UNIVERSITAT DE BARCELONA

Energy and random point processes on two-point homogeneous manifolds

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Tesi de doctorat

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Víctor de la Torre Estévez

Certifico que la present memòria ha estat desenvolupada per Víctor de la Torre Estévez i dirigida per mi.

Dr. Jordi Marzo Sánchez
Barcelona, setembre de 2023

Abstract

We study discrete energy minimization problems on two-point homogeneous manifolds. Since finding N-point configurations with optimal energy is highly challenging, recent approaches have involved examining random point processes with low expected energy to obtain good N-point configurations.

In Chapter 2, we compute the second joint intensity of the random point process given by the zeros of elliptic polynomials, which enables us to recover the expected logarithmic energy on the 2-dimensional sphere previously computed by Armentano, Beltrán, and Shub. Moreover, we obtain the expected Riesz s-energy, which is remarkably close to the conjectured optimal energy. The expected energy serves as a bound for the extremal s-energy, $s \neq 0$, thereby improving upon the bounds derived from the study of the spherical ensemble by Alishahi and Zamani. Among other additional results, we get a closed expression for the expected separation distance between points sampled from the zeros of elliptic polynomials.

In Chapter 3, we explore the average discrepancies and worst-case errors of random point configurations on the sphere $\mathbb{S}^d$. We find that the points drawn from the so called spherical ensemble and the zeros of elliptic polynomials achieve optimal spherical L^2 cap discrepancy on average. Additionally, we provide an upper bound for the L^∞ discrepancy for N-point configurations drawn from the harmonic ensemble on any two-point homogeneous space, thereby generalizing the previous findings for the sphere $\mathbb{S}^d$ by Beltrán, Marzo and Ortega-Cerdà. We introduce a nondeterministic version of the Quasi Monte Carlo (QMC) strength for random sequences of points and compute its value for the spherical ensemble, the zeros of elliptic polynomials, and the harmonic ensemble. Finally, we compare our results with the conjectured QMC strengths of certain deterministic distributions associated with these random point processes.

In Chapter 4, our focus shifts to the Green energy minimization problem. Firstly, we extend the work by Beltrán and Lizarte on spheres to establish a close to sharp lower bound for the minimal Green energy on any two-point homogeneous manifold, improving on the existing lower bounds on projective spaces. Secondly, by adapting a method introduced by Wolff, we deduce an upper bound for the L^∞ discrepancy of N-point sets that minimize the Green energy.

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Contents

Notation

$\mathbb{R}$	The set of real numbers
$\mathbb{C}$	The set of complex numbers
$\mathbb{H}$	The set of quaternions
$\mathbb{O}$	The set of octonions
$\mathbb{F}$	$\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$ or $\mathbb{O}$
$\mathcal{M}$	A compact connected two-point homogeneous manifold, unless stated otherwise
d	The real dimension of the manifold $\mathcal{M}$
$\vartheta(x, y)$	The Riemannian distance between $x, y \in \mathcal{M}$
D	The diameter of the manifold $\mathcal{M}$
σ	The normalized uniform measure on the manifold $\mathcal{M}$
α	$\frac{d}{2} - 1$
β	α for $\mathbb{S}^d$ and $\frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1$ for $\mathbb{FP}^n$
κ	$1/2$ for $\mathbb{S}^d$ and 1 for $\mathbb{FP}^n$
$\mathbb{S}^d$	The d-dimensional unit sphere on $\mathbb{R}^{d+1}$
$\mathbb{FP}^n$	The projective space over $\mathbb{F}$
$P_\ell^{(\alpha,\beta)}(x)$	The Jacobi polynomial of degree ℓ and parameters (α, β)
$P_\ell^{(d)}(x)$	The Gegenbauer polynomial of degree ℓ and parameter d
λ_ℓ	The ℓ-th eigenvalue (in increasing order) of the Laplace-Beltrami operator on $\mathcal{M}$
m_ℓ	The multiplicity of λ_ℓ
V_ℓ	The eigenspace of the Laplace-Beltrami operator on $\mathcal{M}$ corresponding to λ_ℓ

$\pi_L^{(\alpha,\beta)}$	The dimension of the subspace $\Pi_L = \bigoplus_{\ell=0}^{L} V_\ell \subset \mathcal{M}$
$K_L^{(\alpha,\beta)}$	The reproducing kernel of the subspace $\Pi_L = \bigoplus_{\ell=0}^{L} V_\ell \subset \mathcal{M}$
χ_A	The characteristic function of the set A
$\Gamma(x)$	The gamma function
$\psi(x)$	The digamma function, $\psi(x) = \frac{\Gamma'(x)}{\Gamma(x)}$
$\zeta(x)$	The Riemann zeta function
$\zeta(x,a)$	The Hurwitz zeta function
$(x)_n$	The Pochhammer symbol, $(x)_0 = 1$ and $(x)_n = x(x+1)\cdots(x+n-1)$ for $n \geq 1$
γ	The Euler-Mascheroni constant, $\gamma = -\psi(1)$
δ_x	The Dirac's delta at x
$x_n \lesssim y_n$	$\limsup_{n\to\infty} \frac{x_n}{y_n} \leq C$ for some $C \geq 0$ independent of n. Also written as $x_n = O(y_n)$
$x_n \approx y_n$	$x_n \lesssim y_n$ and $y_n \lesssim x_n$
$x_n \sim y_n$	$\lim_{n\to\infty} \frac{x_n}{y_n} = 1$

Introduction

In this dissertation, we study energy minimization problems on two-point homogeneous manifolds, with special attention to the case of the sphere $\mathbb{S}^2 \subset \mathbb{R}^3$. Given a configuration $X_N = \{x_1, \ldots, x_N\}$ of N points in a manifold $\mathcal{M}$ interacting pairwise through some potential $K : \mathcal{M} \times \mathcal{M} \to \mathbb{R} \cup \{+\infty\}$, the *discrete K-energy of X_N* is defined by

$$E_K(X_N) = \sum_{i \neq j} K(x_i, x_j). \tag{1}$$

We ask for N-point extremal configurations of this energy under some hypotheses on the potential.

Some instances of this general problem have been studied from long time ago. For example, the Coulomb potential $K(x, y) = 1/|x - y|$ gives rise to the most famous problem in this context, the *Thomson problem*, which looks for the minimal possible energy of N electrons restricted to the sphere $\mathbb{S}^2$ that repel each other according to Coulomb's law. The problem arose in 1904 after the physicist J. Thomson proposed his atomic model. In a system of charged particles, the equilibrium configurations are those on which the forces acting on each particle are balanced, resulting in a state of minimum energy. Finding these equilibrium configurations provides insights into the geometric arrangement of charges, which may have implications in molecular structure determination and crystallography. Despite being a centenary problem, the exact solution to the Thomson problem is only known for $N = 2, 3, 4, 5, 6$ or 12 points. The problem becomes computationally demanding as the number of points increases, requiring efficient algorithms and computational resources, see [BHS19]. Beyond electrostatics, the problem has applications in various fields such as condensed matter physics, chemistry and material science, see [Ser15].

In the present work, we study the generalization of this problem to *Riesz potentials*

$$K_s(x, y) = \frac{1}{|x - y|^s}, \quad s \neq 0, \tag{2}$$

for which we define the *extremal (minimal or maximal) s-energy* by

$$\mathcal{E}_s(N) = \begin{cases} \min_{X_N \subset \mathbb{S}^2} E_{K_s}(X_N) & \text{if } s > 0, \\ \max_{X_N \subset \mathbb{S}^2} E_{K_s}(X_N) & \text{if } s < 0. \end{cases}$$

For $s = 0$, defining the potential K_0 by (2) would yield a trivial minimal discrete energy, since $E_{K_0}(X_N) = N(N-1)$ for any N-point configuration. The derivative of

$1/|x-y|^s$ with respect to s at the origin suggests the definition

$$K_0(x,y) = \log \frac{1}{|x-y|},$$

which is known as the *logarithmic potential.* The *minimal discrete logarithmic energy* is given by

$$\mathcal{E}_0(N) = \min_{X_N \subset \mathbb{S}^2} E_{K_0}(X_N).$$

The study of this energy has received a lot of attention during the last years. Since points minimizing the logarithmic energy are points maximizing the product of mutual distances, these points are also called *elliptic Fekete points.*

Similar to what happens with the Thomson problem, which corresponds to $s=1$ in our context, finding N-point configurations with optimal s-energy is exceedingly difficult, except for a few select values of N. As the number of points increases, the problem becomes analytically intractable due to its computational complexity. Therefore, developing algorithms that can generate N-point configurations with low energy is of great interest. In fact, the 7th problem listed by Smale for the XXI century [Sma00] asks for an algorithm that produces N points $X_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^2$ satisfying the inequality

$$E_{K_0}(X_N) - \mathcal{E}_0(N) \leq c \log N$$

for some universal constant c. The problem is far from being solved, see [Bel13] for a survey. One capital problem is the insufficient current knowledge of the asymptotic expansion of the minimal logarithmic energy, which is

$$\mathcal{E}_0(N) = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{1}{2} N \log N + C_{\log} N + o(N), \quad N \to +\infty, \tag{3}$$

with $C_{\log}$ a constant such that

$$-0.0569\ldots \leq C_{\log} \leq 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.0556\ldots, \tag{4}$$

see [BS18, Lau21] and [BL22] for a recent direct computation of the lower bound. The upper bound for $C_{\log}$ has been conjectured to be an equality by two different approaches, [BHS12, BS18]. The setting of this constant is one of the main problems in the area.

For other values of the parameter s, the situation is similar. In particular, for $0 < |s| < 2$, it is known that there exist $c_s, C_s > 0$ (depending on s) such that

$$-c_s N^{1+s/2} \leq \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s} N^2 \leq -C_s N^{1+s/2}, \tag{5}$$

see [RSZ94, Wag90, Wag92]. The asymptotic expansion of the optimal Riesz s-energy has been conjectured in [BHS12] to be

$$\mathcal{E}_s(N) = \frac{2^{1-s}}{2-s} N^2 + \frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}} N^{1+\frac{s}{2}} + o(N^{1+\frac{s}{2}}), \quad N \to +\infty, \tag{6}$$

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

Observe that in both the Riesz and logarithmic cases the first term in the expansion corresponds to the continuous energy of the normalized uniform measure σ on $\mathbb{S}^2$,

$$\int_{\mathbb{S}^2}\int_{\mathbb{S}^2} \frac{1}{|x-y|^s}\, \mathrm{d}\sigma(x)\, \mathrm{d}\sigma(y) = \frac{2^{1-s}}{2-s}, \quad s \neq 0,$$

and

$$\int_{\mathbb{S}^2}\int_{\mathbb{S}^2} \log\frac{1}{|x-y|}\, \mathrm{d}\sigma(x)\, \mathrm{d}\sigma(y) = \frac{1}{2} - \log 2.$$

We will provide more details about this relationship in Section 1.2.

In the pursuit of algorithms generating N-point configurations of our interest, recent approaches have focused on exploring random point processes with low expected energy. In fact, by sampling N independent points from the uniform probability measure on $\mathbb{S}^2$, we already capture the leading term in the asymptotic expansion of the optimal energy. For instance, in the case of $s \neq 0$, the expected energy is

$$\mathbb{E}[E_{K_s}(X_N)] = \frac{2^{1-s}}{2-s}N^2 - \frac{2^{1-s}}{2-s}N.$$

Nonetheless, this simple approach tends to yield suboptimal energy due to the independence of the points, allowing the possibility of two points being very close to each other, which is heavily penalized by the Riesz s-energy.

To overcome this limitation, one effective strategy is to partition the sphere $\mathbb{S}^2$ into N equal-area regions and select one random point from each cell. This procedure, known as *jittered sampling*, captures the correct second-order behavior in the asymptotic expansion (6) and provides upper and lower bounds as in (5) for $0 < s < 2$ and $-2 < s < 0$, respectively. However, the constants in these bounds significantly differ from the conjectured value, see [BHS19, Chapter 6].

Although jittered sampling partially mitigates the issue of closely located points, there remains a possibility of adjacent cells containing randomly chosen points near their shared edge. To further enhance the quality of configurations, it has been explored the use of random point processes that incorporate point repulsion, mimicking the behavior of electrons or fermions. Notable examples of such processes include determinantal point processes, introduced by Macchi [Mac75], and the zero sets of Gaussian analytic functions, as discussed in [HKPV09]. Moreover, since the potential $K_s(x, y)$ depends solely on the distance between points x and y, it is natural to choose processes exhibiting distributional invariance under rotations of the sphere.

The *spherical ensemble* is a determinantal point process on $\mathbb{S}^2$ with rotational invariance. In their work [AZ15], Alishahi and Zamani computed the expected Riesz and logarithmic energies for N-point configurations X_N sampled from the spherical ensemble,

$$\mathbb{E}[E_{K_s}(X_N)] = \begin{cases} \dfrac{2^{1-s}}{2-s}N^2 - \dfrac{\Gamma(1-s/2)}{2^s}N^{1+\frac{s}{2}} + o\left(N^{1+\frac{s}{2}}\right), & 0 < |s| < 2, \\ \left(\frac{1}{2} - \log 2\right)N^2 - \frac{1}{2}N\log N + \left(\log 2 - \frac{\gamma}{2}\right)N + o\left(N\right), & s = 0. \end{cases} \tag{7}$$

One advantage of the spherical ensemble over the jittered sampling is the possibility of explicitly computing the expected energy. In the Riesz case, the $N^{1+s/2}$-coefficient in (7) is closer to the corresponding coefficient in the conjectured asymptotic expansion (6) for $s \neq 0$. In the logarithmic case, the spherical ensemble captures the first two terms of the expansion (3), whereas the N-coefficient is still far from the conjectured one.

Besides telling us whether a random point process yields low energy configurations on average, the computation of the expected energy automatically provides an upper (lower) bound for the minimal (maximal) energy. This idea was used in [AZ15] to improve the previously known constants in (5), getting

$$\begin{aligned} \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s} &\leq -\frac{\Gamma(1-s/2)}{2^s} N^{1+s/2}, \quad 0 < s < 2, \\ \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s} &\geq -\frac{\Gamma(1-s/2)}{2^s} N^{1+s/2}, \quad -2 < s < 0. \end{aligned} \tag{8}$$

Among all Gaussian analytic functions (GAFs), there are ones particularly interesting to consider when our objective is to obtain points on the sphere, because their zero sets exhibit distribution invariance under rotations of the sphere. These functions are known as the *elliptic polynomials* P_N,

$$P_N(z) = \sum_{n=0}^{N} a_n \sqrt{\binom{N}{n}} z^n,$$

where a_n are i.i.d. random variables with standard complex Gaussian distribution. These polynomials appeared first in the mathematical physics literature [BBL92, BBL96, Han96] and were quickly studied from a mathematical point of view, [Kos93, SS93a]. Among the random point processes obtained from the zeros of a GAF, this one stands out as the unique process invariant under rotations when stereographically projected onto the sphere $\mathbb{S}^2$, see [Sod00].

In [SS93a], the authors proved that elliptic polynomials are well conditioned with high probability, whereas in [SS93b] they showed that points of almost minimal logarithmic energy are the roots of well conditioned polynomials. It was therefore natural to study the expected energy of the $X_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^2$ zeros of elliptic polynomials stereographically projected to the sphere. This was done in [ABS11], where the following closed expression for the expected logarithmic energy was derived,

$$\mathbb{E}[E_{K_0}(X_N)] = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{1}{2} N \log N - \left(\frac{1}{2} - \log 2\right) N. \tag{9}$$

This asymptotic expression is very close to the minimal logarithmic energy of N points on the sphere and outperforms the result obtained with the spherical ensemble (7). From this, a natural question that arises is whether this process also yields smaller (resp. higher) expected energy for any $s > 0$ (resp. $s < 0$). We address this question in Chapter 2.

Specifically, by computing the second joint intensity of the random point process given by the zeros of elliptic polynomials, in Chapter 2 we recover the previous result (9) and obtain the expected Riesz energy (Theorem 2.1.1), which is remarkably close to the optimal energy described in (6). Similar to the approach in [AZ15], the expected energy provides an upper (resp. lower) bound for the minimal (resp. maximal) s-energy

(Corollary 2.4.1), improving upon those presented in (8). Additionally, we derive a closed expression for the expected separation distance between points sampled from the zeros of elliptic polynomials (Theorem 2.10).

It is well known that any sequence (X_N) of N-point configurations in $\mathbb{S}^d$ optimizing the s-energy for $s > -2$ is *uniformly distributed*, meaning that for any Borel subset $B \subset \mathbb{S}^d$,

$$\lim_{N\to\infty} \frac{|X_N \cap B|}{N} = \sigma(B),$$

see [BHS19, Theorem 6.1.7]. In other words, every region on $\mathbb{S}^d$ receives its corresponding proportion of points from X_N.

We recall that the spherical L^2 cap discrepancy of $X_N \subset \mathbb{S}^d$ is defined by

$$\mathbb{D}_2(X_N) = \left(\int_0^\pi \int_{\mathbb{S}^d} \left| \frac{|X_N \cap B(x,r)|}{N} - \sigma(B(x,r)) \right|^2 \mathrm{d}\sigma(x) \sin r \, \mathrm{d}r \right)^{1/2},$$

where $B(x,r)$ denotes the ball centered at x of radius r with respect to the geodesic distance, and the spherical L^∞ cap discrepancy is defined by

$$\mathbb{D}_\infty(X_N) = \sup_{x\in\mathbb{S}^d, r>0} \left| \frac{|X_N \cap B(x,r)|}{N} - \sigma(B(x,r)) \right|.$$

It is well known that a sequence (X_N) is uniformly distributed if and only if its discrepancy satisfies $\lim_{N\to+\infty} \mathbb{D}_p(X_N) = 0$, for $p = \infty$ or $p = 2$, [BHS19, Section 6.1]. The speed of this convergence is commonly used to measure the degree of uniformity of an N-point set $X_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^d$. According to [Ale72, Sto73, Bec84b], the optimal order of the spherical L^2 cap discrepancy is $N^{-\frac{d+1}{2d}}$, i.e., there exist constants $c_d, C_d > 0$ such that

$$c_d N^{-\frac{d+1}{2d}} \le \inf_{|X_N|=N} \mathbb{D}_2(X_N) \le C_d N^{-\frac{d+1}{2d}}.$$

With respect to the spherical L^∞ cap discrepancy, Beck determined in [Bec84b, Bec84a] its optimal order up to a logarithmic factor,

$$c'_d N^{-\frac{d+1}{2d}} \le \inf_{|X_N|=N} \mathbb{D}_\infty(X_N) \le C'_d N^{-\frac{d+1}{2d}} \sqrt{\log N}.$$

An alternative but related measure of the quality of a distribution is provided by the so called *worst-case error*. Given $s > d/2$, a sequence (X_N) of N-point configurations $X_N \subset \mathbb{S}^d$ is a *sequence of QMC designs for the Sobolev space* $\mathbb{H}^s(\mathbb{S}^d)$ (or an *s-QMC design*) if there exists $C_{d,s} > 0$ such that for all $N \ge 1$,

$$\mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d)) \le C_{d,s} N^{-s/d}, \tag{10}$$

where the *worst-case error of* X_N is defined by

$$\mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d)) = \sup_{\|f\|_{\mathbb{H}^s(\mathbb{S}^d)} \le 1} \left\{ \left| \frac{1}{N} \sum_{x\in X_N} f(x) - \int_{\mathbb{S}^d} f(x)\, \mathrm{d}\sigma(x) \right| \;:\; f \in \mathbb{H}^s(\mathbb{S}^d) \right\}.$$

The exponent in (10) cannot be larger than s/d, since it has been shown that there exists a constant $c_{d,s}$ depending on the $\mathbb{H}^s(\mathbb{S}^d)$-norm such that for any N-point configuration X_N in $\mathbb{S}^d$,

$$c_{d,s}N^{-s/d} \leq \mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d)),$$

see [BCC+14, Result (D)].

From [BCC+14, Theorem 3.1] it follows that if (X_N) is a sequence of QMC designs for $\mathbb{H}^s(\mathbb{S}^d)$ it is also a QMC design for all $\mathbb{H}^{s'}(\mathbb{S}^d)$ for $\frac{d}{2} < s' < s$, see also [BSSW14, Lemma 23]. The maximal $s^* > \frac{d}{2}$ where (10) holds for all $\frac{d}{2} < s < s^*$ is the *QMC strength of the sequence* (X_N), [BSSW14]. The strength can be seen as a measure of the regularity of the sequence.

In Chapter 3, we study the average discrepancies and worst-case errors of some random point configurations on the sphere $\mathbb{S}^d$. These two concepts are connected through Stolarsky's formula. In particular, the worst-case error with $s = (d+1)/2$ corresponds to the spherical L^2 cap discrepancy up to a constant. On the one hand, we show that the spherical ensemble and the zeros of elliptic polynomials have optimal spherical L^2 cap discrepancy on average and we compute their expected L^2 *hemisphere discrepancy*, another version of discrepancy studied in [BDM18]. On the other hand, we give a non-deterministic version of the definition (10) and define the *average QMC strength of a random sequence* (X_N). We find this value for the spherical ensemble, the zeros of elliptic polynomials and the *harmonic ensemble*, a determinantal point process on $\mathbb{S}^d$ described in [BMOC16]. Lastly, we compare our findings with the conjectured QMC strengths of certain deterministic distributions associated with these random point processes.

In recent years, there has been a growing interest in exploring the kind of problems previously described in this introduction in spaces beyond the sphere. One natural direction for further investigation is to consider projective spaces, which along with the sphere form the class of compact connected two-point homogeneous spaces. In particular, they are the real, complex and quaternionic projective spaces $\mathbb{RP}^n$ $\mathbb{CP}^n$, $\mathbb{HP}^n$ and the Cayley plane $\mathbb{OP}^2$. For results in this direction see [BCCdR19, Skr19, Skr20b, ADG+22].

In particular, in [ADG+22] the authors study the energy minimization problem on projective spaces, using adapted versions of the Riesz and logarithmic potentials. They extend the harmonic ensemble introduced in [BMOC16] to any two-point homogeneous space, allowing them to derive upper bounds on the minimal energies for some values of N. We conclude Chapter 3 by showing that N-point sets drawn from the harmonic ensemble on projective spaces $\mathbb{FP}^n$ satisfy $\mathbb{D}_\infty(X_N) = O\left(N^{-\frac{d+1}{2d}} \log N\right)$ with overwhelming probability, a result that was already known for spheres $\mathbb{S}^d$, [BMOC16, Corollary 5].

In addition to the Riesz and logarithmic energies, the Green energy is also examined in [ADG+22]. This energy, whose associated potential $K(x, y)$ in (1) is the Green function, was first studied in [BCCdR19], where it was shown that its minimizers are uniformly distributed, as it is well known for the Riesz and logarithmic energies on the sphere. In fact, for the 2-dimensional sphere the Green function is essentially equivalent to the logarithmic potential, up to constants. This property makes the Green function a natural kernel to consider when studying higher-dimensional spheres or projective spaces. Given a two-point homogeneous manifold $\mathcal{M}$, the *minimal Green energy in* $\mathcal{M}$, denoted by

$\mathcal{E}_G(\mathcal{M}, N)$, has an order of $N^{2-2/d}$, where $d = \dim_{\mathbb{R}}(\mathcal{M})$ represents the real dimension of the manifold $\mathcal{M}$. More precisely, it satisfies the following inequality:

$$-c_{\mathcal{M}} N^{2-2/d} \leq \mathcal{E}_G(\mathcal{M}, N) \leq -C_{\mathcal{M}} N^{2-2/d}, \tag{11}$$

provided that $d > 2$. The lower bound, established in [Ste21] (see previous work by Elkies referenced in [Lan88, Lemma 5.2]), is satisfied for general compact Riemannian manifolds without boundary. The upper bound can be deduced by estimating the expected energy of the jittered sampling in the manifold (Proposition 4.1.3) and in particular holds for any two-point homogeneous manifold.

We observe that by the relation mentioned above, the Green energy minimization problem on $\mathbb{S}^2$ reduces to the logarithmic energy minimization problem. Moreover, for $\mathcal{M} = \mathbb{RP}^2$ or $\mathbb{CP}^1$, the corresponding Green energy can be expressed in terms of the Green energy on $\mathbb{S}^2$, as we will detail in Chapter 4. Consequently, the minimal Green energy on these two-point homogeneous manifolds is related to the minimal logarithmic energy on $\mathbb{S}^2$, and there is no need to separately consider the Green energy problem for these cases. For $d > 2$, the Green energy and the Riesz $(d-2)$-energy are related. This relationship is utilized in [ADG+22] to establish upper and lower bounds for the minimal Green energy in projective spaces based on the results they prove for the minimal Riesz energy. Notably, the lower bounds derived in [ADG+22] provide explicit values for the constant $c_{\mathcal{M}}$ in (11), which is in contrast to the general result presented in [Ste21].

Since the Green and logarithmic minimization problems are equivalent on $\mathbb{S}^2$, the lower bound in (3) is essentially giving a lower bound for $\mathcal{E}_G(\mathbb{S}^2, N)$. The most recent lower bound of $C_{\log}$ in (4) was established by Lauritsen in [Lau21] (building on previous works [LN75, SM76]) by considering a renormalized energy in the plane that is related to the energy on the sphere through [BS18, Theorem 1.5]. In [BL22], Beltrán and Lizarte showed that Lauritsen's argument can be adapted to directly work on the sphere $\mathbb{S}^2$ instead of the plane. Furthermore, they extended it to spheres of any dimension $d \geq 2$, obtaining

$$\mathcal{E}_G(\mathbb{S}^d, N) \geq -\frac{d^{1+2/d}}{d^2-4}\left(\frac{V_{\mathbb{S}^d}}{V_{\mathbb{S}^{d-1}}}\right)^{2/d} N^{2-2/d} + o(N^{2-2/d})$$

for the minimal Green energy on $\mathbb{S}^d$, where $V_{\mathbb{S}^d}$ denotes the volume of the d-dimensional sphere.

In Chapter 4, we present a simplified proof of the previous lower bound and extend it to cover any two-point homogeneous manifold (Theorem 4.1.1). This extension improves the lower bounds of the minimal Green energy established in [ADG+22]. Our proof follows Lauritsen's argument and is based on a decomposition of the discrete Green energy, revealing its connection with a discrepancy measure defined in terms of Sobolev norms (Definition 4.1.6). The derived results lead to an upper bound for this Sobolev discrepancy (Theorem 4.1.7). As a consequence, by adapting a method introduced by Wolff in an unpublished manuscript, we are able to establish an upper bound for the L^∞ discrepancy of N-point sets that minimize the Green energy (Theorem 4.1.4). Even for $\mathcal{M} = \mathbb{S}^2$, the Wolff's approach gives the best result in terms of L^∞ discrepancy of logarithmic (or Green) energy minimizers.

Part of the results in this thesis are contained in the following preprints:

1. C. Beltrán, V. de la Torre, and F. Lizarte. Lower bound for the green energy of point configurations in harmonic manifolds, 2022, arXiv:2212.12526.

2. V. de la Torre and J. Marzo. Expected energy of zeros of elliptic polynomials, 2022, arXiv:2211.07599.

3. V. de la Torre and J. Marzo. QMC strength for some random configurations on the sphere, 2023, arXiv:2302.01001. To appear in: A. Hinrichs, P. Kritzer, F. Pillichshammer (eds.). Monte Carlo and Quasi-Monte Carlo Methods 2022. Springer Verlag.

Chapter 1

Preliminaries

In this chapter, we present the key elements that form the basis of this thesis: the two-point homogeneous manifolds and the point processes we are going to study. Additionally, we gather some fundamental results concerning energy, expressed in the context of the energies that will be explored throughout the thesis: the Riesz and logarithmic energy on the sphere $\mathbb{S}^d$ and the Green energy on any two-point homogeneous manifold.

1.1 Two-point homogeneous manifolds

Let $\mathcal{M}$ be a Riemannian manifold with Riemannian distance ϑ and let G be its group of isometries. In this thesis, we will always deal with compact connected two-point homogeneous spaces, i.e., spheres and projective spaces.

Definition 1.1.1. A connected Riemannian manifold $\mathcal{M}$ is said to be *two-point homogeneous* if for every two pairs (x_1, x_2) and (y_1, y_2) of points in $\mathcal{M}$ satisfying $\vartheta(x_1, x_2) = \vartheta(y_1, y_2)$, there exists an isometry $g \in G$ such that $g(x_i) = y_i$, $i = 1, 2$.

