Energy of determinantal point processes in the torus and the sphere

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The torus

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The dual lattice

$$\Lambda^* = \{x \in \mathbb{R}^d : \forall \lambda \in \Lambda \ \ \langle x, \lambda \rangle \in \mathbb{Z}\},$$

is given by the matrix $(A^t)^{-1}$.
We denote by $|\Lambda| = |\det A|$, the co-volume of Λ and $d\mu$ is the normalized measure in Ω

The periodic potential

For $s > d$, the Epstein Hurwitz zeta function for the lattice Λ defined by

$$\zeta_\Lambda(s;x) = \sum_{v\in\Lambda} \frac{1}{|x+v|^s}, \quad x \in \mathbb{R}^d,$$

is the Λ-periodic potential generated by the Riesz s-energy $|x|^{-s}$.

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$$\sum_{v\in\Lambda}\int_1^{+\infty} e^{-|x+v|^2 t}\frac{t^{\frac{s}{2}-1}}{\Gamma\left(\frac{s}{2}\right)}dt + \frac{1}{|\Lambda|}\sum_{w\in\Lambda^*\setminus\{0\}} e^{2\pi i\langle x,w\rangle}\int_0^1 \frac{\pi^{d/2}}{t^{d/2}}e^{-\frac{\pi^2|w|^2}{t}}\frac{t^{\frac{s}{2}-1}}{\Gamma\left(\frac{s}{2}\right)}dt$$

The energy in the torus

For $\omega \in \Omega^N$ define, for $0 < s < d$, the periodic Riesz s-energy of $\omega = (x_1, \ldots, x_N)$ by

$$E_{s,\Lambda}(\omega) = \sum_{k \neq j} F_{s,\Lambda}(x_k - x_j),$$

and the minimal periodic Riesz s-energy by

$$\mathcal{E}_{s,\Lambda}(N) = \inf_{\omega \in (\mathbb{R}^d)^N} E_{s,\Lambda}(\omega_N).$$

This was considered by Hardin, Saff and Simanek who computed the leading terms.

Known results in the torus

Hardin, Saff, Simanek and Su proved that for $0 < s < d$ there exists a constant $C_{s,d}$ independent of Λ such that for $N \to \infty$

$$\mathcal{E}_{s,\Lambda}(N) = \frac{2\pi^{d/2}|\Lambda|^{-1}}{\Gamma\left(\frac{s}{2}\right)(d-s)} N^2 + C_{s,d}|\Lambda|^{-s/d} N^{1+\frac{s}{d}} + o(N^{1+\frac{s}{d}}).$$

It is also shown that for $0 < s < d$

$$C_{s,d} \le \inf_{\Lambda} \zeta_{\Lambda}(s),$$

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It is also shown that for $0 < s < d$

$$C_{s,d} \leq \inf_{\Lambda} \zeta_\Lambda(s),$$

where Λ runs on the lattices with $|\Lambda| = 1$. The Epstein zeta function $\zeta_\Lambda(s)$ defined by

$$\zeta_\Lambda(s) = \sum_{v \in \Lambda \setminus \{0\}} \frac{1}{|v|^s}, \quad s > d,$$

can be extended analytically to $\mathbb{C} \setminus \{d\}$.

Some estimates

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But all explicitly known lattices in large dimensions are such that the corresponding Epstein zeta function have a zero in $0 < s < d$.
The value of $C_{s,d}$ it is known only for $d = 1$ and $C_{s,1} = \zeta_{\mathcal{Z}}(s) = 2\zeta(s)$. For $d = 2$ it is known that $\inf_\Lambda \zeta_\Lambda(s)$ is attained for the triangular lattice.

Determinantal point process

Definition

A determinantal point process A is a random point process such that the joint intensities have the form:

$$\rho_n(x_1, \ldots, x_n) = det(K(x_i, x_j)_{i,j \le n}).$$

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Recall that the joint intensities ρ_k satisfy:

$$\mathbb{E} \sum_{x_1, \ldots, x_k \in A} f(x_1, \ldots, x_k) = \int f(x_i, \ldots, x_k) \rho_k(x_i, \ldots, x_k)$$

for any f symmetric bounded and of compact support.

To define the processes we will consider only projection kernels.

