai, R. Matzke (2018),
- H. He, K. Basu, Q. Zhao, A. Owen (2019)

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Versions:

- two-point homogeneous spaces (M. Skriganov),
- Hamming cube (A. Barg),
- Geodesic distance on the sphere (DB, F. Dai, R. Matzke; M. Skriganov): **hemisphere discrepancy** \rightarrow **geodesic distance**
- General energies on the sphere (DB, F. Dai, R. Matzke)
- Energies on metric spaces (DB, R. Matzke, O. Vlasiuk)
- ... and more

Theorem (Stolarsky invariance principle)

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Easy corollaries:

- i.i.d. random points: $\mathbb{E} D_{L^2, \text{cap}}^2(Z) \lesssim N^{-1}$
- jittered sampling: $\mathbb{E} D_{L^2, \text{cap}}^2(Z) \lesssim N^{-1-\frac{1}{d}}$
- $\frac{1}{N^2} \sum_{i,j=1}^N \|z_i - z_j\| \leq \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\| d\sigma(x) d\sigma(y)$

Theorem (Stolarsky invariance principle)

For any finite set $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$

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- $\int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\| d\mu(x) d\mu(y) \leq \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\| d\sigma(x) d\sigma(y)$

Which regular Borel probability measure μ on a compact domain $\Omega \subset \mathbb{R}^n$ **maximizes** the energy integral

$$I_\alpha(\mu) = \int_{\Omega} \int_{\Omega} \|x - y\|^\alpha d\mu(x) d\mu(y)$$

for a given $\alpha > 0$?

Theorem (Björck (1956))

- $0 < \alpha < 2$: *unique maximizer.*
- $\alpha > 2$: *discrete maximizers with at most $n + 1$ points in the support.*

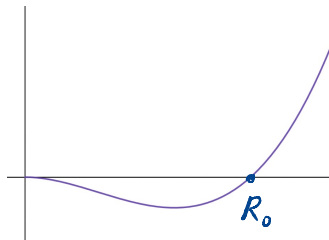
Discreteness of minimizers for mild repulsion

For a kernel $W : \mathbb{R}_+ \rightarrow \mathbb{R}$ define

$$I_W(\mu) = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} W(\|x - y\|) d\mu(x) d\mu(y)$$

- $W(0) = 0$
- $W(r) < 0$ for $r < R_0$.
- $W(r) > 0$ for $r > R_0$

(attractive-repulsive interaction)



Theorem (Carillo, Figalli, Patacchini, '17)

Assume that $W(r) \approx -r^\alpha$ as $r \rightarrow 0$ with $\alpha > 2$ (*mild repulsion*).
Then all global minimizers of I_W are discrete with finite support.

Arthur Schopenhauer



“A number of porcupines huddled together for warmth on a cold day in winter; but, as they began to prick one another with their quills, they were obliged to disperse. However the cold drove them together again, when just the same thing happened. At last, after many turns of huddling and dispersing, they discovered that they would be best off by remaining at a little distance from one another. In the same way the need of society drives the human porcupines together, only to be mutually repelled by the many prickly and disagreeable qualities of their nature. The moderate distance which they at last discover to be the only tolerable condition of intercourse, is the code of politeness and fine manners; and those who transgress it are roughly told—in the English phrase—to keep their distance. By this arrangement the mutual need of warmth is only very moderately satisfied; but then people do not get pricked. A man who has some heat in himself prefers to remain outside, where he will neither prick other people nor get pricked himself.”