The complete list of compact connected Riemannian manifolds was given in [Wan52]: the sphere $\mathbb{S}^d$, the real, complex and quaternionic projective spaces $\mathbb{RP}^n, \mathbb{CP}^n, \mathbb{HP}^n$ and the Cayley plane $\mathbb{OP}^2$. Before defining the projective spaces, we recall that

$$\begin{aligned}
&\mathbb{O} = \{x = x_0 + x_1 i_1 + \ldots + x_7 i_7 : \ x_i \in \mathbb{R}\} \text{ are the } \textit{octonions},\\
&\mathbb{H} = \{x \in \mathbb{O} : \ x_4 = x_5 = x_6 = x_7 = 0\} \text{ are the } \textit{quaternions},\\
&\mathbb{C} = \{x \in \mathbb{H} : \ x_2 = x_3 = 0\} \text{ are the } \textit{complex numbers},\\
&\mathbb{R} = \{x \in \mathbb{C} : \ x_1 = 0\} \text{ are the } \textit{real numbers}.
\end{aligned}$$

The first three types of projective spaces $\mathbb{FP}^n$, $\mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}$, can be thought as the spaces of lines passing through the origin in $\mathbb{F}^{n+1}$:

$$\mathbb{FP}^n = \{p(a) = a\mathbb{F} : \ a \in \mathbb{F}^{n+1}, |a| = 1\}.$$

This description does not extend to $\mathbb{OP}^2$, because the algebra $\mathbb{O}$ is not associative. However, there is another model for the projective spaces $\mathbb{FP}^n$, $\mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}$, that admits a

	$\mathbb{S}^d$	$\mathbb{FP}^n$
α	$\frac{d}{2}-1$	
β	α	$\frac{\dim_{\mathbb{R}}(\mathbb{F})}{2}-1$
κ	$1/2$	1

Table 1.1: Parameters α, β, κ associated to each two-point homogeneous manifold.

generalization to $\mathbb{OP}^2$, see [Skr20b] and references therein for details. The Cayley plane can be described then as the subset of 3×3 Hermitian matrices Π over $\mathbb{O}$ with $\Pi^2=\Pi$ and $\operatorname{Tr}\Pi = 1$.

Furthermore, since for each of these spaces its group of isometries G is transitive, from [Lee13, Theorem 21.18] we have a quotient representation of $\mathcal{M}$ as an homogeneous space G/G_a, where $G_a := \{g \in G : \; ga = a\}$ is the isotropy group of an arbitrary point $a \in \mathcal{M}$.

Following the notation from [ADG+22, Section 2], each two-point homogeneous space has associated parameters α, β, κ given by Table 1.1 and is equipped with its corresponding G-invariant volume form $\tilde{\sigma}$ and geodesic distance ϑ, normalized to take values in $\left[0, \frac{\pi}{2\kappa}\right]$. We will usually consider the normalized uniform measure $\sigma = \tilde{\sigma}/V$, where V stands for the total volume of $\mathcal{M}$, i.e., $V = V_{\mathcal{M}} = \tilde{\sigma}(\mathcal{M})$.

Given a sphere $S(x,a) = \{y \in \mathcal{M} : \vartheta(x,y) = a\}$ centered at x of radius a, its surface measure is

$$A(a) = V_{\mathbb{S}^{d-1}} \kappa^{-2\alpha-1} \sin^{2\alpha+1}(\kappa a)\cos^{2\beta+1}(\kappa a),$$

see [Hel65, Proposition 5.6 and p.171]. Then the ball $B(x,a) = \{y \in \mathcal{M} : \vartheta(x,y) < a\}$ has volume

$$\tilde{\sigma}(B(x,a)) = \int_0^a A(r)\,\mathrm{d}r = V_{\mathbb{S}^{d-1}}\kappa^{-2\alpha-1}\int_0^a \sin^{2\alpha+1}(\kappa r)\cos^{2\beta+1}(\kappa r)\,\mathrm{d}r. \tag{1.1}$$

Both quantities are independent of the point $x \in \mathcal{M}$ due to the symmetry of two-point homogeneous manifolds.

If $D = D_{\mathcal{M}} = \frac{\pi}{2\kappa}$ is the diameter of $\mathcal{M}$, that is, the maximum distance between two points in $\mathcal{M}$, from the previous formula with $a = D$ we get the total volume of $\mathcal{M}$:

$$\begin{aligned} V_{\mathcal{M}} = \tilde{\sigma}(B(x,D)) &= V_{\mathbb{S}^{d-1}}\kappa^{-2\alpha-1}\int_0^D \sin^{2\alpha+1}(\kappa r)\cos^{2\beta+1}(\kappa r)\,\mathrm{d}r \\ &= V_{\mathbb{S}^{d-1}}\kappa^{-d}\int_0^{\kappa D=\pi/2} \sin^{2\alpha+1} r\cos^{2\beta+1} r\,\mathrm{d}r \\ &= V_{\mathbb{S}^{d-1}}\kappa^{-d}\gamma_{\alpha,\beta}, \end{aligned} \tag{1.2}$$

where

$$\gamma_{\alpha,\beta} = \int_0^{\pi/2} \sin^{2\alpha+1} r\cos^{2\beta+1} r\,\mathrm{d}r = \frac{\mathrm{B}(\alpha+1,\beta+1)}{2}. \tag{1.3}$$

In particular,

$$V_{\mathbb{S}^d} = V_{\mathbb{S}^{d-1}} 2^{d-1} \,\mathrm{B}\left(\frac{d}{2}, \frac{d}{2}\right) = \frac{2\pi^{\frac{d+1}{2}}}{\Gamma\left(\frac{d+1}{2}\right)},$$
$$V_{\mathbb{FP}^n} = V_{\mathbb{S}^{d-1}} \gamma_{\alpha,\beta}.$$

Instead of working with the surface area measure $A(a)$, we will take its normalized version $v(a) = v_{\mathcal{M}}(a) = A(a)/V$,

$$v(a) = \frac{\kappa}{\gamma_{\alpha,\beta}} \sin^{2\alpha+1}(\kappa a) \cos^{2\beta+1}(\kappa a). \tag{1.4}$$

Thus, if $V(a) = V_{\mathcal{M}}(a) = \sigma(B(x,a))$ is the normalized volume of the ball $B(x,a)$, we have

$$V(a) = \int_0^a v(r)\,\mathrm{d}r.$$

More generally, for any integrable function $F : \mathcal{M} \to \mathbb{R}$ such that $F(x) = f(\vartheta(x, x_0))$ for some point $x_0 \in \mathcal{M}$, the formula

$$\int_{\mathcal{M}} F(x)\,\mathrm{d}\sigma(x) = \int_0^D f(r) v(r)\,\mathrm{d}r \tag{1.5}$$

holds.

1.1.1 The Laplace-Beltrami operator and its eigenfunctions

In this thesis we will follow the convention that the Laplace-Beltrami operator is given by $\Delta = -\mathrm{div}\nabla$. Then, the operator will have non-negative eigenvalues $0 = \lambda_0 < \lambda_1 < \cdots$ that satisfy $\lambda_\ell \to \infty$. For each $\ell \in \mathbb{N}$, let V_ℓ be the corresponding eigenspace, with dimension m_ℓ. In the sphere case, these are the vector spaces of spherical harmonics of degree ℓ. The eigenvalues and their respective multiplicities are given by

$$\lambda_\ell = 4\kappa^2 \ell(\ell + \alpha + \beta + 1), \tag{1.6}$$

$$m_\ell = \frac{2\ell + \alpha + \beta + 1}{\alpha + \beta + 1} \frac{(\alpha + \beta + 1)_\ell (\alpha + 1)_\ell}{\ell! (\beta + 1)_\ell}. \tag{1.7}$$

For the Hilbert space $L^2(\mathcal{M}, \sigma)$ of real-valued square integrable functions in $\mathcal{M}$ with the inner product

$$\int_{\mathcal{M}} f(x) g(x)\,\mathrm{d}\sigma(x), \tag{1.8}$$

the decomposition $L^2(\mathcal{M}, \sigma) = \bigoplus_{\ell \geq 0} V_\ell$ holds.

For each $\ell \geq 0$, let $\{Y_{\ell,k}\}_{k=1}^{m_\ell}$ be an orthonormal basis of V_ℓ with respect to the inner product (1.8). The reproducing kernel of V_ℓ is given by the addition formula:

$$Z_\ell^{(\alpha,\beta)}(x, y) = \sum_{k=1}^{m_\ell} Y_{\ell,k}(x) Y_{\ell,k}(y) = \frac{m_\ell}{P_\ell^{(\alpha,\beta)}(1)} P_\ell^{(\alpha,\beta)}(\cos(2\kappa\vartheta(x, y))). \tag{1.9}$$

Here $P_\ell^{(\alpha,\beta)}(t)$ are the Jacobi polynomials, see Section 1.1.2 for the definition and details on the normalization.

The following result tells us how finite-dimensional G-invariant subspaces $H \subset L^2(\mathcal{M},\sigma)$ are. The importance of these subspaces for us lies in the fact that they induce G-invariant determinantal point processes.

Proposition 1.1.2 ([ADG+22, Proposition 2.7])**.** *Let H be a-finite dimensional G-invariant subspace of $L^2(\mathcal{M},\sigma)$. Then there exist $0 \leq \ell_1 < \cdots < \ell_m$ such that*

$$H = V_{\ell_1} \oplus \cdots \oplus V_{\ell_m}.$$

A particular instance of these G-invariant subspaces is the space of eigenfunctions with eigenvalue at most λ_L,

$$\Pi_L = V_0 \oplus \cdots \oplus V_L. \tag{1.10}$$

By the mutual orthogonality of V_ℓ, (1.9) and the summation formula (1.13), its reproducing kernel is

$$\begin{aligned} K_L^{(\alpha,\beta)}(x,y) &= \sum_{\ell=0}^{L} Z_\ell^{(\alpha,\beta)}(x,y) \\ &= \sum_{\ell=0}^{L} \frac{m_\ell}{P_\ell^{(\alpha,\beta)}(1)} P_\ell^{(\alpha,\beta)}(\cos(2\kappa\vartheta(x,y))) \\ &= \frac{(\alpha+\beta+2)_L}{(\beta+1)_L} P_\ell^{(\alpha+1,\beta)}(\cos(2\kappa\vartheta(x,y))), \quad x,y \in \mathcal{M}. \end{aligned} \tag{1.11}$$

The dimension of Π_L can be deduced by taking an arbitrary pair (x,x), $x \in \mathcal{M}$, in the previous expression:

$$\begin{aligned} \pi_L^{(\alpha,\beta)} := \dim(\Pi_L) &= \sum_{\ell=0}^{L} m_\ell \\ &= \frac{(\alpha+\beta+2)_L}{(\beta+1)_L} P_\ell^{(\alpha+1,\beta)}(1) \\ &= \frac{(\alpha+\beta+2)_L(\alpha+2)_L}{(\beta+1)_L L!} \approx L^{2\alpha+2}. \end{aligned} \tag{1.12}$$

1.1.2 Jacobi polynomials

The classical Jacobi polynomials will appear in this thesis as the reproducing kernels of the eigenspaces V_ℓ of the Laplace-Beltrami operator. The Jacobi polynomials $P_\ell^{(\alpha,\beta)}(t)$ are the orthogonal polynomials for the weight function $(1-t)^\alpha(1+t)^\beta$ on the interval $[-1,1]$, normalized as

$$P_\ell^{(\alpha,\beta)}(1) = \binom{\ell+\alpha}{\ell}.$$

The summation formula [Sze39, Formula 4.5.3]

$$\sum_{\ell=0}^{L} \frac{2\ell+\alpha+\beta+1}{\alpha+\beta+1} \frac{(\alpha+\beta+1)_\ell}{(\beta+1)_\ell} P_\ell^{(\alpha,\beta)}(t) = \frac{(\alpha+\beta+2)_L}{(\beta+1)_L} P_\ell^{(\alpha+1,\beta)}(t) \tag{1.13}$$

gives the reproducing kernel of $\Pi_L = \bigoplus_{\ell=0}^{L} V_\ell$, see Section 1.1.1.

1.2 Energies

In this thesis we will be interested in N-point configurations optimizing certain energies. Except for some specific low values of N, this is an almost impossible problem to solve exactly, so in general our goal is to say something about the asymptotic expansion of these energies or the behaviour of their minimizers.

Let $\mathcal{M}$ be a compact connected two-point homogeneous manifold and $K : \mathcal{M} \times \mathcal{M} \to \mathbb{R} \cup \{+\infty\}$ a lower semicontinuous and symmetric function that we call a *potential*. In particular, we will always work with potentials depending on the Riemannian distance, i.e., $K(x, y) = f(\vartheta(x, y))$ for some function f.

Let $X_N = \{x_1, \dots, x_N\} \subset \mathcal{M}$ be an N-point configuration in $\mathcal{M}$. The *discrete K-energy of X_N* is defined by

$$\lim_{N\to\infty} E_K(X_N) = \sum_{i\neq j} K(x_i, x_j).$$

Since $\mathcal{M}$ is compact and K is lower semicontinuous, the *minimal discrete N-point K-energy of $\mathcal{M}$*

$$\mathcal{E}_K(\mathcal{M}, N) := \min_{X_N \subset \mathcal{M}} E_K(X_N)$$

is achieved by some N-point configuration $X_N^* \subset \mathcal{M}$.

The discrete energy has a continuous version. Let $\mathbb{P}(\mathcal{M})$ denote the set of Borel probability measures on $\mathcal{M}$. For any $\mu \in \mathbb{P}(\mathcal{M})$, the *continuous K-energy of μ* is

$$I_K(\mu) = \int_{\mathcal{M}} \int_{\mathcal{M}} K(x, y)\, \mathrm{d}\mu(x)\, \mathrm{d}\mu(y).$$

The *Wiener constant* is the smallest such energy, i.e., $W_K(\mathcal{M}) = \inf_{\mu\in\mathbb{P}(\mathcal{M})} I_K(\mu)$. We say that the probability measure $\mu_{\mathcal{M}} \in \mathbb{P}(\mathcal{M})$ is an equilibrium measure for $\mathcal{M}$ relative to the kernel K if $I_K[\mu] = W_K(\mathcal{M})$.

Both versions of the energy are intimately related for the class of potentials we will consider in this thesis.

Theorem 1.2.1 ([BHS19, Section 4.2])**.** *Let K be a symmetric, lower semicontinuous and conditionally strictly positive definite kernel on $\mathcal{M} \times \mathcal{M}$ for which $W_K(\mathcal{M}) < \infty$. Then*

$$\lim_{N\to\infty} \frac{\mathcal{E}_K(\mathcal{M}, N)}{N^2} = W_K(\mathcal{M}).$$

Moreover, the equilibrium measure $\mu_{\mathcal{M}}$ is unique and if (X_N) is any sequence of N-point minimizers of the discrete K-energy, then the sequence of normalized counting measures

$$\nu(X_N) := \frac{1}{N} \sum_{x \in X_N} \delta_x$$

converges to $\mu_{\mathcal{M}}$ in the weak sense.*

Although the proofs in [BHS19] are for compact subsets of $\mathbb{R}^d$, they can be generalized to compact metric spaces. The last part of the theorem says that the sequence of N-point minimizers is uniformly distributed, that is, every region on $\mathcal{M}$ gets its fair share of points as N grows, while the first part gives the leading term of the asymptotic expansion of $\mathcal{E}_K(\mathcal{M}, N)$.

Next we explore this connection for the potentials considered in this thesis.

1.2.1 Riesz and logarithmic energy on $\mathbb{S}^d$

Let $\mathcal{M} = \mathbb{S}^d$ be the unit sphere. For $s \neq 0$, the *Riesz s-potential* is defined by

$$K_s(x, y) := |x - y|^{-s}.$$

For $s = 0$, instead of taking this potential, that would yield a trivial energy independent of the N-point configuration, one considers its derivative, i.e.,

$$K_0(x, y) = \frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0^+} |x - y|^{-s} = -\log |x - y|.$$

This is the *logarithmic potential.*

We define the *Riesz s-energy* (*logarithmic energy* if $s = 0$) of $X_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^d$ by

$$E_s(X_N) = \sum_{i \neq j} K_s(x_i, x_j).$$

The *optimal N-point energy* is given by

$$\mathcal{E}_s(N) = \begin{cases} \min_{X_N \subset \mathbb{S}^d} E_s(X_N), & \text{if } s \geq 0, \\ \max_{X_N \subset \mathbb{S}^d} E_s(X_N), & \text{if } s < 0. \end{cases}$$

The *continuous Riesz s-energy* (*logarithmic energy* if $s = 0$) of a Borel probability measure μ on $\mathbb{S}^d$ is

$$I_s[\mu] = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} f_s(|x - y|) \, \mathrm{d}\mu(x) \, \mathrm{d}\mu(y),$$

with the *optimal continuous s-energy* being

$$V_s(\mathbb{S}^d) = \begin{cases} \min_{\mu \in \mathbb{P}(\mathbb{S}^d)} I_s[\mu], & \text{if } s \geq 0, \\ \max_{\mu \in \mathbb{P}(\mathbb{S}^d)} I_s[\mu], & \text{if } s < 0. \end{cases}$$

Classical potential theory yields that $V_s(\mathbb{S}^d) = +\infty$ for $s \geq d$ and that for $-2 < s < d$ the unique optimizer of $I_s[\mu]$ is the normalized surface measure σ, with

$$V_s(\mathbb{S}^d) = \begin{cases} 2^{d-s-1}\frac{\Gamma\left(\frac{d+1}{2}\right)\Gamma\left(\frac{d-s}{2}\right)}{\sqrt{\pi}\,\Gamma\left(d-\frac{s}{2}\right)}, & -2 < s < d,\ s \neq 0, \\ \frac{1}{2} - \log 2, & s = 0,\ d = 2. \end{cases} \tag{1.14}$$

We have omitted here the logarithmic case for $d \geq 3$, because we will restrict our interest to $d = 2$ for this potential.

For $s \geq 0$, the potential K_s is a symmetric, lower semicontinuous and conditionally strictly positive definite kernel and satisfies $W_{K_s}(\mathbb{S}^d) < \infty$ (see [BHS19, Chapter 4] for proofs of these facts), the conclusions in Theorem 1.2.1 hold. For $s < 0$, the same is true for the potential $-K_s$. Therefore, any sequence (X_N) of N-point minimizers (maximizers if $s < 0$) is uniformly distributed on $\mathbb{S}^d$, i.e., σ is the weak* limit of the sequence of normalized counting measures of the sets X_N. Moreover, for $-2 < s < d$,

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(N)}{N^2} = V_s(\mathbb{S}^d).$$

Thus, we get the leading term of the asymptotic expansion $\mathcal{E}_s(N)$ in the *potential-theoretic regime* $-2 < s < d$:

$$\mathcal{E}_s(N) = V_s(\mathbb{S}^d)N^2 + o(N^2), \quad N \to \infty.$$

Observe that in the *hypersingular case* $s \geq d$, since $V_s(\mathbb{S}^d) = +\infty$, the leading term cannot be justified as before.

In Chapter 2 we will give more details on the next-order term of $\mathcal{E}_s(N)$ in the potential-theoretic regime. For a complete overview on this topic we refer to [BHS19, Chapter 6].

1.2.2 Green energy

For a general Riemannian manifold $\mathcal{M}$, the study of the energy given by a potential based on the Green function was initiated in [BCCdR19]. Although one could take the definition of Riesz and logarithmic energy as in the sphere, the Green function is somehow a more intrinsic object to the manifold.

We recall the definition of the Green function from [Aub98, Section 4.2]. Let $\mathcal{M}$ be any compact Riemannian manifold without boundary. The *Green function* is the unique function $G : \mathcal{M} \times \mathcal{M} \to \mathbb{R} \cup \{\infty\}$ with the properties:

1. In the sense of distributions, $\Delta_y G = \delta_x - 1$, where δ_x is Dirac's delta.
2. G is $\mathcal{C}^\infty$ on $\mathcal{M} \times \mathcal{M}$ minus the diagonal.
3. Symmetry: $G_\mathcal{M}(x, y) = G_\mathcal{M}(y, x)$.
4. The mean of $G_\mathcal{M}(x, \cdot)$ is zero for all $x \in \mathcal{M}$, i.e., $\int_{y\in\mathcal{M}} G_\mathcal{M}(x, y)\, \mathrm{d}\sigma(y) = 0$.

For an N-point configuration $X_N = \{x_1, \ldots, x_N\} \subset \mathcal{M}$, the *discrete Green energy of* X_N is defined by

$$E_\mathcal{M}(X_N) = \sum_{i\neq j} G_\mathcal{M}(x_i, x_j).$$

By the lower semicontinuity, there exists some N-point configuration X_N^* reaching the *minimal Green energy*,

$$\mathcal{E}_G(\mathcal{M}, N) = \min_{X_N \subset \mathcal{M}} E_{\mathcal{M}}(X_N).$$

The *continuous Green energy of a measure* $\mu \in \mathbb{P}(\mathcal{M})$ is defined by

$$I_G(\mu) = \int_{\mathcal{M}} \int_{\mathcal{M}} G(x, y) \, \mathrm{d}\mu(x) \, \mathrm{d}\mu(y).$$

In the context of two-point homogeneous manifolds, it was proved in [BCCdR19] that G is a conditionally strictly positive kernel, so one can apply Theorem 1.2.1 to conclude that the N-point minimizers are equidistributed and

$$\lim_{N \to \infty} \frac{\mathcal{E}_G(\mathcal{M}, N)}{N^2} = W_G(\mathcal{M}). \tag{1.15}$$

The equilibrium measure, which by the theorem is unique, turns out to be the normalized uniform measure σ on $\mathcal{M}$. By our normalization of G, its energy is zero and then $W_G(\mathcal{M}) = 0$. Therefore, in this case (1.15) does not reveal the leading term of the minimal Green energy and it only yields that

$$\mathcal{E}_G(\mathcal{M}, N) = o(N^2), \quad N \to \infty.$$

In Chapter 4 we will state the correct order of the leading term of the expansion and we will obtain a lower bound of the main coefficient for two-point homogeneous manifolds.

1.3 Point processes

Let Λ be a locally compact Polish space, i.e., a topological space that can be topologized by a complete and separable metric. In this dissertation, Λ is going to be either $\mathbb{C}$ or a two-point homogeneous manifold $\mathcal{M}$. We consider also a Radon measure μ on Λ. For the concepts in this section we follow [HKPV09].

Definition 1.3.1. A *simple point process* $\mathcal{X}$ *on* Λ is a random discrete subset of Λ.

Given a subset $D \subset \Lambda$, we denote by $\mathcal{X}(D)$ or n_D the random variable counting the number of points that fall in D. A way to define the distribution of a point process is through its joint intensities.

Definition 1.3.2. Let $\mathcal{X}$ be a simple point process on Λ. The *joint intensities* ρ_k *of* $\mathcal{X}$ *w.r.t.* μ are functions defined on Λ^k such that for any family of mutually disjoint subsets $D_1, \ldots, D_k \subset \Lambda$,

$$\mathbb{E}\left[\prod_{i=1}^{k} \mathcal{X}(D_i)\right] = \int_{\prod_i D_i} \rho_k(x_1, \ldots, x_k) \, \mathrm{d}\mu(x_1) \cdots \mathrm{d}\mu(x_k). \tag{1.16}$$

If $x_i = x_j$ for some $i \neq j$, $\rho_k(x_1, \ldots, x_k)$ is required to vanish.

Let $\mathcal{X}^{\wedge k}$ be the set of ordered k-tuples of distinct points of $\mathcal{X}$. As a consequence of (1.16) it follows that for any Borel set $B \subset \Lambda^k$,

$$\mathbb{E}\left[|B \cap \mathcal{X}^{\wedge k}|\right] = \int_B \rho_k(x_1, \ldots, x_k)\, \mathrm{d}\mu(x_1) \cdots \mathrm{d}\mu(x_k), \tag{1.17}$$

see [HKPV09, Formula 1.2.2]. Finally, a standard application of the monotone convergence theorem yields

$$\mathbb{E}\left[\sum_{i_1, \ldots, i_k \text{ distinct}} \phi(x_{i_1}, \ldots, x_{i_k})\right] = \int_{\Lambda^k} \phi(x_1, \ldots, x_k)\rho_k(x_1, \ldots, x_k)\, \mathrm{d}\mu(x_1) \cdots \mathrm{d}\mu(x_k) \tag{1.18}$$

for any measurable function $\phi : \Lambda^k \to [0, +\infty)$. This formula is used to compute the expected energies of points drawn from some random point processes. Since the energies we consider involve pairwise interactions between points, we will need the first and the second joint intensity of these processes.

For a general point process, the number of points can depend on the realization. Since we are interested in producing random N-point configurations, we will need to restrict to processes giving N points almost surely.

Zeros of random polynomials

A natural way to obtain random point processes is to take the zero set of random functions.

Definition 1.3.3. Let f be a random variable taking values in the space of analytic functions on a region $\Lambda \subset \mathbb{C}$. We say that f is a Gaussian analytic function (GAF) on Λ if $(f(z_1), \ldots, f(z_n))$ has a mean zero complex Gaussian distribution for any $n \geq 1$ and every $z_1, \ldots, z_n \in \Lambda$. The covariance kernel K is defined by $K(z, w) = \mathbb{E}[f(z)\overline{f}(w)]$.

The following lemma provides a recipe to construct GAFs.

Lemma 1.3.4 ([HKPV09, Lemma 2.2.3])**.** *Let ψ_n be holomorphic functions on Λ. Assume that $\sum_n |\psi_n(z)|^2$ converges uniformly on compact sets in Λ. Let a_n be i.i.d. random variables with standard complex Gaussian distribution. Then $f(z) := \sum_n a_n\psi_n(z)$ is a GAF with covariance kernel $K(z, w) = \sum_n \psi_n(z)\overline{\psi}_n(w)$.*

Once we have this random analytic function, we can take the random subset $\mathcal{X} = f^{-1}(0)$, which by [HKPV09, Lemma 2.4.1] is a simple point process. The following formula for the joint intensities of $\mathcal{X}$ was deduced by Hammersley.

Theorem 1.3.5 ([HKPV09, Corollary 3.4.2])**.** *Let f be a GAF on $\Lambda \subset \mathbb{C}$ with covariance kernel K. If $\det\left(K(z_i, z_j)\right)_{i,j\leq k}$ does not vanish anywhere on Λ, then the k-point intensity function ρ_k with respect to the Lebesgue measure exists and is given by*

$$\rho_k(z_1, \ldots, z_k) = \frac{\operatorname{per}(C - BA^{-1}B^*)}{\det(\pi A)},$$

where A, B, C are the $k \times k$ matrices with entries

$$\begin{aligned} A(i,j) &= \mathbb{E}[f(z_i)\overline{f}(z_j)], \\ B(i,j) &= \mathbb{E}[f'(z_i)\overline{f}(z_j)], \\ C(i,j) &= \mathbb{E}[f'(z_i)\overline{f'}(z_j)]. \end{aligned}$$

For the first intensity we have a simpler expression, known as Edelman-Kostlan formula [HKPV09, Formula 2.4.8]:

$$\rho_1(z) = \frac{1}{4\pi}\Delta \log K(z,z), \tag{1.19}$$

with respect to the Lebesgue measure on $\mathbb{C}$.

Determinantal point processes

In the previous setting, in general it is difficult to derive the joint intensities of the zero set. Even though they can be obtained through the Hammersley's formula, in practice the computation of ρ_k becomes hard already for $k \geq 2$. Now we consider a kind of point processes whose joint intensities are given by the determinant of the Gram matrix of a kernel.

Definition 1.3.6. Let $K : \Lambda^2 \to \mathbb{C}$ be a measurable function. A simple point process $\mathcal{X}$ on Λ is a *determinantal point process with kernel* K if, for every $k \geq 1$ and $x_1, \ldots, x_k \in \Lambda$,

$$\rho_k(x_1, \ldots, x_k) = \det\left(K(x_i, x_j)\right)_{1 \leq i,j \leq k} \tag{1.20}$$

with respect to the background measure μ.

In general, given such a function K, it is not clear whether a determinantal point process with kernel K exists. However, it is the case for the particular kind of determinantal processes we are going to consider throughout this thesis.

Definition 1.3.7. A *determinantal projection process* is a determinantal point process whose kernel K_H defines a projection operator onto a subspace $H \subset L^2(\Lambda, \mu)$ or, equivalently, $K_H(x,y) = \sum \varphi_k(x)\overline{\varphi}_k(y)$, where $\{\varphi_k\}_k$ is any orthonormal basis for H.