Definition

We say that K is a projection kernel if it is a Hermitian projection kernel, i.e. the integral operator in $L^2(\mu)$ with kernel K is selfadjoint and has eigenvalues 1 and 0.

A projection kernel $K(x, y)$ defines a determinantal process with N points a.s. if the trace for the corresponding integral operator equals N, i.e. if

$$\int_\Omega K(x, x)d\mu(x) = N.$$

Translation invariant kernels

For $w \in \Lambda^*$, the Laplace-Beltrami eigenfunctions $f_w(u) = e^{2\pi i \langle u,w \rangle}$ of eigenvalue $-4\pi^2\langle w, w\rangle$ i.e. satisfying

$$\Delta f_w + 4\pi^2 \langle w, w\rangle f_w = 0,$$

are ortonormal in $L^2(\Omega)$, with respect to the normalized lebesgue measure μ,

$$\int_\Omega f_w(u)\overline{f_{w'}(u)} d\mu(u) = \delta_{w,w'}$$

for $w, w' \in \Lambda^*$.

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We consider functions $\kappa = (\kappa_N)_{N \geq 0}$ where each $\kappa_N : \Lambda^* \longrightarrow \{0, 1\}$ has compact support define the kernels

$$K_N(u, v) = \sum_{w \in \Lambda^*} \kappa_N(w) e^{2\pi i \langle u - v, w \rangle},$$

Expected Energies

The expected periodic Riesz s-energy of T_N points is

$$\mathbb{E}(E_{s,\Lambda}(x)) = \int_{\Omega^2} (T_N^2 - |K_N(u,v)|^2) F_{s,\Lambda}(u-v) d\mu(u) d\mu(v).$$

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Theorem

Let $x = (x_1, \ldots, x_{T_N})$ be drawn from the determinantal process Then, for $0 < s < d$, the expected energy is

$$\frac{2\pi^{d/2}}{\Gamma\left(\frac{s}{2}\right)(d-s)|\Lambda|^{-1}}({T_N}^2 - T_N) - \frac{\pi^{s-\frac{d}{2}}\Gamma\left(\frac{d-s}{2}\right)}{\Gamma\left(\frac{s}{2}\right)|\Lambda|} \sum_{\substack{w,w' \in \Lambda^* \\ w \neq w'}} \frac{\kappa_N(w)\kappa_N(w')}{|w - w'|^{d-s}}.$$

Frequencies in an open set

Definition

Let $\mathcal{D} \subset \mathbb{R}^d$ be open, bounded with $|\partial D| = 0$. Take

$$k_N(w) = \begin{cases} 1 & \text{if } w \in \Lambda^* \cap N^{1/d}\mathcal{D}, \\ 0 & \text{otherwise.} \end{cases}$$

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Proposition

Let $|\Lambda||\mathcal{D}| = 1$. *Then* $\mathbb{E}_{x \in (\mathbb{R}^d)^{N_*}}(E_{s,\Lambda}(x))$ *is*

$$\frac{2\pi^{d/2}|\Lambda|^{-1}}{\Gamma\left(\frac{s}{2}\right)(d-s)} {N_*}^2 - \frac{\pi^{s-\frac{d}{2}}\Gamma\left(\frac{d-s}{2}\right)}{\Gamma\left(\frac{s}{2}\right)|\Lambda|} I_{\mu^*}^{\mathcal{D}} N_*^{1+s/d} + o(N_*^{1+s/d}),$$

$$I_{\mu^*}^{\mathcal{D}} = \int_{\mathcal{D}\times\mathcal{D}} \frac{1}{|x-y|^{d-s}} d\mu^*(x) d\mu^*(y),$$

Ω^* *is a fundamental domain for* Λ^* *and* $\mu^*(\Omega^*) = 1$.

Final optimization

A natural question is now, given a fixed lattice Λ, to find the optimal $\mathcal{D} \subset \mathbb{R}^d$.

Theorem (Riesz inequality)

Given f, g, H nonnegative functions in $\mathbb{R}^d$ with $h(x) = H(|x|)$ symmetrically decreasing. Then

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(x)g(y)H(|x-y|)dxdy \leq \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \widetilde{f}(x)\widetilde{g}(y)H(|x-y|)dxdy,$$

where $\widetilde{f}, \widetilde{g}$ are the symmetric decreasing rearrangements of f and g.

