# ENERGY AND DISCREPANCY OF ROTATIONALLY INVARIANT DETERMINANTAL POINT PROCESSES IN HIGH DIMENSIONAL SPHERES

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ABSTRACT. We study expected Riesz $s$-energies and linear statistics of some determinantal processes on the sphere $\mathbb{S}^d$. In particular, we compute the expected Riesz and logarithmic energies of the determinantal processes given by the reproducing kernel of the space of spherical harmonics. This kernel defines the so called harmonic ensemble on $\mathbb{S}^d$. With these computations we improve previous estimates for the discrete minimal energy of configurations of points in the sphere. We prove a comparison result for Riesz 2-energies of points defined through determinantal point processes associated with isotropic kernels. As a corollary we get that the Riesz 2-energy of the harmonic ensemble is optimal among ensembles defined by isotropic kernels with the same trace. Finally, we study the variance of smooth and rough linear statistics for the harmonic ensemble and compare the results with the variance for the spherical ensemble (in $\mathbb{S}^2$).

## 1. INTRODUCTION

Let $\mathbb{S}^d$ be the unit sphere in the Euclidean space $\mathbb{R}^{d+1}$ and let $\mu$ be the normalized Lebesgue surface measure. We study Riesz $s$-energies and the uniformity (discrepancy and separation) of random configurations of points on the sphere $\mathbb{S}^d$ given by some determinantal point processes.

### 1.1. Riesz energies.

For a given collection of points $x_1, \dots, x_n \in \mathbb{S}^d$ and $s > 0$ the discrete $s$-energy associated with the tuple $x = (x_1, \dots, x_n)$ is

$$E_s(x) = \sum_{i \neq j} \frac{1}{\|x_i - x_j\|^s}.$$

The minimal Riesz $s$-energy is the value $\mathcal{E}(s, n) = \inf_x E_s(x)$, where $x$ runs through the $n$-point subsets of $\mathbb{S}^d$. The limiting case $s = 0$, given (through $(t^s - 1)/s \to \log t$ when $s \to 0$) by

$$E_0(x) = \sum_{i \neq j} \log \frac{1}{\|x_i - x_j\|},$$

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is the discrete logarithmic energy associated with $x$ and $\mathcal{E}(0,n) = \inf_x E_0(x)$, is the minimal discrete logarithmic energy for $n$ points on the sphere.

The asymptotic behavior of these energies, in the spherical and in other settings, has been extensively studied. See for example the survey papers [8, 9]. One problem in studying these quantities is to get computable examples. It is natural then to study random configurations of points and try to estimate asymptotically their energies on average. The next natural question is how to get good random configurations on the sphere. It is clear that uniform random points are not good candidates to have low energies because there is no local repulsion between points and the sets exhibit clumping.

A method to get better distributed random points is to take sets of zeros of certain random holomorphic polynomials on the plane with independent coefficients and transport them to the sphere via the stereographic projection. As the zeros repel each other, the configurations exhibit no clumping. This idea was used in [3] and the authors managed to get, in $\mathbb{S}^2$, the average behavior of the logarithmic energy (other relations between the logarithmic energy and polynomial roots are known, see [39]). See the works of Zelditch et al. [35, 43, 44, 15] for an extension to several complex variables.

We consider instead random sets of points given by a determinantal process. Random points drawn from a determinantal process exhibit local repulsion, they can be built in any dimension and they are computationally feasible, as proven in [11] and implemented in [32].

1.2. **Determinantal processes.** In this section we follow [11, Chap. 4]. See also [2, 32] or [38].

We denote as $\mathcal{X}$ a simple random point process in $\mathbb{S}^d$, that is a random discrete subset of $\mathbb{S}^d$ (the definition of a point process which is not "simple" is a little more involved, see [11, Sec. 1.2]). A way to describe the process is to specify the random variable counting the number of points of the process in $D$, for all Borel sets $D \subset \mathbb{S}^d$. We denote this random variable as $\mathcal{X}(D)$ or $n_D$. In many cases the point process is conveniently characterized by the so–called joint intensity functions, see [20, 21].

The joint intensities $\rho_k(x_1, \ldots, x_k)$ are functions defined in $(\mathbb{S}^d)^k$ such that for any family of mutually disjoint subsets $D_1, \ldots, D_k \subset \mathbb{S}^d$

$$\mathbb{E}\left[\mathcal{X}(D_1) \cdots \mathcal{X}(D_k)\right] = \int_{D_1 \times \cdots \times D_k} \rho_k(x_1, \ldots, x_k) d\mu(x_1) \ldots d\mu(x_k),$$

we assume that $\rho_k(x_1, \ldots, x_k) = 0$ when $x_i = x_j$ for $i \neq j$.

A random point process on the sphere is called determinantal with kernel $K : \mathbb{S}^d \times \mathbb{S}^d \to \mathbb{C}$, if it is simple and the joint intensities with respect to a background measure $\mu$ (the normalized surface measure in our case) are given by

$$\rho_k(x_1, \ldots, x_k) = \det(K(x_i, x_j))_{1 \le i,j \le k},$$

for every $k \geq 1$ and $x_1, \ldots, x_k \in \mathbb{S}^d$.

We will mostly restrict ourselves to a special class of determinantal point processes, induced by the so called projection kernels.

**Definition 1.** 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 its trace equals $n$, i.e.

$$\int_{\mathbb{S}^d} K(x,x)d\mu(x) = n.$$

In this case, the random vector in $(\mathbb{S}^d)^n$ with density $\frac{1}{n!}\det(K(x_i,x_j))_{1\le i,j\le k}$ is a determinantal process with the right marginals i.e. the joint intensities are given by determinants of the kernel [2, Remark 4.2.6].

Determinantal processes on $\mathbb{S}^2$ have been considered before. In [1] the authors study the so called spherical ensemble. The points of this process correspond to the generalized eigenvalues of certain random matrices, mapped to the surface of the sphere by the stereographic projection. It was shown by Krishnapur [18] that this process is determinantal and the kernel is the reproducing kernel of a weighted space of polynomials on the plane. In [1] the authors obtain, among other results, the expected Riesz logarithmic and $s$-energies (for $s$ in some range) and they use it to improve previous bounds for the minimal discrete energies. This point process does not have an immediate extension to arbitrary dimensions.

To compute the expected energy of a determinantal process we use the following well known result:

**Proposition 1.** *A projection kernel $K$, with trace $n$, defines a determinantal point process on $\mathbb{S}^d$ which generates $n$ points at random in $\mathbb{S}^d$. Moreover, let $x=(x_1,\dots,x_n)$ be generated by the associated point process. Then, for any measurable $f:\mathbb{S}^d\times\mathbb{S}^d\to[0,\infty)$ we have*

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}\left(\sum_{i\ne j} f(x_i,x_j)\right) = \int_{x,y\in\mathbb{S}^d} \left(K(x,x)K(y,y)-|K(x,y)|^2\right) f(x,y)\, d\mu(x)\, d\mu(y).$$

The fact that $K$ defines a determinantal point process in $\mathbb{S}^d$ is granted by Macchi-Soshnikov's theorem [11, Theorem 4.5.5] and from [11, Formula (1.2.2)] the formula above follows.

We will be interested in the values of the Riesz $s$-energy and the logarithmic energy of points coming from the determinantal point process with a projection kernel $K$, in particular we will use the following corollary.

**Corollary 1.** *The expected value of the Riesz $s$-energy and the logarithmic energy of $n$ points given by the determinantal point process associated with $K$ are given by:*

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) = \int_{x,y\in\mathbb{S}^d} \frac{K(x,x)K(y,y)-|K(x,y)|^2}{|x-y|^s}\, d\mu(x)\, d\mu(y),$$

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_0(x)) = \int_{x,y\in\mathbb{S}^d} \left(K(x,x)K(y,y)-|K(x,y)|^2\right)\log|x-y|^{-1}\, d\mu(x)\, d\mu(y).$$

*In particular, if we let $g(s)=\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x))$ then $\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_0(x)) = g'(0)$.*

1.3. **Spherical harmonics.** For a classical introduction to shperical harmonics see for example [40, Ch. IV]. Given an integer $\ell \geq 0$, let $\mathcal{H}_\ell$ be the vector space of spherical harmonics of degree $\ell$, and let $h_\ell = \dim \mathcal{H}_\ell$. It is known that

$$h_\ell = \frac{2\ell+d-1}{\ell+d-1}\binom{\ell+d-1}{\ell} = \frac{2}{\Gamma(d)}\ell^{d-1} + o(\ell^{d-1}).$$

For the Hilbert space $L^2(\mathbb{S}^d)$ of square integrable functions in $\mathbb{S}^d$ with the inner product

$$\langle f, g\rangle = \int_{\mathbb{S}^d} f(x)g(x)d\mu(x), \quad f, g \in L^2(\mathbb{S}^d),$$

one has that $L^2(\mathbb{S}^d) = \bigoplus_{\ell\geq 0}\mathcal{H}_\ell$ and therefore the expansion in an orthonormal basis of spherical harmonics provides a generalization of Fourier series.

The Gegenbauer polynomials $C_k^\alpha(t)$ are orthogonal polynomials in $[-1,1]$ with respect to the weight $(1-t^2)^{\alpha-\frac{1}{2}}$. We assume the normalization $C_k^\alpha(1) = \binom{2\alpha+k-1}{k}$. Let $\{Y_{\ell,k}\}_{k=1}^{h_\ell}$ be an orthonormal basis with respect to the norm in $L^2(\mathbb{S}^d)$. The reproducing kernel $Z_\ell(x,y)$ in $\mathcal{H}_\ell$ is then

$$Z_\ell(x,y) = \sum_{k=1}^{h_\ell} Y_{\ell,k}(x)Y_{\ell,k}(y) = \frac{2\ell+d-1}{d-1}C_\ell^{\frac{d-1}{2}}(\langle x,y\rangle), \quad x, y \in \mathbb{S}^d,$$

where $\langle x, y\rangle$ is the scalar product in $\mathbb{R}^{d+1}$. Observe that $d(x,y) = \arccos\langle x,y\rangle$ is the geodesic distance in $\mathbb{S}^d$. The function $Z_\ell$ is also known as the zonal harmonic of degree $\ell$.

We denote by $\Pi_L$ the vector space of spherical harmonics of degree at most $L$ in $\mathbb{S}^d$ (which equals the space of polynomials of degree at most $L$ in $\mathbb{R}^{d+1}$ restricted to $\mathbb{S}^d$). Its dimension is

$$\dim \Pi_L = \pi_L = \frac{2L+d}{d}\binom{d+L-1}{L} = \frac{2}{\Gamma(d+1)}L^d + o(L^d). \tag{1}$$

As the spaces $\mathcal{H}_\ell$ are mutually orthogonal one can see using the Christoffel-Darboux formula that the reproducing kernel $K_L(x,y)$ of $\Pi_L$ is

$$K_L(x,y) = \sum_{\ell=0}^{L} Z_\ell(x,y) = \frac{\pi_L}{\binom{L+\frac{d}{2}}{L}}P_L^{(1+\lambda,\lambda)}(\langle x,y\rangle), \quad x, y \in \mathbb{S}^d,$$

where $\lambda = \frac{d-2}{2}$ and the Jacobi polynomials $P_L^{(1+\lambda,\lambda)}(t)$ are normalized as

$$P_L^{(1+\lambda,\lambda)}(1) = \binom{L+\frac{d}{2}}{L} = \frac{\Gamma\left(L+\frac{d}{2}+1\right)}{\Gamma(L+1)\Gamma\left(\frac{d}{2}+1\right)}.$$

The following classical asymptotic estimate is a particular case from [41, Theorem 8.21.13]

$$P_L^{(1+\lambda,\lambda)}(\cos\theta) = \frac{k(\theta)}{\sqrt{L}}\left\{\cos\left((L+\lambda+1)\theta+\gamma\right) + \frac{O(1)}{L\sin\theta}\right\}, \tag{2}$$

if $c/L \le \theta \le \pi - (c/L)$, where $c$ is a fixed positive constant and

$$k(\theta) = \pi^{-1/2}\left(\sin\frac{\theta}{2}\right)^{-\lambda-3/2}\left(\cos\frac{\theta}{2}\right)^{-\lambda-1/2}, \quad \gamma = -\left(\lambda+\frac{3}{2}\right)\frac{\pi}{2}.$$

Near the end points, the asymptotic behavior of the Jacobi polynomials is given by the Mehler-Heine formulas

$$\lim_{L\to\infty} L^{-1-\lambda}P_L^{(1+\lambda,\lambda)}\left(\cos\frac{z}{L}\right) = \left(\frac{z}{2}\right)^{-1-\lambda} J_{1+\lambda}(z),$$
$$\lim_{L\to\infty} L^{-\lambda}P_L^{(1+\lambda,\lambda)}\left(\cos\left(\pi-\frac{z}{L}\right)\right) = \left(\frac{z}{2}\right)^{-\lambda} J_{\lambda}(z), \tag{3}$$

where the limits are uniform on compact subsets of $\mathbb{C}$, [41, p. 192] and the $J_\nu$ are Bessel functions of the first kind (see the paragraph before Proposition 6).

By definition of reproducing kernel

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

for $P \in \Pi_L$. Observe that $K_L(x,x) = \pi_L$ for every $x \in \mathbb{S}^d$.

**Definition 2.** The harmonic ensemble is the determinantal point process in $\mathbb{S}^d$ with $\pi_L$ points a.s. induced by the reproducing kernel $K_L(x,y)$.

1.4. **Linear statistics and spherical cap discrepancy.** Given a simple point process $\mathcal{X}$ on the sphere and a measurable function $\phi : \mathbb{S}^d \to \mathbb{C}$, the corresponding linear statistic is the random variable

$$\mathcal{X}(\phi) = \int_{\mathbb{S}^d} \phi\, d\mathcal{X} = \sum_j \phi(x_j).$$

When $\phi = \chi_A$ is the characteristic function of a Borel set $A \subset \mathbb{S}^d$, we have that $\mathcal{X}(\chi_A) = \mathcal{X}(A)$ is just the number of points of the process $\mathcal{X}$ in $A$. Characteristic functions define rough linear statistics, when $\phi$ is an smooth function we talk about smooth linear statistics.

A measure of the uniformity of the distribution of a finite set of points is the spherical cap discrepancy defined by

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

where $x = (x_1,\dots,x_n) \in (\mathbb{S}^d)^n$ and $A$ runs through the spherical caps (i.e. balls with respect to the geodesic distance) of $\mathbb{S}^d$.

It is well known that a system of points $\{x^{(n)}\}_n$, where $x^{(n)} \in (\mathbb{S}^d)^{m_n}$, is asymptotically uniformly distributed if and only if $\lim_{n\to\infty}\mathbb{D}(x^{(n)}) = 0$. Therefore, a measure of the similarity between the atomic measures $\frac{1}{m_n}\sum_{i=1}^{m_n}\delta_{x_i^{(n)}}$ and the Lebesgue surface measure, $\mu$, is the speed of this convergence.