We will restrict ourselves to finite-dimensional subspaces H, in which case the kernel is given by a finite sum $K_H(x,y) = \sum_{k=1}^N \varphi_k(x)\overline{\varphi}_k(y)$. Then, by [HKPV09, Lemmas 4.2.6, 4.4.1, 4.5.1], there exists a unique determinantal projection process on Λ with kernel K_H. Moreover, the number of points in $\mathcal{X}$ is equal to $N = \dim(H)$, almost surely. This fact makes determinantal projection processes a useful method to pick N random points from Λ; otherwise the number of points could depend on the realization of the point process.

1.3.1 Zeros of elliptic polynomials

As explained above, a source of simple point processes are the zero sets of Gaussian analytic functions. In this section, we introduce a GAF on $\mathbb{C}$ satisfying two conditions:

(i) The number of points in $\mathcal{X}$ is N, almost surely.

(ii) If we send $\mathcal{X}$ to the sphere $\mathbb{S}^2$ through the stereographic projection, the resulting point process is invariant in distribution under rotations of the sphere. This condition can also be verified directly on $\mathbb{C}$, see [HKPV09, Section 2.3] for the expression of these rotations on the complex plane.

It turns out that, up to a constant, there is only one GAF on $\mathbb{C}$ satisfying (ii), [HKPV09, Proposition 2.3.4, Theorem 2.5.2]:

$$P_N(z) = \sum_{n=0}^{N} a_n \sqrt{\binom{N}{n}} z^n, \tag{1.21}$$

where a_n are i.i.d. random variables with standard complex Gaussian distribution. These are the *elliptic polynomials*, also called Kostlan-Shub-Smale or $SU(2)$ polynomials. In terms of Lemma 1.3.4, they correspond to taking $\psi_n(z) = \sqrt{\binom{N}{n}} z^n$ for $n \leq N$ and $\psi_n(z) = 0$ for $n > N$ and have covariance kernel $K(z,w) = (1 + z\overline{w})^N$. Observe that condition (i) automatically holds, so the images by the stereographic projection of the zeros of the elliptic polynomial P_N give N random points on the sphere.

Applying the Edelman-Kostlan formula (1.19), we can obtain the first intensity of the process:

$$\rho_1(z) = \frac{1}{4\pi} \Delta \log \left(1 + |z|^2\right)^N = N \frac{1}{\pi(1+|z|^2)^2},$$

with respect to the Lebesgue measure dz. In other words, the intensity is N with respect to the Lebesgue surface measure of the sphere, which means that the expected number of points in a subset $A \subset \mathbb{S}^2$ is proportional to its area.

Since this process is not determinantal, as will be seen in Chapter 2, there is no simple expression for the joint intensities ρ_k, $k \geq 2$, and this complicates the application of formula (1.18) to compute expected energies. However, in [ABS11] Armentano, Beltrán and Shub managed to obtain the expected logarithmic energy without computing the second joint intensity: if $X_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^2$ are the images by the stereographic projection of the N zeros of the elliptic polynomial P_N in (1.21),

$$\mathbb{E}[E_0(X_N)] = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{1}{2} N \log N - \left(\frac{1}{2} - \log 2\right) N.$$

Their arguments do not seem to extend to the Riesz energy, so in Chapter 2 we will compute the second joint intensity ρ_2 in order to apply formula (1.18).

1.3.2 Spherical ensemble

Given A, B independent $N \times N$ random matrices with i.i.d. complex standard entries, the eigenvalues $\{\lambda_1, \dots, \lambda_N\}$ of $A^{-1}B$ are a simple point process on $\mathbb{C}$. Krishnapur [Kri09] proved that this process is determinantal on the complex plane with kernel $(1 + z\overline{w})^{N-1}$ with respect to the background measure

$$\frac{N}{\pi(1+|z|^2)^{N+1}}\, \mathrm{d}z.$$

Moreover, its kernel defines a projection operator to the subspace

$$H = \operatorname{span}\left\{ \frac{z^k}{(1+|z|^2)^{\frac{N+1}{2}}} \,:\, 0 \le k \le N-1 \right\},$$

so it is a determinantal projection process.

The process $X_N = \{x_1, \dots, x_N\} \subset \mathbb{S}^2$ obtained when mapping the eigenvalues λ_i to the sphere $\mathbb{S}^2$ through the stereographic projection is known as the *spherical ensemble*. If the points $x_1, \dots, x_N$ are taken in uniform random order, they have density

$$C \prod_{i<j} |x_i - x_j|^2$$

with respect to the surface measure σ in $\mathbb{S}^2$. Thus, the process is invariant in distribution under rotations of $\mathbb{S}^2$. Furthermore, the kernel with respect to σ of the spherical ensemble as a determinantal point process on $\mathbb{S}^2$ satisfies

$$|K_N(x_1, x_2)|^2 = N^2 \left(1 - \frac{|x_1 - x_2|^2}{4}\right)^{N-1}. \tag{1.22}$$

Alishahi and Zamani computed in [AZ15] the expected Riesz and logarithmic energies of N points X_N sampled from the spherical ensemble. In particular, one of their main results is the following estimate for $s < 4$,

$$\mathbb{E}[E_s(X_N)] = \begin{cases} \dfrac{2^{1-s}}{2-s} N^2 - \dfrac{\Gamma(N)\Gamma(1-s/2)}{2^s \Gamma(N+1-s/2)} N^2, & s \ne 0, 2, \\ \left(\frac{1}{2} - \log 2\right) N^2 - \frac{1}{2} N \log N + \left(\log 2 - \frac{\gamma}{2}\right) N - \frac{1}{4} + O\left(\frac{1}{N}\right), & s = 0, \\ \frac{1}{4} N^2 \log N + \frac{\gamma}{4} N^2 - \frac{N}{8} - \frac{1}{48} + O\left(\frac{1}{N^2}\right), & s = 2. \end{cases} \tag{1.23}$$

1.3.3 Harmonic ensembles

We finally introduce the class of determinantal point processes that we are going to study on two-point homogeneous spaces. As seen in Section 1.2, the potentials we are considering in this dissertation are invariant under the isometries of the manifold $\mathcal{M}$. Thus, when choosing a subspace $H \subset L^2(\mathcal{M}, \sigma)$ to induce a determinantal point process, a natural condition is that the resulting process also exhibits invariance. By Proposition

1.1.2, this happens if H is an orthogonal sum of eigenspaces V_ℓ of the Laplace-Beltrami operator on $\mathcal{M}$.

Beltrán, Marzo and Ortega-Cerdà [BMOC16] defined in this way the *harmonic ensemble*, a determinantal projection process in $\mathbb{S}^d$ given by the projection onto

$$\Pi_L = V_0 \oplus \cdots \oplus V_L,$$

which makes the process invariant under rotations of the sphere. The subspace Π_L is the vector space of spherical harmonics of degree at most L in $\mathbb{S}^d$ and coincides with the space of polynomials of degree at most L in $\mathbb{R}^{d+1}$ restricted to $\mathbb{S}^d$.

More recently, in [ADG+22], a version of this process has been proposed for projective spaces: the determinantal projection process induced by the subspace $\Pi_L = \bigoplus_{\ell=0}^{L} V_\ell$, where V_ℓ are the eigenspaces of the Laplace-Beltrami operator on $\mathbb{FP}^n$. By analogy with the spherical case, the authors call these processes *harmonic ensembles*.

Thus, for any two-point homogeneous manifold $\mathcal{M}$ with parameters (α, β), the harmonic ensemble is a determinantal point process with $\pi_L^{(\alpha,\beta)} = \dim(\Pi_L) = \frac{(\alpha+\beta+2)_L(\alpha+2)_L}{(\beta+1)_L L!} \approx L^d$ a.s. points whose kernel

$$K_L^{(\alpha,\beta)}(x, y) = \frac{(\alpha + \beta + 2)_L}{(\beta + 1)_L} P_L^{(\alpha+1,\beta)}(\cos(2\kappa\vartheta(x, y))) \tag{1.24}$$

defines a projection operator onto the subspace Π_L.

Chapter 2

Expected energy of zeros of elliptic polynomials

In 2011, Armentano, Beltrán and Shub obtained in [ABS11] a closed expression for the expected logarithmic energy of the random point process on the sphere given by the roots of random elliptic polynomials. We consider a different approach which allows us to extend the study to the Riesz energies and to compute the expected separation distance.

This chapter is based on [dlTM22].

2.1 Introduction and main results

In Section 1.3.1 we have introduced the elliptic polynomials P_N, which are Gaussian analytic functions defined by

$$P_N(z) = \sum_{n=0}^{N} a_n \sqrt{\binom{N}{n}} z^n,$$

where a_n are i.i.d. random variables with standard complex Gaussian distribution.

As defined in Section 1.2, the Riesz or logarithmic energy of a set of N different points $X_N = \{x_1, \ldots, x_N\}$ on the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$ is

$$E_s(X_N) = \sum_{i \neq j} f_s(|x_i - x_j|),$$

where $f_s(r) = r^{-s}$ for $s \neq 0$ and $f_0(r) = -\log r$ are, respectively, the Riesz and logarithmic potentials. We denote the extremal (minimal or maximal) energy attained by a set of N points on the sphere by

$$\mathcal{E}_s(N) = \begin{cases} \min_{X_N \subset \mathbb{S}^2} E_s(X_N) & \text{if } s \geq 0, \\ \max_{X_N \subset \mathbb{S}^2} E_s(X_N) & \text{if } s < 0. \end{cases}$$

In [ABS11], the authors obtained the following closed expression for the expected logarithmic energy of random points $X_N = \{x_1, \dots, x_N\} \subset \mathbb{S}^2$, images by the stereographic projection of zeros of elliptic polynomials,

$$\mathbb{E}[E_0(X_N)] = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{1}{2} N \log N - \left(\frac{1}{2} - \log 2\right) N. \tag{2.1}$$

The asymptotic expression above is very close to the minimal logarithmic energy of N points on the sphere, see Section 2.4. Working in a more general setting, in [Zho08, ZZ10] the same expression (2.1) was obtained but with a $o(N)$ remainder. Our main result in this chapter is an extension of the above result (2.1) to the Riesz s-energies for $s < 4$.

Theorem 2.1.1. *Let $X = \{x_1, \dots, x_N\} \subset \mathbb{S}^2$ be the image by the stereographic projection of N points drawn from zeros of elliptic polynomials. Then,*

(i) for $s < 4$, $s \neq 0, 2$ and a fixed $m \geq 1$,

$$\begin{aligned}\mathbb{E}[E_s(X_N)] &= \frac{2^{1-s}}{2-s} N^2 \\ &+ \frac{\Gamma\left(1 - \frac{s}{2}\right)}{2^{s+1}} \left[s\left(1 + \frac{s}{2}\right) \sum_{j=0}^{m-1} \frac{B_{2j}^{(\frac{s}{2})}(\frac{s}{4})(1 - \frac{s}{2})_{2j}}{(2j)!} N^{\frac{s}{2}+1-2j} \zeta\left(1 - \frac{s}{2} + 2j, 1 + \frac{4-s}{4N}\right) \right. \\ &+ \left. s\left(1 - \frac{s}{2}\right) \sum_{j=0}^{m-1} \frac{B_{2j}^{(\frac{s}{2}-1)}(\frac{s-2}{4})(2 - \frac{s}{2})_{2j}}{(2j)!} N^{\frac{s}{2}-2j} \zeta\left(2 - \frac{s}{2} + 2j, 1 + \frac{2-s}{4N}\right) \right] \\ &+ O\left(N^{\frac{s}{2}+1-2m}\right),\end{aligned} \tag{2.2}$$

for $N \to +\infty$.

(ii) Moreover, the energies with $s = -2n$ for an integer $n \geq -1$ can be computed exactly:

For $s = 0$,

$$\mathbb{E}[E_0(X_N)] = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{N \log N}{2} - \left(\frac{1}{2} - \log 2\right) N. \tag{2.3}$$

For $s = 2$,

$$\mathbb{E}[E_2(X_N)] = -\frac{N\pi}{4} \sum_{j=1}^{N-1} \frac{j}{N} \cot\left(\frac{\pi j}{N}\right) + \frac{3N^2}{8} - \frac{3N}{8}. \tag{2.4}$$

For $s = -2n$, $n \geq 1$,

$$\begin{aligned}\mathbb{E}[E_{-2n}(X_N)] &= 2^{2n} N^2 \left(\frac{1}{n+1} - \frac{n(n-1)}{n+1} - n \sum_{m=1}^{n+1} \frac{1}{m} \right) \\ &+ 2^{2n} n N \left(-\gamma + \sum_{m=1}^{n+1} \binom{n+1}{m} (-1)^m \psi\left(\frac{m}{N}\right) \left(\frac{n-1}{n+1} m + 1\right) \right).\end{aligned} \tag{2.5}$$

In the above result, γ is the Euler-Mascheroni constant, $B_{2j}^{(2\rho)}(\rho)$ are the generalized Bernoulli polynomials defined by

$$\left(\frac{t}{e^t-1}\right)^{2\rho} e^{\rho t} = \sum_{j=0}^{\infty} \frac{t^{2j}}{(2j)!} B_{2j}^{(2\rho)}(\rho),$$

for $|t| < 2\pi$, with $B_0^{(2\rho)}(\rho) = 1$,

$$\zeta(s,a) = \sum_{j=0}^{\infty} \frac{1}{(j+a)^s}, \quad \Re s > 1, \ a \notin \mathbb{Z}_{\leq 0}$$

is the Hurwitz Zeta function and $\psi(z) = \Gamma'(z)/\Gamma(z)$ is the digamma function.

By considering two terms of the asymptotic expansion of the Hurwitz Zeta function

$$\zeta(s,1+a) = \sum_{k=0}^{\infty} \frac{(-1)^k (s)_k \zeta(s+k)}{k!} a^k,$$

for $|a| < 1$ and $s \neq 1$ [DLMF, 25.11.10] and taking $m = 1$ in (2.2) we get, for $0, 2 \neq s < 4$,

$$\mathbb{E}[E_s(X_N)] = \frac{2^{1-s}}{2-s} N^2 + C(s) N^{1+s/2} + \frac{s}{16} C(s-2) N^{s/2} + O(N^{-1+s/2}), \tag{2.6}$$

when $N \to \infty$, where

$$C(s) = \frac{1}{2^s} \frac{s}{2} \left(1 + \frac{s}{2}\right) \Gamma\left(1 - \frac{s}{2}\right) \zeta\left(1 - \frac{s}{2}\right). \tag{2.7}$$

Remark 2.1.2. The result above for the expected Riesz energy allows us to compare the zeros of elliptic polynomials with other point processes, for example in terms of expected p-moments of averages. Indeed, from Khintchine's inequality [KK01, Theorem 3], it follows that

$$\mathbb{E}\left[\left|\sum_{i=1}^{N} x_i\right|^p\right] \sim N^{p/2}$$

when $x_1, \ldots, x_N$ are uniform i.i.d. points on the sphere $\mathbb{S}^2$ and $1 \leq p < \infty$. For points drawn from the spherical ensemble, for which there is repulsion between points, it follows from

$$\sum_{i,j=1}^{N} |x_i - x_j|^2 = 2N^2 - 2\left|\sum_{i=1}^{N} x_i\right|^2 \tag{2.8}$$

and the result about the expected Riesz energy $s = -2$ in (1.23) that the expected 2-moment is bounded. Hence, for the spherical ensemble $\mathbb{E}\left[\left|\sum_{i=1}^{N} x_i\right|^p\right]$ is bounded for $1 \leq p \leq 2$, and numerical simulations suggest that the same holds for $p > 2$. In our case, for zeros of elliptic polynomials mapped to the sphere by the stereographic projection, it follows from (2.5) that

$$\mathbb{E}\left[\left|\sum_{i=1}^{N} x_i\right|^2\right] = 4\frac{\zeta(3)}{N} + o(N^{-1}), \tag{2.9}$$

for $N \to +\infty$, and the average p-moments for $1 \le p \le 2$ converge to zero. Again, numerical simulations suggest the same behavior for $p > 2$. It is well known that minimal logarithmic points have center of mass in the center of the sphere, i.e. have zero dipole, [BHS19, Corollary 6.7.5], [BBPM94]. Therefore, the behavior of the expected p-moments matches the particularly low logarithmic energy of zeros of elliptic polynomials. For the comparison with minimal and expected energies of other point processes, see discussion in Section 2.4.

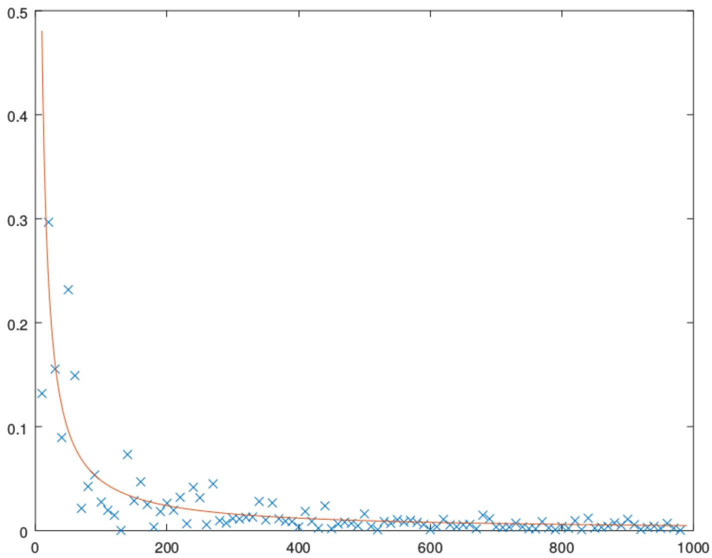

Figure 2.1: Plot of $4\zeta(3)/N$ and realizations of $|\sum_{i=1}^N x_i|^2$ for natural N up to 1000.

In our last result, we compute a closed expression for the expected separation distance between points drawn from zeros of elliptic polynomials. The separation distance of the configuration $X_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^2$ is defined by

$$\operatorname{sep}(X_N) = \min_{i \neq j} |x_i - x_j|,$$

and its counting version by $G(t, X_N) = |\{i < j : |x_i - x_j| \le t\}|$. Recall that energy minimizers have a separation distance of order $N^{-1/2}$, [BHS19, Section 6.9].

Theorem 2.1.3. *Let X_N be a set of $N-$points drawn from zeros of elliptic polynomials mapped to the sphere by the stereographic projection. Then*

$$\mathbb{E}[G(t, X_N)] = \frac{t^2N^2}{8} - \frac{N}{2} + \frac{t^2N^2}{8(4-t^2)\left(\left(\frac{4}{4-t^2}\right)^N - 1\right)}\left[8 - t^2 - t^2N - \frac{t^2N}{\left(\frac{4}{4-t^2}\right)^N - 1}\right]. \tag{2.10}$$

Therefore,

$$\mathbb{E}[G(t, X_N)] = \frac{N^3t^4}{128}(1 + o(1)), \tag{2.11}$$

if $t = o(1/\sqrt{N})$, *and moreover*

$$\mathbb{E}[G(t, X_N)] \leq \frac{N^3 t^4}{128}, \tag{2.12}$$

for $t \leq 2$.

Note that $\text{sep}(X_N) \leq t$ implies $G(t, X_N) \geq 1$, hence

$$\mathbb{P}(\text{sep}(X_N) \leq t) \leq \mathbb{P}(G(t, X_N) \geq 1) \leq \mathbb{E}(G(t, X_N))$$

and therefore, as in the harmonic case, see [BMOC16], an N-tuple drawn from the zeros of elliptic polynomials likely satisfies $\text{sep}(X_N) \gtrsim N^{-3/4}$, Figure 2.2. See also [AZ15, Corollary 1.6] for the analogue result for the spherical ensemble.

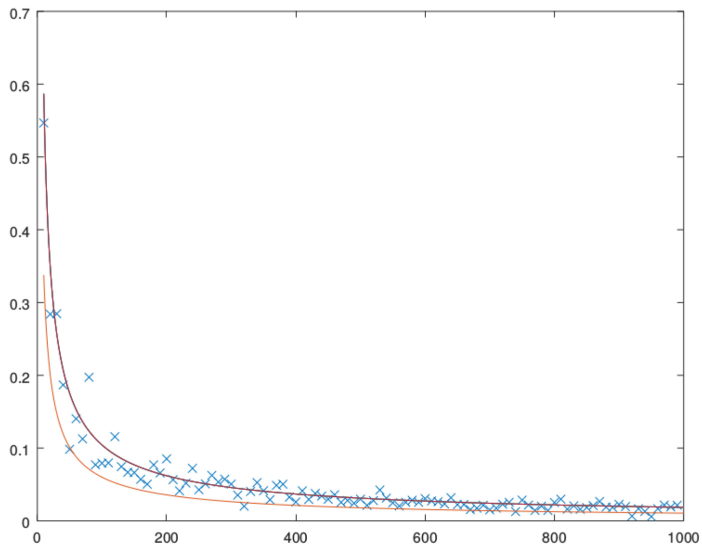

Figure 2.2: x marks correspond to the values of the minimal separation for realizations of N elliptic zeros for natural N from 10 up to 1000. The continuous graph are $cN^{-3/4}$ for $c = 1.89$ (yellow) and 3.27 (brown): using Chebyshev's inequality at least 90% of the realizations are above yellow and at least 10% above brown.

2.2 Intensity function

In this section we compute the 2-point intensity function of the random point process on $\mathbb{C}$ given by the roots of random elliptic polynomials P_N. With this intensity function, we will be able to compute the expected energy for N points drawn from this point process.

Let $F(x, y)$ be a measurable function defined on $\mathbb{S}^2 \times \mathbb{S}^2$ whose variables will be considered in $\mathbb{C}$ through the stereographic projection, i.e., $F(z, w) = F(x(z), y(w))$, with the points $x, y \in \mathbb{S}^2$ corresponding to $z, w \in \mathbb{C}$. By (1.18), if $x_1, \dots x_N \in \mathbb{S}^2$ are the images of the zeros $z_1, \dots, z_N$ of elliptic polynomials, then

$$\mathbb{E}\left[\sum_{i\neq j} F(x_i, x_j)\right] = \mathbb{E}\left[\sum_{i\neq j} F(z_i, z_j)\right] = \int_{\mathbb{C}}\int_{\mathbb{C}} F(z,w)\rho_2(z,w)\,\mathrm{d}z\,\mathrm{d}w, \tag{2.13}$$

with $\rho_2(z,w)$ the 2-point intensity function given by (1.3.5),

$$\rho_2(z_1, z_2) = \frac{\operatorname{per}(C - BA^{-1}B^*)}{\det(\pi A)}, \tag{2.14}$$

where A, B, C are the 2×2 matrices

$$\begin{aligned} A(i,j) &= \mathbb{E}[P_N(z_i)\overline{P_N}(z_j)], \\ B(i,j) &= \mathbb{E}[P_N'(z_i)\overline{P_N}(z_j)], \\ C(i,j) &= \mathbb{E}[P_N'(z_i)\overline{P_N'}(z_j)]. \end{aligned}$$

Here, ρ_2 denotes the 2-point intensity with respect to the Lebesgue measure $\mathrm{d}z$ on $\mathbb{C}$. By the rotational invariance of the process, it is also natural to rewrite the intensity function in terms of the spherical measure

$$\mathrm{d}\sigma(z) = \frac{\mathrm{d}z}{\pi(1+|z|^2)^2}.$$

In fact, as explained in Section 1.3.1, the first intensity is then constant. If ρ_k^*, $k = 1, 2$, denotes the k-intensity function with respect to σ, we have $\rho_1^*(z) = N$ and

$$\rho_2^*(z,w) = \pi^2\rho_2(z,w)(1+|z|^2)^2(1+|w|^2)^2, \tag{2.15}$$

as can be checked by rewriting the integral in (2.13) as

$$\int_{\mathbb{C}}\int_{\mathbb{C}} F(z,w)\overbrace{\pi^2\rho_2(z,w)(1+|z|^2)^2(1+|w|^2)^2}^{\rho_2^*(z,w)}\underbrace{\frac{\mathrm{d}z}{\pi(1+|z|^2)^2}}_{\mathrm{d}\sigma(z)}\underbrace{\frac{\mathrm{d}w}{\pi(1+|w|^2)^2}}_{\mathrm{d}\sigma(w)}.$$

The relevance of ρ_2^* comes from its rotational invariance. Thus, if we assume that F is also invariant by rotations, we have

$$\begin{aligned} &\mathbb{E}\left[\sum_{i\neq j} F(x_i, x_j)\right] \\ &= \int_{\mathbb{C}}\int_{\mathbb{C}} F(z,w)\rho_2(z,w)\,\mathrm{d}z\,\mathrm{d}w && \text{by (2.13)} \\ &= \int_{\mathbb{C}}\mathrm{d}\sigma(w)\int_{\mathbb{C}} F(z,w)\rho_2^*(z,w)\,\mathrm{d}\sigma(z) && \text{by (2.15)} \\ &= \int_{\mathbb{C}}\mathrm{d}\sigma(w)\int_{\mathbb{C}} F(\varphi_w(z),0)\rho_2^*(\varphi_w(z),0)\,\mathrm{d}\sigma(z) && F, \rho_2^* \text{ inv. by rotations} \\ &= \int_{\mathbb{C}}\mathrm{d}\sigma(w)\int_{\mathbb{C}} F(z,0)\rho_2^*(z,0)\,\mathrm{d}\sigma(z) && \sigma \text{ invariant by rotations} \\ &= \pi\int_{\mathbb{C}} F(z,0)\rho_2(z,0)\,\mathrm{d}z, \end{aligned} \tag{2.16}$$

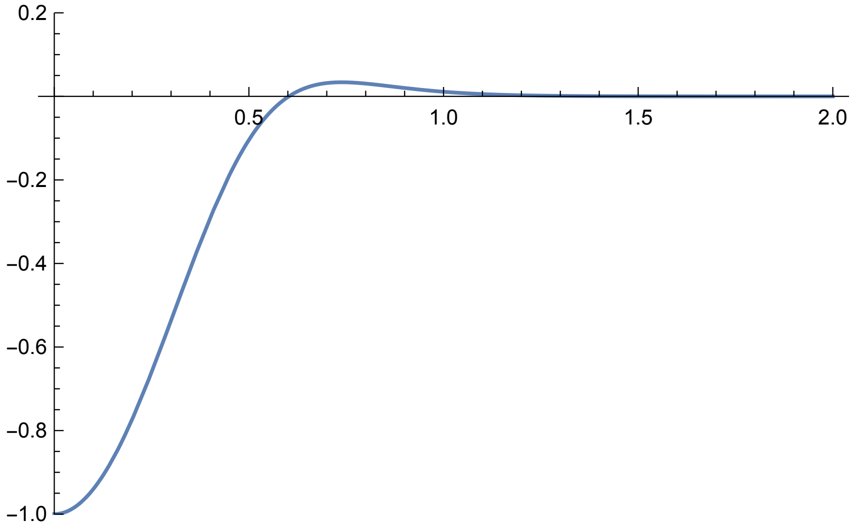

Figure 2.3: $\frac{\pi^2}{N^2}(\rho_2(r,0)-\rho_1(r)\rho_1(0))$ for $r>0$ and $N=10$.

where φ_w is any rotation of the sphere that sends the fixed w to 0.

Therefore, it is enough to compute $\rho_2(z_1,z_2)$ for $z_1=z\in\mathbb{C}$ and $z_2=0$. The matrices in (2.14) are then

$$A=\begin{pmatrix}(1+|z|^2)^N & 1\\ 1 & 1\end{pmatrix},$$

$$B=N\begin{pmatrix}\overline{z}(1+|z|^2)^{N-1} & 0\\ \overline{z} & 0\end{pmatrix},$$

$$C=N\begin{pmatrix}(1+|z|^2)^{N-2}(1+N|z|^2) & 1\\ 1 & 1\end{pmatrix},$$

and we obtain

$$\rho_2(z,0)=\frac{N^2\left[\left(1-\frac{N|z|^2}{(1+|z|^2)^N-1}\right)^2(1+|z|^2)^{N-2}+\left(1-\frac{N|z|^2(1+|z|^2)^{N-1}}{(1+|z|^2)^N-1}\right)^2\right]}{\pi^2[(1+|z|^2)^N-1]},$$

see [Han96] and Figure 2.3 where one can notice that this point process is not determinantal ([HKPV09, p.83]).