Upper bounds for the minimal Energy

Proposition

If we take

$$\mathcal{D} = \mathbb{B}_d(0, r_d), \ \textit{with} \ \ r_d = \left(\frac{d}{\omega_{d-1} |\det A|} \right)^{1/d}.$$

Then

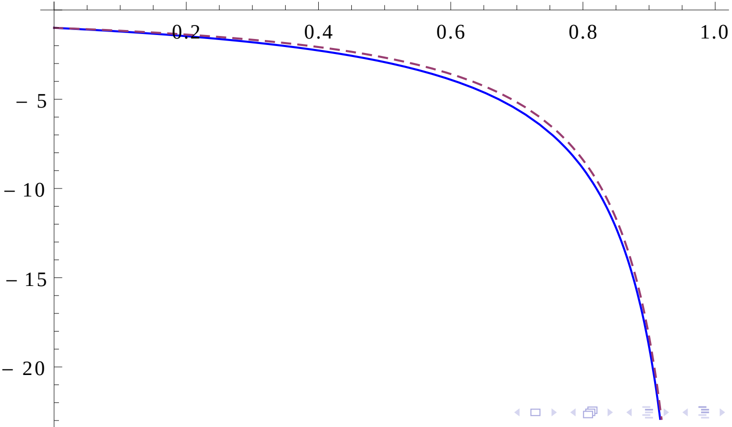
$$\frac{\pi^{s-\frac{d}{2}} \Gamma\left(\frac{d-s}{2}\right)}{\Gamma\left(\frac{s}{2}\right) |\Lambda|^{1-\frac{s}{d}}} I_{\mu^*}^{\mathcal{D}} =$$

$$\frac{\Gamma\left(\frac{d-s}{2}\right) \Gamma(d+1) \Gamma\left(\frac{s+1}{2}\right)}{2^{d+1} \Gamma\left(\frac{d}{2}+1\right) \Gamma\left(\frac{s}{2}+1\right) \Gamma\left(\frac{d+s}{2}+1\right) \Gamma\left(\frac{d+1}{2}\right)}.$$

$d = 1$

In the one-dimensional case $C_{s,1} = 2\zeta(s)$ and our bound is

$$-\frac{\pi^{s-1/2}\Gamma\left(\frac{1-s}{2}\right)}{\Gamma\left(\frac{s}{2}\right)}\frac{2}{s(s+1)}.$$



Riesz Potentials in the sphere

Given a Riesz potential:

$$K_\alpha(x,y) = \begin{cases} |x-y|^{-\alpha} & \text{if } \alpha > 0 \\ \log|x-y|^{-1} & \text{if } \alpha = 0, \end{cases}$$

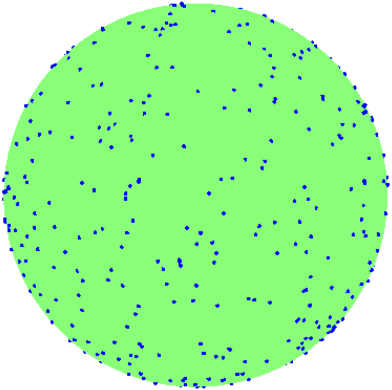
and given n points $\mathcal{P}_n$ at the sphere, we want to minimize the energy

$$E_\alpha = \sum_{x,y\in\mathcal{P}_n,\ x\neq y} K_\alpha(x,y),$$

among all collections of points $\mathcal{P}_n \subset \mathbb{S}^d$. When $\alpha = d-2$ we have the Newtonian potential that corresponds to the Thomson problem. When $\alpha \to \infty$, we recover Tammes problem.