It was shown by Beck in [5] that there exists an $n$-point set in $\mathbb{S}^d$ with spherical cap discrepancy smaller than a constant times $n^{-\frac{1}{2}(1+\frac{1}{d})}\sqrt{\log n}$. To prove this result Beck uses a random distribution of points and the proof is therefore nonconstructive. The known explicit constructions are still far from this bound, see

[23, 24] and [4] for the $\mathbb{S}^2$ case. The random configuration used by Beck consist of taking points uniformly in each set of a, so called, area-regular partition of the sphere, see [19, 29]. For other interesting properties of this random process see [10].

The upper bound above is almost optimal because, in [5, p. 35], Beck shows that the spherical cap discrepancy of an $n$ point set is bounded below by (a constant times) $n^{-\frac{1}{2}(1+\frac{1}{d})}$.

Following Beck [5], see also [1], we will deduce information about the spherical cap discrepancy of a random set of points drawn from the harmonic ensemble by using the rough linear statistic defined above.

1.5. **Separation distance.** We discuss also another measure of how well distributed a collection $x = (x_1, \dots, x_n) \in (\mathbb{S}^d)^n$ of spherical point is, namely, the separation distance

$$\operatorname{sep\_dist}(x) = \min_{i \neq j} \|x_i - x_j\|.$$

A well distributed collection of points should have all of its points well-separated, so one can search for $x$ maximizing $\operatorname{sep\_dist}(x)$. This is a classical problem known as the hard spheres problem, the best packing problem or Tammes problem since [42]. In the 2-dimensional case, a surprisingly sharp result [34] is known:

$$\min_{x=(x_1,\dots,x_n)\in(\mathbb{S}^2)^n} \operatorname{sep\_dist}(x) = \sqrt{\frac{8\pi}{\sqrt{3}}} n^{-1/2} + O(n^{-2/3}).$$

For the $d$-dimensional case the precise value of the constant is unknown but we still have that the minimal separation distance $\min_{x=(x_1,\dots,x_n)\in(\mathbb{S}^d)^n} \operatorname{sep\_dist}(x)$ is of order $n^{-1/d}$. Collections of points minimizing the Riesz energy for $s = d-1$ have been proven to satisfy this bound with constant $2^{1/d}$, see [13]. Following [1] we will obtain a bound on the separation distance of points choosen at random from the harmonic ensemble.

1.6. **Notation.** For two sequences $x_n$, $y_n$ of positive real numbers the expressions

$$x_n \lesssim y_n, \quad x_n = O(y_n) \text{ and } y_n = \Omega(x_n),$$

all mean that there is a constant $C \geq 0$ independent of $n$ such that

$$\limsup_{n\to\infty} \frac{x_n}{y_n} \leq C.$$

We sometimes write the inequality in the opposite order $x_n \gtrsim y_n$ (which means $y_n \lesssim x_n$). Finally, if both $x_n \lesssim y_n$ and $x_n \gtrsim y_n$ we simply write $x_n \sim y_n$. We also recall that $x_n = o(y_n)$ means that

$$\limsup_{n\to\infty} \frac{x_n}{y_n} = 0.$$

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## 2. Main results

2.1. **Riesz and logarithmic energies of the harmonic ensemble.** Our first result is the computation of the expected Riesz $s$-energy (in this section for $0 < s < d$) of the determinantal process given by the reproducing kernel $K_L(x, y)$ of the space of polynomials of degree at most $L$, i.e. for points from the harmonic ensemble. The closed expression for the energy is given in terms of a generalized hypergeometric function.

Recall that for integer $p, q \geq 0$ and complex values $a_i, b_j$ the generalized hypergeometric function is defined by the power series

$$ {}_pF_q(a_1, \ldots, a_p; b_1, \ldots, b_q; z) = \sum_{n=0}^{\infty} \frac{(a_1)_n \ldots (a_p)_n}{(b_1)_n \ldots (b_q)_n} \frac{z^n}{n!}, \tag{4} $$

where $(\cdot)_n$ is the rising factorial or Pochhammer symbol given by $(x)_0 = 1$ for $x \in \mathbb{C}$ and

$$ (x)_n = x(x+1)\cdots(x+n-2)(x+n-1) = \frac{\Gamma(x+n)}{\Gamma(x)}, \quad n \geq 1. $$

(Note that the formula involving the Gamma function is not defined for integer $x \leq 0$, but the finite product always is.)

The continuous $s$-energy for the normalized Lebesgue measure is defined as

$$ V_s(\mathbb{S}^d) = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \frac{1}{\|x-y\|^s} \, d\mu(x) \, d\mu(y) = 2^{d-s-1} \frac{\Gamma\left(\frac{d+1}{2}\right) \Gamma\left(\frac{d-s}{2}\right)}{\sqrt{\pi}\Gamma\left(d - \frac{s}{2}\right)}. \tag{5} $$

Then (recall that $\lambda = (d-2)/2$) one can write this quantity in terms of the beta function

$$ V_s(\mathbb{S}^d) = \frac{\omega_{d-1} 2^{d-s-1}}{\omega_d} B\left(\lambda + 1, \lambda + 1 - \frac{s}{2}\right), \tag{6} $$

where

$$ \omega_d = 2 \frac{\pi^{\frac{d+1}{2}}}{\Gamma\left(\frac{d+1}{2}\right)} \tag{7} $$

is the surface area of $\mathbb{S}^d$.

**Theorem 1.** *Let $x = (x_1, \ldots, x_n) \in (\mathbb{S}^d)^n$, where $n = \pi_L$, be $n$ points drawn from the harmonic ensemble. Then, $\mathbb{E}_{x \in (\mathbb{S}^d)^n}(E_s(x))$ is finite iff $s < d + 2$. Moreover, for $0 < s < d$,*

$$ \mathbb{E}_{x \in (\mathbb{S}^d)^n}(E_s(x)) = n^2 V_s(\mathbb{S}^d) - \frac{2^{d-1-s}\omega_{d-1} n^2}{\binom{L+\frac{d}{2}}{L}^2 \omega_d} \frac{\Gamma\left(\frac{d-s}{2}\right)}{\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(1+\frac{s}{2}\right)} $$

$$ \times C_{s,d}(L) {}_4F_3\left(-L, d+L, \frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1, d - \frac{s}{2} + L, -\frac{s}{2} - L; 1\right), $$

*where the constant $C_{s,d}(L)$ satisfies:*

$$ C_{s,d}(L) = \frac{\Gamma\left(L+\frac{d}{2}\right)\Gamma\left(L+\frac{d}{2}+1\right)\Gamma\left(L+\frac{s}{2}+1\right)}{\Gamma(L+1)^2 \Gamma\left(L - \frac{s}{2} + d\right)} \sim L^s, \quad L \to \infty. $$

The expression in Theorem 1 does not directly give us an insight on the dependence of the expected value with respect to the number of points $n$, since $L$ and $n$ are related and appear in different places of the formula. In order to get the asymptotic expansion of the expected Riesz $s$-energy we show that the generalized hypergeometric function converges to a hypergeometric function and then we use Gauss's theorem. To prove this convergence we use classical estimates of the Jacobi polynomials to get Proposition 6 which we think may be of independent interest. With this result we get the following asymptotic behavior, which clarifies the dependence on $n$ of the formula in Theorem 1.

**Theorem 2.** *Let $x = (x_1, \dots, x_n) \in (\mathbb{S}^d)^n$, where $n = \pi_L$, be $n$ points drawn from the harmonic ensemble. Then, for $0 < s < d$,*

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

*where*

$$C_{s,d} = 2^{s-s/d}V_s(\mathbb{S}^d)\,(d!)^{-1+\frac{s}{d}}\,\frac{d\,\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(\frac{1+s}{2}\right)\Gamma\left(d-\frac{s}{2}\right)}{\sqrt{\pi}\Gamma\left(1+\frac{s}{2}\right)\Gamma\left(1+\frac{s+d}{2}\right)}. \tag{8}$$

The correct order of growth for the second term of the minimal Riesz $s$-energy is known (see [19]) i.e. for $d \geq 2$ and $0 < s < d$ there exist constants $C, c > 0$ such that

$$-cn^{1+s/d} \leq \mathcal{E}(s,n) - V_s(\mathbb{S}^d)n^2 \leq -Cn^{1+s/d}, \tag{9}$$

for $n \geq 2$.

It has been conjectured in ([8, Conjecture 3]) that 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 $d = 2, 4, 8, 24$

$$A_{s,d} = |\Lambda_d|^{s/d}\zeta_{\Lambda_d}(s), \tag{10}$$

where $|\Lambda_d|$ stands for the co-volume and $\zeta_{\Lambda_d}(s)$ for the Epstein zeta function of the lattice $\Lambda_d$. Here $\Lambda_d$ 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 $d = 24$.

In the particular case of $d = 2$ the conjecture reduces to

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

where $\zeta_{\Lambda_2}(s)$ is the zeta function of the hexagonal lattice. This zeta function can be evaluated by using its relation with a particular Dirichlet L-series, see [8].

When $n$ is of the form $\pi_L$, since $\mathcal{E}(s,n) \leq \mathbb{E}E_s(n)$, we get from Theorem 2 an upper bound for the minimal energy, for $d \geq 2$ and $0 < s < d$:

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

for $C_{s,d}$ as in (8).

For $d = 2$ this bound is a bit worse ($C_{s,2}$ is smaller) than the lower constant $2^{-s}\Gamma(1-\frac{s}{2})$ from [1, Corollary 1.4] given by the spherical ensemble, see figure 1.

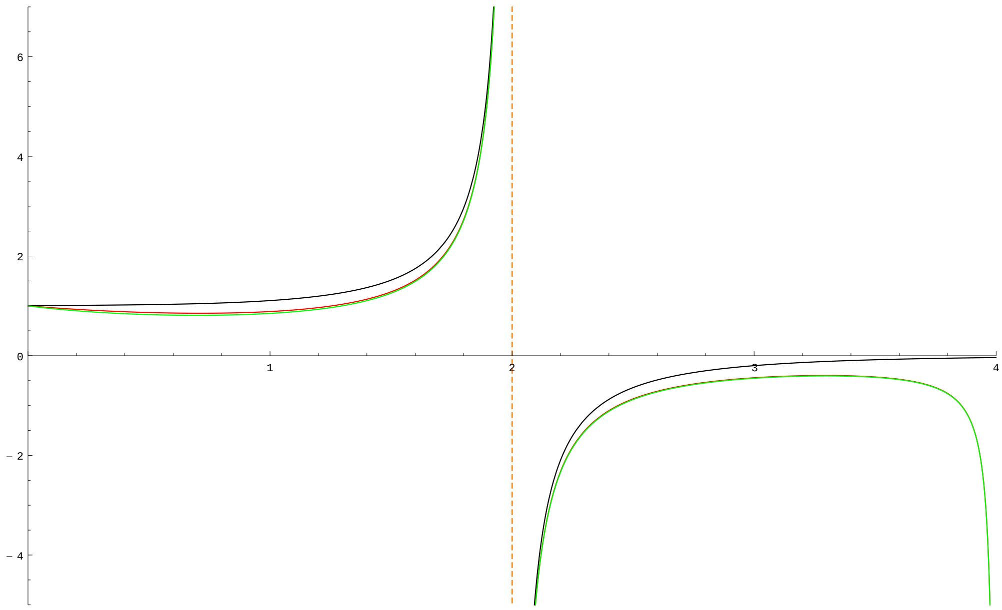


FIGURE 1. Graphic of $-\frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}}$ in black, $2^{-s}\Gamma(1-\frac{s}{2})$ in red and the constant $C_{s,2}$ of (8) in green (case $d=2$). Note that Theorem 2 only involves this constant for $s<2$. We plot the constants in a larger interval for illustration purposes.

For larger $d$, according to [22, Theorem 3.8.2] and [29], the known upper bound, $C$ in (9), equals $1/Q^s$ where $Q$ is the minimal constant such that one can construct an area-regular partition $\{D_j\}$ of $\mathbb{S}^d$ with diameter $\operatorname{diam}(D_j) \le Qn^{-1/d}$. Observe that the area of the spherical cap of (small) radius $r$ is essentially equal to $\frac{r^d}{d}\omega_{d-1}$ and therefore the radius of a spherical cap of area $\omega_d/n$ is approximately $(d\omega_d/\omega_{d-1})^{1/d}n^{-1/d}$. This implies, together with the fact that the spherical cap has the smallest diameter among the sets with the same area, that $Q \ge 2(d\omega_d/\omega_{d-1})^{1/d}$. In fact, it is known how to construct area-regular partitions with diameter $8(d\omega_d/\omega_{d-1})^{1/d}$ (for $d=2$ one can get better constants but always with $Q \ge 4$). These constants are worse than the constant given by Theorem 2.

It has been recently shown, [28], that in the case of $\mathbb{R}^d$ and $d-2<s<d$ the second term of the minimal energy has indeed the form $B_{s,d}n^{1+s/d}$ for a constant $B_{s,d}$.

In the range $d-1<s<d$ we get the following result.

**Corollary 2.** *For any $n \ge 1$ (not necessarily of the form $\pi_L$) for $d-1<s<d$ we have that*

$$\mathcal{E}(s,n) \le V_s(\mathbb{S}^d)n^2 - C_{s,d}n^{1+s/d} + o(n^{1+s/d}),$$

*where $C_{s,d}$ is the constant in (8).*

Indeed, this Corollary follows easily from the fact that for $n \in (\pi_L, \pi_{L+1})$

$$\mathcal{E}(s,n) \le \mathcal{E}(s,\pi_{L+1}) \le \mathbb{E}_{x\in(\mathbb{S}^d)^{\pi_{L+1}}}(E_s(x)),$$

and both $\mathbb{E}_{x\in(\mathbb{S}^d)^{\pi_L}}(E_s(x))$ and $\mathbb{E}_{x\in(\mathbb{S}^d)^{\pi_{L+1}}}(E_s(x))$ have the same two first asymptotic terms. More precisely, if $\pi_L = A_d L^d + O(L^{d-1})$, also $\pi_{L+1} = A_d L^d + O(L^{d-1})$, and

$$\begin{aligned}\mathbb{E}_{x\in(\mathbb{S}^d)^{\pi_{L+1}}}(E_s(x)) &= V_s(\mathbb{S}^d)A_d^2 L^{2d} + O(L^{2d-1}) - C_{s,d}A_d^{1+s/d}L^{d+s} + o(L^{d+s}) \\ &= V_s(\mathbb{S}^d)A_d^2 L^{2d} - C_{s,d}A_d^{1+s/d}L^{d+s} + o(L^{d+s}) \\ &= V_s(\mathbb{S}^d)n^2 - C_{s,d}n^{1+s/d} + o(n^{1+s/d}),\end{aligned}$$

when $d-1 < s < d$ and $n \in (\pi_L, \pi_{L+1})$.

For the logarithmic potential the continuous energy is

$$V_{\log}(\mathbb{S}^d) = \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} \log\frac{1}{\|x-y\|}\,d\mu(x)\,d\mu(y) = \frac{1}{2}(\psi_0(d) - \psi_0(d/2)) - \log 2,$$

where $\psi_0 = (\log\Gamma)'$ is the digamma function. Note that we have

$$V_{\log}(\mathbb{S}^d) = \frac{d}{ds}\Big|_{s=0}\left(V_s(\mathbb{S}^d)\right). \tag{11}$$

In the computation of the derivative of the generalized hypergeometric function in Theorem 1 most of the terms vanish, and we get a closed expression for the expected energy.