Thus, if $F(x,y)=f(|x-y|)$ for some function f, the following expression for the chordal metric

$$|x-y|=\frac{2|z-w|}{\sqrt{1+|z|^2}\sqrt{1+|w|^2}} \tag{2.17}$$

yields $F(z,0)=f\left(\frac{2|z|}{\sqrt{1+|z|^2}}\right)$ and from formula (2.16) we get

$$\begin{aligned}\mathbb{E}\left[\sum_{i\neq j}F(x_i,x_j)\right]&=\pi\int_{\mathbb{C}}f\left(\frac{2|z|}{\sqrt{1+|z|^2}}\right)\rho_2(z,0)\,\mathrm{d}z\\&=2N^2\int_0^\infty r\,f\left(\frac{2r}{\sqrt{1+r^2}}\right)\gamma(r)\,\mathrm{d}r,\end{aligned}\tag{2.18}$$

where

$$\gamma(r)=\frac{\left(1-\frac{Nr^2}{(1+r^2)^N-1}\right)^2(1+r^2)^{N-2}+\left(1-\frac{Nr^2(1+r^2)^{N-1}}{(1+r^2)^N-1}\right)^2}{(1+r^2)^N-1}.\tag{2.19}$$

2.3 Expected logarithmic and Riesz energy

In this section we apply (2.18) to compute the expected energies for X_N, the N zeros of random elliptic polynomials stereographically projected to $\mathbb{S}^2$. In the logarithmic case, the result (2.1) follows immediately, since the resulting integrand in (2.18) has a primitive function:

$$\mathbb{E}[E_0(X_N)]=-2N^2\int_0^\infty r\log\left(\frac{2r}{\sqrt{1+r^2}}\right)\gamma(r)\,\mathrm{d}r=\frac{N^2}{2}\left[g_N(r)\right]_0^\infty,$$

with

$$\begin{aligned}g_N(r)=&\frac{r^2\left(2\left((N-1)r^2-2\right)\log\left(\frac{2r}{\sqrt{1+r^2}}\right)+1\right)}{(1+r^2)\left((1+r^2)^N-1\right)}+\frac{2\log\left(\frac{2r}{\sqrt{1+r^2}}\right)}{1+r^2}\\&+\frac{2Nr^4\log\left(\frac{2r}{\sqrt{1+r^2}}\right)}{(1+r^2)\left((1+r^2)^N-1\right)^2}-\frac{1}{1+r^2}+\frac{\log\left((1+r^2)^N-1\right)}{N}-2\log(r).\end{aligned}$$

Evaluating at the endpoints,

$$\begin{aligned}&\lim_{r\to+\infty}g_N(r)\\&=\lim_{r\to+\infty}\left(\frac{2(N-1)r^4\log 2}{r^{2+2N}}+\frac{2\log 2}{1+r^2}+\frac{2Nr^4\log 2}{r^{2+4N}}-\frac{1}{1+r^2}+2\log(r)-2\log(r)\right)=0\end{aligned}$$

and

$$\begin{aligned}&\lim_{r\to 0}g_N(r)\\&=\lim_{r\to 0}\left(\frac{r^2\left(-4\log(2r)+1\right)}{Nr^2}+2\log(2r)+\frac{2Nr^4\log(2r)}{N^2r^4}-\frac{1}{1+r^2}+\frac{\log(Nr^2)}{N}-2\log(r)\right)\\&=\lim_{r\to 0}\left(\frac{1}{N}\left(-2\log 2+1+\log N\right)+2\log 2-\frac{1}{1+r^2}\right)\\&=-1+2\log 2+\frac{1}{N}\left(\log N+1-2\log 2\right).\end{aligned}$$

Then

$$\mathbb{E}[E_0(x_1,\ldots,x_N)] = -\frac{N^2}{2}\left(-1+2\log 2+\frac{1}{N}(\log N+1-2\log 2)\right)$$
$$= \left(\frac{1}{2}-\log 2\right)N^2 - \frac{N}{2}\log N - \left(\frac{1}{2}-\log 2\right)N.$$

Next we study the expected Riesz energy. For $s \neq 0$, (2.18) yields

$$\mathbb{E}[E_s(X_N)] = 2^{1-s}N^2\int_0^\infty r^{1-s}(1+r^2)^{s/2}\gamma(r)\,\mathrm{d}r. \tag{2.20}$$

Theorem 2.1.1 deals with this integral to provide the exact Riesz energy for some specific values of s and its asymptotic expansion as $N \to \infty$ for any value. We also recover the expected logarithmic energy as a limit when $s \to 0$.

2.3.1 Proof of Theorem 2.1.1

In this section we prove first our general result (2.2) with the auxiliary Proposition 2.3.1. Then we prove the cases (2.4),(2.5) and finally (2.3).

Proof. To simplify the notation we write $\mathbb{E}[E_s]$ instead of $\mathbb{E}[E_s(X_N)]$. The change of variables $r = \sqrt{x}$ in (2.20) yields

$$\mathbb{E}[E_s] = \frac{N^2}{2^s}\int_0^\infty \frac{x^{-s/2}(1+x)^{s/2}}{[(1+x)^N-1]^3}$$
$$\left[\left((1+x)^N-1-Nx\right)^2(1+x)^{N-2} + \left((1+x)^N-1-Nx(1+x)^{N-1}\right)^2\right]\mathrm{d}x.$$

The integrand is equivalent to x^{-2} at infinity, which is integrable, and to $x^{1-s/2}$ at $x=0$, which is integrable iff $1-s/2 > -1$. Then, the energy will be finite iff $s < 4$.

Now let us compute the integral. We take $r = s/2$ for simplicity, so we will be assuming $r < 2$ throughout the proof. Using that $\frac{1}{(x-1)^3} = \frac{1}{2}\sum_{k=2}^\infty k(k-1)x^{-(k+1)}$ for $x > 1$ and the fact that all the terms are positive, we get

$$\mathbb{E}[E_{2r}] = \frac{N^2}{2^{2r+1}}\sum_{k=2}^\infty k(k-1)\int_0^\infty \frac{(1+x)^{r-N(k+1)}}{x^r} \tag{2.21}$$
$$\left[\left((1+x)^N-1-Nx\right)^2(1+x)^{N-2} + \left((1+x)^N-1-Nx(1+x)^{N-1}\right)^2\right]\mathrm{d}x$$
$$= \frac{N^2}{2^{2r+1}}\lim_{M\to\infty}\sum_{k=2}^M k(k-1)\Bigg[\underbrace{\int_0^\infty \frac{\left[(1+x)^{r-2-Nk}+(1+x)^{r-N(k+1)}\right]\left((1+x)^N-1\right)^2}{x^r}\mathrm{d}x}_{A_k}$$
$$-2N\underbrace{\int_0^\infty x^{1-r}\left[(1+x)^{r-2-Nk}+(1+x)^{r-1-Nk}\right]\left((1+x)^N-1\right)\mathrm{d}x}_{B_k}$$
$$+N^2\underbrace{\int_0^\infty x^{2-r}\left[(1+x)^{r-2-Nk}+(1+x)^{r-2-N(k-1)}\right]\mathrm{d}x}_{C_k}\Bigg].$$

Using the following integral representation for the beta function [GR07, 8.380 (3)],

$$B(x,y)=\frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}=\int_0^\infty \frac{t^{x-1}}{(1+t)^{x+y}}\,dt \qquad x,y>0, \tag{2.22}$$

it is immediate to obtain B_k, C_k in (2.21)

$$B_k=B(2-r,N(k-1))-B(2-r,Nk)+B(2-r,N(k-1)-1)-B(2-r,Nk-1), \tag{2.23}$$

$$C_k=B(3-r,Nk-1)+B(3-r,N(k-1)-1), \tag{2.24}$$

so

$$\begin{aligned}&-2NB_k+N^2C_k\\&=\Gamma(2-r)\left[-2N\left(\frac{\Gamma(N(k-1))}{\Gamma(N(k-1)+2-r)}-\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)}+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+1-r)}\right.\right.\\&\left.\left.-\frac{\Gamma(Nk-1)}{\Gamma(Nk+1-r)}\right)+N^2(2-r)\left(\frac{\Gamma(Nk-1)}{\Gamma(Nk+2-r)}+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+2-r)}\right)\right].\end{aligned}$$

To compute A_k we integrate by parts. Let $\beta\in\{r-2-Nk, r-N(k+1)\}$ denote the exponent in $(1+x)$. If $r\neq 1$,

$$\begin{aligned}I_\beta&:=\int_0^\infty \frac{(1+x)^\beta\left((1+x)^N-1\right)^2}{x^r}\,\mathrm{d}x=\frac{1}{1-r}x^{1-r}(1+x)^\beta\left((1+x)^N-1\right)^2\Big|_0^\infty\\&-\frac{1}{1-r}\int_0^\infty x^{1-r}\left[\beta(1+x)^{\beta-1}\left((1+x)^N-1\right)^2+2N(1+x)^{\beta+N-1}\left((1+x)^N-1\right)\right]\mathrm{d}x,\end{aligned}$$

with the evaluation in the first line vanishing, so

$$\begin{aligned}I_\beta=\frac{-1}{1-r}&\left[\beta\int_0^\infty x^{1-r}(1+x)^{\beta-1}\left((1+x)^{2N}-2(1+x)^N+1\right)\mathrm{d}x\right.\\&\left.+2N\int_0^\infty x^{1-r}(1+x)^{\beta+N-1}\left((1+x)^N-1\right)\mathrm{d}x\right]\end{aligned}$$

and from (2.22),

$$\begin{aligned}I_\beta&=\frac{-1}{1-r}\left[\beta(B(2-r,-\beta-2N-1+r)\right.\\&-2B(2-r,-\beta-N-1+r)+B(2-r,-\beta-1+r))\\&\left.+2N\left(B(2-r,-\beta-2N-1+r)-B(2-r,-\beta-N-1+r)\right)\right]\\&=B(1-r,-\beta-2N-1+r)-2B(1-r,-\beta-N-1+r)+B(1-r,-\beta-1+r).\end{aligned}$$

Then

$$\begin{aligned}A_k&=I_{r-2-Nk}+I_{r-N(k+1)}\\&=B(1-r,N(k-2)+1)-2B(1-r,N(k-1)+1)+B(1-r,Nk+1)\\&+B(1-r,N(k-1)-1)-2B(1-r,Nk-1)+B(1-r,N(k+1)-1),\end{aligned} \tag{2.25}$$

or, in terms of the gamma function,

$$A_k = \Gamma(1-r)\left[\frac{\Gamma(N(k-2)+1)}{\Gamma(N(k-2)+2-r)} - 2\frac{\Gamma(N(k-1)+1)}{\Gamma(N(k-1)+2-r)} + \frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)}\right.$$
$$\left. + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)-r)} - 2\frac{\Gamma(Nk-1)}{\Gamma(Nk-r)} + \frac{\Gamma(N(k+1)-1)}{\Gamma(N(k+1)-r)}\right],$$

provided that $r \neq 1$. The case $r = 1$ will be studied as the limit $r \to 1$.

Therefore, for $r \neq 1$, writing all together

$$\begin{aligned}\mathbb{E}[E_{2r}] = \frac{N^2}{2^{2r+1}} \lim_{M\to\infty} &\left[\sum_{k=2}^{M} k(k-1)\Gamma(1-r)\left(\frac{\Gamma(N(k-2)+1)}{\Gamma(N(k-2)+2-r)} - 2\frac{\Gamma(N(k-1)+1)}{\Gamma(N(k-1)+2-r)}\right.\right.\\ &+\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)-r)} - 2\frac{\Gamma(Nk-1)}{\Gamma(Nk-r)} + \left.\frac{\Gamma(N(k+1)-1)}{\Gamma(N(k+1)-r)}\right)\\ &+\sum_{k=2}^{M} k(k-1)\Gamma(2-r)\left(-2N\left(\frac{\Gamma(N(k-1))}{\Gamma(N(k-1)+2-r)} - \frac{\Gamma(Nk)}{\Gamma(Nk+2-r)}\right.\right.\\ &+\left.\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+1-r)} - \frac{\Gamma(Nk-1)}{\Gamma(Nk+1-r)}\right)\\ &\left.\left.+N^2(2-r)\left(\frac{\Gamma(Nk-1)}{\Gamma(Nk+2-r)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+2-r)}\right)\right)\right].\end{aligned} \tag{2.26}$$

The sums get simplified by using the property $\Gamma(z+1) = z\Gamma(z)$ and changing the indices in such a way that all quotients have the form $\Gamma(Nk+1)/\Gamma(Nk+2-r)$

$$\begin{aligned}\mathbb{E}[E_{2r}] = &\frac{\Gamma(1-r)N^2}{2^{2r+1}}\\ &\lim_{M\to\infty}\left[\frac{2}{\Gamma(2-r)} + \sum_{k=1}^{M}(1-r+Nk(1+r))\frac{2r\Gamma(Nk)}{\Gamma(Nk+2-r)} - (M+1)M\frac{\Gamma(N(M-1)+1)}{\Gamma(N(M-1)+2-r)}\right.\\ &-\frac{(M+1)\left(r\left(N\left(N(4M-3)-2M+2\right)-1\right)-2(N-1)N(M-1)+(N-1)^2r^2\right)}{N(NM-1)}\\ &\left.\frac{\Gamma(NM+1)}{\Gamma(NM+2-r)} + \frac{M(M-1)(N(M+1)-r)(N(M+1)+1-r)}{N(M+1)(N(M+1)-1)}\frac{\Gamma(N(M+1)+1)}{\Gamma(N(M+1)+2-r)}\right].\end{aligned}$$

Taking the asymptotic expansion of the terms in M as $M \to \infty$, we get

$$\begin{aligned}\mathbb{E}[E_{2r}] = \frac{\Gamma(1-r)N^2}{2^{2r+1}} \lim_{M\to\infty} &\left[\frac{2}{\Gamma(2-r)} + 2r(1+r)\sum_{k=1}^{M}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)}\right.\\ &\left.+2r(1-r)\sum_{k=1}^{M}\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)} - 2(1+r)N^{r-1}M^r - r(N+r+Nr-r^2)N^{r-2}M^{r-1}\right].\end{aligned} \tag{2.27}$$

Applying Proposition 2.3.1 below we obtain the following expression for every $r \neq 0, 1$

with $r<2$,

$$\mathbb{E}[E_{2r}] = \frac{\Gamma(1-r)N^2}{2^{2r+1}}$$
$$\left[\frac{2}{\Gamma(2-r)} + 2r(1+r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}\zeta\left(1-r+2j, 1+\frac{2-r}{2N}\right)N^{r-1-2j}\right.$$
$$\left.+2r(1-r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!}\zeta\left(2-r+2j, 1+\frac{1-r}{2N}\right)N^{r-2-2j} + O\left(N^{r-1-2m}\right)\right].$$

Writing the expression in terms of $s=2r$ yields the result (2.2).

Now we prove (2.4) from the case $r\neq 1$. By continuity, the evaluation of the integral at the beginning of (2.21) can be performed by taking the limit $r\to 1$ in A_k, B_k, C_k, that is, in both sums in (2.26). The only tricky limit is the first one. It can be computed using the asymptotic expansion

$$\frac{1}{\Gamma(a+\gamma)} = \frac{1}{\Gamma(a)} - \frac{\psi(a)}{\Gamma(a)}\gamma + o\left(\gamma\right),$$

for $\gamma\to 0$, where a will be a natural number. Considering $\gamma = 1-r$,

$$\begin{aligned}
\lim_{\gamma\to 0}\Gamma(\gamma)&\left[\frac{\Gamma(N(k-2)+1)}{\Gamma(N(k-2)+1+\gamma)} - \frac{2\Gamma(N(k-1)+1)}{\Gamma(N(k-1)+1+\gamma)} + \frac{\Gamma(Nk+1)}{\Gamma(Nk+1+\gamma)}\right.\\
&\left.+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)-1+\gamma)} - 2\frac{\Gamma(Nk-1)}{\Gamma(Nk-1+\gamma)} + \frac{\Gamma(N(k+1)-1)}{\Gamma(N(k+1)-1+\gamma)}\right]\\
&= -\psi(N(k-2)+1) + 2\psi(N(k-1)+1) - \psi(Nk+1)\\
&\quad - \psi(N(k-1)-1) + 2\psi(Nk-1) - \psi(N(k+1)-1),
\end{aligned}$$

and we get from (2.26)

$$\begin{aligned}
\mathbb{E}[E_2] = \frac{N^2}{2^3}\lim_{M\to\infty}&\left[\sum_{k=2}^{M}k(k-1)(-\psi(N(k-2)+1) + 2\psi(N(k-1)+1)\right. \qquad (2.28)\\
&-\psi(Nk+1) - \psi(N(k-1)-1) + 2\psi(Nk-1) - \psi(N(k+1)-1))\\
&+\sum_{k=2}^{M}k(k-1)\left(-2N\left(\frac{\Gamma(N(k-1))}{\Gamma(N(k-1)+1)} - \frac{\Gamma(Nk)}{\Gamma(Nk+1)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1))}\right.\right.\\
&\left.\left.\left.-\frac{\Gamma(Nk-1)}{\Gamma(Nk)}\right) + N^2\left(\frac{\Gamma(Nk-1)}{\Gamma(Nk+1)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+1)}\right)\right)\right].
\end{aligned}$$

The first sum in (2.28),

$$\begin{aligned}
\Sigma_1 := \sum_{k=2}^{M}k(k-1)(&-\psi(N(k-2)+1) + 2\psi(N(k-1)+1) - \psi(Nk+1)\\
&-\psi(N(k-1)-1) + 2\psi(Nk-1) - \psi(N(k+1)-1)),
\end{aligned}$$

can be rewritten as

$$\begin{aligned}\Sigma_1 &= (M+2)(M+1)\psi(NM+1) + (M+1)M\psi(N(M-1)+1)\\ &\quad - 2(M+1)M\psi(NM+1) - 2\sum_{k=0}^{M}\psi(Nk+1)\\ &\quad + (M+1)M\psi(NM-1) - M(M-1)\psi(N(M+1)-1) - 2\sum_{k=1}^{M}\psi(Nk-1),\end{aligned}$$

while the second

$$\begin{aligned}\Sigma_2 := \sum_{k=2}^{M} k(k-1)\Bigg(-2N\left(\frac{\Gamma(N(k-1))}{\Gamma(N(k-1)+1)} - \frac{\Gamma(Nk)}{\Gamma(Nk+1)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1))}\right.\\ \left. - \frac{\Gamma(Nk-1)}{\Gamma(Nk)}\right) + N^2\left(\frac{\Gamma(Nk-1)}{\Gamma(Nk+1)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+1)}\right)\Bigg)\end{aligned}$$

becomes

$$\begin{aligned}\Sigma_2 = \sum_{k=2}^{M} k(k-1)\Bigg(-2N\left(\frac{1}{N(k-1)} - \frac{1}{Nk} + \frac{1}{N(k-1)-1} - \frac{1}{Nk-1}\right)\\ + N^2\left(\frac{1}{Nk-1} - \frac{1}{Nk} + \frac{1}{N(k-1)-1} - \frac{1}{N(k-1)}\right)\Bigg),\end{aligned}$$

which after playing with the indices gets simplified to

$$\begin{aligned}\Sigma_2 &= \sum_{k=2}^{M} k(k-1)\left(\frac{2N-N^2}{Nk} - \frac{2N+N^2}{N(k-1)} + \frac{(2N+N^2)}{Nk-1} - \frac{(2N-N^2)}{N(k-1)-1}\right)\\ &= -\sum_{k=1}^{M-1}\frac{2kN(2+kN)}{Nk} + \frac{M(M-1)}{NM}(2N-N^2)\\ &\quad + \sum_{k=1}^{M-1}\frac{2kN(-2+kN)}{Nk-1} + \frac{M(M-1)}{NM-1}(2N+N^2)\\ &= -(M-1)(4+N) - \frac{2}{N}\sum_{k=1}^{M-1}\frac{1}{k-\frac{1}{N}} + \frac{M(M-1)N(2+N)}{NM-1}.\end{aligned}$$

Now we will use the functional relation $\psi(x+1) = \psi(x) + \frac{1}{x}$ for the digamma function, which allows us to obtain, for instance,

$$\sum_{k=1}^{M-1}\frac{1}{k-\frac{1}{N}} = \psi\left(M-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right).$$

Using this we get

$$\Sigma_2 = -(M-1)(4+N) - \frac{2}{N}\left(\psi\left(M-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right)\right) + \frac{M(M-1)N(2+N)}{NM-1}.$$

We can simplify Σ_1 with the same property. Since

$$\sum_{k=1}^{M} \psi(Nk-1) = \sum_{k=1}^{M} \left(\psi(Nk+1) - \frac{1}{Nk-1} - \frac{1}{Nk} \right),$$

then

$$\begin{aligned}
-2\sum_{k=0}^{M} \psi(Nk+1) - 2\sum_{k=1}^{M} \psi(Nk-1) &= 2\gamma - 4\sum_{k=1}^{M} \psi(Nk+1) + 2\sum_{k=1}^{M} \frac{1}{Nk-1} + 2\sum_{k=1}^{M} \frac{1}{Nk} \\
&= 2\gamma - 4\sum_{k=1}^{M} \psi(Nk+1) + \frac{2}{N}\left(\psi\left(M+1-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right)\right) + \frac{2}{N}(\psi(M+1)+\gamma).
\end{aligned}$$

Therefore,

$$\begin{aligned}
\Sigma_1 + \Sigma_2 &= (M+2)(M+1)\psi(NM+1) + (M+1)M\psi(N(M-1)+1) \\
&- 2(M+1)M\psi(NM+1) + (M+1)M\psi(NM-1) - M(M-1)\psi(N(M+1)-1) + 2\gamma \\
&+ \frac{2}{N}\left(\psi\left(M+1-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right)\right) + \frac{2}{N}(\psi(M+1)+\gamma) - (M-1)(4+N) \\
&- \frac{2}{N}\left(\psi\left(M-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right)\right) + \frac{M(M-1)N(2+N)}{NM-1} - 4\sum_{k=1}^{M} \psi(Nk+1).
\end{aligned}$$

From the relation [GR07, 8.365 (6)],

$$\sum_{k=1}^{M} \psi(Nk+1) = \frac{1}{N}\sum_{k=1}^{M}\sum_{j=1}^{N} \psi\left(k+\frac{j}{N}\right) + M\log N = \frac{1}{N}\sum_{j=1}^{N}\sum_{k=1}^{M} \psi\left(k+\frac{j}{N}\right) + M\log N.$$

Summation by parts gives

$$\begin{aligned}
\sum_{k=1}^{M} \psi\left(k+\frac{j}{N}\right) &= M\psi\left(M+\frac{j}{N}\right) - \sum_{l=1}^{M-1}\left(\psi\left(l+1+\frac{j}{N}\right) - \psi\left(l+\frac{j}{N}\right)\right) l \\
&= M\psi\left(M+\frac{j}{N}\right) - \sum_{l=1}^{M-1} \frac{l}{l+\frac{j}{N}} = M\psi\left(M+\frac{j}{N}\right) - (M-1) + \frac{j}{N}\sum_{l=1}^{M-1} \frac{1}{l+\frac{j}{N}} \\
&= M\psi\left(M+\frac{j}{N}\right) - (M-1) + \frac{j}{N}\left(\psi\left(M+\frac{j}{N}\right) - \psi\left(1+\frac{j}{N}\right)\right) \\
&= \left(M+\frac{j}{N}\right)\psi\left(M+\frac{j}{N}\right) - \frac{j}{N}\psi\left(1+\frac{j}{N}\right) - (M-1),
\end{aligned}$$

for every $1 \leq j \leq N$. Thus,

$$\begin{aligned}
&\Sigma_1 + \Sigma_2 = (M+2)(M+1)\psi(NM+1) + (M+1)M\psi(N(M-1)+1) \\
&- 2(M+1)M\psi(NM+1) + (M+1)M\psi(NM-1) - M(M-1)\psi(N(M+1)-1) \\
&+ 2\gamma + \frac{2}{N}\left(\psi\left(M+1-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right)\right) + \frac{2}{N}(\psi(M+1)+\gamma) \\
&- (M-1)(4+N) - \frac{2}{N}\left(\psi\left(M-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right)\right) + \frac{M(M-1)N(2+N)}{NM-1} \\
&- \frac{4}{N}\sum_{j=1}^{N}\left(M+\frac{j}{N}\right)\psi\left(M+\frac{j}{N}\right) + \frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(1+\frac{j}{N}\right) + 4(M-1) - 4M\log N
\end{aligned}$$

and simplifying

$$\begin{aligned}
&\Sigma_1 + \Sigma_2 = -M(M-1)\psi(N(M+1)-1) + 2(M+1)\psi(NM+1) \\
&+ (M+1)M\psi(N(M-1)+1) - \frac{M(M+1)}{NM} + \frac{(M-1)\left(\left(N^2+2N-1\right)M-2\right)}{NM-1} \\
&+ \frac{2}{N}\psi(M+1) - N(M-1) - 4M\log N - \frac{4}{N}\sum_{j=1}^{N}\left(M+\frac{j}{N}\right)\psi\left(M+\frac{j}{N}\right) \\
&+ \frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(1+\frac{j}{N}\right) + 2\gamma\left(1+\frac{1}{N}\right).
\end{aligned}$$

Using the asymptotic expansion $\psi(z) = \log z - \frac{1}{2z} - \frac{1}{12z^2} + O\left(z^{-4}\right)$ as $z \to \infty$, we obtain

$$\Sigma_1 + \Sigma_2 = -1 - \frac{3}{N} + 2\log N + O\left(M^{-1}\right) + \frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(1+\frac{j}{N}\right) + 2\gamma\left(1+\frac{1}{N}\right).$$

Then

$$\begin{aligned}
\mathbb{E}[E_2] &= \frac{N^2}{2^3}\lim_{M\to\infty}\Big[\Sigma_1+\Sigma_2\Big] \\
&= \frac{N^2}{2^3}\left(-1-\frac{3}{N}+2\log N+\frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(1+\frac{j}{N}\right)+2\gamma\left(1+\frac{1}{N}\right)\right) \\
&= \frac{N^2}{2^3}\left(-1-\frac{3}{N}+2\log N+\frac{4}{N}\underbrace{\sum_{j=1}^{N}\frac{j}{N}\frac{1}{j/N}}_{=N}+\frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(\frac{j}{N}\right)+2\gamma\left(1+\frac{1}{N}\right)\right) \\
&= \frac{N}{2^3}\left(3N-3+2N\log N+4\sum_{j=1}^{N}\frac{j}{N}\psi\left(\frac{j}{N}\right)+2\gamma\Big(N+1\Big)\right) \\
&= \frac{N}{2^3}\left(3N-3+2N\log N+4\sum_{j=1}^{N-1}\frac{j}{N}\psi\left(\frac{j}{N}\right)+2\gamma(N-1)\right).
\end{aligned}$$

Finally, using

$$\sum_{j=1}^{N-1} \frac{j}{N}\psi\left(\frac{j}{N}\right) = -\frac{\gamma}{2}(N-1) - \frac{N}{2}\log N - \frac{\pi}{2}\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right),$$

[Bla15, (B.11)], we get (2.4)

$$\mathbb{E}[E_2] = -\frac{N\pi}{4}\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) + \frac{3N^2}{8} - \frac{3N}{8}.$$

To compute $\mathbb{E}[E_{-2n}]$ and $\mathbb{E}[E_0]$, we start observing that for $r < 0$ formula (2.27) yields

$$\mathbb{E}[E_{2r}] = \frac{\Gamma(1-r)N^2}{2^{2r}} \left(\frac{1}{\Gamma(2-r)} + r(1+r)\sum_{k=1}^{\infty}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)} + r(1-r)\sum_{k=1}^{\infty}\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)}\right),$$

since both sums are convergent in this case. Using the expression of the beta function in terms of gamma function and the monotone convergence theorem, we get

$$\mathbb{E}[E_{2r}] = \frac{N^2}{2^{2r}}\left(\frac{1}{1-r} + r(1+r)\int_0^1 (1-t)^{-r}\frac{t^N}{1-t^N}\,dt + r\int_0^1 (1-t)^{1-r}\frac{t^{N-1}}{1-t^N}\,dt\right). \tag{2.29}$$

For $r = -n$, the energy is

$$\mathbb{E}[E_{-2n}] = 2^{2n}N^2\left(\frac{1}{n+1} - n(1-n)\underbrace{\int_0^1 (1-t)^n\frac{t^N}{1-t^N}\,dt}_{I_1} - n\underbrace{\int_0^1 (1-t)^{1+n}\frac{t^{N-1}}{1-t^N}\,dt}_{I_2}\right). \tag{2.30}$$

To compute I_1 and I_2 we will use the following integral representation [GR07, 8.361 (7)] for the digamma function

$$\psi(z) = \int_0^1 \frac{t^{z-1}-1}{t-1}\,dt - \gamma, \qquad z > 0,$$

from which we get

$$\int_0^1 \frac{t^a - 1}{1-t^N}\,dt = \frac{1}{N}\int_0^1 \frac{y^{(a+1)/N-1} - y^{1/N-1}}{1-y}\,dt = -\frac{1}{N}\left(\psi\left(\frac{a+1}{N}\right) - \psi\left(\frac{1}{N}\right)\right), \tag{2.31}$$

for any $a > -1$. Then

$$\begin{aligned} I_1 &= \int_0^1 \sum_{m=0}^{n}\binom{n}{m}(-1)^m\frac{t^{N+m}}{1-t^N}\,dt = \int_0^1 \sum_{m=0}^{n}\binom{n}{m}(-1)^m\frac{t^{N+m}-1}{1-t^N}\,dt \\ &= -\frac{1}{N}\sum_{m=0}^{n}\binom{n}{m}(-1)^m\left(\psi\left(\frac{m+1}{N}+1\right) - \psi\left(\frac{1}{N}\right)\right) \\ &= -\frac{1}{N}\sum_{m=0}^{n}\binom{n}{m}(-1)^m\psi\left(\frac{m+1}{N}+1\right), \end{aligned}$$

where we have used $\sum_{m=0}^{n}\binom{n}{m}(-1)^m = 0$ in the second and last equality. Applying $\psi(x+1)=\psi(x)+1/x$,

$$I_1 = -\frac{1}{N}\sum_{m=0}^{n}\binom{n}{m}(-1)^m\psi\left(\frac{m+1}{N}\right)+\sum_{m=0}^{n}\binom{n}{m}(-1)^{m+1}\frac{1}{m+1}$$

and it is trivial to check that the second sum equals $-1/(n+1)$.