"Well distributed" points on the sphere

$$\mathbb{S}^d = \{x = (x_1, \dots, x_{d+1}) \in \mathbb{R}^{d+1} \; : \; x_1^2 + \cdots + x_{d+1}^2 = 1\}$$



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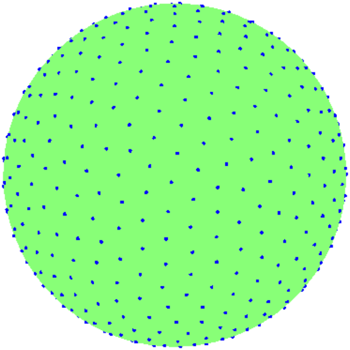

: R. Womersley web http://web.maths.unsw.edu.au/ rsw/Sphere/ 529 Fekete points

It is known that (Alexander, Stolarsky, Wagner, Kuijlaars, Saff, Brauchart) for $d \geq 2$ and $0 < s < d$ there exist constants $C, c > 0$ such that

$$-cn^{1+s/d} \leq \mathcal{E}(s, n) - V_s(\mathbb{S}^d)n^2 \leq -Cn^{1+s/d},$$

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Conjecture (BHS) : there is a constant $A_{s,d}$ such that

$$\mathcal{E}(s,n) = V_s(\mathbb{S}^d)n^2 + \frac{A_{s,d}}{\omega_d^{s/d}} n^{1+s/d} + o(n^{1+s/d}).$$

Furthermore, when $d = 2, 4, 8, 24$

$$A_{s,d} = |\Lambda_d|^{s/d} \zeta_{\Lambda_d}(s), \tag{1}$$

where $|\Lambda_d|$ stands for the co-volume and $\zeta_{\Lambda_d}(s)$ for the Epstein zeta function of the lattice Λ_d. Here Λ_d denotes the hexagonal lattice for $d = 2$, the root lattices D_4 for $d = 4$ and E_8 for $d = 8$ and the Leech lattice for $d = 24$.

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Recall that in the logarithmic case the constant exist.

Spherical ensembles

Krishnapur considered the following point process: Let A, B be n by n random matrices with i.i.d. Gaussian entries. Then he proved that the generalized eigenvalues associated to the pair (A, B), i.e. the eigenvalues of $A^{-1}B$ have joint probability density (wrt Lebesgue measure):

$$C_n \prod_{k=1}^{n} \frac{1}{(1+|z_k|^2)^{n+1}} \prod_{i<j} |z_i - z_j|^2.$$

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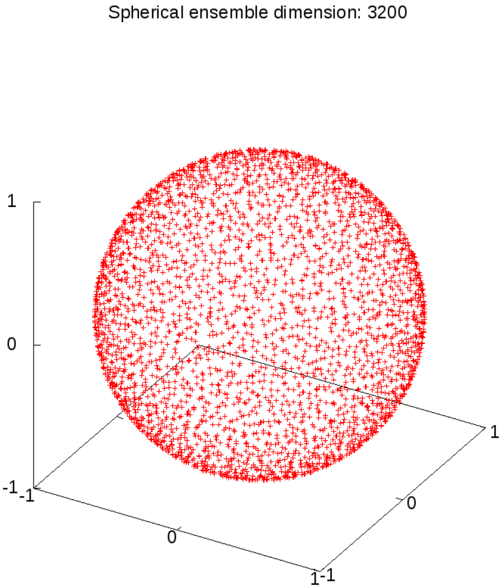
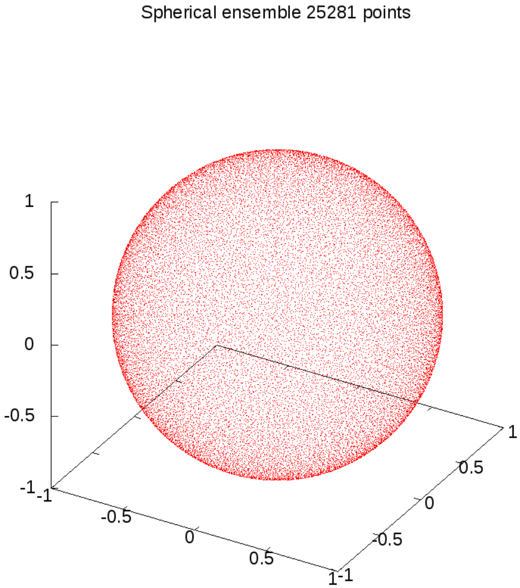
If we consider the stereographic projection to the sphere $\mathbb{S}^2$, then the joint density (with respect to the product area measure in the sphere) is

$$K_n \prod_{i<j} \|P_i - P_j\|^2_{\mathbb{R}^3}.$$


Spherical ensemble dimension: 3200
1
0
-1
-1
0
1
-1
0
1


Spherical ensemble 25281 points
1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1
-1
-0.5
0
0.5
1

The harmonic ensemble in $\mathbb{S}^d$

Let Π_L of spherical harmonics of degree at most L in $\mathbb{S}^d$.