– Arthur Schopenhauer, *Parerga and Paralipomena*

Eine Gesellschaft Stachelschweine drängte sich, an einem kalten Wintertage, recht nahe zusammen, um durch die gegenseitige Wärme, sich vor dem Erfrieren zu schützen. Jedoch bald empfanden sie die gegenseitigen Stacheln; welches sie dann wieder von einander entfernte. Wann nun das Bedürfnis der Erwärmung sie wieder näher zusammen brachte, wiederholte sich jenes zweite Uebel; so daß sie zwischen beiden Leiden hin und hergeworfen wurden, bis sie eine mäßige Entfernung von einander herausgefunden hatten, in der sie es am besten aushalten konnten. —

So treibt das Bedürfnis der Gesellschaft, aus der Leere und Monotonie des eigenen Innern entsprungen, die Menschen zu einander; aber ihre vielen widerwärtigen Eigenschaften und unerträglichen Fehler stoßen sie wieder von einander ab. Die mittlere Entfernung, die sie endlich herausfinden, und bei welcher ein Beisammenseyn bestehen kann, ist die Höflichkeit und feine Sitte. Dem, der sich nicht in dieser Entfernung hält, ruft man in England zu: keep your distance! — Vermöge derselben wird zwar das Bedürfnis gegenseitiger Erwärmung nur unvollkommen befriedigt, dafür aber der Stich der Stacheln nicht empfunden. — Wer jedoch viel eigene, innere Wärme hat bleibt lieber aus der Gesellschaft weg, um keine Beschwerde zu geben, noch zu empfangen.

Which regular Borel probability measure μ on a compact domain $\Omega \subset \mathbb{R}^n$ **maximizes** the energy integral

$$I_\alpha(\mu) = \int_{\Omega} \int_{\Omega} \|x - y\|^\alpha d\mu(x) d\mu(y)$$

for a given $\alpha > 0$?

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- $0 < \alpha < 2$: *unique maximizer.*
- $\alpha > 2$: *discrete maximizers with at most $d + 1$ points in the support.*

Euclidean distance energy integrals: sphere

Which regular Borel probability measure μ on the sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$ **maximizes** the energy integral

$$I_\alpha(\mu) = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\|^\alpha d\mu(x) d\mu(y)$$

for a given $\alpha > 0$?

Theorem (Björck (1956))

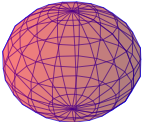
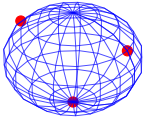
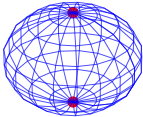
- $0 < \alpha < 2$: *unique maximizer is surface measure σ .*
- $\alpha = 2$: *any measure with center of mass at 0.*
- $\alpha > 2$: *mass $\frac{1}{2}$ at two opposite poles.*

- $-d < \alpha \leq 0$: unique minimizer is surface measure σ .



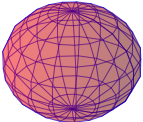
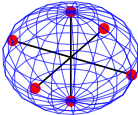
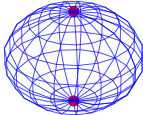
The Euclidean Distance on \mathbb{S}^d

Björck (1956)

| $-d < \alpha < 2$ | $\alpha = 2$ | $\alpha > 2$ |
|---|---|--|
| σ | center of mass at 0 | $\frac{1}{2}(\delta_p + \delta_{-p})$ |
|  |  |  |

The Geodesic Distance on \mathbb{S}^d

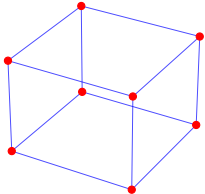
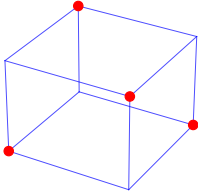
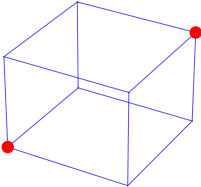
DB, Dai (2019)

| $-d < \alpha < 1$ | $\alpha = 1$ | $\alpha > 1$ |
|---|---|---|
| uniform σ | centrally symmetric | $\frac{1}{2}(\delta_p + \delta_{-p})$ |
|  |  |  |