The integral I_2 can be computed in a similar way

$$\begin{aligned} I_2 &= \int_0^1 \sum_{m=0}^{n+1}\binom{n+1}{m}(-1)^m\frac{t^{N-1+m}-1}{1-t^N}\,dt = -\frac{1}{N}\sum_{m=0}^{n+1}\binom{n+1}{m}(-1)^m\psi\left(\frac{m}{N}+1\right) \\ &= \frac{1}{N}\left(\gamma-\sum_{m=1}^{n+1}\binom{n+1}{m}(-1)^m\psi\left(\frac{m}{N}\right)\right)+\sum_{m=1}^{n+1}\binom{n+1}{m}(-1)^{m+1}\frac{1}{m}, \end{aligned}$$

where the second sum is $\sum_{m=1}^{n+1}\frac{1}{m}$, as stated in [GR07, 0.155 (4)].

Finally from (2.30) we get (2.5)

$$\begin{aligned} \mathbb{E}[E_{-2n}] &= 2^{2n}N^2\Bigg[\frac{1}{n+1}-n(1-n)\left(-\frac{1}{N}\sum_{m=0}^{n}\binom{n}{m}(-1)^m\psi\left(\frac{m+1}{N}\right)-\frac{1}{n+1}\right) \\ &-n\left(\frac{1}{N}\left(\gamma-\sum_{m=1}^{n+1}\binom{n+1}{m}(-1)^m\psi\left(\frac{m}{N}\right)\right)+\sum_{m=1}^{n+1}\frac{1}{m}\right)\Bigg] \\ &= 2^{2n}N^2\left(\frac{1}{n+1}-\frac{n(n-1)}{n+1}-n\sum_{m=1}^{n+1}\frac{1}{m}\right) \\ &+2^{2n}nN\left(-\gamma+\sum_{m=1}^{n+1}\binom{n+1}{m}(-1)^m\psi\left(\frac{m}{N}\right)\left(\frac{n-1}{n+1}m+1\right)\right). \end{aligned}$$

In order to compute $\mathbb{E}[E_0]$, i.e. formula (2.3) from [ABS11], we take the derivative of $\mathbb{E}[E_s]$ at $s=0$. Consider the continuous function

$$g(r)=\begin{cases}\mathbb{E}[E_{2r}], & \text{for } r\neq 0,\\ N^2-N, & \text{for } r=0,\end{cases}$$

where $r=0$ matches the Riesz 0-energy, which trivially is N^2-N for any configuration of points. Then

$$\mathbb{E}[E_0]=\frac{1}{2}g'(0).$$

Since $g'(0)$ exists, we can derive it by restricting to $r<0$

$$g'(0)=\lim_{r\to 0^-}\frac{g(r)-g(0)}{r},$$

where according to (2.29),

$$g(r) = 2^{-2r} N^2 \left(\frac{1}{1-r} + r(1+r) \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt + r \int_0^1 (1-t)^{1-r} \frac{t^{N-1}}{1-t^N}\, dt \right).$$

Then

$$\begin{aligned}\lim_{r\to 0^-} g(r) &= N^2 + N^2 \lim_{r\to 0^-} r(1+r) \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt \\ &\quad + N^2 \lim_{r\to 0^-} r \int_0^1 (1-t)^{1-r} \frac{t^{N-1}}{1-t^N}\, dt = N^2 + N^2 \lim_{r\to 0^-} r(1+r) \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt,\end{aligned}$$

because $(1-t)^{1-r} \uparrow (1-t)$ when $r \to 0^-$ and $\int_0^1 (1-t) \frac{t^{N-1}}{1-t^N}\, dt < \infty$. By continuity, we also have $\lim_{r\to 0^-} g(r) = g(0) = N^2 - N$, so we deduce that

$$\lim_{r\to 0^-} r \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt = -\frac{1}{N}. \tag{2.32}$$

Therefore,

$$\begin{aligned}\frac{g'(0)}{N^2} &= (1-\log 4) + \lim_{r\to 0^-} \frac{\frac{r(1+r)}{2^{2r}} \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt + \frac{1}{N}}{r} + \lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{1-r} \frac{t^{N-1}}{1-t^N}\, dt}{r} \\ &= (1-\log 4) + \lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt + \frac{1}{N}}{r} + \underbrace{\lim_{r\to 0^-} r \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt}_{=-1/N \text{ by (2.32)}} \\ &\quad + \int_0^1 (1-t) \frac{t^{N-1}}{1-t^N}\, dt = (1-\log 4) + \underbrace{\lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt + \frac{1}{N}}{r}}_{I_3} \\ &\quad - \frac{1}{N} - \frac{1}{N} \left(\psi(1) - \psi\left(1 + \frac{1}{N}\right) \right),\end{aligned} \tag{2.33}$$

by (2.31).

It remains to compute the limit I_3

$$\begin{aligned} I_3 &= \lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{-r} \left(\frac{t^N}{1-t^N} - \frac{1}{N(1-t)} \right) dt}{r} + \frac{1}{N} \lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{-r} \frac{1}{1-t}\, dt + 1}{r} \\ &= \lim_{r\to 0^-} \int_0^1 (1-t)^{-r} \left(\frac{t^N}{1-t^N} - \frac{1}{N(1-t)} \right) dt + \frac{1}{N} \lim_{r\to 0^-} \frac{-2^{-2r}+1}{r} \\ &= \underbrace{\int_0^1 \left(\frac{t^N}{1-t^N} - \frac{1}{N(1-t)} \right) dt}_{I_4} + \frac{2}{N} \log 2,\end{aligned}$$

where the limit of the last integral is justified by monotone convergence theorem. Using (2.31), we obtain

$$
\begin{aligned}
I_4 &= \frac{1}{N}\int_0^1 \frac{Nt^N - \sum_{j=0}^{N-1} t^j}{1-t^N}\,dt = \frac{1}{N}\sum_{j=0}^{N-1}\int_0^1 \frac{t^N - t^j}{1-t^N}\,dt \\
&= -\frac{1}{N^2}\sum_{j=0}^{N-1}\left(\psi\left(1+\frac{1}{N}\right) - \psi\left(\frac{j+1}{N}\right)\right) = -\frac{1}{N}\psi\left(1+\frac{1}{N}\right) + \frac{1}{N^2}\sum_{j=0}^{N-1}\psi\left(\frac{j+1}{N}\right) \\
&= -\frac{1}{N}\psi\left(1+\frac{1}{N}\right) - \frac{1}{N}\left(\log N + \gamma\right),
\end{aligned}
$$

where we have used that $\sum_{j=0}^{N-1}\psi\left(\frac{j+1}{N}\right) = -N\log N - \gamma N$.

From (2.33) we finally get

$$
\begin{aligned}
2\mathbb{E}[E_0] = g'(0) &= (1-\log 4)\,N^2 + N^2\left(-\frac{1}{N}\psi\left(1+\frac{1}{N}\right) - \frac{1}{N}\left(\log N + \gamma\right) + \frac{2}{N}\log 2\right) \\
&\quad - N - N\left(\psi(1) - \psi\left(1+\frac{1}{N}\right)\right) = (1-\log 4)\,N^2 - N\log N - (1-\log 4)\,N.
\end{aligned}
$$

□

The following auxiliary result is used in the proof of Theorem 2.1.1.

Proposition 2.3.1. *Let $1 \neq r < 2$ and $m \geq 1$. Then*

$$
\begin{aligned}
&\lim_{M\to\infty}\Bigg[2r(1+r)\sum_{k=1}^{M}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)} + 2r(1-r)\sum_{k=1}^{M}\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)} \\
&- 2(1+r)N^{r-1}M^r - r(N+r+Nr-r^2)N^{r-2}M^{r-1}\Bigg] \\
&= 2r(1+r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}N^{r-1-2j}\zeta\left(1-r+2j, 1+\frac{2-r}{2N}\right) \\
&+ 2r(1-r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!}N^{r-2-2j}\zeta\left(2-r+2j, 1+\frac{1-r}{2N}\right) + O\left(N^{r-1-2m}\right),
\end{aligned}
\tag{2.34}
$$

when $N \to +\infty$.

Proof. We will use the following Fields' approximation for the quotient of gamma functions, see [DLMF, Eq. 5.11.14] or [Fie66]

$$
\frac{\Gamma(z+a)}{\Gamma(z+b)} = \sum_{j=0}^{m-1}\frac{B_{2j}^{(2\rho)}(\rho)(b-a)_{2j}w^{a-b-2j}}{(2j)!} + O\left(w^{a-b-2m}\right),
$$

as $w \to \infty$ with $|\arg(w+\rho)| < \pi$ where a and b are fixed complex numbers, $w = z + \rho$ and $2\rho = 1 + a - b$. Then,

$$\sum_{k=1}^{M} \frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)} = \sum_{k=1}^{M} \left(Nk + \frac{2-r}{2}\right)^{r-1} + \sum_{j=1}^{m-1} \frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!} \sum_{k=1}^{M} \left(Nk + \frac{2-r}{2}\right)^{r-1-2j} + \sum_{k=1}^{M} O\left(\left(Nk + \frac{2-r}{2}\right)^{r-1-2m}\right)$$

and factorising,

$$\sum_{k=1}^{M} \frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)} = N^{r-1} \underbrace{\sum_{k=1}^{M} \left(k + \frac{2-r}{2N}\right)^{r-1}}_{D} \tag{2.35}$$

$$+ \sum_{j=1}^{m-1} \frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!} N^{r-1-2j} \underbrace{\sum_{k=0}^{M-1} \frac{1}{\left(k+1+\frac{2-r}{2N}\right)^{1-r+2j}}}_{E_j} + O\left(N^{r-1-2m}\right) \underbrace{\sum_{k=1}^{M} \frac{1}{k^{1-r+2m}}}_{F}.$$

In the same way,

$$\sum_{k=1}^{M} \frac{\Gamma(Nk)}{\Gamma(Nk+2-r)} = \sum_{k=1}^{M} \left(Nk + \frac{1-r}{2}\right)^{r-2} + \sum_{j=1}^{m-1} \frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!} \sum_{k=1}^{M} \left(Nk + \frac{1-r}{2}\right)^{r-2-2j} + \sum_{k=1}^{M} O\left(\left(Nk + \frac{1-r}{2}\right)^{r-2-2m}\right)$$

and

$$\sum_{k=1}^{M} \frac{\Gamma(Nk)}{\Gamma(Nk+2-r)} = N^{r-2} \underbrace{\sum_{k=0}^{M-1} \frac{1}{\left(k+1+\frac{1-r}{2N}\right)^{2-r}}}_{G} \tag{2.36}$$

$$+ \sum_{j=1}^{m-1} \frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!} N^{r-2-2j} \underbrace{\sum_{k=0}^{M-1} \frac{1}{\left(k+1+\frac{1-r}{2N}\right)^{2-r+2j}}}_{H_j} + O\left(N^{r-2-2m}\right) \underbrace{\sum_{k=1}^{M} \frac{1}{k^{2-r+2m}}}_{I}.$$

To compute the limit as $M \to \infty$, observe that $E_j \to \zeta\left(1-r+2j, 1+\frac{2-r}{2N}\right)$ and $H_j \to \zeta\left(2-r+2j, 1+\frac{1-r}{2N}\right)$ for $j \geq 1$, since $1-r+2j, 2-r+2j > 1$. The sums F and I are convergent and G can be written as (see [DLMF, Eq. 25.11.5])

$$\sum_{k=1}^{M} \frac{1}{\left(k+\frac{1-r}{2N}\right)^{2-r}} = \zeta\left(2-r, 1+\frac{1-r}{2N}\right) - \frac{\left(M+\frac{1-r}{2N}\right)^{r-1}}{1-r} - (2-r)\int_{M-1}^{\infty} \frac{x - \lfloor x \rfloor}{\left(x+1+\frac{1-r}{2N}\right)^{3-r}}\, dx. \tag{2.37}$$

The same formula holds to approximate D for $r < 1$,

$$\sum_{k=1}^{M} \frac{1}{\left(k+\frac{2-r}{2N}\right)^{1-r}} = \zeta\left(1-r, 1+\frac{2-r}{2N}\right) + \frac{\left(M+\frac{2-r}{2N}\right)^{r}}{r} - (1-r)\int_{M-1}^{\infty} \frac{x-\lfloor x\rfloor}{\left(x+1+\frac{2-r}{2N}\right)^{2-r}}\,\mathrm{d}x, \tag{2.38}$$

while if $r > 1$, by the Euler-Maclaurin formula,

$$\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1} = \int_{1}^{M}\left(x+\frac{2-r}{2N}\right)^{r-1}\mathrm{d}x + \frac{1}{2}\left[\left(M+\frac{2-r}{2N}\right)^{r-1} + \left(1+\frac{2-r}{2N}\right)^{r-1}\right] + (r-1)\int_{1}^{M}\frac{x-\lfloor x\rfloor-1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\,\mathrm{d}x,$$

which after computing the first integral and rewritting the second as a difference of integrals is

$$\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1} = \frac{\left(M+\frac{2-r}{2N}\right)^{r}}{r} + \frac{\left(M+\frac{2-r}{2N}\right)^{r-1}}{2} - \frac{\left(1+\frac{2-r}{2N}\right)^{r}}{r} + \frac{\left(1+\frac{2-r}{2N}\right)^{r-1}}{2} + (r-1)\int_{-\left(\frac{2-r}{2N}\right)}^{M}\frac{x-\lfloor x\rfloor-1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\,\mathrm{d}x - (r-1)\int_{-\left(\frac{2-r}{2N}\right)}^{1}\frac{x-\lfloor x\rfloor-1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\,\mathrm{d}x.$$

Solving the last integral, we finally get

$$\begin{aligned}\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1} &= \frac{\left(M+\frac{2-r}{2N}\right)^{r}}{r} + \frac{\left(M+\frac{2-r}{2N}\right)^{r-1}}{2} - \frac{\left(1+\frac{2-r}{2N}\right)^{r}}{r} + \frac{\left(1+\frac{2-r}{2N}\right)^{r-1}}{2} \\ &+ (r-1)\int_{-\left(\frac{2-r}{2N}\right)}^{M}\frac{x-\lfloor x\rfloor-1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\,\mathrm{d}x - \left(\frac{2-r}{2N}\right)^{r-1} + \frac{\left(1+\frac{2-r}{2N}\right)^{r}}{r} - \frac{\left(1+\frac{2-r}{2N}\right)^{r-1}}{2} \\ &= \frac{\left(M+\frac{2-r}{2N}\right)^{r}}{r} + \frac{\left(M+\frac{2-r}{2N}\right)^{r-1}}{2} + (r-1)\int_{-\left(\frac{2-r}{2N}\right)}^{M}\frac{x-\lfloor x\rfloor-1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\,\mathrm{d}x - \left(\frac{2-r}{2N}\right)^{r-1},\end{aligned} \tag{2.39}$$

where the last integral converges for $1 < r < 2$ to $\zeta\left(1-r, \frac{2-r}{2N}\right)$ when $M \to +\infty$, see [DLMF, Eq. 25.11.26].

Thus, if we denote

$$\begin{aligned} g_{r,N}(M) :=& 2r(1+r)\sum_{k=1}^{M}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)} + 2r(1-r)\sum_{k=1}^{M}\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)} \\ &- 2(1+r)N^{r-1}M^{r} - r(N+r+Nr-r^2)N^{r-2}M^{r-1},\end{aligned}$$

from (2.35), (2.36) and (2.37) we have

$$g_{r,N}(M) = 2r(1+r)\left(N^{r-1}\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1}\right.$$
$$+\sum_{j=1}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}\sum_{k=0}^{M-1}\frac{N^{r-1-2j}}{\left(k+1+\frac{2-r}{2N}\right)^{1-r+2j}}+O\left(N^{r-1-2m}\right)\left.\sum_{k=1}^{M}\frac{1}{k^{1-r+2m}}\right)$$
$$+2r(1-r)\left(N^{r-2}\left(\zeta\left(2-r,1+\frac{1-r}{2N}\right)-\frac{\left(M+\frac{1-r}{2N}\right)^{r-1}}{1-r}\right.\right.$$
$$\left.-\int_{M-1}^{\infty}\frac{(2-r)(x-\lfloor x\rfloor)}{\left(x+1+\frac{1-r}{2N}\right)^{3-r}}\,\mathrm{d}x\right)+\sum_{j=1}^{m-1}\frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!}\sum_{k=0}^{M-1}\frac{N^{r-2-2j}}{\left(k+1+\frac{1-r}{2N}\right)^{2-r+2j}}$$
$$\left.+O\left(N^{r-2-2m}\right)\sum_{k=1}^{M}\frac{1}{k^{2-r+2m}}\right)-2(1+r)N^{r-1}M^{r}-r(N+r+Nr-r^2)N^{r-2}M^{r-1}.$$

Then, using all the previous computations, we get

$$\lim_{M\to\infty}g_{r,N}(M)=\lim_{M\to\infty}\left[2r(1+r)N^{r-1}\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1}-2(1+r)N^{r-1}M^{r}\right.$$
$$\left.-2rN^{r-2}\left(M+\frac{1-r}{2N}\right)^{r-1}-r(N+r+Nr-r^2)N^{r-2}M^{r-1}\right] \tag{2.40}$$
$$+2r(1-r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!}N^{r-2-2j}\zeta\left(2-r+2j,1+\frac{1-r}{2N}\right)$$
$$+2r(1+r)\sum_{j=1}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}N^{r-1-2j}\zeta\left(1-r+2j,1+\frac{2-r}{2N}\right)+O\left(N^{r-1-2m}\right).$$

Everything reduces to compute the limit appearing in (2.40). Let us define

$$h_{r,N}(M):=2r(1+r)N^{r-1}\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1}-2(1+r)N^{r-1}M^{r}$$
$$-2rN^{r-2}\left(M+\frac{1-r}{2N}\right)^{r-1}-r(N+r+Nr-r^2)N^{r-2}M^{r-1}.$$

If $r<1$, using (2.38),

$$\lim_{M\to\infty}h_{r,N}(M)=\lim_{M\to\infty}\left[2r(1+r)N^{r-1}\left(\zeta\left(1-r,1+\frac{2-r}{2N}\right)\right.\right.$$
$$\left.\left.+\frac{\left(M+\frac{2-r}{2N}\right)^{r}}{r}-(1-r)\int_{M-1}^{\infty}\frac{x-\lfloor x\rfloor}{\left(x+1+\frac{2-r}{2N}\right)^{2-r}}\,\mathrm{d}x\right)-2(1+r)N^{r-1}M^{r}\right],$$

where the integral tends to 0. Consequently,

$$\begin{aligned}
&\lim_{M\to\infty} h_{r,N}(M)\\
&= 2r(1+r)N^{r-1}\zeta\left(1-r, 1+\frac{2-r}{2N}\right) + 2(1+r)N^{r-1}\lim_{M\to\infty}\left(\left(M+\frac{2-r}{2N}\right)^r - M^r\right)\\
&= 2r(1+r)N^{r-1}\zeta\left(1-r, 1+\frac{2-r}{2N}\right).
\end{aligned}$$

If $r>1$, using (2.39),

$$\begin{aligned}
h_{r,N}(M) = 2r(1+r)N^{r-1}&\left(\frac{\left(M+\frac{2-r}{2N}\right)^r}{r} + \frac{\left(M+\frac{2-r}{2N}\right)^{r-1}}{2}\right.\\
&\left.+\int_{-\left(\frac{2-r}{2N}\right)}^{M} \frac{(r-1)(x-\lfloor x\rfloor - \frac{1}{2})}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\,\mathrm{d}x - \left(\frac{2-r}{2N}\right)^{r-1}\right) - 2(1+r)N^{r-1}M^r\\
&- 2rN^{r-2}\left(M+\frac{1-r}{2N}\right)^{r-1} - r(N+r+Nr-r^2)N^{r-2}M^{r-1}.
\end{aligned}$$

Factorising terms and taking into account that the integral tends to $\zeta\left(1-r, \frac{2-r}{2N}\right)$,

$$\begin{aligned}
&\lim_{M\to\infty} h_{r,N}(M) = \lim_{M\to\infty}\left[2(1+r)N^{r-1}M^r\left(\left(1+\frac{2-r}{2NM}\right)^r - 1\right)\right.\\
&\left.+ rN^{r-2}M^{r-1}\left((1+r)\left(1+\frac{2-r}{2NM}\right)^{r-1}N - 2\left(1+\frac{1-r}{2NM}\right)^{r-1} - \left(N+r+Nr-r^2\right)\right)\right]\\
&+ 2r(1+r)N^{r-1}\left(\zeta\left(1-r, \frac{2-r}{2N}\right) - \left(\frac{2-r}{2N}\right)^{r-1}\right).
\end{aligned}$$

The function inside the limit has asymptotic expansion

$$rN^{r-2}M^{r-1}\underbrace{[(1+r)(2-r)+(1+r)N-2-(N+r+Nr-r^2)]}_{=0} + O\left(M^{r-2}\right)$$

as $M\to\infty$, so the limit is 0 and

$$\begin{aligned}
\lim_{M\to\infty} h_{r,N}(M) &= 2r(1+r)N^{r-1}\left(\zeta\left(1-r, \frac{2-r}{2N}\right) - \left(\frac{2-r}{2N}\right)^{r-1}\right)\\
&= 2r(1+r)N^{r-1}\zeta\left(1-r, 1+\frac{2-r}{2N}\right),
\end{aligned}$$

where we have used that $\zeta(s,a) - a^{-s} = \zeta(s, 1+a)$.

Therefore,

$$\lim_{M\to\infty} h_{r,N}(M) = 2r(1+r)N^{r-1}\zeta\left(1-r, 1+\frac{2-r}{2N}\right)$$

independently of r. Applying this limit on (2.40) we get the desired result. □

2.4 Bounds for the minimal energy asymptotic expansion

In this section we compare our results with minimal and expected energies of other point processes. We will start recalling some known results and conjectures about the asymptotic expansion of the extremal energy $\mathcal{E}_s(N)$ attained by a set of N points on the sphere $\mathbb{S}^2$. For a more complete picture see [BHS19].

The current knowledge about the asymptotic expansion of the minimal energy is far from complete even in $\mathbb{S}^2$, but for $s \leq -2$ the situation is well known. Indeed, the minimizers of the Riesz energy for $s < -2$ are points placed at each of the two endpoints of some diameter (for even N), [Bjö56], and for $s = -2$, formula (2.8) shows that any configuration with center of mass at the origin attains the maximum $2N^2$.

For $0 < |s| < 2$, it is known that there exist $c, C > 0$ (depending on s) such that

$$-cN^{1+s/2} \leq \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2 \leq -CN^{1+s/2}, \tag{2.41}$$

see [RSZ94, Wag90, Wag92] and [Bra06, AZ15] for improvements in the value of the constants leading to the bounds

$$\begin{aligned} \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s} &\leq -\frac{\Gamma(1-s/2)}{2^s}N^{1+s/2}, \quad \text{if } 0 < s < 2, \\ \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s} &\geq -\frac{\Gamma(1-s/2)}{2^s}N^{1+s/2}, \quad \text{if } -2 < s < 0, \end{aligned} \tag{2.42}$$

which were obtained with the bound given by the expected energy of random points from the spherical ensemble [AZ15].

In the boundary case $s = 2$, it was shown in [BHS12, Proposition 3] that

$$-\frac{1}{4}N^2 + O(N) \leq \mathcal{E}_2(N) - \frac{1}{4}N^2 \log N \leq \frac{1}{4}N^2 \log\log N + O(N^2),$$

and the upper bound was improved in [AZ15] to

$$\mathcal{E}_2(N) - \frac{1}{4}N^2 \log N \leq \frac{\gamma}{4}N^2, \tag{2.43}$$

where γ is the Euler–Mascheroni constant.

For the logarithmic potential, it is known that there exists a constant $C_{\log}$ such that

$$-0.0569\ldots \leq C_{\log} \leq 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.0556\ldots,$$

for which

$$\mathcal{E}_0(N) = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{1}{2}N\log N + C_{\log}N + o(N), \quad N \to +\infty, \tag{2.44}$$

see [BS18, Lau21] and [BL22] for a recent direct computation of the lower bound. The upper bound for $C_{\log}$ has been conjectured to be an equality by two different approaches, [BHS12, BS18].

For $-2 < s < 4$, $s \neq 0, 2$, the asymptotic expansion of the optimal Riesz s-energy has been conjectured in [BHS12] to be

$$\mathcal{E}_s(N) = \frac{2^{1-s}}{2-s}N^2 + \frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}}N^{1+\frac{s}{2}} + o(N^{1+\frac{s}{2}}), \quad N \to +\infty, \tag{2.45}$$

where $\zeta_{\Lambda_2}(s)$ is the zeta function of the hexagonal lattice, while for $s = 2$ the conjectured expansion is

$$\mathcal{E}_2(N) = \frac{1}{4}N^2 \log N + DN^2 + O(1), \quad N \to +\infty, \tag{2.46}$$

where $D = \frac{1}{4}\left(\gamma - \log(2\sqrt{3}\pi)\right) + \frac{\sqrt{3}}{4\pi}(\gamma_1(2/3) - \gamma_1(1/3)) \approx -0.08577$. Here, $\gamma_n(a)$ is the generalized Stieltjes constant in the Laurent expansion of the Hurwitz zeta function $\zeta(s, a)$ around $s = 1$.

It is clear that the minimal (maximal) energy is always bounded from above (below) by the expected energy with respect to a given random configuration. Therefore, one can bound the asymptotic expansion of the minimal energy by the asymptotic expansion of the expected energy. This idea was used in [ABS11] to get bounds for the minimal logarithmic energy using (2.1) and in [AZ15] to get (2.42) and (2.43). For other computations of expected energies in different settings, see [BS13, BMOC16, BE18, MOC18, BE19, BF20, BDFSL22, ADG+22]. From our main result, Theorem 2.1.1, we obtain the asymptotic expansion (2.6), which is close to the conjectured expansion for the minimal energy, see Figure 2.4, and we can prove the following bounds.

Corollary 2.4.1. *Let $C(s)$ be the constant in (2.7). Then,*

(i) for $0 < s < 2$, there exists an $N_0 = N_0(s)$ such that, for any $N \geq N_0$,

$$\mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2 \leq C(s)N^{1+s/2}.$$

(ii) For $-2 < s < 0$ and a given $\epsilon > 0$, there exists an $N_1 = N_1(\epsilon, s)$ such that, for any $N \geq N_1$,

$$\mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2 \geq C(s)(1+\epsilon)N^{1+s/2}.$$

(iii) For any $N \geq 2$,

$$\mathcal{E}_2(N) - \frac{N^2 \log N}{4} \leq \frac{1}{4}\left(\frac{3}{2} - \log(2\pi) + \gamma\right)N^2. \tag{2.47}$$

Remark 2.4.2. The bound (2.47) improves (2.43), since $\frac{1}{4}\left(\frac{3}{2} - \log(2\pi) + \gamma\right) \approx 0.0598$ and $\frac{\gamma}{4} \approx 0.1443$. In the proof we show also that

$$\mathbb{E}[E_2] = \frac{N^2 \log N}{4} + \frac{1}{4}\left(\frac{3}{2} - \log(2\pi) + \gamma\right)N^2 - \frac{N}{8} + O(1), \quad N \to +\infty,$$

see (2.51).