**Theorem 3.** *Let $x = (x_1, \ldots, x_n) \in (\mathbb{S}^d)^n$, where $n = \pi_L$, be $n$ points drawn from the harmonic ensemble. Then,*

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_0(x)) = n^2 V_{\log}(\mathbb{S}^d) - \frac{n}{2}\left(\sum_{k=1}^{L}\frac{1}{\frac{d}{2}+k} + H_{L+d-1} + \psi_0(1/2) - \psi_0(d/2)\right),$$

*where $H_k = \sum_{j=1}^{k}\frac{1}{j}$ stands for the $k$th harmonic number.*

**Corollary 3.** *Let $x = (x_1, \ldots, x_n) \in (\mathbb{S}^d)^n$, where $n = \pi_L$, be $n$ points drawn from the harmonic ensemble. Then,*

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_0(x)) = n^2 V_{\log}(\mathbb{S}^d) - \frac{1}{d}n\log n + C_d n + o(n),$$

*where*

$$C_d = \frac{1}{d}\log\frac{2}{d!} + \log 2 + \psi_0\left(\frac{d}{2}\right) + \frac{1}{d}.$$

*In particular, for $d = 2$, we have $C_2 = 1/2 + \log 2 - \gamma \approx 0.6159...$, where $\gamma$ is the Euler-Mascheroni constant.*

For the logarithmic case it is known that

$$\mathcal{E}(0,n) = V_{\log}(\mathbb{S}^d)n^2 - \frac{1}{d}n\log n + O(n).$$

There is a conjecture about the value of the asymptotic coefficient of $n$ for $d = 2, 4, 8$ and 24 which is similar to the one above, see [8]. For $d \geq 3$ there is a lower bound for this coefficient, see [7], and it is negative. But for $d \geq 3$, it is not known if the limit $\lim_{n\to\infty}\left[\mathcal{E}_{log}(n) - V_{\log}(\mathbb{S}^d)n^2 + \frac{1}{d}n\log n\right]/n$ exists. For $d = 2$, Bétermin and Sandier [6] show that the corresponding limit exists and that the conjectured value

$$\frac{1}{d}\log\frac{\omega_d}{|\Lambda_d|}+\zeta'_{\Lambda_d}(0)=-0.0556...,$$

would be correct if the triangular lattice was a minimizer of the Coulombian renormalized energy introduced by Sandier and Serfaty, [31].

As before, we can easily get upper bounds for the constant involved in the above conjectures but, as the constant seems to be negative (it is for $d=2$), we think these bounds are not so interesting. For the sake of illustration:

When $d=2$ we get $C_2=\log 2+\frac{1}{2}-\gamma\approx 0.6159...$ while the constant is known to lie in $(-0.2254,-0.0556)$, see [6]. By taking the expected logarithmic energy of the point process in $\mathbb{S}^2$ given by the zeros of polynomials with random coefficients via the stereographic projection, the authors in [3] get the value $\log 2-\frac{1}{2}=0.1931....$ By using the determinantal process with exponential decay introduced by Krishnapur, i.e. the spherical ensemble, the authors in [1] get $\log 2-\frac{\gamma}{2}\approx 0.4045....$

A final remark is in order: in the case $d=1$ we have that $V_{\log}(\mathbb{S}^1)=0$ and

$$\mathbb{E}_{x\in(\mathbb{S}^1)^n}(E_0(x))=-n\log n+(1-\gamma)n+o(n),$$

while the minimal energy is known to be $\mathcal{E}(0,n)=-n\log n$ (the energy of the roots of unity).

In the limiting case $s=d$ the optimal continuous energy is not finite and this case is called singular. In the discrete setting it is known from [19] that

$$\lim_{n\to\infty}\frac{\mathcal{E}(d,n)}{n^2\log n}=\frac{\omega_{d-1}}{d\omega_d}.$$

It was shown in [8, Proposition 2] that

$$-c(d)n^2+O(n^{2-2/d}\log n)\le\mathcal{E}(d,n)-\frac{\omega_{d-1}}{d\omega_d}n^2\log n\le\frac{\omega_{d-1}}{d\omega_d}n^2\log\log n+o(n^2),$$

with

$$c(d)=\frac{\omega_{d-1}}{d\omega_d}\left(1-\log\frac{\omega_{d-1}}{d\omega_d}+d[\psi_0(d/2)-\psi(1)-\log 2]\right).$$

And it was conjectured [8, Conjecture 5] that

$$\mathcal{E}(d,n)=\frac{\omega_{d-1}}{d\omega_d}n^2\log n+A_{d,d}n^2+O(1),$$

where

$$A_{d,d}=\lim_{s\to d}\left[V_s(\mathbb{S}^d)+\frac{A_{s,d}}{\omega_d^{s/d}}\right],$$

and $A_{s,d}$ is the constant in (10). Observe that when $d=2$ we have $A_{2,2}=-0.0857....$

In the case $d=2$ it was shown in [1] that the correct order of the second term is indeed $n^2$ by showing that the expected 2-energy of the spherical ensemble is

$$\frac{1}{4}n^2\log n+\frac{\gamma}{4}n^2-\frac{n}{8}-\frac{1}{48}+O(n^{-2}).$$

We get a similar result.

**Theorem 4.** *Let $x = (x_1, \dots, x_n) \in (\mathbb{S}^d)^n$, where $n = \pi_L$, be $n$ points drawn from the harmonic ensemble. Then*

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_d(x)) = \frac{\omega_{d-1}}{d\omega_d} n^2 \log n + C_{d,d} n^2 + o(n^2),$$

*where*

$$C_{d,d} = \frac{\omega_{d-1}}{2\omega_d}\left(\psi_0(d+1) - \psi_0\left(\frac{d}{2}+1\right)\right) - \psi_0\left(\frac{d}{2}\right) - \frac{1}{d} - \frac{1}{d}\log\frac{2}{d!}. \tag{12}$$

For example, when $d = 2$ we get

$$\mathbb{E}_{x\in(\mathbb{S}^2)^n}(E_2(x)) = \frac{1}{4} n^2 \log n + \left(\gamma - \frac{3}{8}\right) n^2 + o(n^2),$$

so a larger energy than in [1], as $\gamma - \frac{3}{8} = 0.2022...$ and $\frac{\gamma}{4} = 0.1443....$

As in Corollary 2, we get a bound for $\mathcal{E}(d,n)$ for all $n$ (not only of the form $\pi_L$) and we get the correct order for the second asymptotic term.

**Corollary 4.** *For any $n \geq 1$ (not necessarily of the form $n = \pi_L$),*

$$\mathcal{E}_d(n) \leq \frac{\omega_{d-1}}{d\omega_d} n^2 \log n + C_{d,d} n^2 + o(n^2).$$

*where $C_{d,d}$ is the constant in* (12).

Indeed, see discussion after Corollary 2 and observe that the computation works when $s = d$.

2.2. **Optimality for isotropic projection kernels.** In our next results we deal with more general kernels. We assume that our kernel is invariant by rotations i.e.

$$\text{when } \ d(x,y) = d(z,t) \ \text{ then } \ K(x,y) = K(z,t), \quad x,y,z,t \in \mathbb{S}^d.$$

This implies that the random point field is invariant by rotations, or isotropic, and that it can be written as $K(\langle x,y\rangle)$ for some $K : [-1,1] \to \mathbb{C}$. If we want that this kernel generates a determinantal process, the function $K$ should be positive definite in $\mathbb{S}^d$ and by Schoenberg's Theorem we get that, see [33] or [12, Th. 1, p. 123], it has the form

$$K(x,y) = K(\langle x,y\rangle), \quad K(t) = \sum_{k=0}^{\infty} a_k C_k^{\frac{d-1}{2}}(t), \tag{13}$$

where $C_k^{\frac{d-1}{2}}$ is the Gegenbauer polynomial and the $a_k \geq 0$ satisfy:

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

From the Macchi-Soshknikov theorem [11, Theorem 4.5.5] the fact that $0 \leq a_k \leq \frac{2k+d-1}{d-1}$ is needed also to get a determinantal process as the operator has to have spectrum in $[0,1]$ and $\frac{2k+d-1}{d-1} C_k^{\frac{d-1}{2}}(\langle x,y\rangle)$ (the zonal harmonic of degree $k$) is the projection kernel onto $\mathcal{H}_k$.

As we want the process to have $n$ points a.s. and it is known that the total number of points in the process has the distribution of a sum of independent Bernoulli's with parameters $a_k \frac{d-1}{2k+d-1}$, see [11, Theorem 4.5.3], we impose that our kernel is a projection kernel and therefore

$$a_k = \begin{cases} \frac{2k+d-1}{d-1} & \text{for finitely many } k, \\ 0 & \text{otherwise,} \end{cases} \tag{14}$$

with

$$\sum_{k=0}^{\infty} a_k \binom{d+k-2}{k} = n. \tag{15}$$

Note that such a sequence $a_k$ does not exist for all values of $n$. It does however exist for an infinite sequence of $n$ (which depends on $d$) including those $n$ of the form $n = \pi_L$ for some positive integer $L$.

In such a general setup we get an expression in terms of the integral of the kernel.

**Theorem 5.** *Let $x = (x_1, \ldots, x_n) \in (\mathbb{S}^d)^n$ be $n$ points generated by the determinantal random point process associated with the kernel $K$. Then, for $0 < s < d$,*

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) = V_s(\mathbb{S}^d)n^2 - \frac{\omega_{d-1}}{\omega_d 2^{s/2}} \int_{-1}^{1} \frac{|K(t)|^2(1-t^2)^{d/2-1}}{(1-t)^{s/2}}\, dt.$$

In the particular case of the Riesz 2-energy and $\mathbb{S}^d$ for $d \geq 3$ one can get, after lengthy computations, the following explicit expression for the energy in terms of the coefficients of the kernel. We haven't been able to get simple expressions like this one for other energies.

**Theorem 6.** *In the setting of Theorem 5, for $s = 2$ and $d \geq 3$ we have*

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_2(x)) = V_2(\mathbb{S}^d)\left(n^2 - \sum_{\ell=0}^{\infty} a_\ell \binom{d+\ell-2}{\ell}\left(a_\ell + 2\sum_{j>\ell} a_j\right)\right).$$

The following result provides a criterion to compare energies given by different kernels. In particular it implies that the harmonic kernel gives the smallest expected 2-energy among the different isotropic kernels with the same trace.

**Theorem 7.** *Let $K_a$ and $K_b$ be two kernels with coefficients $a = (a_0, a_1, \ldots)$ and $b = (b_0, b_1, \ldots)$ satifying conditions (14), (15). Let $\mathbb{E}_a$ and $\mathbb{E}_b$ denote respectively the expected value of $E_2(x)$ when $x$ is given by the determinantal point process associated with $K_a$ and $K_b$. Assume that for every $i, j \in \mathbb{N}$ we have:*

$$\text{if } i < j, a_i = 0 \text{ and } a_j > 0 \text{ then } b_i = 0. \tag{16}$$

*Then, $\mathbb{E}_a \leq \mathbb{E}_b$, with strict inequality unless $a = b$. In particular, the harmonic kernel is optimal since (16) is trivially satisfied in that case.*

*Remark* 1. Note that the hypotheses (16) just means that, if there are "holes" (i.e. intermediate zeros) in the sequence $a_0, a_1, \ldots$ then the sequence $b_0, b_1, \ldots$ must also have these holes (thus, informally, Theorem 7 means that more holes imply larger energy).

It is natural to ask if the optimality of the harmonic kernel remains true for general $s$. We thus propose the following conjecture.

**Conjecture 1.** *The harmonic kernel is optimal for all $s \geq 0$ in the sense that if $K$ is another isotropic kernel producing $n = \pi_L$ points in $\mathbb{S}^d$, then the expected value of $E_s(x)$ when $x$ is drawn from the point process given by $K$, is larger than the expected value of $E_s(x)$ when $x$ is drawn from the harmonic ensemble.*

In [26, Theorem 4.4] the authors show that among isotropic kernels the harmonic kernel is optimal with respect to some measures of repulsiveness defined in terms of the second intensity function (as in our case).

2.3. **Expectation and Variance of linear statistics.** Another measure of the uniformity of the distribution of the harmonic ensemble is the computation of the variance of linear statistics.

Let $\mathcal{X}$ the point process with $\pi_L$ points a.s. in $\mathbb{S}^d$ defined by the harmonic ensemble. We denote by $\mu_L$ the empirical measure associated with a realization $x_1, \ldots, x_{\pi_L} \in \mathbb{S}^d$ of this process i.e.

$$\mu_L = \sum_{1 \leq j \leq \pi_L} \delta_{x_j}.$$

Recall: given a function $\phi$ on the sphere, we denote by $\mathcal{X}(\phi) = \sum_{1 \leq j \leq \pi_L} \phi(x_j)$ the linear statistic associated with $\phi$. The expected value of $\mathcal{X}(\phi)$ is easily computed with the first intensity function of the harmonic ensemble:

$$\mathbb{E}(\mathcal{X}(\phi)) = \pi_L \int_{\mathbb{S}^d} \phi d\mu \sim L^d.$$

When $\phi$ is the characteristic function of a spherical cap $\phi = \chi_A$, the random variable $\mathcal{X}(\chi_A)$ is the number of points in $A$ that we denote as $n_A$. For this case of a rough linear statistic we get the following result.

**Proposition 2.** *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 $n_A$ be the number of points in $A$ among $\pi_L$ points drawn from the harmonic ensemble. Then*

$$\operatorname{Var}(n_A) \lesssim L^{d-1} \log L + O(L^{d-1}),$$

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

From the proposition above one can deduce, following Beck [5, Theorem 2] or [1, Theorem 1.1] for this determinantal setting, the following result about the spherical cap discrepancy.

**Corollary 5.** *For every $M > 0$, the spherical cap discrepancy of a set of $n = \pi_L$ points $x = (x_1, \ldots, x_n) \in (\mathbb{S}^d)^n$ drawn from the harmonic ensemble satisfies*

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

*with probability $1 - \frac{1}{n^M}$, i.e. with overwhelming probability.*

When $\phi$ is a smooth function on the sphere we have a better result.

**Proposition 3.** *Let $\phi \in \mathcal{C}^1(\mathbb{S}^d)$ then*

$$\mathrm{Var}(\mathcal{X}(\phi)) \lesssim L^{d-1}.$$

*Moreover this cannot be improved in general. If $\phi(x) = x_i$ where $x_i$ is any coordinate function then*

$$\mathrm{Var}(\mathcal{X}(\phi)) \sim L^{d-1}.$$

Thus in the harmonic setting there is a gain of a $\log L$ term when we move from rough linear statistics to smooth linear statistics.