Hamming Distance on the Hamming Cube

$$H^d = \{\pm 1\}^d \subset \sqrt{d}\mathbb{S}^{d-1}.$$

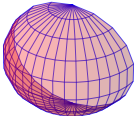
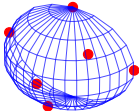
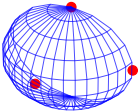
Hamming distance: $d_H(x, y) = \#\{i : x_i \neq y_i\} = \frac{1}{4}\|x - y\|^2$

| $0 < \alpha < 1$ | $\alpha = 1$ | $\alpha > 1$ |
|---|---|--|
| uniform σ_H | Center of Mass 0 | $\frac{1}{2}(\delta_p + \delta_{-p})$ |
|  |  |  |

Barg, DB, Matzke

Chordal Distance on \mathbb{RP}^d

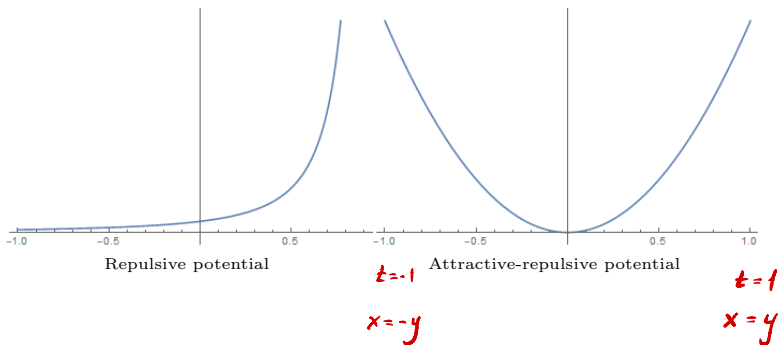
Chordal distance on \mathbb{RP}^d : $\rho(x, y) = \sqrt{1 - |x \cdot y|^2}$

| $-d < \alpha < 2$ | $\alpha = 2$ | $\alpha > 2$ |
|---|---|---|
| uniform σ | isotropic probability measures | μ_{ONB} |
|  |  |  |

**Anderson, Dostert, Grabner, Matzke, Stepaniuk;
DB, Ferizović, Glazyrin, Matzke, Park, Vlasiuk.**

Repulsive vs. attractive-repulsive potentials

Graph of $F(t)$, $t = x \cdot y$



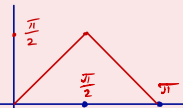
Sum of acute angles

Fejes Tóth Problem about the sum of acute angles

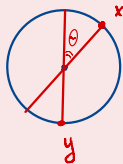
Find the configurations of N points on the sphere \mathbb{S}^d which **maximize** the sum

$$\sum_{i \neq j} \theta(z_i, z_j),$$

where



$$\theta(x, y) = \min\{d(x, y), \pi - d(x, y)\}$$



is the **acute (non-obtuse) angle** between the lines generated by vectors $x, y \in \mathbb{S}^d$. It is conjectured that the periodically repeated orthonormal basis of \mathbb{R}^{d+1} is a maximizer, e.g., for $d = 2$, $N = 5$,

$$\{e_1, e_2, e_3, e_1, e_2\} \text{ is a maximizer.}$$

- Fejes Tóth solved for small values of $N \leq 6$ on \mathbb{S}^2 .
- Solved on \mathbb{S}^1 . Open for $d \geq 2$.

Conjecture

The energy integral

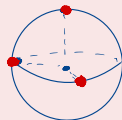
$$I_{\theta}(\mu) = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \theta(x, y) d\mu(x) d\mu(y),$$

where

$$\theta(x, y) = \min\{d(x, y), \pi - d(x, y)\}$$

is the acute (non-obtuse) angle between the lines generated by vectors $x, y \in \mathbb{S}^d$, is maximized by the uniform measure on an orthonormal basis