By Christoffel-Darboux formula the reproducing kernel of Π_L

$$K_L(x,y) = \frac{\pi_L}{\binom{L+\frac{d}{2}}{L}} P_L^{(1+\lambda,\lambda)}(\langle x,y\rangle), \quad x,y \in \mathbb{S}^d,$$

where $\lambda = \frac{d-2}{2}$ and the Jacobi polynomials are
$P_L^{(1+\lambda,\lambda)}(1) = \binom{L+\frac{d}{2}}{L}$.
By definition

$$P(x) = \langle P, K_L(\cdot,x)\rangle = \int_{\mathbb{S}^d} K_L(x,y)P(y)d\mu(y), \text{ for } P \in \Pi_L.$$

Π_L is the space of polynomials in $\mathbb{R}^{d+1}$ restricted to $\mathbb{S}^d$,

$$\dim \Pi_L = \pi_L = \frac{2}{\Gamma(d+1)} L^d + o(L^d),$$

and $K_L(x,x) = \pi_L$ for every $x \in \mathbb{S}^d$.

The harmonic ensemble in $\mathbb{S}^d$

The harmonic ensemble is the determinantal point process in $\mathbb{S}^d$ with π_L points a.s. induced by the kernel

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We study different aspects of this process:

- Expected Riesz energies
- Linear statistics and spherical cap discrepancy
- Separation distance
- Energy optimality among isotropic processes

Let $x = (x_1, \ldots, x_n)$ where $n = \pi_L$ be drawn from the harmonic ensemble. Then, for $0 < s < d$,

$$\mathbb{E}_{x \in (\mathbb{S}^d)^n}(E_s(x)) = V_s(\mathbb{S}^d) n^2 - C_{s,d} n^{1+s/d} + o(n^{1+s/d}),$$

for some explicit constant $C_{s,d} > 0$.

The general case (and the limiting cases) are more difficult: we improve the constants or match the order (s=d).

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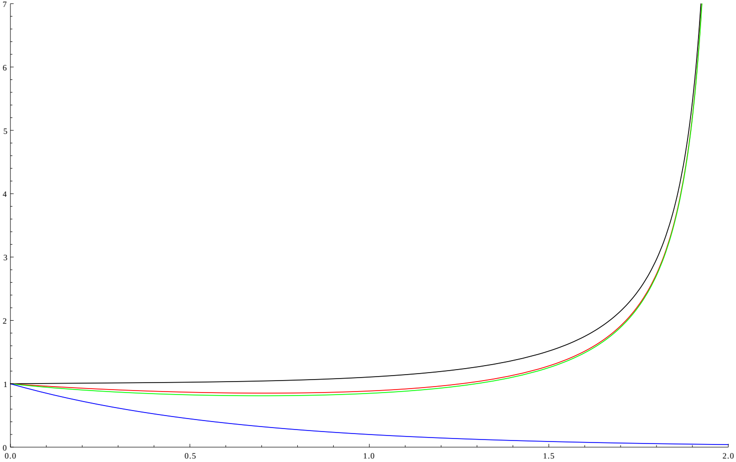
The general case (and the limiting cases) are more difficult: we improve the constants or match the order (s=d).
For $d = 2$ the BHS conjecture is

$$\mathcal{E}(s,n) = V_s(\mathbb{S}^2)n^2 + \frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}}n^{1+s/2} + o(n^{1+s/2}),$$

where $\zeta_{\Lambda_2}(s)$ is the zeta function of the hexagonal lattice (Dirichlet L-series).

d=2



: Graphic of $-\frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}}$ in black, $2^{-s}\Gamma(1-\frac{s}{2})$ (spherical) in red, the constant $C_{s,2}$ (harmonic) in green and $1/(2\sqrt{2\pi})^s$ in blue.

Optimality

Can we find the best determinantal process? i.e. the kernel such that the expected energy is minimal?