This is in contrast with the spherical ensemble setting in $\mathbb{S}^2$, for which one can see that the improvement is much better. Indeed, all we need to use is that the kernel associated with the spherical ensemble, denoted as $S_n(x, y)$, satisfies the estimate

$$|S_n(x,y)| = \frac{n}{4\pi}\left(1 - \frac{\|x-y\|^2}{4}\right)^{\frac{n-1}{2}} \lesssim n \exp(-Cnd^2(x,y)),$$

see [1, Formula (4.2)]. For the rough case, the variance of the number of points in a spherical cap of constant radius, for $n$ points drawn from the spherical ensemble, was computed in [1, Lemma 2.1] and it is of order $n^{1/2}$. In the smooth case, if we take a Lipschitz linear statistic with symbol $\phi$ and $\mathcal{X}$ is the point process with $n$ points defined by the spherical ensemble we have that

$$\mathrm{Var}(\mathcal{X}(\phi)) \lesssim \int_{\mathbb{S}^2\times\mathbb{S}^2} |S_n(x,y)|^2\, d^2(x,y) d\mu(x) d\mu(y)$$

$$\lesssim \int_{\mathbb{S}^2} n^2 d^2(x, \mathbf{n}) \exp(-Cnd^2(x,\mathbf{n})) d\mu(x) \le C,$$

where $\mathbf{n} = (0, 0, 1) \in \mathbb{S}^2$ stands for the north pole. Therefore, in the spherical ensemble, there is a gain of a power $n^{1/2}$ when we consider smooth statistics instead of rough statistics.

All this information has been condensed in Table 1. For reference it is also included the variance of linear statistics of the point process generated by random elliptic polynomials which was studied in [36]. To get a fair comparison between processes it is convenient to consider the case of $n = L^2$ points in the spherical ensemble and in the random polynomial case.

2.4. **Separation distance.** Following [1] we also consider the probability distribution of the separation distance sep_dist$(x)$ of a given $x \in (\mathbb{S}^d)^n$, and its counting version

$$G(t, x) = \sharp\{(i, j) : i < j, \|x_i - x_j\| \le t\}.$$

We have the following result which gives a sharp bound on the expected value of $G(t, x)$ for the harmonic kernel.

TABLE 1. Expectation and Variance of linear statistics with different rotation–invariant random point processes in the sphere

| | Harmonic ensemble ($n \sim L^d$) | Spherical ensemble with $n$ points ($d=2$) | Zeros of random polynomials of degree $n$ ($d=2$) |
|---|---|---|---|
| Expectation | $L^d$ | $n$ | $n$ |
| Var. Rough | $L^{d-1}\log L$ | $n^{1/2}$ | $n^{1/2}$ |
| Var. Smooth | $L^{d-1}$ | $n^0$ | $n^{-1}$ |

**Proposition 4.** *Let $x=(x_1,\ldots,x_n)\in(\mathbb{S}^d)^n$ be $n=\pi_L$ points drawn from the harmonic ensemble. Then, for*

$$t\le\frac{d+6}{(2L+d)L},$$

*we have*

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(G(t,x))\le\frac{L(L+d)\pi_L^2\omega_{d-1}}{2(d+2)^2\omega_d}t^{d+2}=C_dn^{2+2/d}t^{d+2}+o(n^{2+2/d})t^{d+2},$$

*where*

$$C_d=\frac{\Gamma(d+1)^{2/d}\omega_{d-1}}{2^{1+2/d}(d+2)^2\omega_d}.$$

Observe that $C_d$ above behaves asymptotically (for large $d$) as $\frac{\sqrt{d}}{2^{3/2}e^2\pi^{1/2}}$. Note that $\text{sep\_dist}(x)\le t$ implies $G(t,x)\ge 1$, hence $\mathbb{P}(\text{sep\_dist}(x)\le t)\le\mathbb{P}(G(t,x)\ge 1)\le\mathbb{E}(G(t,x))$. We thus have:

**Corollary 6.** *Let $x=(x_1,\ldots,x_n)\in(\mathbb{S}^d)^n$ be $n=\pi_L$ points drawn from the harmonic ensemble. For $\alpha\in(0,\frac{d+6}{(2L+d)L})$ we have*

$$\mathbb{P}\left(\text{sep\_dist}(x)\le\alpha n^{-\frac{2d+2}{d^2+2d}}\right)\le\mathbb{E}_{x\in(\mathbb{S}^d)^n}(G(\alpha n^{-\frac{2d+2}{d^2+2d}},x))\le C_d\alpha^{d+2}+o(1).$$

From Corollary 6, an $n$-tuple $(x_1,\ldots,x_n)\in(\mathbb{S}^d)^n$ drawn from the harmonic ensemble likely satisfies

$$\text{sep\_dist}(x)=\Omega\left(n^{-\frac{2d+2}{d^2+2d}}\right).$$

If each point is generated randomly and uniformly in the sphere $\mathbb{S}^d$ it is easy to see that one can just expect $\text{sep\_dist}(x)=\Omega(n^{-2/d})$ which is a worse estimate since

$$\frac{2d+2}{d^2+2d}<\frac{2}{d},\quad d\ge 1.$$

In the two-dimensional case , $d=2$, the spherical ensemble studied in [1] satisfies $\text{sep\_dist}(x)=\Omega(n^{-3/4})$ for large $n$ (see [1, Corollary 1.6]). For the harmonic ensemble we have also $\text{sep\_dist}(x) = \Omega(n^{-3/4})$ for $d = 2$. Moreover, the expected value of $G(\alpha/n^{3/4}, x)$ in both cases satisfies (assymptotically for $n \to \infty$)

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}\left(G\left(\frac{\alpha}{n^{3/4}}, x\right)\right) \leq \frac{\alpha^4}{64}.$$

However, as pointed out before, the optimal separation distance is of order $n^{-1/d}$. Therefore, the separation distance of the harmonic ensemble is better (larger) than the one obtained by uniform points in $\mathbb{S}^d$, but it is still far from the optimal value.

## 3. Proofs

3.1. **Riesz $s$-energy. From Theorem 1 to Theorem 4.** We start with a lemma about integration of zonal functions.

**Lemma 1.** *Let $v \in \mathbb{S}^d$ and let $f : \mathbb{S}^d \to [0, \infty)$ be such that $f(u) = g(\langle u, v\rangle)$ for some measurable function $g$ defined in $[-1, 1]$. Then*

$$\int_{\mathbb{S}^d} f(u)\, d\mu(u) = \frac{\omega_{d-1}}{\omega_d}\int_{-1}^{1} g(t)(1-t^2)^{d/2-1}\, dt.$$

*Proof.* This is a particular case of Funck-Hecke formula, see [27, Theorem 6]. It can also be proved directly using the change of variables theorem for the projection parallel to the space $v^\perp$ defined from the sphere to the cylinder. □

We thus have:

**Lemma 2.** *Let $\mathbf{n} = (0, \dots, 0, 1) \in \mathbb{S}^d$ be the north pole. For $0 < s < d$,*

$$\int_{x\in\mathbb{S}^d} \frac{P_L^{(1+\lambda,\lambda)}(\langle x, \mathbf{n}\rangle)^2}{\|x-\mathbf{n}\|^s}\, d\mu(x) = \frac{\omega_{d-1}}{2^{s/2}\omega_d}\int_{-1}^{1} P_L^{(1+\lambda,\lambda)}(t)^2(1-t)^{\lambda-\frac{s}{2}}(1+t)^{\lambda}\, dt =$$

$$\frac{2^{d-1-s}\omega_{d-1}C_{s,d}(L)\Gamma\left(\frac{d-s}{2}\right)}{\omega_d\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(1+\frac{s}{2}\right)}\cdot {}_4F_3\big(-L, d+L, \frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1, d-\frac{s}{2}+L, -\frac{s}{2}-L; 1\big).$$

*Proof.* The first equality follows directly from Lemma 1. The value of that integral can be found in standard integral tables, see for example [14, p. 288]. This finishes the proof of the lemma. □

*Proof of Theorem 1.* From Corollary 1 we have

$$\begin{aligned}\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) =&\pi_L^2\int_{u,v\in\mathbb{S}^d} \frac{1-\frac{1}{\binom{L+\frac{d}{2}}{L}^2}P_L^{(1+\lambda,\lambda)}(\langle u, v\rangle)^2}{\|u-v\|^s}\, d\mu(u)\, d\mu(v)\\ =&\pi_L^2\int_{u\in\mathbb{S}^d}\frac{1}{\|u-\mathbf{n}\|^s} - \frac{P_L^{(1+\lambda,\lambda)}(\langle u, \mathbf{n}\rangle)^2}{\binom{L+\frac{d}{2}}{L}^2\|u-\mathbf{n}\|^s}\, d\mu(u), \qquad (17)\end{aligned}$$

where $\mathbf{n} = (0, \dots, 0, 1) \in \mathbb{S}^d$ is the north pole. The last equality follows from the rotation invariance of the functions involved. Now we see from (17) that the expected value of the energy $E_s(x)$ is finite if and only if $s < d+2$. Indeed, sending a small cap around the north pole $\mathbf{n}$ to $\mathbb{R}^d$ through the projection onto the first $d$

coordinates and using some trivial bounds, the integral in (17) is finite if and only if for some $\epsilon > 0$ we have

$$\int_{x\in\mathbb{R}^d, \|x\|<\epsilon} \frac{1}{\|x\|^s} \left(1 - \frac{P_L^{(1+\lambda,\lambda)}(1-\|x\|^2/2)^2}{\binom{L+\frac{d}{2}}{L}^2}\right) dx < \infty. \tag{18}$$

An elementary bound on the value of Jacobi polynomials is shown in Lemma 4. Using that result we have

$$\frac{P_L^{(1+\lambda,\lambda)}(1-\|x\|^2/2)}{\binom{L+\frac{d}{2}}{L}} = 1 - \frac{L(L+d)}{2d+4}\|x\|^2 + O(\|x\|^4).$$

We thus have

$$\frac{1}{\|x\|^s} \left(1 - \frac{P_L^{(1+\lambda,\lambda)}(1-\|x\|^2/2)^2}{\binom{L+\frac{d}{2}}{L}^2}\right) \sim \|x\|^{2-s},$$

and passing to polar coordinates the integral in (18) is finite if and only if $s < d+2$.

Now we center in the case $0 < s < d$. From the definition of $V_s(\mathbb{S}^d)$, see (5), and the invariance under rotations of $\|\cdot\|$ we get that

$$\int_{\mathbb{S}^d} \frac{1}{\|x-\mathbf{n}\|^s}\, d\mu(x) = V_s(\mathbb{S}^d).$$

For the second summand in (17) we use Lemma 2. This, together with the asymptotic formula for the gamma function, to get the asymptotic behavior $C_{s,d}(L) \sim L^s$, finishes the proof of Theorem 1. □

Our goal is to study the first terms of the asymptotic expansion of the energy. To some extent, it is possible to get information from the generalized hypergeometric function but we will use estimates of the Jacobi polynomials to get a complete answer.

*Remark* 2. Observe that our generalized hypergeometric function is a terminating balanced series because $(-L)_k = 0$ if $k > L$. Note also that using $(-x)_k = (-1)^k(x-k+1)_k$ we have

$$(-L)_k = (-1)^k(L-k+1)_k = (-1)^k \frac{\Gamma(L+1)}{\Gamma(L-k+1)}, \quad 0 \le k \le L.$$

We drop the dependence on the dimension $d$ and write

$$\begin{aligned} F_L(s) &= {}_4F_3\left(-L, d+L, \frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1, d-\frac{s}{2}+L, -\frac{s}{2}-L; 1\right) \\ &= \sum_{k=0}^{L} \frac{(-L)_k (d+L)_k (\frac{d-s}{2})_k (-\frac{s}{2})_k}{(\frac{d}{2}+1)_k (d-\frac{s}{2}+L)_k (-\frac{s}{2}-L)_k} \frac{1}{k!}. \end{aligned} \tag{19}$$

Observe that, as a function of the variable $s$, $F_L(0) = F_L(d) = 1$.

By induction it is not difficult to show the following

**Proposition 5.** *For $0 < s \leq d$, $L \geq 1$ and $0 \leq k \leq L$ we have*

$$0 < \frac{(-L)_k (d+L)_k}{(d-\frac{s}{2}+L)_k(-\frac{s}{2}-L)_k} \leq 1, \tag{20}$$

*and the quotient is decreasing in $k$.*

From this proposition it is easy to deduce that when $\left(-\frac{s}{2}\right)_k < 0$ for all $k \geq 1$, for example when $0 < s < 2$, we have

$${}_2F_1\left(\frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1; 1\right) \leq F_L(s) \leq 1,$$

where ${}_2F_1$, is the (standard) hypergeometric function. By Gauss theorem (as $s > -1$)

$${}_2F_1\left(\frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1; 1\right) = \frac{\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(1+s\right)}{\Gamma\left(1+\frac{s}{2}\right)\Gamma\left(1+\frac{d+s}{2}\right)}.$$

In fact, when $s$ is even, $s = 2m$ for some $m \in \mathbb{N}$, the sum in the generalized hypergeometric function (19) is just up to $m$ because $\left(-\frac{s}{2}\right)_k = (-m)_k = 0$, when $k > m$.

From the asymptotic property of the gamma function

$$\lim_{n\to\infty} \frac{\Gamma(n+\alpha)}{\Gamma(n)n^\alpha} = 1, \quad \alpha \in \mathbb{R},$$

and the observation above, it follows that for even $s$

$$F_L(s) \to {}_2F_1\left(\frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1; 1\right) \tag{21}$$

when $L$ goes to $+\infty$. We will see from our next results that this limit holds for all $0 < s < d$.

Now we prove the asymptotic expansion of Riesz $s$-energy. The main ingredient in the proof of Theorem 2 is the following estimate in terms of Bessel functions $J_\nu$ of the first kind. Recall that for $\nu \in \mathbb{C}$, Bessel functions of the first kind of order $\nu$ are the canonical solutions of the second order differential equation

$$\frac{d^2y}{dz^2} + \frac{1}{z}\frac{dy}{dz} + \left(1 - \frac{\nu^2}{z^2}\right) y = 0.$$

**Proposition 6.**

$$\begin{aligned}
&\lim_{L\to\infty} \frac{1}{L^s} \int_{-1}^{1} P_L^{(1+\lambda,\lambda)}(t)^2 (1-t)^{\lambda-\frac{s}{2}}(1+t)^\lambda \, dt = 2^{\frac{s}{2}+d} \int_0^\infty \frac{J_{1+\lambda}(x)^2}{x^{1+s}} dx \\
&= 2^{\frac{s}{2}-1} \frac{\Gamma\left(\frac{d-s}{2}\right)}{\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(1+\frac{s}{2}\right)} {}_2F_1\left(\frac{d-s}{2}, \frac{d+1}{2}; d+1; 1\right) \\
&= 2^{d+\frac{s}{2}-1} \frac{\Gamma\left(\frac{d-s}{2}\right)\Gamma\left(\frac{1+s}{2}\right)}{\sqrt{\pi}\Gamma\left(1+\frac{s}{2}\right)\Gamma\left(1+\frac{s+d}{2}\right)}.
\end{aligned}$$

Observe that from Proposition 6 we get the following

**Corollary 7.** *Given $F_L(s)$ as in* (19) *then for* $0 < s < d$

$$\lim_{L\to+\infty} F_L(s) = {}_2F_1\left(\frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1; 1\right).$$

*Proof.* From Lemma 2 we get that

$$F_L(s) = \frac{\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(1+\frac{s}{2}\right)}{2^{d-s/2-1}C_{s,d}(L)\Gamma\left(\frac{d-s}{2}\right)}\int_{-1}^{1} P_L^{(1+\lambda,\lambda)}(t)^2(1-t)^{\lambda-\frac{s}{2}}(1+t)^{\lambda}\,dt.$$

Now from the Proposition above and Legendre's duplication formula

$$\sqrt{\pi}\Gamma(x) = 2^{x-1}\Gamma\left(\frac{x+1}{2}\right)\Gamma\left(\frac{x}{2}\right) \tag{22}$$

we get the result. □

*Proof of Proposition 6.* The second equality is from [14, p.47, (4)]. For the last equality use Gauss theorem about the hypergeometric function and the duplication formula (22).