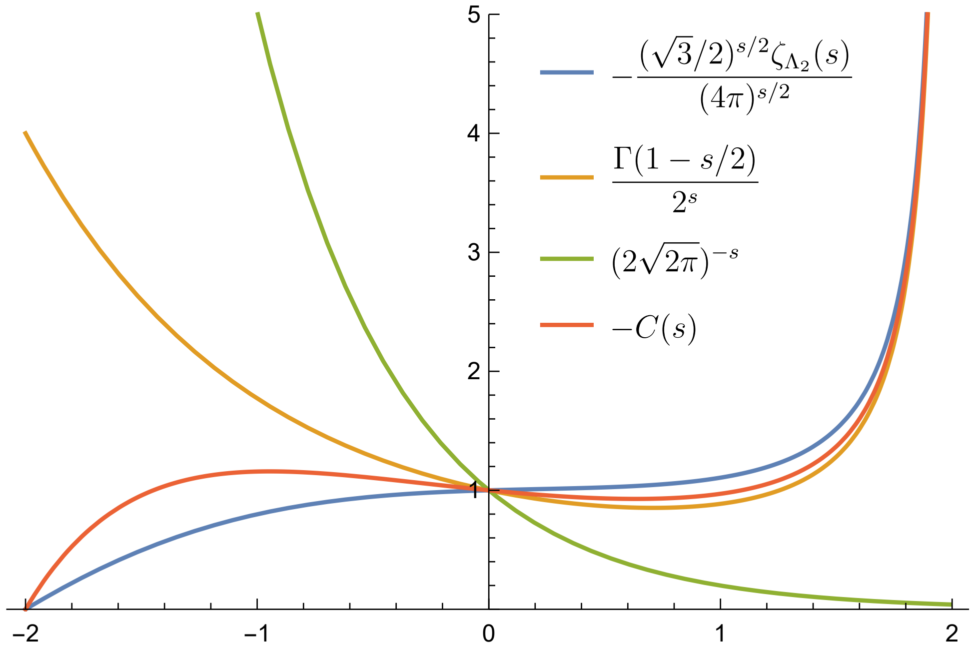

Figure 2.4: Absolute value of the second order coefficient of the asymptotic expansion of $\mathcal{E}_s(N)$ in several works. The blue curve is given by the conjectured valued (2.45). The green and yellow curves corresponds to [RSZ94] and [AZ15], respectively, and the red is our constant (2.7).

Proof. For $0 < s < 2$, from (2.6),

$$\frac{\mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2}{N^{1+s/2}} \leq \frac{\mathbb{E}[E_s] - \frac{2^{1-s}}{2-s}N^2}{N^{1+s/2}} = C(s) + \frac{s}{16}C(s-2)N^{-1} + O(N^{-2}), \quad N \to \infty.$$

Since $C(s-2)$ is negative, the last expression is bounded above by $C(s)$ for N big enough.

For $-2 < s < 0$, using (2.6) again,

$$\frac{\mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2}{N^{1+s/2}} \geq \frac{\mathbb{E}[E_s] - \frac{2^{1-s}}{2-s}N^2}{N^{1+s/2}} \xrightarrow[N\to\infty]{} C(s).$$

Therefore, given $\delta > 0$, for N large enough the right-hand side is bounded from below by $C(s) - \delta$. Since the constant $C(s)$ is negative, we can choose $\delta = -\epsilon C(s)$ to obtain the result.

For $s = 2$, the energy is (2.4):

$$\mathbb{E}[E_2] = -\frac{N\pi}{4}\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) + \frac{3N^2}{8} - \frac{3N}{8}.$$

We can rewrite the sum as

$$-\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) = \underbrace{\sum_{j=1}^{N-1}\left[-\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) - \frac{1}{\pi(1-j/N)}\right]}_{A} + \underbrace{\sum_{j=1}^{N-1}\frac{1}{\pi(1-j/N)}}_{B}, \quad (2.48)$$

in such a way that the term corresponding to $j = N$ in the first sum is well-defined. Let us apply the Euler-Maclaurin formula to $f(x) = g(x/N)$, with $g(x) = -x\cot(\pi x) - \frac{1}{\pi(1-x)}$:

$$\begin{aligned} A &= \sum_{j=0}^{N} f(j) - f(0) - f(N) \\ &= \int_0^N f(x)\,\mathrm{d}x - \frac{f(0)+f(N)}{2} + \frac{B_2}{2!}[f'(N) - f'(0)] + \frac{B_4}{4!}[f^{(3)}(N) - f^{(3)}(0)] + R_N^A \\ &= N\int_0^1 g(x)\,\mathrm{d}x - \frac{g(0)+g(1)}{2} + \frac{1}{12N}[g'(1) - g'(0)] - \frac{1}{720N^3}[g^{(3)}(1) - g^{(3)}(0)] + R_N^A, \end{aligned}$$

where B_j are the Bernoulli numbers and R_N^A is the remainder term, that satisfies

$$|R_N^A| \le \frac{2\zeta(5)}{(2\pi)^5}\int_0^N |f^{(5)}(x)|\,\mathrm{d}x = \frac{2\zeta(5)}{(2\pi)^5 N^4}\int_0^1 |g^{(5)}(x)|\,\mathrm{d}x. \tag{2.49}$$

We get

$$A = -\frac{\log(2\pi)}{\pi}N + \frac{3}{2\pi} + \frac{\pi^2+3}{36\pi N} - \frac{\pi^4+45}{5400\pi N^3} + R_N^A.$$

The second sum in (2.48) is

$$B = \frac{N}{\pi}\sum_{j=1}^{N-1}\frac{1}{N-j} = \frac{N}{\pi}\sum_{j=1}^{N-1}\frac{1}{j} = \frac{N}{\pi}\left(H_N - \frac{1}{N}\right),$$

where H_N is the N-th harmonic number. Its expansion as $N \to \infty$, see [Boa77], is

$$H_N = \log N + \gamma + \frac{1}{2N} - \frac{1}{12N^2} + R_N^H,$$

where

$$0 < R_N^H < \frac{1}{120N^4}. \tag{2.50}$$

With these expansions, formula (2.48) reads

$$\begin{aligned} &-\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) \\ &\quad = -\frac{\log(2\pi)}{\pi}N + \frac{3}{2\pi} + \frac{\pi^2+3}{36\pi N} - \frac{\pi^4+45}{5400\pi N^3} + R_N^A \\ &\quad + \frac{N}{\pi}\left(\log N + \gamma - \frac{1}{2N} - \frac{1}{12N^2} + R_N^H\right) \\ &\quad = \frac{1}{\pi}\left[N\log N + (-\log(2\pi)+\gamma)N + 1 + \frac{\pi^2}{36N} + NR_N^H - \frac{\pi^4+45}{5400N^3} + \pi R_N^A\right]. \end{aligned}$$

Plugging this into the formula (2.4), we obtain

$$\begin{aligned}\mathbb{E}[E_2(x_1,\ldots,x_N)] &= \frac{N}{4}\left[N\log N + \left(\frac{3}{2}-\log(2\pi)+\gamma\right)N - \frac{1}{2}\right.\\ &\left.+\frac{\pi^2}{36N} + NR_N^H - \frac{\pi^4+45}{5400}\frac{1}{N^3} + \pi R_N^A\right]\\ &= \frac{N^2\log N}{4} + \frac{1}{4}\left(\frac{3}{2}-\log(2\pi)+\gamma\right)N^2 - \frac{1}{8}N\\ &+ \underbrace{\frac{\pi^2}{144} + \frac{N^2 R_N^H}{4}}_{C} + \frac{1}{4}\Bigg(\underbrace{-\frac{\pi^4+45}{5400}\frac{1}{N^2} + \pi N R_N^A}_{D}\Bigg).\end{aligned} \tag{2.51}$$

Finally, from (2.50), we have

$$C \leq \frac{\pi^2}{144} + \frac{1}{480N^2} \leq \frac{\pi^2}{144} + \frac{1}{480} < 0.25 \leq \frac{N}{8}$$

for any $N \geq 2$, and $D \leq 0$ because

$$\pi N|R_N^A| \leq \frac{2\pi\zeta(5)}{(2\pi)^5 N^3}\int_0^1 |g^{(5)}(x)|\,\mathrm{d}x \leq \frac{2\pi\zeta(5)}{(2\pi)^5 N^3}|g^{(5)}(1)| \leq \frac{\pi^4+45}{5400}\frac{1}{N^2},$$

if $N \geq 2$. This proves (2.47). □

2.5 Proof of Theorem 2.1.3

Proof. We use formula (2.18) with $F(p,q) = \chi_{\{|p-q|\leq t\}}$:

$$\begin{aligned}2\mathbb{E}[G(t,X_N)] &= \mathbb{E}\left[\sum_{i\neq j}\chi_{\{|x_i-x_j|\leq t\}}\right] = 2N^2\int_0^\infty r\,\chi_{\left\{\frac{2r}{\sqrt{1+r^2}}\leq t\right\}}(r)\gamma(r)\,\mathrm{d}r\\ &= N^2\int_0^{\frac{t^2}{4-t^2}} \frac{\left[\left((1+x)^N-1-Nx\right)^2(1+x)^{N-2} + \left((1+x)^N-1-Nx(1+x)^{N-1}\right)^2\right]}{[(1+x)^N-1]^3}\,\mathrm{d}x,\end{aligned}$$

where we have applied the change of variables $r = \sqrt{x}$. As in the proof of Theorem 2.1.1, we use the identity $\frac{1}{(x-1)^3} = \frac{1}{2}\sum_{k=2}^{\infty} k(k-1)x^{-(k+1)}$ for $x > 1$ to get

$$
\begin{aligned}
4\mathbb{E}[G(t, X_N)] = N^2 \lim_{M\to\infty} \sum_{k=2}^{M} k(k-1) \\
\Bigg[\underbrace{\int_0^{\frac{t^2}{4-t^2}} \left[(1+x)^{-2-Nk} + (1+x)^{-N(k+1)}\right] \left((1+x)^N - 1\right)^2 \mathrm{d}x}_{A_k} \\
- 2N \underbrace{\int_0^{\frac{t^2}{4-t^2}} x \left[(1+x)^{-2-Nk} + (1+x)^{-1-Nk}\right] \left((1+x)^N - 1\right) \mathrm{d}x}_{B_k} \\
+ N^2 \underbrace{\int_0^{\frac{t^2}{4-t^2}} x^2 \left[(1+x)^{-2-Nk} + (1+x)^{-2-N(k-1)}\right] \mathrm{d}x}_{C_k} \Bigg].
\end{aligned}
$$

The expression is the same than (2.21) with $r = 0$, but changing the upper limit of integration. We can take advantage of our previous computations using the following representation for the incomplete beta function

$$
B_{s/(s+1)}(x, y) = \int_0^s \frac{t^{x-1}}{(1+t)^{x+y}}\, dt \qquad s, x, y > 0, \tag{2.52}
$$

which follows from

$$
B_z(x, y) := \int_0^z u^{x-1}(1-u)^{y-1}\, du \qquad 0 \le z \le 1,\ x, y > 0
$$

and the change of variables $u = t/(t+1)$.

Therefore, if $s = \frac{t^2}{4-t^2}$ and $s' = \frac{s}{s+1}$, we have the analogues of (2.25), (2.23) and (2.24)

$$
\begin{aligned}
A_k = B_{s'}(1, N(k-2)+1) - 2B_{s'}(1, N(k-1)+1) + B_{s'}(1, Nk+1) \\
+ B_{s'}(1, N(k-1)-1) - 2B_{s'}(1, Nk-1) + B_{s'}(1, N(k+1)-1),
\end{aligned}
$$

$$
B_k = B_{s'}(2, N(k-1)) - B_{s'}(2, Nk) + B_{s'}(2, N(k-1)-1) - B_{s'}(2, Nk-1),
$$

and

$$
C_k = B_{s'}(3, Nk-1) + B_{s'}(3, N(k-1)-1).
$$

Then, changing indices as in the proof of Theorem 2.1.1, we get

$$\begin{aligned}
&4\mathbb{E}[G(t,X_N)] = N^2 \lim_{M\to\infty} \sum_{k=2}^{M} k(k-1)\Big[B_{s'}(1,N(k-2)+1) - 2B_{s'}(1,N(k-1)+1)\\
&+ B_{s'}(1,Nk+1) + B_{s'}(1,N(k-1)-1) - 2B_{s'}(1,Nk-1) + B_{s'}(1,N(k+1)-1)\\
&- 2N\big(B_{s'}(2,N(k-1)) - B_{s'}(2,Nk) + B_{s'}(2,N(k-1)-1) - B_{s'}(2,Nk-1)\big)\\
&+ N^2\big(B_{s'}(3,Nk-1) + B_{s'}(3,N(k-1)-1)\big)\Big]\\
&= N^2 \lim_{M\to\infty}\left(2\sum_{k=0}^{M} B_{s'}(1,Nk+1) + 2\sum_{k=1}^{M} B_{s'}(1,Nk-1) - 4N\sum_{k=1}^{M} kB_{s'}(2,Nk)\right.\\
&\left. - 4N\sum_{k=1}^{M} kB_{s'}(2,Nk-1) + 2N^2\sum_{k=1}^{M} k^2B_{s'}(3,Nk-1) + g_{N,s}(M)\right),
\end{aligned}$$

where

$$\begin{aligned}
g_{N,s}(M) &= (M+1)(M-2)B_{s'}(1,NM+1) - (M+1)MB_{s'}(1,N(M-1)+1)\\
&- (M+1)MB_{s'}(1,NM-1) + M(M-1)B_{s'}(1,N(M+1)-1)\\
&+ 2N(M+1)MB_{s'}(2,NM) + 2N(M+1)MB_{s'}(2,NM-1)\\
&- N^2(M+1)MB_{s'}(3,NM-1).
\end{aligned}$$

Observe that for any $n \geq 1$,

$$B_{s'}(1,n) = \int_0^s \frac{1}{(1+t)^{n+1}}\,dt = -\frac{(1+s)^{-n}}{n} + \frac{1}{n}.$$

Integrating by parts, one can also check that

$$B_{s'}(2,n) = -\frac{s(1+s)^{-n-1}}{n+1} - \frac{(1+s)^{-n}}{(n+1)n} + \frac{1}{(n+1)n}$$

and

$$B_{s'}(3,n) = -\frac{s^2(1+s)^{-n-2}}{n+2} - \frac{2s(1+s)^{-n-1}}{(n+2)(n+1)} - \frac{2(1+s)^{-n}}{(n+2)(n+1)n} + \frac{2}{(n+2)(n+1)n}.$$

If we replace this expressions in $g_{N,s}(M)$, we see that only the last term survives when we take the limit. For instance,

$$\begin{aligned}
2N(M+1)MB_{s'}(2,NM) &= -\frac{2N(M+1)Ms(1+s)^{-NM-1}}{NM+1}\\
&\quad - \frac{2N(M+1)M(1+s)^{-NM}}{(NM+1)NM} + \frac{2N(M+1)M}{(NM+1)NM},
\end{aligned}$$

and all the terms containing the factor $(1+s)^{-NM+m}$ go to 0 as $M\to\infty$. Therefore,

$$\lim_{M\to\infty} g_{s,N}(M) = \lim_{M\to\infty}\left[\frac{(M+1)(M-2)}{NM+1} - \frac{(M+1)M}{N(M-1)+1} - \frac{(M+1)M}{NM-1}\right.$$
$$+ \frac{M(M-1)}{N(M+1)-1} + \frac{2N(M+1)M}{(NM+1)NM} + \frac{2N(M+1)M}{NM(NM-1)}$$
$$\left.- \frac{2N^2(M+1)M}{(NM+1)NM(NM-1)}\right] = \lim_{M\to\infty}\left(-\frac{2}{N} + O\left(\frac{1}{M}\right)\right) = -\frac{2}{N}.$$

On the other hand, we have

$$2\sum_{k=0}^{M} B_{s'}(1,Nk+1) + 2\sum_{k=1}^{M} B_{s'}(1,Nk-1) - 4N\sum_{k=1}^{M} kB_{s'}(2,Nk)$$
$$- 4N\sum_{k=1}^{M} kB_{s'}(2,Nk-1) + 2N^2\sum_{k=1}^{M} k^2B_{s'}(3,Nk-1)$$
$$= 2\sum_{k=0}^{M}\frac{1-(1+s)^{-Nk-1}}{Nk+1} + 2\sum_{k=1}^{M}\frac{1-(1+s)^{-Nk+1}}{Nk-1}$$
$$- 4N\sum_{k=1}^{M} k\left(-\frac{s(1+s)^{-Nk-1}}{Nk+1} + \frac{1-(1+s)^{-Nk}}{(Nk+1)Nk}\right)$$
$$- 4N\sum_{k=1}^{M} k\left(-\frac{s(1+s)^{-Nk}}{Nk} + \frac{1-(1+s)^{-Nk+1}}{Nk(Nk-1)}\right)$$
$$+ 2N^2\sum_{k=1}^{M} k^2\left(-\frac{s^2(1+s)^{-Nk-1}}{Nk+1} - \frac{2s(1+s)^{-Nk}}{(Nk+1)Nk} + \frac{2-2(1+s)^{-Nk+1}}{(Nk+1)Nk(Nk-1)}\right)$$
$$= 2\left(1-(1+s)^{-1}\right) + 2s\sum_{k=1}^{M}(1+s)^{-Nk-1}(2+s-sNk).$$

Hence,

$$4\mathbb{E}[G(t,X_N)] = N^2\left(2\left(1-(1+s)^{-1}\right) + 2s\sum_{k=1}^{\infty}(1+s)^{-Nk-1}(2+s-sNk) - \frac{2}{N}\right)$$
$$= N^2\left(\frac{2s}{1+s} - \frac{2}{N} + \frac{2s(2+s)}{(1+s)\left((1+s)^N-1\right)} - \frac{2Ns^2(1+s)^N}{(1+s)\left((1+s)^N-1\right)^2}\right)$$

and with the change $s = t^2/(4-t^2)$ we get the result (2.10).

Now we prove inequality (2.12). In terms of s, since $t^2 = 4s/(1+s)$, it reads

$$\frac{N^2}{4}\left(-\frac{2}{N} + \frac{2s}{1+s} + \frac{2s(2+s)}{(1+s)\left((1+s)^N-1\right)} - \frac{2Ns^2(1+s)^N}{(1+s)\left((1+s)^N-1\right)^2}\right) \le \frac{N^3s^2}{8(1+s)^2},$$

or, by regrouping terms,

$$s^2 + \frac{4}{N^2}(1+s)\left(1 - \frac{Ns}{(1+s)^N - 1}\right)\left(1 - \frac{Ns}{(1+s)^N - 1} - (N-1)s\right) \geq 0.$$

Then, if we multiply by $((1+s)^N - 1)^2 N^2$, we have to prove

$$\begin{aligned} f_N(s) &:= s^2 N^2 ((1+s)^N - 1)^2 \\ &\quad + 4(1+s)\left((1+s)^N - 1 - Ns\right)\left((1+s)^N - 1 - Ns - (N-1)s((1+s)^N - 1)\right) \geq 0. \end{aligned}$$

We expand the polynomial $(1+s)^N$ and rearrange terms in order to identify the coefficients of the polynomial f_N

$$\begin{aligned} f_N(s) &= s^2 N^2 \sum_{j=1}^{N} \binom{N}{j} s^j \sum_{k=1}^{N} \binom{N}{k} s^k \\ &\quad + 4(1+s) \sum_{j=2}^{N} \binom{N}{j} s^j \left(\sum_{k=2}^{N} \binom{N}{k} s^k - (N-1)s \sum_{k=1}^{N} \binom{N}{k} s^k \right) \\ &= s^4 N^2 \sum_{j=0}^{N-1} \binom{N}{j+1} s^j \sum_{k=0}^{N-1} \binom{N}{k+1} s^k \\ &\quad + 4s^4 \underbrace{(1+s) \sum_{j=0}^{N-2} \binom{N}{j+2} s^j \left(\sum_{k=0}^{N-2} \binom{N}{k+2} s^k - (N-1) \sum_{k=0}^{N-1} \binom{N}{k+1} s^k \right)}_{A}. \end{aligned}$$

Using that $\binom{n}{k} = 0$ if $k > n$, the expression A can be expanded in the following way

$$\begin{aligned} A &= (1+s) \sum_{j=0}^{N-2} \binom{N}{j+2} s^j \left(\sum_{k=0}^{N-1} \binom{N}{k+2} s^k - (N-1) \sum_{k=0}^{N-1} \binom{N}{k+1} s^k \right) \\ &= \left(\sum_{j=0}^{N-1} \left(\binom{N}{j+2} + \binom{N}{j+1} \right) s^j - N \right) \left(\sum_{k=0}^{N-1} \binom{N}{k+2} s^k - (N-1) \sum_{k=0}^{N-1} \binom{N}{k+1} s^k \right) \\ &= \sum_{j=0}^{N-1} \binom{N}{j+2} s^j \sum_{k=0}^{N-1} \binom{N}{k+2} s^k - (N-1) \sum_{j=0}^{N-1} \binom{N}{j+2} s^j \sum_{k=0}^{N-1} \binom{N}{k+1} s^k \\ &\quad + \sum_{j=0}^{N-1} \binom{N}{j+1} s^j \sum_{k=0}^{N-1} \binom{N}{k+2} s^k - (N-1) \sum_{j=0}^{N-1} \binom{N}{j+1} s^j \sum_{k=0}^{N-1} \binom{N}{k+1} s^k \\ &\quad - N \sum_{k=0}^{N-1} \left(\binom{N}{k+2} - (N-1) \binom{N}{k+1} \right) s^k, \end{aligned}$$

and then $g_N(s) := f_N(s)/s^4$ becomes

$$g_N(s) = (N-2)^2 \sum_{j=0}^{N-1} \binom{N}{j+1} s^j \sum_{k=0}^{N-1} \binom{N}{k+1} s^k - 4(N-2) \sum_{j=0}^{N-1} \binom{N}{j+1} s^j \sum_{k=0}^{N-1} \binom{N}{k+2} s^k$$
$$+ 4 \sum_{j=0}^{N-1} \binom{N}{j+2} s^j \sum_{k=0}^{N-1} \binom{N}{k+2} s^k - 4N \sum_{k=0}^{N-1} \left(\binom{N}{k+2} - (N-1)\binom{N}{k+1} \right) s^k.$$

Now we compute the products of sums. For instance, for the first product,

$$\sum_{j=0}^{N-1} \binom{N}{j+1} s^j \sum_{k=0}^{N-1} \binom{N}{k+1} s^k = \sum_{m=0}^{2N-2} \sum_{j=0}^{m} \binom{N}{j+1} \binom{N}{m-j+1} s^m.$$

The same can be done with the others, yielding

$$g_N(s) = \sum_{m=0}^{2N-2} \Bigg[(N-2)^2 \underbrace{\sum_{j=0}^{m} \binom{N}{j+1}\binom{N}{m-j+1}}_{B} - 4(N-2) \underbrace{\sum_{j=0}^{m} \binom{N}{j+1}\binom{N}{m-j+2}}_{C}$$
$$+ 4 \underbrace{\sum_{j=0}^{m} \binom{N}{j+2}\binom{N}{m-j+2}}_{D} - 4N \left(\binom{N}{m+2} - (N-1)\binom{N}{m+1} \right) \Bigg] s^m.$$

Next, we apply Vandermonde's identity, [GR07, 0.156], to obtain the sums B, C and D:

$$\begin{aligned}
B &= \sum_{k=1}^{m+1} \binom{N}{k}\binom{N}{m+2-k} = \sum_{k=0}^{m+2} \binom{N}{k}\binom{N}{m+2-k} - 2\binom{N}{m+2} \\
&= \binom{2N}{m+2} - 2\binom{N}{m+2} \\
C &= \binom{2N}{m+3} - 2\binom{N}{m+3} - N\binom{N}{m+2} \\
D &= \binom{2N}{m+4} - 2\binom{N}{m+4} - 2N\binom{N}{m+3}.
\end{aligned}$$

Then

$$\begin{aligned}
g_N(s) = \sum_{m=0}^{2N-2} \Bigg[& (N-2)^2 \left(\binom{2N}{m+2} - 2\binom{N}{m+2} \right) \\
& - 4(N-2) \left(\binom{2N}{m+3} - 2\binom{N}{m+3} - N\binom{N}{m+2} \right) \\
& + 4 \left(\binom{2N}{m+4} - 2\binom{N}{m+4} - 2N\binom{N}{m+3} \right) \\
& -4N \left(\binom{N}{m+2} - (N-1)\binom{N}{m+1} \right) \Bigg] s^m =: \sum_{m=0}^{2N-2} c_{N,m} s^m.
\end{aligned}$$

Remember that our goal is to check that $g_N(s) \geq 0$ for $s \geq 0$. In fact, we will see that the coefficients of this polynomial are all positive for any $N \geq 2$. To prove this, let us successively apply the identity $\binom{n}{k} = \frac{n-k+1}{k}\binom{n}{k-1}$ to get

$$c_{N,m} = \frac{1}{(m+2)(m+3)(m+4)} \left(\binom{N}{m+1} h^A(N,m) + \binom{2N}{m+1} h^B(N,m) \right),$$

where

$$\begin{aligned} h^A(N,m) &= 2N^3(m^2+7m+8) + 2N^2(m^3+8m^2+23m+4) \\ &\quad - 4N(m^2+m+10) + 16(m+1), \\ h^B(N,m) &= 2N^3(m^2-m-4) - N^2(m^3+3m-20) + 4N(m^2-m+2) - 8(m+1). \end{aligned}$$

Using the trivial inequality

$$2N^2(m^3+8m^2+23m) - 4N(m^2+m) + 16(m+1) \geq 0,$$

we have

$$c_{N,m} \geq \frac{1}{(m+2)(m+3)(m+4)} \left(\binom{N}{m+1} h^C(N,m) + \binom{2N}{m+1} h^B(N,m) \right), \quad (2.53)$$

where

$$h^C(N,m) = 2N^3(m^2+7m+8) + 8N^2 - 40N.$$

Now we check that $c_{N,m} \geq 0$, for any $0 \leq m \leq 2N-2$, $N \geq 2$. Let $m \geq 3$. Then, both h^C and h^B are positive. Indeed, for the first one,

$$h^C(N,m) \geq 16N^3 + 8N^2 - 40N = 8N(2N^2+N-5) \geq 0.$$

For the second one, taking into account that we restrict to $m \leq 2N-2$, which means $N \geq (m+2)/2$, it is easy to see that $h^B(N,m)$ is increasing as a function of N and therefore

$$h^B(N,m) \geq h^B(\lceil m/2 \rceil + 1, m) \geq h^B(m/2+1, m) = \frac{1}{4}(m-2)^2\left(m^2+7m+12\right) \geq 0.$$

Finally, from (2.53), we also have

$$(m+2)(m+3)(m+4)c_{N,m} \geq \begin{cases} 8N\left(6N^2-3N-2\right), & m=0, \\ 4N\left(7N^3-6N^2-5N+4\right), & m=1, \\ 2N/3(5N^5-13N^4+20N^3-56N^2+68N-24), & m=2, \end{cases}$$

which are positive for any $N \geq 2$, and we are done. □

Chapter 3

Average worst-case error and discrepancies

In this chapter, we study how well-distributed are N-point configurations on the sphere $\mathbb{S}^d$ given by some random point processes from two different perspectives: the QMC strength and the discrepancy.

Following [BSSW14], a sequence $(X_N) \subset \mathbb{S}^d$ of N-point sets on the d-dimensional sphere has QMC strength $s^* > d/2$ if it has worst-case error of optimal order, which turns out to be $N^{-s/d}$, for Sobolev spaces of order s for all $d/2 < s < s^*$, and the order is not optimal for $s > s^*$. In the same paper, conjectured values of the QMC strength are given for some well known point families in $\mathbb{S}^2$ based on numerical results. We study the average QMC strength for somehow related random configurations.

In addition, we consider different notions of discrepancy: with respect to spherical caps, which measures the asymptotic equidistribution, and with respect to hemispheres, which measures the symmetry. We compute the expected discrepancies for some random point processes on the spheres. As a final result, we extend a discrepancy result from [BMOC16] for point configurations drawn from the harmonic ensemble on the sphere to any two-point homogeneous manifold. As a corollary, we show that with high probability realizations of the harmonic ensemble on any two-point homogeneous manifold have almost optimal L^∞ discrepancy.