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- Invariant by rotations i.e.

$$d(x,y) = d(z,t) \Longrightarrow K(x,y) = K(z,t), \quad x,y,z,t \in \mathbb{S}^d,$$

  and then $K(\langle x,y\rangle)$ for some $K : [-1,1] \mapsto \mathbb{C}$.

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- We need that for any $x_1,\ldots,x_k \in \mathbb{S}^d$ the matrix

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  is nonnegative definite.
- If we want n points a.s. in $\mathbb{S}^d$ then all the eigenvalues must be 1 (projection kernel).

Schoenberg theorem

We must have

$$K(x, y) = K(\langle x, y \rangle), \quad K(t) = \sum_{k=0}^{\infty} a_k C_k^{d/2-1/2}(t),$$

where $C_k^{d/2-1/2}$ is a Gegenbauer polynomial and the $a_k \in \left[0, \frac{2k+d-1}{d-1}\right]$ satisfy:

$$\text{trace}(K) = K(1) = \sum_{k=0}^{\infty} a_k \binom{d+k-2}{k} < \infty.$$

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To have a projection kernel with with n points we take

$$a_k \in \left\{0, \frac{2k+d-1}{d-1}\right\} \ \text{ with } \ \sum_{k=0}^{\infty} a_k \binom{d+k-2}{k} = n. \ \ (*)$$

Theorem

Let K_a and K_b be two kernels with coefficients $a = (a_0, a_1, \dots)$ and $b = (b_0, b_1, \dots)$ satisfying conditions $(*)$. Let $\mathbb{E}_a$ and $\mathbb{E}_b$ denote respectively the expected value of

$$E_2(x) = \sum_{i \neq j} \frac{1}{\|x_i - x_j\|^2},$$

when $x = (x_1, \dots, x_n)$ is given by the determinantal point process associated to K_a and K_b. Assume that for every $i, j \in \mathbb{N}$ we have:

$$\text{if } i < j,\, a_i = 0 \text{ and } a_j > 0 \text{ then } b_i = 0. \tag{2}$$

Then, $\mathbb{E}_a \leq \mathbb{E}_b$, with strict inequality unless $a = b$. In particular, the harmonic kernel is optimal since (2) is trivially satisfied in that case.

Discrepancy

There are other ways of quantifying the "equidistribution" of the point process: A measure of the uniformity of the distribution of a set $x = \{x_1, \ldots, x_n\} \subset \mathbb{S}^d$ of n points is the spherical cap discrepancy. We denote as $d(x, y) = \arccos\langle x, y\rangle$ the geodesic distance in $\mathbb{S}^d$. A spherical cap is a ball with respect to the geodesic distance.
The spherical cap discrepancy of the set x is

$$\mathbb{D}(x) = \sup_A \left| \frac{1}{n} \sum_{i=1}^{n} \chi_A(x_i) - \mu(A) \right|,$$

where A runs on the spherical caps of $\mathbb{S}^d$.
Lubotzky, Philips and Sarnak found (a deterministic) construction with discrepancy smaller than $\frac{(\log n)^{2/3}}{n^{1/3}}$.
This was improved by T. Wolff to $\frac{c}{n^{1/3}}$ and by Beck to $n^{-\frac{1}{2}(1+\frac{1}{d})} \log n$

Theorem

Let $A = A_L$ be a spherical cap of radius $\theta_L \in [0, \pi)$ with

$$\lim_{L\to\infty} \theta_L \in [0, \pi),$$

and $L\theta_L \to \infty$ when $L \to \infty$. Let $\phi = \chi_A$. Then

$$\mathrm{Var}(\mathcal{X}(\phi)) \lesssim L^{d-1} \log L + O(L^{d-1}),$$

where the constant is $\lim_{L\to\infty} {\theta_L}^{d-1} \frac{4}{2^d \pi \Gamma\left(\frac{d}{2}\right)^2}$.

Corollary

For every $M > 0$ the spherical cap discrepancy of a set of $n = \pi_L$ points $x = (x_1, \ldots, x_n)$ drawn from the harmonic ensemble satisfies

$$\mathbb{D}(x) = O(L^{-\frac{d+1}{2}} \log L) = O(n^{-\frac{1}{2}(1+\frac{1}{d})} \log n)$$