For the first equality, we split the integral

$$\begin{aligned}&\int_{-1}^{1} L^{-s}P_L^{(1+\lambda,\lambda)}(t)^2(1-t)^{\lambda-\frac{s}{2}}(1+t)^{\lambda}\,dt\\ &=\left[\int_{-1}^{-\cos\frac{c}{L}} + \int_{-\cos\frac{c}{L}}^{\cos\frac{c}{L}} + \int_{\cos\frac{c}{L}}^{1}\right] L^{-s}P_L^{(1+\lambda,\lambda)}(t)^2(1-t)^{\lambda-\frac{s}{2}}(1+t)^{\lambda}\,dt\\ &=A(c,L)+B(c,L)+C(c,L),\end{aligned}$$

where $c > 0$ is fixed and $c < \pi L$. For the boundary parts we do a change of variables $t = \cos(x/L)$ to get

$$C(c,L) =$$

$$2^{s/2}\int_0^c L^{-2-2\lambda}P_L^{(1+\lambda,\lambda)}\left(\cos\frac{x}{L}\right)^2\left(\frac{\sin\frac{x}{L}}{\frac{x}{L}}\right)^{2\lambda+1}\left(\frac{1-\cos\frac{x}{L}}{\frac{1}{2}\left(\frac{x}{L}\right)^2}\right)^{-s/2} x^{2\lambda+1-s}\,dx.$$

Using the Mehler-Heine estimates (3) and the elementary limits

$$\lim_{L\to\infty}\frac{\sin\frac{x}{L}}{\frac{x}{L}} = 1, \quad \lim_{L\to\infty}\frac{1-\cos\frac{x}{L}}{\frac{1}{2}\left(\frac{x}{L}\right)^2} = 1,$$

we conclude:

$$\lim_{L\to\infty} C(c,L) = 2^{\frac{s}{2}+d}\int_0^c \frac{J_{1+\lambda}(x)^2}{x^{1+s}}dx.$$

For the other end of the interval, using the change of variables $t = -\cos(x/L)$ we get

$$A(c,L) = \int_0^c L^{-2-2\lambda}P_L^{(1+\lambda,\lambda)}\left(-\cos\frac{x}{L}\right)^2\left(\frac{\sin\frac{x}{L}}{\frac{x}{L}}\right)^{2\lambda+1}\left(\frac{1+\cos\frac{x}{L}}{\left(\frac{x}{L}\right)^2}\right)^{-s/2} x^{2\lambda+1}dx,$$

and, again using (3), this expression converges to zero when $L \to \infty$. For the middle integral we get, after the change of variables $t = -\cos\theta$ and the use of the asymptotic estimate for Jacobi polynomials (2)

$$0 \le B(c,L) \lesssim \frac{1}{L^{s+1}} \int_{\frac{c}{L}}^{\pi-\frac{c}{L}} \frac{1}{(\sin\frac{\theta}{2})^{s+2}} d\theta \lesssim \frac{1}{L^{s+1}} \int_{\frac{c}{L}}^{\pi-\frac{c}{L}} \frac{1}{\theta^{s+2}} d\theta$$
$$\le \frac{1}{L^{s+1}} \int_{\frac{c}{L}}^{+\infty} \frac{1}{\theta^{s+2}} d\theta = \frac{1}{(s+1)c^{s+1}}.$$

We have then proved that for all $c > 0$,

$$2^{\frac{s}{2}+d} \int_0^c \frac{J_{1+\lambda}(x)^2}{x^{1+s}} dx \le \lim_{L\to\infty} \left( \int_{-1}^1 L^{-s} P_L^{(1+\lambda,\lambda)}(t)^2 (1-t)^{\lambda-\frac{s}{2}} (1+t)^\lambda \, dt \right)$$
$$\le \frac{R(s,d)}{(s+1)c^{s+1}} + 2^{\frac{s}{2}+d} \int_0^\infty \frac{J_{1+\lambda}(x)^2}{x^{1+s}} \, dx,$$

with $R(s,d)$ a constant independent of $c$. Taking the limit as $c \to \infty$, the result follows. □

*Proof of Theorem 2.* From Theorem 1 we get that

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) = \pi_L^2 V_s(\mathbb{S}^d) - \frac{\pi_L^2 \omega_{d-1}}{\binom{L+\frac{d}{2}}{L}^2 2^{s/2}\omega_d} \int_{-1}^1 P_L^{(1+\lambda,\lambda)}(t)^2 (1-t)^{\lambda-\frac{s}{2}} (1+t)^\lambda \, dt.$$

When $L \to \infty$

$$\frac{\pi_L}{\binom{L+\frac{d}{2}}{L}^2} = \frac{2\Gamma\left(1+\frac{d}{2}\right)^2}{d!} + o(1) \text{ and } \pi_L^{s/d} = \left(\frac{2}{d!}\right)^{s/d} L^s(1+o(1)).$$

From

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) - \pi_L^2 V_s(\mathbb{S}^d) = \pi_L^{1+\frac{s}{d}} \left(\frac{d!}{2}\right)^{-1+\frac{s}{d}} \Gamma\left(1+\frac{d}{2}\right)^2 \frac{\omega_{d-1}}{2^{s/2}\omega_d}$$
$$\times (1+o(1)) \int_{-1}^1 L^{-s} P_L^{(1+\lambda,\lambda)}(t)^2 (1-t)^{\lambda-\frac{s}{2}} (1+t)^\lambda \, dt,$$

and Proposition 6 we get the result with

$$C_{s,d} = \left(\frac{d!}{2}\right)^{-1+\frac{s}{d}} \frac{\omega_{d-1}}{\omega_d} 2^{d-1} \frac{\Gamma\left(1+\frac{d}{2}\right)^2 \Gamma\left(\frac{d-s}{2}\right) \Gamma\left(\frac{1+s}{2}\right)}{\sqrt{\pi}\Gamma\left(1+\frac{s}{2}\right) \Gamma\left(1+\frac{s+d}{2}\right)}.$$

Finally, recall the value of $V_s(\mathbb{S}^d)$ from (6) which yields

$$\frac{\omega_{d-1}}{\omega_d} 2^{d-1} \Gamma\left(\frac{d}{2}\right) \Gamma\left(\frac{d-s}{2}\right) = 2^s V_s(\mathbb{S}^d) \Gamma\left(d - \frac{s}{2}\right).$$

□

*Proof of Theorem 3.* We compute the derivative at $s=0$ of the expression given in Theorem 1, which according to Corollary 1 equals the expected value of the logarithmic energy. We then have (using (11) for the first term):

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_0(x)) = \pi_L^2 V_{\log}(\mathbb{S}^d) - C_L\frac{d}{ds}\mid_{s=0^+}(D_L(s)E_L(s)F_L(s)),$$

where

$$\begin{aligned}
C_L &= \frac{2^{d-1}\omega_{d-1}\pi_L^2\Gamma\left(L+\frac{d}{2}\right)\Gamma\left(L+\frac{d}{2}+1\right)}{\binom{L+\frac{d}{2}}{L}^2\omega_d\Gamma(L+1)^2\Gamma\left(1+\frac{d}{2}\right)},\\
D_L(s) &= \frac{\Gamma\left(L+\frac{s}{2}+1\right)}{\Gamma\left(1+\frac{s}{2}\right)},\\
E_L(s) &= \frac{2^{-s}\Gamma\left(\frac{d-s}{2}\right)}{\Gamma\left(L-\frac{s}{2}+d\right)},\\
F_L(s) &= {}_4F_3\left(-L, d+L, \frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1, d-\frac{s}{2}+L, -\frac{s}{2}-L; 1\right)\\
&= \sum_{k=0}^{L}\frac{(-L)_k(d+L)_k(\frac{d-s}{2})_k(-\frac{s}{2})_k}{(\frac{d}{2}+1)_k(d-\frac{s}{2}+L)_k(-\frac{s}{2}-L)_k}\frac{1}{k!}.
\end{aligned}$$

We have that

$$D_L(0) = L!,\quad E_L(0) = \frac{\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(d+L\right)},\quad F_L(0)=1.$$

The derivatives at 0 of $D_L$ and $E_L$ are:

$$\begin{aligned}
D_L'(0) &= \frac{1}{2}\left(\Gamma'\left(L+1\right)-\Gamma\left(L+1\right)\Gamma'\left(1\right)\right) = \frac{L!}{2}H_L,\\
E_L'(0) &= \frac{B(0)}{2}\left(H_{L+d-1}-\gamma-\psi_0(d/2)-2\log 2\right),
\end{aligned}$$

where $\gamma = -\psi_0(1) = -\Gamma'(1)$ is the Euler-Mascheroni constant.

Finally, from the series expression of $F_L(s)$ and using that $(0)_k = 0$ when $k>0$ we deduce that

$$F_L'(0) = \sum_{k=1}^{L}\frac{(-L)_k(d+L)_k(\frac{d}{2})_k\frac{d}{ds}[(-\frac{s}{2})_k]_{s=0}}{(\frac{d}{2}+1)_k(d+L)_k(-L)_k}\frac{1}{k!} = \sum_{k=1}^{L}\frac{d}{ds}\Big[\left(-\frac{s}{2}\right)_k\Big]_{s=0}\frac{d}{d+2k}\frac{1}{k!}.$$

For $k\geq$ we have:

$$\frac{d}{ds}\Big[\left(-\frac{s}{2}\right)_k\Big] = -\frac{1}{2}\left(-\frac{s}{2}\right)_k\left(\psi_0\left(k-\frac{s}{2}\right)-\psi_0\left(-\frac{s}{2}\right)\right)\to -\frac{1}{2}\Gamma(k),\ s\to 0^+,$$

and conclude that

$$F_L'(0) = -\frac{d}{2}\sum_{k=1}^{L}\frac{1}{k(d+2k)}.$$

We have then proved that

$$\frac{d}{ds}\mid_{s=0^+}(D_L(s)E_L(s)F_L(s))$$

$$= \frac{\Gamma\left(\frac{d}{2}\right) L!}{2\Gamma\left(d+L\right)} \left( H_L + H_{L+d-1} + \psi_0(1/2) - \psi_0(d/2) - d\sum_{k=1}^{L} \frac{1}{k(d+2k)} \right).$$

Note that

$$d\sum_{k=1}^{L} \frac{1}{k(d+2k)} = \sum_{k=1}^{L} \left( \frac{1}{k} - \frac{1}{\frac{d}{2}+k} \right) = H_L - \sum_{k=1}^{L} \frac{1}{\frac{d}{2}+k}.$$

We have proved that

$$\begin{aligned}&\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_0(x))\\ =&\pi_L^2 V_{\log}(\mathbb{S}^d) - \frac{C_L\Gamma\left(\frac{d}{2}\right) L!}{2\Gamma\left(d+L\right)} \left( \sum_{k=1}^{L} \frac{1}{\frac{d}{2}+k} + H_{L+d-1} + \psi_0(1/2) - \psi_0(d/2) \right).\end{aligned}$$

Finally, by using the duplication formula (22) one can easily check that

$$\frac{C_L\Gamma\left(\frac{d}{2}\right) L!}{\Gamma\left(d+L\right)} = \pi_L.$$

□

*Proof of Corollary 3.* We compute the asymptotic behavior based on the equality of Theorem 3. From the recurrence relation

$$\psi_0(x+1) = \psi_0(x) + \frac{1}{x}$$

we get that

$$\sum_{k=1}^{L} \frac{1}{\frac{d}{2}+k} = \psi_0\left(\frac{d}{2}+1+L\right) - \psi_0\left(\frac{d}{2}\right) - \frac{2}{d}$$

Recall the asymptotic expansions (for $x, n \to \infty$):

$$\psi_0(x) = \log x - \frac{1}{2x} + o(x^{-1}), \qquad H_n = \psi_0(n+1) + \gamma = \log n + \gamma + \frac{1}{2n} + o(n^{-1})$$

So when $L \to \infty$ we have from Theorem 3 ($\psi_0(1/2) = -\gamma - 2\log 2$)

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_0(x)) = \pi_L^2 V_{\log}(\mathbb{S}^d) - \pi_L \left( \log L - \log 2 - \psi_0\left(\frac{d}{2}\right) - \frac{1}{d} + o(1) \right).$$

From the asymptotic expression (1) we have as $L \to \infty$:

$$\log L = \frac{\log \pi_L}{d} - \frac{\log(2/d!)}{d} + o(1), \tag{23}$$

so we have proved:

$$\begin{aligned}\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_0(x)) &= \pi_L^2 V_{\log}(\mathbb{S}^d) - \frac{1}{d}\pi_L \log \pi_L \\ &\quad + \left( \frac{1}{d}\log\frac{2}{d!} + \log 2 + \psi_0\left(\frac{d}{2}\right) + \frac{1}{d} \right) \pi_L + o(\pi_L),\end{aligned}$$

as wanted. □

To prove Theorem 4 we use the following result.