Part of the results in this chapter are based on [dlTM23].

3.1 Introduction and main results

3.1.1 QMC strength

Let $\mathbb{S}^d = \{x \in \mathbb{R}^{d+1} : |x| = 1\}$ be the unit sphere with the normalized Lebesgue measure σ. Recall from Section 1.1 that V_ℓ denotes the vector space of spherical harmonics of degree $\ell \geq 0$, that is, the space of eigenfunctions of the Laplace-Beltrami operator Δ with eigenvalue

$$\lambda_\ell = \ell(\ell + d - 1)$$

and dimension

$$m_\ell = \frac{2\ell + d - 1}{d-1}\binom{d+\ell-2}{\ell},$$

as follows from (1.6) with $\alpha = \beta = \frac{d-2}{2}$. In this chapter we denote $\lambda := \frac{d-2}{2}$.

Let $L^2(\mathbb{S}^d) = L^2(\mathbb{S}^d, \sigma)$ be the Hilbert space of real-valued square integrable functions in $\mathbb{S}^d$ with the inner product

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

One has that $L^2(\mathbb{S}^d) = \bigoplus_{\ell\geq 0} V_\ell$ and the Fourier series expansion of a function $f \in L^2(\mathbb{S}^d)$ is given by

$$f = \sum_{\ell,k} f_{\ell,k}Y_{\ell,k}, \qquad f_{\ell,k} = \langle f, Y_{\ell,k}\rangle = \int_{\mathbb{S}^d} f\,Y_{\ell,k}\,\mathrm{d}\sigma,$$

where $\{Y_{\ell,k}\}_{k=1}^{m_\ell}$ is an orthonormal basis of V_ℓ.

For $s \geq 0$, we define the $L^2(\mathbb{S}^d)$-based Sobolev spaces of order s as the Hilbert space

$$\mathbb{H}^s(\mathbb{S}^d) = \left\{ f \in L^2(\mathbb{S}^d) : \sum_{\ell=0}^{+\infty}\sum_{k=1}^{m_\ell}(1+\lambda_\ell)^s|f_{\ell,k}|^2 < +\infty \right\},$$

with the norm

$$\|f\|_{\mathbb{H}^s(\mathbb{S}^d)} = \left(\sum_{\ell=0}^{+\infty}\sum_{k=1}^{m_\ell}\frac{1}{a_\ell^{(s)}}|f_{\ell,k}|^2\right)^{1/2},$$

where $a_\ell^{(s)} \approx (1+\ell^2)^{-s}$. Although the norm depends on the choice of $a_\ell^{(s)}$, for a fixed s all possible choices lead to equivalent norms. It is well known that $\mathbb{H}^s(\mathbb{S}^d)$ is continuously embedded in $\mathcal{C}(\mathbb{S}^d)$ if $s > d/2$ and it has, in this range, a reproducing kernel given by

$$K^{(s)}(x,y) = K^{(s)}(x\cdot y) = \sum_{\ell=0}^{\infty}\sum_{k=0}^{m_\ell} a_\ell^{(s)}Y_{\ell,k}(x)Y_{\ell,k}(y),$$

i.e., for all $x \in \mathbb{S}^d$ and $f \in \mathbb{H}^s(\mathbb{S}^d)$,

$$f(x) = \langle f, K^{(s)}(x,\cdot)\rangle_{\mathbb{H}^s(\mathbb{S}^d)}.$$

Let $X_N \subset \mathbb{S}^d$ be an N-point configuration. The *worst-case error of* X_N is defined by

$$\operatorname{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d)) = \sup_{\|f\|_{\mathbb{H}^s(\mathbb{S}^d)}\leq 1}\left\{\left|\frac{1}{N}\sum_{x\in X_N} f(x) - \int_{\mathbb{S}^d} f(x)\,\mathrm{d}\sigma(x)\right| \;:\; f \in \mathbb{H}^s(\mathbb{S}^d)\right\}.$$

Given $s > d/2$, there exists a constant $c_{d,s}$ depending on the $\mathbb{H}^s(\mathbb{S}^d)$-norm such that for any N-point configuration X_N in $\mathbb{S}^d$,

$$c_{d,s}N^{-s/d} \leq \operatorname{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d)),$$

see [BCC+14, Result (D)]. This lower bound is the reason for the next definition.

Definition 3.1.1. Given $s > d/2$, a sequence (X_N) of N-point configurations $X_N \subset \mathbb{S}^d$ is a sequence of QMC designs for $\mathbb{H}^s(\mathbb{S}^d)$ (or s-QMC designs) if there exists $C_{d,s} > 0$ such that for all $N \geq 1$,

$$\text{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d)) \leq C_{d,s} N^{-s/d}. \tag{3.1}$$

In the definition (X_N) may be defined only for a subsequence of natural numbers N converging to $+\infty$.

From [BCC$^+$14, Theorem 3.1] it follows that if (X_N) is a sequence of QMC designs for $\mathbb{H}^s(\mathbb{S}^d)$, then it is also a sequence of QMC designs for all $\mathbb{H}^{s'}(\mathbb{S}^d)$ with $d/2 < s' < s$, see also [BSSW14, Lemma 23]. Thus, there exists some value s^* such that (X_N) is a sequence of s-QMC designs for all s with $d/2 < s < s^*$, and is not a QMC design for $s > s^*$.

Definition 3.1.2. Let (X_N) be a sequence of N-point configurations on $\mathbb{S}^d$. The maximal $s^* > \frac{d}{2}$ for which (3.1) holds for all $\frac{d}{2} < s < s^*$ is called the *QMC strength of the sequence* (X_N).

The strength can be seen as a measure of the regularity of the sequence. The problem of determining the strength for a given sequence seems to be quite difficult and its value has been determined only in a few cases. It was shown by Hesse and Sloan [HS05] and by Brauchart and Hesse [BH07] that sequences of optimal quadrature formulas satisfying some regularity property, which in particular is true for quadrature formulas with positive weights, are s-QMC designs for all $s > d/2$, i.e., they have $s^* = +\infty$. It was observed in [BSSW14] that this previous result, together with the existence of optimal spherical designs [BRV13], implies the existence of spherical designs with strength $s^* = +\infty$. Also in [BSSW14, Theorem 14], the authors show that maximizers of the sum of suitable powers of the Euclidean distance between pairs of points have $s^* = d/2 + 1$. To the best of our knowledge these are the only cases where the strength is known.

Values for the strength were conjectured in [BSSW14] for some well known point configurations in $\mathbb{S}^2$ based on numerical results. In particular, for Fekete points the conjecture is $s^* = 3/2$, for equal area points $s^* = 2$ and for minimal logarithmic energy points $s^* = 3$, see next section for definitions. The expected worst-case error of some random configurations was also studied in [BSSW14]. Next we define an average version of the s-QMC design property for random configurations.

Definition 3.1.3. Let (X_N) be a sequence of random N-point configurations on $\mathbb{S}^d$ following some distribution and let $s > d/2$. We say that (X_N) is a sequence of QMC designs for $\mathbb{H}^s(\mathbb{S}^d)$ (or s-QMC designs) on average if there exists $C_{d,s} > 0$ such that for all $N \geq 1$,

$$\sqrt{\mathbb{E}[\text{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d))^2]} \leq C_{d,s} N^{-s/d}. \tag{3.2}$$

As in the deterministic case, we allow the subindex N to follow a subsequence converging to $+\infty$.

The following property shows that if a sequence of random point configurations is a sequence of s-QMC designs on average for some $s > d/2$, then it is also an s'-QMC design for $d/2 < s' < s$.

Proposition 3.1.4. *Given $s > d/2$, if $\mathbb{E}[\mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d))^2] \leq 1$, then there exists a constant $C_{d,s',s} > 0$ such that*

$$\mathbb{E}[\mathrm{wce}(X_N, \mathbb{H}^{s'}(\mathbb{S}^d))^2] \leq C_{d,s',s} \left(\mathbb{E}[\mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d))^2]\right)^{s'/s}, \quad \frac{d}{2} < s' < s.$$

For a proof in the deterministic case, see [BSSW14]. The proof of our average version follows the same lines. From this Proposition we can define the notion of average QMC strength for sequences of random configurations.

Definition 3.1.5. Let (X_N) be a sequence of random N-point configurations on $\mathbb{S}^d$ following some distribution. The maximal $s^* > \frac{d}{2}$ for which (3.2) holds for all $\frac{d}{2} < s < s^*$ is called the *average QMC strength of the sequence* (X_N).

For this average version, it was shown in [BSSW14, Theorem 7] that uniform i.i.d. points on the sphere are not an s-QMC design on average for any $s > d/2$. By contrast, [BSSW14, Theorem 21,Theorem 22] shows that points from jittered sampling (i.e. uniform i.i.d point taken with respect to an area regular partition) have average strength $d/2 + 1$. Observe that in this last case the average strength matches the conjectured value in [BSSW14] mentioned above for the related equal area points in $\mathbb{S}^2$. Now we present the main results about the average QMC strength.

Harmonic ensemble

In our first result we show that points from the harmonic ensemble have average strength $\frac{d+1}{2}$. Observe that the mode of this distribution corresponds to the Fekete points, for which it was conjectured strength 3/2 in [BSSW14]. We refer to Section 3.2.3 for an explanation of this fact and the definition of the harmonic ensemble. The expected worst case error of this process was previously studied in [Hir18].

Theorem 3.1.6. *Let (X_N) be a sequence where X_N is an N-point set drawn from the harmonic ensemble in $\mathbb{S}^d$. Observe that N must be of the form π_L for some natural L. Then (X_N) is a sequence of s-QMC designs on average for $\frac{d}{2} < s < \frac{d+1}{2}$. Moreover*

$$\lim_{N \to +\infty} N^{\frac{d+1}{d}} \mathbb{E}[\mathrm{wce}(X_N; \mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^2))^2] = +\infty, \tag{3.3}$$

therefore (X_N) is not a QMC design on average if $s > \frac{d+1}{2}$ and the average QMC strength is $\frac{d+1}{2}$.

For the harmonic ensemble we can deduce, from results in [BSSW14, BMOC16], see also [Ber19], almost sure optimality of the worst-case error up to a logarithmic factor.

Corollary 3.1.7. *For every $M > 0$ and $\frac{d}{2} < s < \frac{d+1}{2}$, there exists $C_{d,s,M} > 0$ such that*

$$\mathbb{P}\left(\mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^d)) \leq C_{d,s,M} \frac{(\log N)^{\frac{2s}{d+1}}}{N^{\frac{s}{d}}}\right) \geq 1 - \frac{1}{N^M}, \tag{3.4}$$

where X_N is an N-point set drawn from the harmonic ensemble. Therefore, for fixed $\frac{d}{2} < s < \frac{d+1}{2}$ there exists $C_{d,s} > 0$ such that, with probability 1 and for N large enough,

$$\mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^d)) \leq C_{d,s} \frac{(\log N)^{\frac{2s}{d+1}}}{N^{\frac{s}{d}}}.$$

Spherical ensemble

We recall the definition of the spherical ensemble in Section 3.2.4. Applying results from [AZ15] it was shown in [Hir18] that points from the spherical ensemble are s-QMC designs on average for $1 < s < 2$. One can easily see that 2 is indeed the average strength. The mode of this distribution is the set of elliptic Fekete points, i.e., minimizers of the logarithmic energy. In this case there is no coincidence with the conjectured strength from [BSSW14], which was 3.

Theorem 3.1.8. *Let (X_N) be a sequence where X_N is an N-point set drawn from the spherical ensemble. Then (X_N) is a sequence of s-QMC designs on average for $1 < s < 2$, and for $s \in (2, 3)$ there exists a constant $C > 0$ such that*

$$N^2 \mathbb{E}\left[\mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2\right] \geq C,$$

i.e., the average strength is 2.

Remark 3.1.9. A concentration result similar to Corollary 3.1.7 can be proved also for the spherical ensemble or other configurations given by determinantal point processes, like the jittered sampling [BGKZ20], using the concentration results for determinantal point processes in [PP14]. The bounds are far from sharp. For the spherical ensemble a close to optimal bound has been proved using a concentration of measure inequality particular of the spherical ensemble, [Ber19].

Zeros of elliptic polynomials

In our last result, we prove that the average strength for the zeros of the elliptic polynomials behaves better than all these previous random processes and coincides with the conjectured strength in [BSSW14] for the logarithmic energy minimizers. We refer to Section 3.2.5 for the definition of the zeros of elliptic polyonomials.

Theorem 3.1.10. *Let (X_N) be a sequence where X_N is an N-point set drawn from zeros of elliptic polynomials mapped to the sphere by the stereographic projection. Then (X_N) is a sequence of s-QMC designs on average for $1 < s < 3$, and for $s \in (3, 4)$ there exists a constant $C > 0$ such that*

$$N^3 \mathbb{E}\left[\mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2\right] \geq C,$$

i.e., the average strength is 3.

3.1.2 Discrepancies

Discrepancy is a usual way to quantify the degree of uniformity of a finite set of points $X_N = \{x_1, \dots, x_N\} \subset \mathbb{S}^d$. Here we are going to consider the classical L^2 and L^∞ notions of discrepancy. It is well known that a sequence of point sets (X_N) is asymptotically uniformly distributed if and only if $\lim_{N\to+\infty} \mathbb{D}_p(X_N) = 0$, for $p = \infty$ or $p = 2$, [BHS19, Section 6.1]. Next we recall the definitions of both discrepancies.

L^2 discrepancies on the sphere $\mathbb{S}^d$

The L^2 discrepancy of X_N with respect to spherical caps is defined by

$$\mathbb{D}_2(X_N) = \left(\int_0^\pi \int_{\mathbb{S}^d} \left| \frac{|X_N \cap B(x,r)|}{N} - \sigma(B(x,r)) \right|^2 \mathrm{d}\sigma(x) \sin r \, \mathrm{d}r \right)^{1/2}, \tag{3.5}$$

where $B(x,r) = \{y \in \mathbb{S}^d : \vartheta(x,y) < r\}$ is the ball centered at x of radius r with respect to the geodesic distance.

From [Ale72, Sto73, Bec84b] the optimal order of the L^2 spherical cap discrepancy is $N^{-\frac{d+1}{2d}}$, i.e.,

$$c_d N^{-\frac{d+1}{2d}} \leq \inf_{|X_N|=N} \mathbb{D}_2(X_N) \leq c'_d N^{-\frac{d+1}{2d}} \tag{3.6}$$

for some constants $c_d, c'_d > 0$ depending on d.

As an immediate consequence of the results on the expected worst-case error and the Stolarsky formula (see Section 3.2.2), we deduce that the spherical ensemble and the zeros of elliptic polynomials projected to $\mathbb{S}^2$ produce N-point configurations with average L^2 discrepancy of optimal order.

Proposition 3.1.11. *Let (X_N) be a sequence where X_N is an N-point set drawn from the spherical ensemble. Then*

$$\mathbb{E}\left[\mathbb{D}_2(X_N)\right] = O(N^{-3/4}).$$

The same bound holds if the points in (X_N) are drawn from the zeros of elliptic polynomials mapped to the sphere by the stereographic projection.

Observe that this result gives in a very straightforward way the existence of N-point configurations with discrepancy of optimal growth and therefore the upper bound in (3.6).

Bilyk, Dai and Matzke defined in [BDM18] another version of the L^2 discrepancy by replacing the set of all spherical caps by hemispheres, i.e., spherical caps with geodesic radius $\pi/2$. Let $H(x) = D(x, \pi/2)$ denote the hemisphere centered at x. Since $\sigma(H(x)) = 1/2$, the natural L^2 discrepancy of an N-point configuration X_N with respect to hemispheres is

$$\mathbb{D}_{2,\mathrm{hem}}(X_N) = \left(\int_0^\pi \int_{\mathbb{S}^d} \left| \frac{|X_N \cap H(x)|}{N} - \frac{1}{2} \right|^2 \mathrm{d}\sigma(x) \sin r \, \mathrm{d}r \right)^{1/2}. \tag{3.7}$$

Unlike the classical L^2 discrepancy, the hemisphere discrepancy can be very small, even zero, for large N. Indeed, if N is even, this discrepancy vanishes for any centrally symmetric distribution X_N. If N is odd, the minimum value of the discrepancy is $1/2N$, see [BDM18, Theorem 3.2] for the proof and a characterization of all N-point minimizers. Therefore, the hemisphere discrepancy could be seen as a measure of the symmetry of a distribution.

We study the expected L^2 hemisphere discrepancy for the two point processes with optimal L^2 cap discrepancy on average.

Proposition 3.1.12. *Let (X_N) be a sequence where X_N is an N-point set drawn from the spherical ensemble. Then*

$$\mathbb{E}\left[\mathbb{D}_{2,hem}(X_N)^2\right] = \frac{1}{2\sqrt{\pi}}\frac{1}{N^{3/2}} + o\left(\frac{1}{N^{3/2}}\right).$$

If the points are drawn from the zeros of elliptic polynomials mapped to the sphere by the stereographic projection, then

$$\mathbb{E}\left[\mathbb{D}_{2,hem}(X_N)^2\right] = \frac{1}{8\sqrt{\pi}}\zeta\left(\frac{3}{2}\right)\frac{1}{N^{3/2}} + o\left(\frac{1}{N^{3/2}}\right).$$

Both processes have an expected order of decay of $N^{-3/2}$ for $\mathbb{D}^2_{2,\text{hem}}(X_N)$, while the optimal order is N^{-2}. The zeros of elliptic polynomials, however, exhibit a smaller leading coefficient than the spherical ensemble:

$$\frac{1}{8\sqrt{\pi}}\zeta\left(\frac{3}{2}\right) = 0.1842\ldots < 0.2821\ldots = \frac{1}{2\sqrt{\pi}}.$$

Just to see the improvement on the expected hemisphere discrepancy with respect to a trivial random point process, we will show in Section 3.4.1 that if the N points are taken independently and uniformly from $\mathbb{S}^2$, then

$$\mathbb{E}\left[\mathbb{D}_{2,\text{hem}}(X_N)^2\right] = \frac{1}{4N}. \tag{3.8}$$

L^∞ discrepancy on two-point homogeneous manifolds

Now we consider N-point configurations in a two-point homogeneous manifold $\mathcal{M}$. The L^∞ discrepancy of $X_N \subset \mathcal{M}$ is given by

$$\mathbb{D}_\infty(X_N) = \sup_{x\in\mathcal{M}, r>0}\left|\frac{|X_N \cap B(x,r)|}{N} - \sigma(B(x,r))\right|,$$

where σ stands for the normalized surface measure on $\mathcal{M}$. For $\mathcal{M} = \mathbb{S}^d$, $\mathbb{D}_\infty(X_N)$ is called spherical cap discrepancy. In fact, we will refer to geodesic balls $B(x,r)$ as *caps* even when the manifold is not the sphere, so this quantity will also be called *cap discrepancy.*

In [Bec84b, Bec84a], Beck obtained the order of the spherical cap discrepancy up to a logarithmic factor:

$$cN^{-\frac{d+1}{2d}} \leq \inf_{|X_N|=N} \mathbb{D}_\infty(X_N) \leq CN^{-\frac{d+1}{2d}}\sqrt{\log N} \tag{3.9}$$

for constants $c, C > 0$. Bounds of the same order hold for the other two-point homogeneous manifolds, with d standing for the real dimension of the manifold. The upper bound was established in [BCC+19, Corollary 8.6] (see also [Skr20a]), whereas the lower bound comes from [Skr19].

Alishahi and Zamani showed in [AZ15, Theorem 1.1] that the spherical ensemble has discrepancy of order $O(N^{-3/4}\sqrt{\log N})$ with overwhelming probability. The proof, which goes through an estimate of the variance of the number of points in a cap along with an application of Bernstein's inequality, relies on the fact that the spherical ensemble is a determinantal point process. Later on, the same approach was used in [BMOC16] to deduce the order $O(N^{-\frac{d+1}{2d}} \log N)$ for the discrepancy of N points from the harmonic ensemble on $\mathbb{S}^d$.

Next we extend this discrepancy result from [BMOC16] to any two-point homogeneous manifold, which is a corollary of the following bound for the variance of the number of points that fall in a cap.

Proposition 3.1.13. *Let $A = A_L$ be a ball of radius $\theta_L \in [0, \pi/2)$ with*

$$\lim_{L\to\infty} \theta_L \in [0, \pi/2), \quad \lim_{L\to\infty} L\theta_L = \infty.$$

Let n_A be the number of points in A among $N = \pi_L^{(\alpha,\beta)}$ points drawn from the harmonic ensemble on the projective space $\mathbb{FP}^n$, with dimension $d = n \cdot dim_{\mathbb{R}}(\mathbb{F})$ and associated parameters $\alpha = d/2 - 1$ and $\beta = dim_{\mathbb{R}}(\mathbb{F})/2 - 1$, see definitions in Section 3.2.3. Then

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

Following [AZ15, Theorem 1.1], we deduce the following upper bound for the cap discrepancy of the harmonic ensemble on $\mathcal{M}$.

Corollary 3.1.14. *Let $\mathcal{M}$ be a two-point homogeneous manifold. For every $M > 0$, the L^∞ discrepancy of a set of $N = \pi_L^{(\alpha,\beta)} \approx L^d$ points drawn from the harmonic ensemble on $\mathcal{M}$ satisfies*

$$\mathbb{D}_\infty(X_N) = O(L^{-\frac{d+1}{2}} \log L) = O\left(N^{-\frac{d+1}{2d}} \log N\right)$$

with probability $1 - \frac{1}{N^M}$.

3.2 Background

3.2.1 Riesz energy and worst-case error

In Section 1.2 we defined the Riesz (logarithmic) energy of a set $X_N = \{x_1, \ldots, x_N\}$ of N points on the unit sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$ as

$$E_s(X_N) = \sum_{i\neq j} f_s(|x_i - x_j|),$$

where $f_s(r) = r^{-s}$, $s \neq 0$, ($f_0(r) = -\log r$) is the Riesz (logarithmic) potential. From now on, to simplify the notation, we write E_s for $E_s(X_N)$ when the set of points is clear from the context. Recall that this quantity has a continuous version for measures which for the normalized surface measure σ and $0 \neq s < d$ is

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

In [BSSW14], the authors obtained a formula for the worst-case error of an N-point set in terms of Riesz energies, provided s is not a positive integer. When $d/2 < s < d/2+1$, the expression reads

$$\mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d))^2 = -\frac{1}{N^2}\left(E_{d-2s} - V_{d-2s}(\mathbb{S}^d)N^2\right), \tag{3.10}$$

whereas for $d/2+M < s < d/2+M+1$, with M a positive integer,

$$\mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^d))^2 = \frac{1}{N^2}\left[\sum_{j,i=1}^{N} \mathcal{Q}_M(x_j \cdot x_i) + (-1)^{M+1}(E_{d-2s} - V_{d-2s}(\mathbb{S}^d)N^2)\right], \tag{3.11}$$

where

$$\mathcal{Q}_M(x_j \cdot x_i) := \sum_{\ell=1}^{M}\left((-1)^{M+1-\ell} - 1\right)\alpha_\ell^{(s)} m_\ell P_\ell^{(d)}(x_j \cdot x_i),$$

with $P_\ell^{(d)}(x)$ the Gegenbauer polynomial normalized by $P_\ell^{(d)}(1) = 1$ and

$$\alpha_\ell^{(s)} = V_{d-2s}(\mathbb{S}^d)\frac{(-1)^{M+1}(1-s)_\ell}{(1+s)_\ell}. \tag{3.12}$$

3.2.2 Stolarsky invariance principles

A classical result by Stolarsky [Sto73] connects the L^2 discrepancy of an N-point configuration $X_N = \{x_1, \ldots, x_N\} \subset \mathbb{S}^d$ with its discrete energy:

$$\mathbb{D}_2(X_N)^2 = \gamma_d\left(V_{-1}(\mathbb{S}^d) - \frac{1}{N^2}\sum_{i,j=1}^{N}|x_i - x_j|\right), \tag{3.13}$$

where

$$\gamma_d = \frac{\Gamma(\frac{d+1}{2})}{d\sqrt{\pi}\,\Gamma(\frac{d}{2})}.$$

Thus, from (3.10) for $s = (d+1)/2$ one can see that there is a direct relation between energy, discrepancy and worst-case error,

$$\begin{aligned}\mathrm{wce}(X_N; \mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d)) &= \left(V_{-1}(\mathbb{S}^d) - \frac{1}{N^2}E_{-1}(X_N)\right)^{1/2} \\ &= \frac{1}{\sqrt{\gamma_d}}\mathbb{D}_2(X_N).\end{aligned} \tag{3.14}$$

We observe that in [BDM18] the following version of Stolarsky invariance principle was shown for the hemisphere discrepancy:

$$D_{2,\mathrm{hem}}(X_N)^2 = \frac{1}{2\pi}\left(\int_{\mathbb{S}^d}\int_{\mathbb{S}^d}\vartheta(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) - \frac{1}{N^2}\sum_{i,j=1}^{N}\vartheta(x_i,x_j)\right). \tag{3.15}$$

Thus, when considering this notion of discrepancy, the role of the Euclidean distance in the classical discrepancy is replaced by the geodesic distance.

3.2.3 The harmonic ensemble

Let $\mathcal{M}$ be a two-point homogenenous manifold with parameters (α, β) (see Table 1.1). Recall from Section 1.3.3 that the harmonic ensemble is the determinantal point process in $\mathcal{M}$ induced by the projection operator to the space $\Pi_L = \bigoplus_{\ell=0}^N V_\ell$, where V_ℓ are the eigenspaces of the Laplace-Beltrami operator on $\mathcal{M}$. This determinantal point process has $\pi_L^{(\alpha,\beta)} = \frac{(\alpha+\beta+2)_L(\alpha+2)_L}{(\beta+1)_L L!} \approx L^d$ points a.s. and kernel

$$K_L^{(\alpha,\beta)} = \frac{(\alpha+\beta+2)_L}{(\beta+1)_L} P_L^{(\alpha+1,\beta)}(\cos(2\kappa\vartheta(x,y))), \tag{3.16}$$

see Section 1.1 for the notation.

In the particular case $\mathcal{M} = \mathbb{S}^d$, the harmonic ensemble [BMOC16] is the determinantal point process induced by the subspace $\Pi_L = \bigoplus_{\ell=0}^N V_\ell$ of polynomials in $\mathbb{R}^{d+1}$ of degree at most L restricted to $\mathbb{S}^d$ with

$$\pi_L := \dim(\Pi_L) = \pi_L^{(\lambda,\lambda)} = \frac{2L+d}{d}\binom{d+L-1}{L} \approx L^d \tag{3.17}$$

points a.s. and kernel

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

where $\langle\cdot,\cdot\rangle$ denotes the usual inner product in $\mathbb{R}^{d+1}$.

Observe that the mode of the distribution, in some sense the value that appears most often in a set of data values sampled from this DPP, is the maximum of the joint density

$$p(x_1,\ldots,x_{\pi_L}) = \frac{1}{\pi_L!}\det(K_L(x_i,x_j))_{1\le i,j\le\pi_L},$$

for $x_1,\ldots,x_{\pi_L} \in \mathbb{S}^d$. In order to identify these mode points, observe that if $\phi_1,\ldots,\phi_{\pi_L}$ is a basis of the space Π_L, then from

$$K_L(x,y) = \sum_{i=1}^{\pi_L} \phi_i(x)\phi_i(y)$$

we have

$$\det(K_L(x_i,x_j))_{1\le i,j\le\pi_L} = |\det\left(\phi_j(x_i)\right)_{1\le i,j\le\pi_L}|^2.$$

Thus, the mode points maximize the absolute value of the determinant

$$V_L(x_1,\ldots,x_{\pi_L}) = \left|\det(\phi_i(x_j))_{1\le i,j\le\pi_L}\right|.$$

Points maximizing this quantity are known as *Fekete points* or called extremal fundamental systems, [Rei03]. Sloan and Womersley conjectured that they have all positive cubature weights [WS01] and were shown to be asymptotically uniformly equidistributed in [MOC10, BBWN11].

3.2.4 The spherical ensemble

We have introduced the spherical ensemble in Section 1.3.2, together with the expected Riesz energies from [AZ15]. One can see that if we take N points sampled from the spherical ensemble and map them to the sphere $\mathbb{S}^2$ through the stereographic projection, their joint density is

$$C\prod_{i<j}|x_i - x_j|^2$$

with respect to the surface measure in $\mathbb{S}^2$. Therefore, by taking the logarithm of this quantity, we see that the mode of the spherical ensemble is given by the maximizers of $\sum_{i\neq j}\log|x_i - x_j|$ or, equivalently, the minimizers of the logarithmic energy

$$E_0(x_1,\ldots,x_N) = \sum_{i\neq j}\log\frac{1}{|x_i - x_j|},$$

i.e., they are the *elliptic Fekete points*, [BHS19].