$$\mu_{ONB} = \frac{1}{d+1} \sum_{i=1}^{d+1} \delta_{e_i}.$$



- $I_\theta(\mu_{ONB}) = I_\theta\left(\frac{1}{d+1} \sum_{i=1}^{d+1} \delta_{e_i}\right) = \frac{\pi}{2} \cdot \frac{d}{d+1}$.
- F. Fodor, V. Víg, T. Zarnocz (2016): $d = 2$, $I_\theta(\mu) \leq \frac{3\pi}{8}$.
- DB, R. Matzke (2019): $d \geq 2$, $I_\theta(\mu) \leq \frac{\pi}{2} - \frac{69}{50(d+1)}$.
- D. Gorbachev, D. Lepetkov (2022): $d = 2$,
 $I_\theta(\mu) \leq 1.08326\dots$
- In particular, on \mathbb{S}^2 :
$$I_\theta(\mu) < 1.08326\dots < \frac{\pi}{2} - \frac{69}{150} = 1.110796\dots < \frac{3\pi}{8} = 1.178097\dots$$
- Conjectured maximum in $d = 2$ is $\frac{\pi}{3} = 1.047198\dots$

Recent results: continuous version



Theorem

R. McCann, T. Lim (2022)/

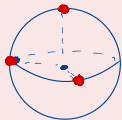
DB, A. Glazyrin, R. Matzke, J. Park, O. Vlasiuk (2022)

There exists $1 \leq \alpha_d < 2$ such that for all $\alpha > \alpha_d$ energy integral

$$\int_{\mathbb{S}^d} \int_{\mathbb{S}^d} (\theta(x, y))^\alpha d\mu(x) d\mu(y)$$

is maximized by the uniform measure on an orthonormal basis

$$\mu = \delta_{ONB} = \frac{1}{d+1} \sum_{i=1}^{d+1} \delta_{e_i}.$$



Theorem (DB, R. Matzke, J. Nathe (2024))

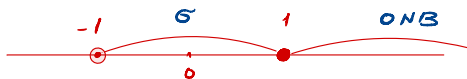
Let $d \geq 2$. For $\alpha \in (-d, -d + 2]$, the uniform surface measure σ on the sphere \mathbb{S}^d minimizes the energy integral $I_\alpha(\mu)$ among all Borel probability measures.

Theorem (DB, R. Matzke, J. Nathe (2024))

Let $d = 1$, i.e. consider the energy $I_\alpha(\mu)$ on the circle \mathbb{S}^1 . For $-1 < \alpha \leq 0$, the uniform measure σ on \mathbb{S}^1 is the unique (up to central symmetry) minimizer of $I_\alpha(\mu)$, while for $0 < \alpha < 1$ it is the unique maximizer.

Geodesic Distance on \mathbb{RP}^d

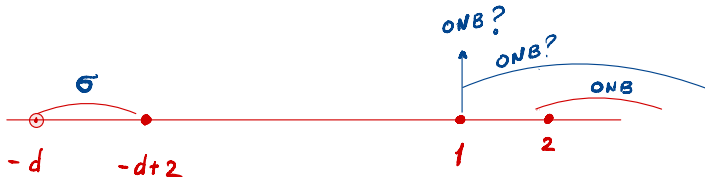
$d=1$



| α | $(-d, -(d-2)]$ | $(-(d-2), 1)$ | 1 | $(1, \infty)$ |
|----------|--------------------------|---------------|-----------------------------------|----------------------------------|
| $d=1$ | σ | N/A | orthogonally symmetric μ | μ_{ONB} |
| $d > 1$ | (abs. cont.) σ | ? | Conjecture: $\{\mu_{ONB}, ?\}$ | $(\alpha \geq 2)$ μ_{ONB} |

Table: The current state of the problem

$d > 1$



Unit norm tight frames (UNTFs)

A set of points $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^{d-1}$ is a tight frame iff for any $x \in \mathbb{R}^d$

$$\sum_k |\langle x, z_k \rangle|^2 = \frac{N}{d} \|x\|^2,$$

or, equivalently,

$$x = \frac{d}{N} \sum \langle x, z_k \rangle z_k.$$

Theorem (Benedetto, Fickus, 2003)