**Proposition 7.** *We have that*

$$\lim_{L\to\infty}\frac{d}{ds}\left[{}_4F_3\left(-L,d+L,\frac{d-s}{2},-\frac{s}{2};\frac{d}{2}+1,d-\frac{s}{2}+L,-\frac{s}{2}-L;1\right)\right]_{s=d}$$
$$=\frac{d}{ds}\left[{}_2F_1\left(\frac{d-s}{2},-\frac{s}{2};\frac{d}{2}+1;1\right)\right]_{s=d}=-\frac{1}{2}\sum_{k=1}^{\infty}\frac{(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k}\frac{1}{k}$$
$$=\frac{1}{2}\left(\psi_0(d+1)-\psi_0\left(\frac{d}{2}+1\right)\right).$$

*Proof.* Let, as before,

$$F_L(s)={}_4F_3\left(-L,d+L,\frac{d-s}{2},-\frac{s}{2};\frac{d}{2}+1,d-\frac{s}{2}+L,-\frac{s}{2}-L;1\right).$$

Then from the fact that

$$\lim_{s\to d^-}\frac{d}{ds}\left[\left(\frac{d-s}{2}\right)_k\right]=-\frac{\Gamma(k)}{2},$$

we get that

$$F_L'(d)=-\frac{1}{2}\sum_{k=1}^{L}\frac{(-L)_k(d+L)_k(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k(\frac{d}{2}+L)_k(-\frac{d}{2}-L)_k}\frac{1}{k}.$$

Observe that, as in the discussion before Proposition 6, when $d$ is even, the sum in the generalized hypergeometric function is up to $d/2$ and then as for all $k=1,\dots,d/2$,

$$\lim_{L\to+\infty}\frac{(-L)_k(d+L)_k}{(\frac{d}{2}+L)_k(-\frac{d}{2}-L)_k}=1,$$

we get that

$$\lim_{L\to+\infty}F_L'(d)=-\frac{1}{2}\sum_{k=1}^{d/2}\frac{(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k}\frac{1}{k}=\frac{d}{ds}\left[{}_2F_1\left(\frac{d-s}{2},-\frac{s}{2};\frac{d}{2}+1;1\right)\right]_{s=d}$$

For odd $d$ also $F_L'(d)$ converges when $L\to+\infty$ to

$$\frac{d}{ds}\left[{}_2F_1\left(\frac{d-s}{2},-\frac{s}{2};\frac{d}{2}+1;1\right)\right]_{s=d}=-\frac{1}{2}\sum_{k=1}^{\infty}\frac{(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k}\frac{1}{k}.$$

Indeed, we have that for $1\le k\le L$,

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

By Euler's reflection formula for the Gamma function and Stirling approximation we get that

$$\left|\Gamma\left(\frac{d}{2}+k+1\right)\Gamma\left(\frac{d}{2}-k+1\right)\right|\sim\pi k^d,$$

and therefore

$$\sum_{k=1}^{\infty}\left|\frac{(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k}\frac{1}{k}\right| \lesssim \sum_{k=1}^{\infty}\frac{1}{k^{d+1}}.$$

Given $\epsilon > 0$, we choose $n_0$ such that

$$\sum_{k=n_0+1}^{\infty}\left|\frac{(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k}\frac{1}{k}\right| < \epsilon,$$

and we get from inequality (20) that for sufficiently large $L > n_0$

$$\left|\sum_{k=n_0+1}^{L}\frac{(-L)_k(d+L)_k(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k(\frac{d}{2}+L)_k(-\frac{d}{2}-L)_k}\frac{1}{k}\right| < \epsilon.$$

Now the result follows as before from the fact that for all $k = 1, \ldots, n_0$,

$$\lim_{L\to+\infty}\frac{(-L)_k(d+L)_k}{(\frac{d}{2}+L)_k(-\frac{d}{2}-L)_k} = 1,$$

and therefore

$$-\frac{1}{2}\sum_{k=1}^{n_0}\frac{(-L)_k(d+L)_k(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k(\frac{d}{2}+L)_k(-\frac{d}{2}-L)_k}\frac{1}{k} \to \sum_{k=1}^{n_0}\frac{(-\frac{d}{2})_k}{(\frac{d}{2}+1)_k}\frac{1}{k},$$

when $L \to +\infty$.

The last equality follows from Gauss theorem

$$\frac{d}{ds}\left[{}_2F_1\left(\frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1; 1\right)\right]_{s=d} = \frac{1}{2}\frac{\Gamma'(d+1)\Gamma\left(\frac{d}{2}+1\right) - \Gamma(d+1)\Gamma'\left(\frac{d}{2}+1\right)}{\Gamma(d+1)\Gamma\left(\frac{d}{2}+1\right)}$$
$$= \frac{1}{2}(\psi_0(d+1) - \psi_0(\frac{d}{2}+1)).$$

□

*Proof of Theorem 4.* The function $V_s(\mathbb{S}^d)$ is meromorphic with a simple pole in $s = d$ (because of the term $\Gamma(\frac{d-s}{2})$) and the residue in $d$ equals

$$\lim_{s\to d} V_s(\mathbb{S}^d)(s-d) = -\frac{\omega_{d-1}}{\omega_d}.$$

We can write from Theorem 1

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) = n^2 V_s(\mathbb{S}^d)\left(1 - U(s)\right),$$

where

$$U(s) = \frac{dF_L(s)\Gamma\left(d-\frac{s}{2}\right)\Gamma\left(L+\frac{s}{2}+1\right)}{(2L+d)\Gamma\left(1+\frac{s}{2}\right)\Gamma\left(L-\frac{s}{2}+d\right)},$$

and $F_L(s) = {}_4F_3\left(-L, d+L, \frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1, d-\frac{s}{2}+L, -\frac{s}{2}-L; 1\right)$. As $U(d) = 1$ we have that

$$\lim_{s\to d}\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) = \frac{\omega_{d-1}}{\omega_d}\pi_L^2 U'(d).$$

We compute this derivative by writing $U(s) = \frac{d}{2L+d} F_L(s) G_L(s)$ with

$$G_L(s) = \frac{(\frac{s}{2}+1)_L}{(d-\frac{s}{2})_L},$$

and using

$$G_L'(d) = \frac{2L+d}{d}\left(\psi_0\left(\frac{d}{2}+L\right) - \psi_0\left(\frac{d}{2}\right) + \frac{1}{d+2L} - \frac{1}{d}\right),$$

and the asymptotic formula for the digamma function

$$\psi_0\left(\frac{d}{2}+L\right) + \frac{1}{d+2L} = \frac{1}{d}\log \pi_L - \frac{1}{d}\log\frac{2}{d!} + o(1).$$

Finally, we get

$$\lim_{s\to d} \mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) = \frac{\omega_{d-1}}{d\omega_d}\pi_L^2 \log \pi_L$$
$$+\pi_L^2\left(\frac{\omega_{d-1}}{\omega_d}F'(d) - \psi_0\left(\frac{d}{2}\right) - \frac{1}{d} - \frac{1}{d}\log\frac{2}{d!} + o(1)\right),$$

where

$$F_L'(d) = \frac{d}{ds}\left[{}_4F_3\left(-L, d+L, \frac{d-s}{2}, -\frac{s}{2}; \frac{d}{2}+1, d-\frac{s}{2}+L, -\frac{s}{2}-L; 1\right)\right]_{s=d}.$$

The result then follows from Proposition 7. ☐

### 3.2. **Optimality among isotropic kernels. Proof of theorems 5, 6 and 7.**

*Proof of Theorem 5.* From Corollary 1 and using the rotational invariance we have

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_s(x)) = \int_{u,v\in\mathbb{S}^d} \frac{n^2 - |K(\langle u,v\rangle)|^2}{(2-2\langle u,v\rangle)^{s/2}}\, d\mu(u)\, d\mu(v) =$$
$$V_s(\mathbb{S}^d)n^2 - \int_{u\in\mathbb{S}^d} \frac{|K(\langle u,\mathbf{n}\rangle)|^2}{(2-2\langle u,\mathbf{n}\rangle)^{s/2}}\, d\mu(u).$$

The theorem follows from Lemma 1. ☐

*Remark* 3. We can substitute $K(t)$ by its expansion (13) to get a formula for the second integral in Theorem 5:

$$\int_{-1}^{1} \frac{|K(t)|^2(1-t^2)^{d/2-1}}{(1-t)^{s/2}}\, dt =$$
$$\sum_{j,k=0}^{\infty} a_k a_j \int_{-1}^{1} (1-t)^{d/2-1-s/2}(1+t)^{d/2-1} C_k^{\frac{d-1}{2}}(t) C_j^{\frac{d-1}{2}}(t)\, dt \tag{24}$$
$$= \sum_{j,k=0}^{\infty} a_k a_j \frac{2^{d-1-s/2}\Gamma\left(\frac{d-s}{2}\right)\Gamma\left(\frac{d}{2}\right)\Gamma\left(\frac{2j+s}{2}\right)\Gamma(d-1+j)\Gamma(d-1+k)}{\Gamma(j+1)\Gamma(k+1)\Gamma\left(\frac{s}{2}\right)\Gamma\left(\frac{2d+2j-s}{2}\right)\Gamma(d-1)^2}\times$$
$${}_4F_3\left(-k, k+d-1, \frac{d-s}{2}, 1-\frac{s}{2}; \frac{d}{2}, d-\frac{s}{2}+j, 1-\frac{s}{2}-j; 1\right).$$

3.2.1. *The special case $s = 2$ and $d \geq 3$. Proof of Theorem 6.* One can use Theorem 5 and (24) to write

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_2(x)) = V_2(\mathbb{S}^d)n^2 - \frac{\omega_{d-1}}{2\omega_d}\sum_{j,k=0}^{\infty} a_k a_j Q^d_{k,j}, \tag{25}$$

where

$$Q^d_{k,j} = \int_{-1}^{1}(1-t)^{d/2-2}(1+t)^{d/2-1}C_k^{\frac{d-1}{2}}(t)C_j^{\frac{d-1}{2}}(t)\,dt.$$

The following lemma shows that these integrals can be solved exactly.

**Lemma 3.** *Let $d \geq 3$ and $s = 2$. Then for all $0 \leq k \leq j$ we have*

$$Q^d_{j,k} = Q^d_{k,j} = Q^d_{k,k} = 2^{d-2}\binom{d+k-2}{k}\mathrm{B}\left(\frac{d}{2},\frac{d}{2}-1\right) = \binom{d+k-2}{k}Q^d_{0,0}.$$

*Remark* 4. The value of the integral in Lemma 3 seems to be known just in the case $k = j$ (see for example [16, p. 803] which gives an alternative but equivalent expression). Note also that we have

$$\frac{\omega_{d-1}}{2\omega_d}Q^d_{0,0} = V_2(\mathbb{S}^d) = \frac{d-1}{2d-4}. \tag{26}$$

The proof of Lemma 3 will be a long computation. We will use the following basic integral, valid for $a, b > 0$:

$$\int_{-1}^{1}(1-t)^a(1+t)^b\,dt \overset{t=2u-1}{=} 2^{a+b+1}\int_0^1(1-u)^a u^b\,du = 2^{a+b+1}\mathrm{B}(a+1,b+1). \tag{27}$$

We will also use Legendre's duplication formula in the following form.

$$\Gamma\left(\frac{d-1}{2}\right) = \frac{\sqrt{\pi}\Gamma(d-2)}{2^{d-3}\Gamma\left(\frac{d}{2}-1\right)}. \tag{28}$$

*Proof of Lemma 3.* We start by computing a few cases for small $k, j$. For $k = j = 0$ we have:

$$Q^d_{0,0} = \int_{-1}^{1}(1-t)^{d/2-2}(1+t)^{d/2-1}\,dt \overset{(27)}{=} 2^{d-2}\mathrm{B}\left(\frac{d}{2},\frac{d}{2}-1\right).$$

For $k = 1, j = 0$ we have:

$$\begin{aligned}
Q^d_{1,0} &= \int_{-1}^{1}(1-t)^{d/2-2}(1+t)^{d/2-1}(d-1)t\,dt\\
&= -(d-1)\left(\int_{-1}^{1}(1-t)^{d/2-2}(1+t)^{d/2-1}(1-t-1)\,dt\right)\\
&= -(d-1)\left(\int_{-1}^{1}(1-t)^{d/2-1}(1+t)^{d/2-1}\,dt - Q^d_{0,0}\right)\\
&\overset{(27)}{=} -(d-1)\left(2^{d-1}\mathrm{B}\left(\frac{d}{2},\frac{d}{2}\right) - Q^d_{0,0}\right) = 2^{d-2}\mathrm{B}\left(\frac{d}{2},\frac{d}{2}-1\right) = Q^d_{0,0}.
\end{aligned}$$

For $k=j=1$ we have:

$$\begin{aligned} Q_{1,1}^d &= \int_{-1}^1 (1-t)^{d/2-2}(1+t)^{d/2-1}(d-1)^2 t^2\, dt \\ &= -(d-1)^2\left(\int_{-1}^1 (1-t)^{d/2-1}(1+t)^{d/2}\, dt - Q_{0,0}^d\right) \\ &\overset{(27)}{=} -(d-1)^2\left(2^d \mathrm{B}\left(\frac{d}{2},\frac{d+1}{2}\right) - Q_{0,0}^d\right) = (d-1)Q_{0,0}^d. \end{aligned}$$

We are now ready to prove the general case. Recall the recurrence relation satisfied by Gegenbauer's polynomials:

$$\ell C_\ell^{d/2-1/2}(t) = (2\ell+d-3)\; t\, C_{\ell-1}^{d/2-1/2}(t) - (\ell+d-3)\, C_{\ell-2}^{d/2-1/2}(t) =$$

$$-(2\ell+d-3)\;(1-t)\, C_{\ell-1}^{d/2-1/2}(t) + (2\ell+d-3)\, C_{\ell-1}^{d/2-1/2}(t) - (\ell+d-3)\, C_{\ell-2}^{d/2-1/2}(t).$$

We thus have

$$\begin{aligned} kQ_{k,j}^d =&\; (2k+d-3)\, Q_{k-1,j}^d - (k+d-3)\, Q_{k-2,j}^d \\ &- \;(2k+d-3)\int_{-1}^1 (1-t^2)^{d/2-1} C_{k-1}^{d/2-1/2}(t) C_j^{d/2-1/2}(t)\, dt, \end{aligned}$$

which implies for $k \geq 2$:

$$k\, Q_{k,j}^d = \begin{cases} (2k+d-3)\, Q_{k-1,j}^d - (k+d-3)\, Q_{k-2,j}^d & k \neq j+1 \\ (2k+d-3)\, Q_{k-1,j}^d - (k+d-3)\, Q_{k-2,j}^d - \frac{\pi 2^{3-d}\Gamma(d+k-2)}{\Gamma(k)\Gamma\left(\frac{d}{2}-\frac{1}{2}\right)^2} & k = j+1 \end{cases} \tag{29}$$

These equalities together with $Q_{k,j}^d = Q_{j,k}^d$ and the values of $Q_{0,0}^d$, $Q_{1,0}^d$ and $Q_{1,1}^d$ define the value of $Q_{k,j}^d$ for all $k, j, d$. We finish the proof with five claims.

**Claim 1.** For all $k \geq 0$ we have $Q_{k,0}^d = Q_{0,0}^d$.

Indeed, we have already proved it for $k=1$. We now use induction, so we let $k \geq 2$ and assume that the claim is true up to $k-1$. From (29), we have

$$Q_{k,0}^d = \frac{1}{k}\left((2k+d-3)\, Q_{k-1,0}^d - (k+d-3)\, Q_{k-2,0}^d\right) = Q_{0,0}^d,$$

as wanted.

**Claim 2.** For all $k \geq 1$ we have $Q_{k,1}^d = Q_{1,1}^d$.

Indeed, we have

$$Q_{2,1}^d = \frac{1}{2}\left((d+1)\, Q_{1,1}^d - (d-1)\, Q_{0,1}^d - \frac{\pi 2^{3-d}\Gamma(d)}{\Gamma\left(\frac{d}{2}-\frac{1}{2}\right)^2}\right) = Q_{1,1}^d,$$

where for the last equality we use (28). Again by induction on $k$ we assume that $k \geq 3$ and the claim is true up to $k-1$. Then, from (29)

$$Q_{k,1}^d = \frac{1}{k}\left((2k+d-3)\, Q_{k-1,j}^d - (k+d-3)\, Q_{k-2,j}^d\right) = Q_{1,1}^d,$$

as wanted.

**Claim 3.** The lemma holds for $0 \le k \le j$.

Indeed, from Claims 1 and 2 we know this for $k = 0, 1$. Again using induction and (29), as long as $k \le j$ we have

$$\begin{aligned} Q^d_{k,1} =& \frac{1}{k}\left((2k+d-3)\, Q^d_{k-1,j} - (k+d-3)\, Q^d_{k-2,j}\right) \\ =& \frac{Q^d_{0,0}}{k}\left((2k+d-3)\binom{d+k-3}{k-1} - (k+d-3)\binom{d+k-4}{k-2}\right) \\ =& \binom{d+k-2}{k} Q^d_{0,0}, \end{aligned}$$

as wanted.

**Claim 4.** For all $j \ge 1$ we have $Q^d_{j+1,j} = Q^d_{j,j}$.

Indeed, using (29) and Claim 3 and denoting

$$R = \frac{\pi 2^{3-d}\Gamma(d+j-1)}{\Gamma(j+1)\Gamma\left(\frac{d}{2}-\frac{1}{2}\right)^2},$$

we have

$$\begin{aligned} Q^d_{j+1,j} =& \frac{Q^d_{0,0}}{j+1}\left((2j+d-1)\binom{d+j-2}{j} - (j+d-2)\binom{d+j-3}{j-1} - R\right) \\ =& \frac{Q^d_{0,0}}{j+1}\left((j+d-1)\binom{d+j-2}{j} - R\right). \end{aligned}$$

From (28) we have

$$R = \frac{\pi 2^{3-d}\Gamma(d+j-1)}{\Gamma(j+1)\Gamma\left(\frac{d}{2}-\frac{1}{2}\right)^2} = (d-2)\binom{d+j-2}{j} Q^d_{0,0}.$$

We have then proved that

$$Q^d_{j+1,j} = \frac{Q^d_{0,0}}{(j+1)}\binom{d+j-2}{j}(j+d-1-(d-2)) = \binom{d+j-2}{j} Q^d_{0,0} = Q^d_{j,j},$$

as claimed.

**Claim 5.** For all $\ell \ge 0$ we have $Q_{j+\ell,j} = Q_{j,j}$.

Indeed, from Claim 4 the equality holds for $\ell = 1$. Reasoning by induction on $\ell$, assume that the equality holds up to $\ell - 1$. From (29) and Claims 3 and 4 we have

$$Q_{j+\ell,j} = \frac{1}{j+\ell}\left((2j+2\ell+d-3)\, Q^d_{j,j} - (j+\ell+d-3)\, Q^d_{j,j}\right) = Q^d_{j,j}.$$

This finishes the proof of Claim 5 and of the lemma.

$\square$

*Proof of Theorem 6.* Note that by reordering the terms:

$$\sum_{j,k=0}^{\infty} a_k a_j Q^d_{k,j} = \sum_{\ell=0}^{\infty}\left(a_\ell^2 Q^d_{\ell,\ell} + \sum_{j>\ell} a_\ell a_j Q^d_{\ell,j} + \sum_{k>\ell} a_k a_\ell Q^d_{k,\ell}\right)$$
$$\underset{\text{Lemma 3}}{=} Q^d_{0,0}\sum_{\ell=0}^{\infty} a_\ell \binom{d+\ell-2}{\ell}\left(a_\ell + 2\sum_{j>\ell} a_j\right).$$

We then have

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_2(x)) = V_2(\mathbb{S}^d)n^2 - \frac{\omega_{d-1}}{2\omega_d}\sum_{j,k=0}^{\infty} a_k a_j Q^d_{k,j} \overset{(26)}{=}$$
$$V_2(\mathbb{S}^d)\left(n^2 - \sum_{\ell=0}^{\infty} a_\ell \binom{d+\ell-2}{\ell}\left(a_\ell + 2\sum_{j>\ell} a_j\right)\right),$$

as wanted. □

The following gives an alternative formula for the expected value computed in Theorem 1 for the case $s = 2$ as well as an asymptotic estimate. Note that the harmonic kernel $K_L$ is obtained when in the general setting of this section we let

$$a_k = \begin{cases} \frac{2k+d-1}{d-1} & k \le L, \\ 0 & k > L. \end{cases} \tag{30}$$

From Theorem 6 we readily have:

**Corollary 8.** *Let $x = (x_1, \dots, x_n) \in (\mathbb{S}^d)^n$ be $n = \pi_L$ points generated by the determinantal random point process associated with harmonic kernel $K_L$. Then, $\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_2(x))$ equals*

$$V_2(\mathbb{S}^d)\left(n^2 - \sum_{\ell=0}^{L}\frac{2\ell+d-1}{d-1}\binom{d+\ell-2}{\ell}\left(\frac{2\ell+d-1}{d-1} + 2\sum_{j=\ell+1}^{L}\frac{2j+d-1}{d-1}\right)\right).$$

*Remark* 5. It is possible to recover the asymptotic estimate of Theorem 2 from Corollary 8 in the case $s = 2$, that is

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(E_2(x)) = V_2(\mathbb{S}^d)\left(n^2 - \frac{4n^{1+2/d}}{(d+2)(d-1)}\left(\frac{d!}{2}\right)^{2/d}\right) + o(n^{1+2/d}).$$

3.2.2. *Optimality of the harmonic kernel. Proof of Theorem 7.* We now prove that the harmonic kernel gives optimal values of the expected 2-energy among rotationally invariant kernels.

*Proof of Theorem 7.* Let $r \in \mathbb{N}$ be such that $a_j = b_j = 0$ for $j \ge r$, and assume that $a \ne b$. Note from (25) and Lemma 3 that $\mathbb{E}_a < \mathbb{E}_b$ is equivalent to $F(a) \ge F(b)$, where

$$F(x) = x^T M x,$$

and where $M = M_r$ is the symmetric matrix given by

$$M = \left(\binom{d+\min(k,j)-2}{\min(k,j)}_{k,j=0,\dots,r}\right) = \begin{pmatrix} \binom{d-2}{0} & \binom{d-2}{0} & \binom{d-2}{0} & \cdots & \binom{d-2}{0} \\ \binom{d-2}{0} & \binom{d-1}{1} & \binom{d-1}{1} & \cdots & \binom{d-1}{1} \\ \binom{d-2}{0} & \binom{d-1}{1} & \binom{d}{2} & \cdots & \binom{d}{2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \binom{d-2}{0} & \binom{d-1}{1} & \binom{d}{2} & \cdots & \binom{d+r-2}{r} \end{pmatrix} \in \mathbb{Z}^{(r+1)\times(r+1)}.$$

We also consider the vector

$$V = \left(\binom{d-2}{0}, \binom{d-1}{1}, \binom{d}{2}, \dots, \binom{d+r-2}{r}\right) \in \mathbb{Z}^{r+1},$$

and, for $0 \le i < j \le r$ we let $w_{ij} \in \mathbb{R}^{r+1}$ be the vector all of whose components are zero except for the $i$th component and the $j$th component that satisfy:

$$(w_{ij})_i = \binom{d+i-2}{i}^{-1}, \quad (w_{ij})_j = -\binom{d+j-2}{j}^{-1}.$$

Note that, for coherence in the exposition, we are numbering the entries of $w_{ij}$ from 0 to $r$ instead of doing it from 1 to $r+1$. Then,

$$w_{ij}^T V = 0, \quad \forall\, i, j,\ 0 \le i < j \le r. \tag{31}$$

An elementary computation shows that if $i < j$ then all the components of the vector $Mw_{ij} \neq 0$ are positive or zero. We thus have

$$x^T M w_{ij} \ge 0 \qquad \text{for all } x \in [0,\infty)^{r+1}.$$

Note now that if $x \in [0,\infty)^{r+1}$ then for all $i, j$ we have

$$DF(x)(w_{ij}) = w_{ij}^T M x + x^T M w_{ij} = 2x^T M w_{ij} \ge 0. \tag{32}$$

Moreover, if $x_i > 0$ then $DF(x)(w_{ij}) > 0$ and the function is strictly increasing in that direction. We will now construct a sequence

$$b = x^0, x^1, \dots, x^t = a$$

with the property that $x^k - x^{k-1}$ is a non-negative multiple of $w_{ij}$ for some $i, j$ with $i < j$. Although the coordinates of $x^0, x^t$ have a particular form given by (14), the coordinates of $x^k$ are just non-negative real numbers. For the construction, let $i$ be the first index such that $a_i \neq 0, b_i = 0$ and let $j$ be the greatest index such that $b_j \neq 0$ and $a_j = 0$ (these $i, j$ exist because $a \neq b$ and the hypotheses $\sum a_i \binom{d+i-2}{i} = \sum b_i \binom{d+i-2}{i} = n$). Note also from (16) that necessarily $j > i$. Then, we define

$$x^1 = x^0 + \left(1 + \frac{2i}{d-1}\right)\binom{d+i-2}{i} w_{ij} \in [0,\infty)^{r+1},$$

and in general to construct $x^{k+1}$ from $x^k$ we let $i$ be the smallest index, among those such that $a_i \neq 0$, such that $x_i^k \neq a_i = 1 + 2i/(d-1)$ and $j$ the greatest index such that, $x_j^k > 0$ and $a_j^k = 0$, if those indices exist. It can be easily seen by induction that (16) is also satisfied changing $b$ to $x^k$ and thus, if such $i, j$ exist, we have $i < j$. Then, we let

$$x^{k+1} = x^k + \lambda w_{ij}, \quad \lambda = \min\left(\binom{d+j-2}{j} x_j^k, \left(1 + \frac{2i}{d-1} - x_i^k\right)\binom{d+i-2}{i}\right).$$

From (32) and the comment after (32) it is clear that

$$F(b) = F(x^0) < F(x^1) \le F(x^2) \le \cdots \le F(x^k), \quad \forall\, k \in \mathbb{N}.$$

We just have to prove that the sequence satisfies $x^k = a$ for some $k \in \mathbb{N}$. First note that from (31) we have for all $k \in \mathbb{N}$:

$$(x^k)^T V = (x^{k-1})^T V = \cdots = x^0 V = n, \quad \text{that is,} \quad \sum_{i=0}^{r} x_i^k \binom{d+i-2}{i} = n. \quad (33)$$

Moreover, by construction we have $x_i^k \in [0, 1 + 2i/(d-1)]$ for all $k$ and $i$. On the other hand, the sequence can only finish if some of the indices $i, j$ in the construction do not exist. Namely, the sequence stops when:

(i) For every $i$ such that $a_i \neq 0$ we have $x_i^k = a_i$, or
(ii) For every $j$ such that $x_j^k \neq 0$ we have $a_j > 0$.

From (33) and the similar equality $\sum_{i=0}^{r} a_i \binom{d+i-2}{i} = n$ it is clear that these two conditions are equivalent and actually imply $x^k = a$. This proves that, if the sequence finishes, then its last element is equal to $a$. Now note that at each iteration $x^k \mapsto x^{k+1}$, either one coordinate of $x^k$ is set to 0 (and in this case, that coordinate remains untouched in further iterations), or one of them is set to its maximum value $1 + 2i/(d-1)$ (which, again, implies that this coordinate remains untouched in further iterations). So the number of iterations of the sequence is at most the total number of coordinates in $a$ or $b$, that is at most $r+1$. This finishes the proof of the theorem. $\square$

3.3. **Linear Statistics. Proof of propositions 2 and 3.** The objective is to estimate the asymptotic behavior of the variance of the number of points of the harmonic ensemble to be found in a spherical cap. To get this estimate we study the trace $\operatorname{tr}(\mathcal{K}_A - \mathcal{K}_A^2)$, where $\mathcal{K}_A$ is the integral operator of concentration on the spherical cap $A \subset \mathbb{S}^d$,

$$\mathcal{K}_A Q(u) = \int_A Q(v) K_L(u, v)\, d\mu(v), \quad Q \in \Pi_L.$$

The proof of Proposition 2 is similar to [25, Proposition 3.1.]. The idea in that paper was, following Landau's work, to study the density of discrete sets (Marcinkiewicz-Zygmund and interpolating arrays) relating the density with spectral properties of the concentration operator in "small" spherical caps. The hypothesis are now different (we consider "big" spherical caps also) so we will sketch the proof.

*Proof of Proposition 2.* It is clear that the variance of the random variable, $n_A$, counting the number of points in $A$, is invariant w.r.t. rotations of $A$, because the process is also invariant. So to compute $\operatorname{Var}(n_A)$ we assume that $A = B(\mathbf{n}, \theta_L)$

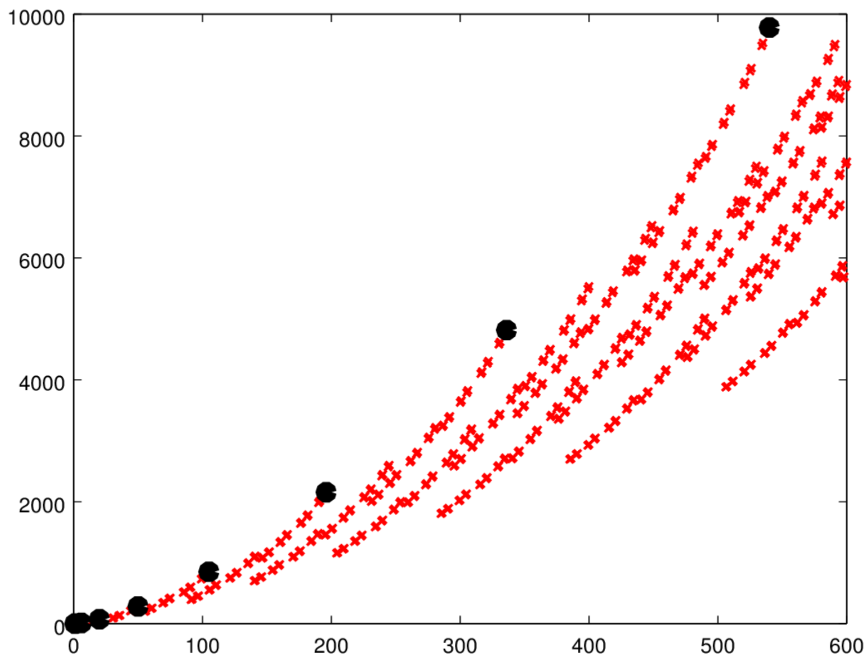


FIGURE 2. Value of $\sum_{\ell=0}^{\infty} a_\ell \binom{d+\ell-2}{\ell}\left(a_\ell + 2\sum_{j>\ell} a_j\right)$ for different kernels in dimension $d=4$. Black dots correspond to the harmonic kernels, i.e. when the $a_k$'s are given by (30), while red crosses correspond to other kernels. For some values of $n$ (for example, $n=4$) there is no kernel that attains this number of points. For other values of $n$ (for example, for $n=6$) there is only one such kernel. For yet another collection of values of $n$ (including for example $n=196$ and $n=540$) there are several choices of kernels which produce this number of points. In these two particular values, one of the choices corresponds to the harmonic kernel. The optimality of the harmonic kernel proved in Theorem 7 is clearly visible: the sum is maximal when the harmonic kernel is used, hence from Theorem 6 the expected value of $E_2$ is minimal.

with $\mathbf{n}$ being the north pole and $\theta_L \in [0,\pi]$. Denote $\theta_L = \alpha_L/L$ with $\alpha_L = O(L)$, and $\alpha_L \to \infty$ when $L \to \infty$. The following formula to compute the covariance can be found in [30, Formula 28]

$$\mathrm{Cov}(f,g) = \frac{1}{2}\int_{\mathbb{S}^d}\int_{\mathbb{S}^d} (f(x)-f(y))(g(x)-g(y))|K_L(x,y)|^2 d\mu(x)d\mu(y), \tag{34}$$

for bounded $f, g$. In particular

$$\mathrm{Var}(n_A) = \mathrm{Cov}(\chi_A,\chi_A) = \int_A\int_{A^c} |K_L(x,y)|^2 d\mu(x)d\mu(y) = \mathrm{tr}(\mathcal{K}_A - \mathcal{K}_A^2).$$

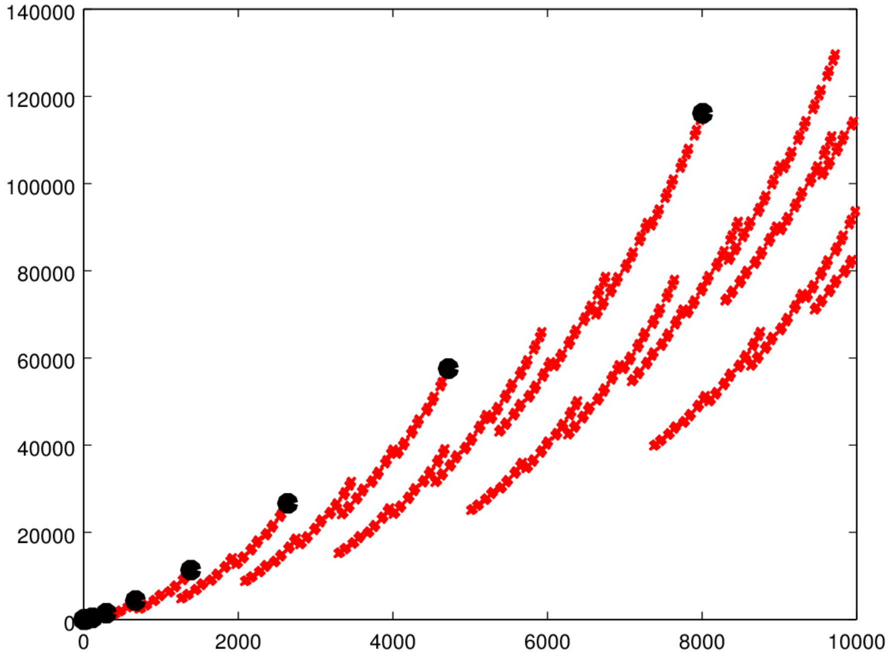


FIGURE 3. Same as Figure 2 but for dimension $d = 6$. Again the optimality of the harmonic kernel is clearly visible.