A set $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^{d-1}$ is a **tight frame** in \mathbb{R}^d if and only if Z is a local minimizer of the frame potential:

$$FP(Z) = \sum_{i,j=1}^N |\langle z_i, z_j \rangle|^2.$$

- **Welch, '74:**

Let $\{z_1, \dots, z_N\}$ be unit vectors in \mathbb{C}^d , $k \in \mathbb{N}$, then

$$\frac{1}{N^2} \sum_{i,j=1}^N |\langle z_i, z_j \rangle|^{2k} \geq \binom{d+k-1}{k}^{-1}.$$

- **Sidelnikov '74, Venkov '81:**

Let $\{z_1, \dots, z_N\} \subset \mathbb{S}^{d-1}$ be unit vectors in \mathbb{R}^d , $k \in \mathbb{N}$, then

$$\frac{1}{N^2} \sum_{i,j=1}^N |\langle z_i, z_j \rangle|^{2k} \geq I_{t^{2k}}(\sigma) = \frac{1 \cdot 3 \dots (2k-1)}{d \cdot (d+2) \dots (d+2k-2)}.$$

- Same for $k = 1$, better for $k > 1$.

Let $F(t) = |t|^p$ with $p > 0$. Consider

$$I_F(\mu) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} |\langle x, y \rangle|^p d\mu(x) d\mu(y)$$

Minimizers:

- $p = 2$: “frame energy” (Benedetto, Fickus, '13)
 - “tight frames” (incl. ONB, simplex)
 - σ (more generally, all isotropic measures μ).
- $0 < p < 2$: ONB (but **not** other frames or σ) (Ehler, Okoudjou, '12)
- $p > 2$, $p = 2k$: σ , spherical designs.
- $p > 2$, but $p \neq 2k$: ???
 - **Conjecture**: all minimizers of the p -frame energy are discrete measures.

Tight designs and 600-cell as Minimizers

Theorem (DB, Glazyrin, M., Park, Vlasiuk)

If C is a tight $(2m + 1)$ -design on \mathbb{S}^{d-1} and $p \in (2m - 2, 2m)$, then $\mu = \frac{1}{\#C} \sum_{x \in C} \delta_x$ is a minimizer of $I_{|t|^p}$.

| d | $ C $ | p -range | Configuration |
|-----|--------|--------------------|-----------------------|
| d | $2d$ | $(0, 2)$ | cross polytope |
| 2 | $2k$ | $(2k - 4, 2k - 2)$ | $2k$ -gon |
| 3 | 12 | $(2, 4)$ | icosahedron |
| 4 | 120 | $(8, 10)$ | 600-cell |
| 7 | 56 | $(2, 4)$ | kissing configuration |
| 8 | 240 | $(4, 6)$ | E_8 roots |
| 23 | 552 | $(2, 4)$ | equiangular lines |
| 23 | 4600 | $(4, 6)$ | kissing configuration |
| 24 | 196560 | $(8, 10)$ | Leech lattice |

Tight designs

A spherical $(2m + 1)$ -design is **tight** if it is centrally symmetric and there are $m + 1$ different distances between its distinct points.

Theorem (DB, Glazyrin, Matzke, Park, Vlasiuk, '19)

If C is a tight $(2m + 1)$ -design on \mathbb{S}^{d-1} and $p \in (2m - 2, 2m)$, then $\mu = \frac{1}{|C|} \sum_{x \in C} \delta_x$ is a minimizer of the p -frame energy.

Minimizers of the p -frame potentials

Tight designs

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Theorem (DB, Glazyrin, Matzke, Park, Vlasiuk, '19)

Suppose $p \notin 2\mathbb{N}$, and μ is a minimizer of the p -frame energy. Then the support of μ has empty interior.