By rotation invariance

$$\begin{aligned}&\int_A \int_{A^c} |K_L(x,y)|^2 d\mu(x) d\mu(y)\\ &= A_{d,L}^2 \int_0^{\theta_L} \sin^{d-1}\eta \left( \int_{\theta_L-\eta}^{\pi} |P_L^{(1+\lambda,\lambda)}(\cos\theta)|^2 \sin^{d-1}\theta d\theta \right) d\eta,\end{aligned}$$

where

$$A_{d,L} = \frac{\pi_L \omega_{d-1}}{\binom{L+\frac{d}{2}}{L}\omega_d} = \frac{2^{1-d}}{\Gamma\left(\frac{d}{2}\right)} L^{d/2} + o(L^{d/2}).$$

For some fixed $c > 0$, we split the inner integral above in three summands corresponding to

$$\left\{ \frac{c}{L} \leq \theta \leq \pi - \frac{c}{L} \right\} = \mathrm{I}, \quad \left\{ \theta > \pi - \frac{c}{L} \right\} = \mathrm{II}, \quad \text{and} \quad \left\{ \frac{c}{L} < \theta \right\} = \mathrm{III}.$$

The integral over I can be bounded above, by using classical estimates for Jacobi polynomials (2)

$$\begin{aligned}&\frac{A_{d,L}^2}{L^d} \int_0^{\alpha_L} \eta^{d-1} \int_{\max(\frac{\alpha_L-\eta}{L}, \frac{c}{L})}^{\pi-\frac{c}{L}} |P_L^{(1+\lambda,\lambda)}(\cos\theta)|^2 \sin^{d-1}\theta d\theta d\eta\\ &\leq \frac{A_{d,L}^2 2^{d-1}}{L^d} \int_0^{\alpha_L} \eta^{d-1} \int_{\max(\frac{\alpha_L-\eta}{L}, \frac{c}{L})}^{\pi-\frac{c}{L}} \frac{1}{\pi L \sin^2\frac{\theta}{2}} d\theta d\eta\end{aligned}$$

$$= \frac{A_{d,L}^2 2^{d-1}}{\pi L^{d+1}} \int_0^{\alpha_L} \eta^{d-1} \left( \cot\left( \frac{\max\{\alpha_L - \eta, c\}}{2L} \right) - \tan\left( \frac{c}{2L} \right) \right) d\eta.$$

The main term comes from the first summand of this last integral because the second is of order $L^{-2}\alpha_L^d$. For the first summand we split the integral again and do a change of variables

$$\int_0^{\alpha_L} \eta^{d-1} \cot\left( \frac{\max\{\alpha_L - \eta, c\}}{2L} \right) d\eta$$
$$= \int_c^{\alpha_L} (\alpha_L - \eta)^{d-1} \cot\left( \frac{\eta}{2L} \right) d\eta + \int_{\alpha_L - c}^{\alpha_L} \eta^{d-1} \cot\left( \frac{c}{2L} \right) d\eta. \qquad (35)$$

The second summand in above is of order $L\alpha_L^{d-1}$. For the first summand in (35) we expand the polynomial in $\eta$ and use the estimate $x \cot x \leq 1$ for $x \in [0, \pi/4]$ to get the bound

$$\alpha_L^{d-1} \int_c^{\alpha_L} \cot\left( \frac{\eta}{2L} \right) d\eta + LO(\alpha_L^{d-1}) = 2L\alpha_L^{d-1} \log \frac{\sin(\frac{\alpha_L}{2L})}{\sin(\frac{c}{2L})} + LO(\alpha_L^{d-1})$$
$$= 2L\alpha_L^{d-1} \log \alpha_L + LO(\alpha_L^{d-1}).$$

For the integral over II we bound the Jacobi polynomial by $CL^{2\lambda}$ getting a term of order $L^{-2}\alpha_L^d = O(\alpha_L^{d-2})$. Finally for the integral over III we bound the Jacobi polynomial by its maximum $CL^{d/2}$ getting another term $O(\alpha_L^{d-1})$.

Putting all together we get

$$\operatorname{Var}(n_A) \leq \frac{2^{2-d}}{\pi \Gamma\left(\frac{d}{2}\right)^2} \alpha_L^{d-1} \log \alpha_L + O(\alpha_L^{d-1}).$$

□

We now turn to the smooth case.

*Proof of Proposition 3.* Given a bounded function $\phi : \mathbb{S}^d \to \mathbb{R}$ we denote by $T_\phi$ the Toeplitz operator on $\Pi_L$ with symbol $\phi$, i.e. $T_\phi(h) := \mathcal{K}_L(\phi h)$ where $\mathcal{K}_L$ denotes the orthogonal projection from $L^2(\mathbb{S}^d)$ to $\Pi_L$

$$\mathcal{K}_L f(x) = \int_{\mathbb{S}^d} K_L(x,y) f(y) d\mu(y), \quad f \in L^2(\mathbb{S}^d),$$

i.e. $T_\phi$ is the self-adjoint operator on $\Pi_L$ determined by

$$\langle T_\phi P, P \rangle = \langle \phi P, P \rangle$$

for any $P \in \Pi_L$. Then it follows from (34) that for $\phi$ Lipschitz

$$\operatorname{Var}(\mathcal{X}(\phi)) \lesssim \frac{1}{2} \int_{\mathbb{S}^d \times \mathbb{S}^d} |K_L(x,y)|^2 d^2(x,y) d\mu(x) d\mu(y).$$

Now, setting $\psi(x) = x_i$ for a fixed index $i \in \{1, \ldots, d\}$, we get

$$\operatorname{Var}(\mathcal{X}(\phi)) \lesssim \int_{\mathbb{S}^d \times \mathbb{S}^d} |K_L(x,y)|^2 (\psi(x) - \psi(y))^2 d\mu(x) d\mu(y).$$

On the other hand, an elementary computation shows that

$$\frac{1}{2}\int_{\mathbb{S}^d\times\mathbb{S}^d} |K_L(x,y)|^2 \left(\psi(x)-\psi(y)\right)^2 d\mu(x)d\mu(y) = \operatorname{tr} T_\psi^2 - \operatorname{tr} T_{\psi^2}.$$

We note that there exists a vector subspace $V_L$ in $\Pi_L$ with dimension $\dim V_L = \pi_L - O(L^{d-1})$ such that when restricted to $V_L$, $T_\psi(P) = P\psi$ and $T_\psi^2(P) = P\psi^2$. We can take $V_L$ to be the space spanned by the restrictions to $\mathbb{S}^d$ of all polynomials of total degree at most $L-2$, i.e. $\Pi_{L-2}$.

If we denote by $W_L$ the orthogonal complement of $V_L$ in $\Pi_L$ then $\dim(W_L) = \pi_L - \pi_{L-2} = O(L^{d-1})$. Setting $A_L := T_\psi^2 - T_{\psi^2}$ gives $A_L = 0$ on $V_L$ and hence

$$\operatorname{tr} T_\psi^2 - \operatorname{tr} T_{\psi^2} = 0 + \operatorname{tr} A_{L|W_L} \lesssim L^{d-1},$$

using that $\langle T_\psi P, P\rangle \le \langle P,P\rangle \sup_{\mathbb{S}^d}|\psi|$ and $\dim W_L = O(L^{d-1})$.

In the other direction, if we take $\phi(x) = x_i$, then

$$\operatorname{Var}(\mathcal{X}(\phi)) = \frac{1}{2}\int_{\mathbb{S}^d\times\mathbb{S}^d} |K_L(x,y)|^2 \left(\phi(x)-\phi(y)\right)^2 d\mu(x)d\mu(y).$$

Therefore (recall that $\mathbf{n}$ stands for the north pole)

$$\operatorname{Var}(\mathcal{X}(\phi)) \gtrsim \int_{\mathbb{S}^d} |K_L(x,\mathbf{n})|^2 d^2(x,\mathbf{n}) d\mu(x) \simeq \int_0^\pi \sin^{d-1}(\theta)|\theta|^2 |P_L^{(1+\lambda,\lambda)}(\cos\theta)|^2 d\theta.$$

Using the classical estimates for Jacobi polynomials as before we get $\operatorname{Var}(\mathcal{X}(\phi)) \gtrsim L^{d-1}$. □

3.4. **Separation distance. Proof of Proposition 4.** Apply Proposition 1 to $f(u,v) = \mathbf{1}_{\|u-v\|\le t}$, which yields

$$2\mathbb{E}_{x\in(\mathbb{S}^d)^n}(G(t,x)) = \int_{u,v\in\mathbb{S}^d, \|u-v\|\le t} \left(K_L(u,u)^2 - |K_L(u,v)|^2\right) d\mu(u)\, d\mu(v).$$

The integrand depends only on the scalar product $\langle u,v\rangle$, so by rotation invariance and using Lemma 1 we have

$$\begin{aligned} 2\mathbb{E}_{x\in(\mathbb{S}^d)^n}(G(t,x)) =& \frac{\pi_L^2\omega_{d-1}}{\omega_d}\int_{1-t^2/2}^{1} \left(1 - \frac{P_L^{(1+\lambda,\lambda)}(s)^2}{\binom{L+d/2}{L}^2}\right)\left(1-s^2\right)^{d/2-1} ds \\ =& \frac{\pi_L^2\omega_{d-1}}{\omega_d}\int_0^{t^2/2} \left(1 - \frac{P_L^{(1+\lambda,\lambda)}(1-s)^2}{\binom{L+d/2}{L}^2}\right)\left(2s-s^2\right)^{d/2-1} ds. \end{aligned}$$

From Lemma 4 below we conclude

$$\mathbb{E}_{x\in(\mathbb{S}^d)^n}(G(t,x)) \le \frac{\pi_L^2\omega_{d-1}}{2\omega_d}\int_0^{t^2/2} \frac{2(L^2+Ld)}{d+2} s\left(2s\right)^{d/2-1} ds = \frac{L(L+d)\pi_L^2\omega_{d-1}}{2(d+2)^2\omega_d} t^{d+2},$$

as claimed.

We have used the following elementary lemma bounding Jacobi polynomials, a short proof is included for completeness:

**Lemma 4.** *Let $L, d \geq 1$. Then, for all $s \in \mathbb{R}$, $0 \leq s \leq \frac{d+6}{(2L+d)L}$ we have*

$$1 - \frac{L^2 + Ld}{d+2} s \leq \frac{P_L^{(1+\lambda,\lambda)}(1-s)}{\binom{L+d/2}{L}} \leq 1 - \frac{L^2 + Ld}{d+2} s + k_0 s^2,$$

*for some constant $k_0 \in (0, \infty)$. In particular,*

$$\frac{2(L^2 + Ld)}{d+2} s - k_0 s^2 \leq 1 - \frac{P_L^{(1+\lambda,\lambda)}(1-s)^2}{\binom{L+d/2}{L}^2} \leq \frac{2(L^2 + Ld)}{d+2} s.$$

*Proof.* Let $q(s) = P_L^{(1+\lambda,\lambda)}(1-s)$. The expansion of $q$ in the standard monomial basis is easy to compute from the derivatives for $0 \leq k \leq L$ (see for example [16, p. 1008]):

$$\frac{d^k}{ds^k} q(0) = (-1)^k \frac{d^k}{ds^k} P_L^{(1+\lambda,\lambda)}(1) = \frac{(-1)^k \Gamma(L+k+d)}{2^k \Gamma(L+d)} \binom{L+d/2}{L-k}.$$

We thus have for $s \in \mathbb{R}$:

$$\begin{aligned}
\frac{q(s)}{\binom{L+d/2}{L}} &= \sum_{k=0}^{L} \frac{(-1)^k \Gamma(L+k+d)}{2^k k! \Gamma(L+d)} \frac{\binom{L+d/2}{L-k}}{\binom{L+d/2}{L}} s^k \\
&= \sum_{k=0}^{L} \frac{(-1)^k \Gamma(L+k+d) \Gamma(L+1) \Gamma(1+d/2)}{2^k k! \Gamma(L+d) \Gamma(L-k+1) \Gamma(k+1+d/2)} s^k \\
&= 1 - \frac{L^2 + Ld}{d+2} s + R,
\end{aligned}$$

where $R$ stands for the terms in the summation from $k = 2$ to $k = L$. We will show that $R \geq 0$, which finishes the proof. The terms of $R$, with the possible exception of the last one if $L$ is even, have alternating signs. It is then sufficient to show that for $k = 2, 4, 6, \ldots$, and $k < L$, the $k$th term in the summation is larger than the (absolute value of the) $(k+1)$th term, that is we have to show that for those values of $k$,

$$\frac{\Gamma(L+k+d)\Gamma(L+1)\Gamma(1+d/2) s^k}{2^k k! \Gamma(L+d)\Gamma(L-k+1)\Gamma(k+1+d/2)} \geq \frac{\Gamma(L+k+d+1)\Gamma(L+1)\Gamma(1+d/2) s^{k+1}}{2^{k+1}(k+1)! \Gamma(L+d)\Gamma(L-k)\Gamma(k+2+d/2)}.$$

This is satisfied whenever

$$s \leq \frac{(k+1)(2k+2+d)}{(L-k)(L+k+d)}.$$

It is a trivial exercise to check that the hypotheses on $s$ guarantee this last inequality. $\square$

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