3.2.5 Zeros of elliptic polynomials

The last point process we are going to consider is the zeros of the elliptic polynomials projected to $\mathbb{S}^2$ through the stereographic projection, which was studied in Chapter 2. In order to compute its expected worst-case error, we will need the expected Riesz energies from Theorem 2.1.1. In particular, for $s < 0$ the asymptotic expansion

$$\mathbb{E}[E_s] = \frac{2^{1-s}}{2-s}N^2 + C(s)N^{1+s/2} + o_{N\to\infty}(N^{1+s/2}), \tag{3.18}$$

$$C(s) = \frac{1}{2^s}\frac{s}{2}\left(1+\frac{s}{2}\right)\Gamma\left(1-\frac{s}{2}\right)\zeta\left(1-\frac{s}{2}\right),$$

which follows from (2.6), will be enough for our propose. Only for $s = -2$ we will require more precision,

$$\mathbb{E}[E_{-2}] = 2N^2 - 8\frac{\zeta(3)}{N} + o_{N\to\infty}\left(\frac{1}{N}\right), \tag{3.19}$$

since in this case $C(-2) = 0$.

3.3 Proofs of average QMC strength results (Section 3.1.1)

3.3.1 Harmonic ensemble

To prove Theorem 3.1.6, we need some preliminaries.

Let $\frac{d}{2} < s < \frac{d}{2} + 1$. From formula (3.10), for $N = \pi_L \approx L^d$ points drawn from the harmonic ensemble on the sphere we get

$$\begin{aligned}\mathbb{E}[\mathrm{wce}(X_N;\mathbb{H}^s(\mathbb{S}^d))^2] &= \frac{1}{N^2}\int_{\mathbb{S}^d}\int_{\mathbb{S}^d} K_L(x,y)^2|x-y|^{2s-d}\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\\ &= \frac{\pi_L^2}{P_L^{(1+\lambda,\lambda)}(1)^2N^2}\int_{\mathbb{S}^d}\int_{\mathbb{S}^d} P_L^{(1+\lambda,\lambda)}(\langle x,y\rangle)^2|x-y|^{2s-d}\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\\ &= \frac{C_d}{P_L^{(1+\lambda,\lambda)}(1)^2}\int_{\mathbb{S}^d} P_L^{(1+\lambda,\lambda)}(\langle x,\mathbf{n}\rangle)^2|x-\mathbf{n}|^{2s-d}\,\mathrm{d}\sigma(x)\\ &= \frac{C_d}{P_L^{(1+\lambda,\lambda)}(1)^2}\int_{-1}^{1} P_L^{(1+\lambda,\lambda)}(t)^2(1-t)^{s-1}(1+t)^{\frac{d}{2}-1}\,\mathrm{d}t,\end{aligned}$$

where $\mathbf{n}$ stands for the north pole of $\mathbb{S}^d$.

From the asymptotic property of the gamma function

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

we get that

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

Therefore we have that for some constant $C_{d,s} > 0$,

$$\mathbb{E}[\mathrm{wce}(X_N;\mathbb{H}^s(\mathbb{S}^d))^2] = \frac{C_{d,s}}{L^d}\int_{-1}^{1} P_L^{(1+\lambda,\lambda)}(t)^2(1-t)^{s-1}(1+t)^{\frac{d}{2}-1}dt. \tag{3.20}$$

The following lemma is an extension to $-1 < a < d$ of a result proved in [BMOC16] for $0 < a < d$.

Proposition 3.3.1. *Given $-1 < a < d$,*

$$\lim_{L\to\infty}\frac{1}{L^a}\int_{-1}^{1} P_L^{(1+\lambda,\lambda)}(t)^2(1-t)^{\lambda-\frac{a}{2}}(1+t)^\lambda\,dt = 2^{\frac{a}{2}+d}\int_0^\infty \frac{J_{1+\lambda}(t)^2}{t^{1+a}}dt$$

and the last integral converges.

Proof. The proof is essentially the same as in [BMOC16, Proposition 6] but with a few changes in the last estimates. We split the integral

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

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

$$\begin{aligned} &C(c, L) \\ &= 2^{a/2} \int_0^c L^{-2-2\lambda} P_L^{(1+\lambda,\lambda)} \left(\cos \frac{x}{L}\right)^2 \left(\frac{\sin \frac{x}{L}}{\frac{x}{L}}\right)^{2\lambda+1} \left(\frac{1-\cos\frac{x}{L}}{\frac{1}{2}\left(\frac{x}{L}\right)^2}\right)^{-a/2} x^{2\lambda+1-a}\, dx. \end{aligned}$$

Using the Mehler-Heine asymptotic formula [Sze39, p. 192] 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:

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

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

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

and using Mehler-Heine again this expression converges to zero when $L \to \infty$. For the middle term we use classical asymptotic estimates of the Jacobi polynomials [Sze39, Theorem 8.21.13]

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

if $c/L \le \theta \le \pi - (c/L)$

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

We get

$$\begin{aligned} 0 \le & B(c, L) \lesssim \frac{1}{L^{a+1}} \int_{\frac{c}{L}}^{\pi-\frac{c}{L}} \frac{1}{(\sin\frac{\theta}{2})^{a+2}}\, \mathrm{d}\theta \lesssim \frac{1}{L^{a+1}} \int_{\frac{c}{L}}^{\pi-\frac{c}{L}} \frac{1}{\theta^{a+2}}\, \mathrm{d}\theta \\ &\le \frac{1}{L^{a+1}} \int_{\frac{c}{L}}^{\pi} \frac{1}{\theta^{a+2}}\, \mathrm{d}\theta = \frac{1}{L^{a+1}(a+1)} \left[\frac{L^{a+1}}{c^{a+1}} - \frac{1}{\pi^{a+1}}\right] = \frac{1}{c^{a+1}(a+1)} + o(L). \end{aligned}$$

Finally, observe that close to zero $J_{1+\lambda}(x) \sim x^{1+\lambda}$ and $J_{1+\lambda}(x) \lesssim x^{-1/2}$ for big x, so the integral above converges precisely for $-1 < a < d$.

□

Proof of Theorem 3.1.6. Now for any $\frac{d}{2} < s < \frac{d+1}{2}$ we apply the proposition above to $-1 < t = d - 2s < 0$ and we get from (3.20) that there exists a (different) constant $C_{d,s} > 0$ such that

$$\lim_{L\to+\infty} L^{2s}\mathbb{E}[\mathrm{wce}(X_N;\mathbb{H}^s(\mathbb{S}^d))^2] = C_{d,s}.$$

This shows that points drawn from the harmonic ensemble form an s-QMC design on average for $\frac{d}{2} < s < \frac{d+1}{2}$.

To get (3.3) we use again (3.20) for $s = \frac{d+1}{2}$ and the representation of the integral in terms of generalized hypergeometric function [EMOT54, p. 288]

$$\mathbb{E}[\mathrm{wce}(X_N;\mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d))^2] \approx L^{-d}\frac{\Gamma\left(\frac{1}{2}+L\right)\Gamma\left(\frac{d}{2}+L\right)\Gamma\left(\frac{d}{2}+L+1\right)}{\Gamma(L+1)^2\Gamma\left(d+\frac{1}{2}+L\right)}$$
$$\times\, {}_4F_3\left(-L, d+L, \frac{d+1}{2}, \frac{1}{2}; \frac{d}{2}+1, d+\frac{1}{2}+L, -L+\frac{1}{2}; 1\right),$$

where the constant depends only on d.

It is easy to see (by induction) that the quotient

$$\frac{(-L)_n(d+L)_n}{(d+\frac{1}{2}+L)_n(-L+\frac{1}{2})_n}$$

is increasing as a function of $0 \le n \le L$ and therefore

$$N^{\frac{d+1}{d}}\mathbb{E}[\mathrm{wce}(X_N;\mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d))^2] \gtrsim \sum_{n=0}^{L}\frac{\left(\frac{d+1}{2}\right)_n\left(\frac{1}{2}\right)_n}{\left(\frac{d}{2}+1\right)_n}\frac{1}{n!}.$$

Finally, this last series diverges when $L \to \infty$ by Gauss test taking $a = (d+1)/2$, $b = 1/2$ and $c = a + b$, because

$$\frac{\frac{(a)_n(b)_n}{(c)_n n!}}{\frac{(a)_{n+1}(b)_{n+1}}{(c)_{n+1}(n+1)!}} = \frac{(c+n)(n+1)}{(a+n)(b+n)} = 1 + \frac{1}{n} + \frac{C_n}{n^2},$$

with C_n a bounded sequence. □

Proof of Corollary 3.1.7. In [BMOC16] it was proved that for every $M > 0$ there exist $C_M > 0$ such that

$$\mathbb{P}\left(\mathbb{D}_\infty(X_N) \le C_M\frac{\log N}{N^{\frac{d+1}{2d}}}\right) \ge 1 - \frac{1}{N^M},$$

where X_N is an N-point set drawn from the harmonic ensemble.

Now it follows from the result above, formula (3.14) and $\mathbb{D}_2(X_N) \lesssim \mathbb{D}_\infty(X_N)$ that there exists (another) $C_M > 0$ such that

$$\mathbb{P}\left(\mathrm{wce}(X_N;\mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d)) \le C_M\frac{\log N}{N^{\frac{d+1}{2d}}}\right) \ge 1 - \frac{1}{N^M}.$$

To get (3.4) it is enough to apply the interpolation result from [BSSW14, Lemma 23], from which we get for $d/2 < s < (d+1)/2$ a constant $C_{d,s} > 0$ such that $\mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^d))^{\frac{d+1}{2s}} \leq C_{d,s}\mathrm{wce}(X_N; \mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d))$ if $\mathrm{wce}(X_N; \mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d)) \leq 1$, see [Ber19, Section 1.5].

Finally, if we take (for example) $M = 2$ in (3.4) we get

$$\sum_N \mathbb{P}\left(\mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^d)) > C_{d,s}\frac{(\log N)^{\frac{2s}{d+1}}}{N^{\frac{s}{d}}}\right) < \infty,$$

and from Borel-Cantelli lemma

$$\mathbb{P}\left(\limsup_{N\to+\infty}\left\{\mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^d)) > C_{d,s}\frac{(\log N)^{\frac{2s}{d+1}}}{N^{\frac{s}{d}}}\right\}\right) = 0.$$

□

3.3.2 Spherical ensemble

Proof of Theorem 3.1.8. The first part is due to [Hir18]. We include it for the sake of completeness. Let $s \in (1, 2)$. Then the worst-case error is given by (3.10). Taking expectations and using (1.23) with $s' = 2 - 2s$,

$$\begin{aligned} N^s\mathbb{E}\left[\mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^2))^2\right] &= -\frac{N^s}{N^2}\left(\mathbb{E}\left[E_{2-2s}\right] - V_{2-2s}(\mathbb{S}^2)N^2\right) \\ &= \frac{2^{2s}\Gamma(s)}{4}\frac{\Gamma(N)}{\Gamma(N+s)}N^s \\ &\xrightarrow[N\to\infty]{} \frac{2^{2s}\Gamma(s)}{4}, \end{aligned}$$

since $\frac{\Gamma(N)}{\Gamma(N+s)} \sim N^{-s}$ as $N \to \infty$ by the asymptotic property of the gamma function. Then $N^s\mathbb{E}\left[\mathrm{wce}(X_N, \mathbb{H}^s(\mathbb{S}^2))^2\right]$ is bounded and (X_N) is a sequence of s-QMC designs on average for $s \in (1, 2)$.

Now we show that $s^* = 2$. Let $s \in (2, 3)$. The expression for the worst-case error is (3.11) with $M = 1$:

$$\mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2 = \frac{1}{N^2}\left[\sum_{j,i=1}^{N}\mathcal{Q}_1(x_j\cdot x_i) + E_{2-2s} - V_{2-2s}(\mathbb{S}^2)N^2\right],$$

with

$$\mathcal{Q}_1(x_j\cdot x_i) = -6\alpha_1^{(s)}x_j\cdot x_i,$$

where we have used that $P_1^{(2)}(x) = x$. Then

$$\begin{aligned} \mathrm{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2 &= \frac{1}{N^2}\left[-6\alpha_1^{(s)}\sum_{j,i=1}^{N}x_j\cdot x_i + E_{2-2s} - V_{2-2s}(\mathbb{S}^2)N^2\right] \\ &= \frac{1}{N^2}\left[-6\alpha_1^{(s)}\sum_{j,i=1}^{N}\left(1 - \frac{|x_j - x_i|^2}{2}\right) + E_{2-2s} - V_{2-2s}(\mathbb{S}^2)N^2\right] \qquad (3.21) \\ &= \frac{1}{N^2}\left[3\alpha_1^{(s)}\left(E_{-2} - 2N^2\right) + E_{2-2s} - V_{2-2s}(\mathbb{S}^2)N^2\right] \end{aligned}$$

Taking expectations and using (1.23) with $s = -2$ and $s' = 2 - 2s$,

$$\begin{aligned} N^2 \mathbb{E}\left[\operatorname{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2\right] &= \left[3\alpha_1^{(s)}\left(\mathbb{E}\left[E_{-2}\right] - 2N^2\right) + \mathbb{E}\left[E_{2-2s}\right] - V_{2-2s}(\mathbb{S}^2)N^2\right] \\ &= -12\alpha_1^{(s)} \frac{N}{N+1} - \frac{2^{2s}\Gamma(s)}{4} \frac{\Gamma(N)}{\Gamma(N+s)} N^2 \\ &\xrightarrow[N\to\infty]{} -12\alpha_1^{(s)} > 0, \end{aligned}$$

since $\frac{\Gamma(N)}{\Gamma(N+s)} N^2 \sim N^{2-s}$. Hence, $N^2\mathbb{E}\left[\operatorname{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2\right]$ is bounded below by a positive constant. □

3.3.3 Zeros of elliptic polynomials

Proof of Theorem 3.1.10. Let $s \in (2, 3)$. We have already seen in (3.21) that the expression for the worst-case error is

$$\operatorname{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2 = \frac{1}{N^2}\left[3\alpha_1^{(s)}\left(E_{-2} - 2N^2\right) + E_{2-2s} - V_{2-2s}(\mathbb{S}^2)N^2\right].$$

Taking expectations and using (3.19) for $\mathbb{E}[E_{-2}]$ and (3.18) with $s' = 2 - 2s$,

$$\begin{aligned} N^s \mathbb{E}\left[\operatorname{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2\right] &= \frac{N^s}{N^2}\left[3\alpha_1^{(s)}\left(\mathbb{E}\left[E_{-2}\right] - 2N^2\right) + \mathbb{E}\left[E_{2-2s}\right] - V_{2-2s}(\mathbb{S}^2)N^2\right] \\ &= N^{s-2}\Bigg[3\alpha_1^{(s)}\left(-8\zeta(3)\frac{1}{N} + o\left(\frac{1}{N}\right)\right) \\ &\quad + C(2-2s)N^{2-s} + o(N^{2-s})\Bigg] \\ &= 3\alpha_1^{(s)}\left(-8\zeta(3)N^{s-3} + o\left(N^{s-3}\right)\right) + C(2-2s) + o(1) \\ &\xrightarrow[N\to\infty]{} C(2-2s). \end{aligned}$$

Then $N^s\mathbb{E}\left[\operatorname{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2\right]$ is bounded for $s \in (2, 3)$. For $1 < s \leq 2$, the result holds automatically from Proposition 3.1.4.

Now we see that the strength is $s^* = 3$. Let $s \in (3, 4)$. By (3.11) with $M = 2$, the square of the worst-case error is

$$\operatorname{wce}(X_N; \mathbb{H}^s(\mathbb{S}^2))^2 = \frac{1}{N^2}\left[\sum_{j,i=1}^{N} \mathcal{Q}_2(x_j \cdot x_i) - (E_{2-2s} - V_{2-2s}(\mathbb{S}^2)N^2)\right],$$

where, using that $P_2^{(2)}(x) = \frac{1}{2}(3x^2 - 1)$,

$$\begin{aligned} \mathcal{Q}_2(x_j \cdot x_i) &= -5\alpha_2^{(s)}[3(x_j \cdot x_i)^2 - 1] \\ &= -5\alpha_2^{(s)}\left[2 - 3|x_j - x_i|^2 + \frac{3}{4}|x_j - x_i|^4\right]. \end{aligned}$$

Then

$$\begin{aligned}\mathrm{wce}(X_N;\mathbb{H}^s(\mathbb{S}^2))^2 =&\frac{1}{N^2}\Big[-5\alpha_2^{(s)}\Big(2N^2-3E_{-2}+\frac{3}{4}E_{-4}\Big)\\&-(E_{2-2s}-V_{2-2s}(\mathbb{S}^2)N^2)\Big].\end{aligned}$$

Taking expectations and using (3.19) for $\mathbb{E}[E_{-2}]$ and (3.18) with $s'=2-2s$,

$$\begin{aligned}\mathbb{E}\left[\mathrm{wce}(X_N;\mathbb{H}^s(\mathbb{S}^2))^2\right] =&\frac{1}{N^2}\Big[-5\alpha_2^{(s)}\Big(2N^2-3\mathbb{E}[E_{-2}]+\frac{3}{4}\mathbb{E}[E_{-4}]\Big)\\&-(\mathbb{E}[E_{2-2s}]-V_{2-2s}(\mathbb{S}^2)N^2)\Big]\\=&\frac{1}{N^2}\Bigg\{-5\alpha_2^{(s)}\left[2N^2-3\left(2N^2-8\zeta(3)\frac{1}{N}+o\left(\frac{1}{N}\right)\right)\right.\\&\left.+\frac{3}{4}\left(\frac{32}{6}N^2+64\zeta(3)\frac{1}{N}+o\left(\frac{1}{N}\right)\right)\right]\\&-\left(C(2-2s)N^{2-s}+o\left(N^{2-s}\right)\right)\Bigg\}\\=&\frac{1}{N^2}\left\{-5\alpha_2^{(s)}\left[72\zeta(3)\frac{1}{N}+o\left(\frac{1}{N}\right)\right]-C(2-2s)N^{2-s}\right\}.\end{aligned}$$

Therefore,

$$\begin{aligned}N^3\mathbb{E}\left[\mathrm{wce}(X_N;\mathbb{H}^s(\mathbb{S}^2))^2\right] &= -5\alpha_2^{(s)}\left[72\zeta(3)+o\left(1\right)\right]-C(2-2s)N^{3-s}\\&\xrightarrow[N\to\infty]{} -360\zeta(3)\alpha_2^{(s)}>0.\end{aligned}$$

Then there exists a constant $B>0$ such that

$$N^3\mathbb{E}\left[\mathrm{wce}(X_N;\mathbb{H}^s(\mathbb{S}^2))^2\right]\geq B.$$

□

3.4 Proofs of discrepancy results (Section 3.1.2)

3.4.1 L^2 discrepancies on the sphere $\mathbb{S}^d$

Any sequence (X_N) of random N-point configurations on $\mathbb{S}^d$ being a sequence of $(d+1)/2$-QMC designs on average automatically yields N-point sets with optimal spherical L^2 cap discrepancy.

Proof of Proposition 3.1.11. From (3.14),

$$\mathbb{D}_2(X_N)^2=\gamma_d\,\mathrm{wce}(X_N;\mathbb{H}^{\frac{3}{2}}(\mathbb{S}^2))^2$$

and applying expectations

$$\mathbb{E}\big[\mathbb{D}_2(X_N)^2\big] = \gamma_d\,\mathbb{E}\big[\mathrm{wce}(X_N;\mathbb{H}^{\frac{3}{2}}(\mathbb{S}^2))^2\big].$$

Since both processes are 3/2-QMC designs on average, $\mathbb{E}\big[\mathrm{wce}(X_N;\mathbb{H}^{\frac{3}{2}}(\mathbb{S}^2))^2\big] = O(N^{-3/2})$ and by the previous equation $\mathbb{E}\big[\mathbb{D}_2(X_N)^2\big] = O(N^{-3/2})$. From Jensen's inequality we get the result. □

All the results concerning the hemisphere discrepancy are obtained from the Stolarsky formula (3.15).

In the case of independent uniform points on $\mathbb{S}^2$, we easily get (3.8):

$$\begin{aligned}\mathbb{E}\big[\mathbb{D}_{2,\mathrm{hem}}(X_N)^2\big] &= \frac{1}{2\pi}\bigg(\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}\vartheta(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) - \frac{1}{N^2}\mathbb{E}\Big[\sum_{i,j=1}^N \vartheta(x_i,x_j)\Big]\bigg)\\ &= \frac{1}{2\pi}\bigg(\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}\vartheta(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) - \frac{N(N-1)}{N^2}\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}\vartheta(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\bigg)\\ &= \frac{1}{2\pi}\int_{\mathbb{S}^2}\vartheta(x,s)\,\mathrm{d}\sigma(x)\frac{1}{N} = \frac{1}{4N},\end{aligned}$$

where $s = (0,0,-1)\in\mathbb{S}^2$ is the south pole. The choice of this point is obviously arbitrary.

Proof of Proposition 3.1.12. First we prove the result for the spherical ensemble. Let $\rho_2^{\mathrm{S}}(x,y)$ and $K_N^{\mathrm{S}}(x,y)$ denote the second joint intensity and the kernel of the spherical ensemble with respect to σ, respectively. By the definition of a determinantal point process and (1.22),

$$\begin{aligned}\rho_2^{\mathrm{S}}(x,y) &= K_N^{\mathrm{S}}(x,x)K_N^{\mathrm{S}}(y,y) - |K_N^{\mathrm{S}}(x,y)|^2\\ &= N^2 - N^2\left(1-\frac{|x-y|^2}{4}\right)^{N-1}\\ &= N^2\left(1-\left(1-\frac{|x-y|^2}{4}\right)^{N-1}\right).\end{aligned}$$

By (1.18) and the rotation invariance of the geodesic distance and $\rho_2^{\mathrm{S}}(x,y)$,

$$\begin{aligned}&\mathbb{E}\big[\mathbb{D}_{2,\mathrm{hem}}(X_N)^2\big]\\ &= \frac{1}{2\pi}\bigg(\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}\vartheta(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) - \frac{1}{N^2}\mathbb{E}\Big[\sum_{i,j=1}^N \vartheta(x_i,x_j)\Big]\bigg)\\ &= \frac{1}{2\pi}\bigg(\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}\vartheta(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) - \frac{1}{N^2}\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}\vartheta(x,y)\rho_2^{\mathrm{S}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\bigg)\\ &= \frac{1}{2\pi}\bigg(\int_{\mathbb{S}^2}\vartheta(x,s)\,\mathrm{d}\sigma(x) - \int_{\mathbb{S}^2}\vartheta(x,s)\bigg(1-\Big(1-\frac{|x-s|^2}{4}\Big)^{N-1}\bigg)\,\mathrm{d}\sigma(x)\bigg)\\ &= \frac{1}{2\pi}\int_{\mathbb{S}^2}\vartheta(x,s)\Big(1-\frac{|x-s|^2}{4}\Big)^{N-1}\,\mathrm{d}\sigma(x),\end{aligned}$$

where $s = (0,0,-1) \in \mathbb{S}^2$ is the south pole.

Since $\vartheta(x,s) = \arccos\langle x,s\rangle$ and $|x-s|^2 = 2 - 2\langle x,s\rangle$, the integrand in the previous equation only depends on the inner product with s. We apply the particular case of Funck-Hecke formula in [BMOC16, Lemma 1] to get

$$\begin{aligned}
\mathbb{E}\left[\mathbb{D}_{2,\mathrm{hem}}(X_N)^2\right] &= \frac{1}{2^N\pi}\int_{\mathbb{S}^2} \arccos\langle x,s\rangle \left(1+\langle x,s\rangle\right)^{N-1} \mathrm{d}\sigma(x) \\
&= \frac{1}{2^{N+1}\pi}\int_{-1}^{1} \arccos t \left(1+t\right)^{N-1} \mathrm{d}t \\
&= \frac{1}{2^{N+1}\pi}\int_0^{\pi} \theta \left(1+\cos\theta\right)^{N-1} \sin\theta \,\mathrm{d}\theta
\end{aligned}$$

where we have applied the change of variables $t = \cos\theta$. Using the trigonometric identities $1+\cos\theta = 2\cos^2(\theta/2)$ and $\sin\theta = 2\sin(\theta/2)\cos(\theta/2)$ and putting $x = \theta/2$, we obtain the result:

$$\begin{aligned}
\mathbb{E}\left[\mathbb{D}_{2,\mathrm{hem}}(X_N)^2\right] &= \frac{2^N}{2^{N+1}\pi}\int_0^{\pi} \theta \cos^{2N-1}\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) \mathrm{d}\theta \\
&= \frac{2}{\pi}\int_0^{\pi} x \cos^{2N-1} x \sin x \,\mathrm{d}x \\
&= \frac{2}{\pi}\frac{\mathrm{B}(1/2, N+1/2)}{4N} \\
&= \frac{1}{2\sqrt{\pi}}\frac{\Gamma(N+1/2)}{N^2\Gamma(N)} \\
&= \frac{1}{2\sqrt{\pi}}\frac{1}{N^{3/2}} + o\left(\frac{1}{N^{3/2}}\right),
\end{aligned}$$

where we have used [PBM03, 2.5.13(14)] for the integral.

Now we get the result for the zeros of elliptic polynomials. In (2.18) we have provided a formula to compute the expected value of $\sum_{i\neq j} F(x_i,x_j)$ when $F(x,y) = f(|x-y|)$ for some function f. Since the Riemannian distance is related to the Euclidean distance by $\vartheta(x,y) = 2\arcsin\frac{|x-y|}{2}$, the formula yields

$$\mathbb{E}\left[\sum_{i,j=1}^{N} \vartheta(x_i,x_j)\right] = 4N^2\int_0^{\infty} r \arcsin\left(\frac{r}{\sqrt{1+r^2}}\right)\gamma(r)\,\mathrm{d}r,$$

where $\gamma(r)$ has been defined in (2.19).

On the other hand, if $s = (0,0,-1) \in \mathbb{S}^2$, by rotation invariance we have

$$\begin{aligned}
\int_{\mathbb{S}^2}\int_{\mathbb{S}^2} \vartheta(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) &= \int_{\mathbb{S}^2} \vartheta(x,s)\,\mathrm{d}\sigma(x) \\
&= 2\int_{\mathbb{S}^2} \arcsin\frac{|x-s|}{2}\,\mathrm{d}\sigma(x) \\
&= 2\int_{\mathbb{C}} \arcsin\left(\frac{|z|}{\sqrt{1+|z|^2}}\right)\frac{1}{\pi(1+|z|^2)^2}\,\mathrm{d}z \\
&= 4\int_0^{\infty} r\arcsin\left(\frac{r}{\sqrt{1+r^2}}\right)\frac{1}{(1+r^2)^2}\,\mathrm{d}r,
\end{aligned}$$

where we have stereographically projected x to z (and s to 0), taking into account the expression (2.17) for the chordal distance between two points on $\mathbb{S}^2$ in terms of their projections on $\mathbb{C}$.

Putting all together

$$\begin{aligned}\mathbb{E}\big[\mathbb{D}_{2,\text{hem}}(X_N)^2\big] &= \frac{1}{2\pi}\bigg(\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}\vartheta(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) - \frac{1}{N^2}\mathbb{E}\Big[\sum_{i,j=1}^{N}\vartheta(x_i,x_j)\Big]\bigg)\\ &= \frac{2}{\pi}\int_0^\infty r\arcsin\left(\frac{r}{\sqrt{1+r^2}}\right)\left(\frac{1}{(1+r^2)^2}-\gamma(r)\right)\mathrm{d}r\\ &= \frac{1}{\pi N}\int_0^\infty \arcsin\left(\sqrt{\frac{x}{N+x}}\right)\left(\frac{1}{\left(1+\frac{x}{N}\right)^2}-\gamma\left(\sqrt{x/N}\right)\right)\mathrm{d}x.\end{aligned}$$

In the last line we have applied the change of variables $r^2 = x/N$. By considering the series of the integrand at $N=\infty$, we obtain

$$\mathbb{E}\big[\mathbb{D}_{2,\text{hem}}(X_N)^2\big] = -\frac{1}{\pi N^{3/2}}\int_0^\infty \sqrt{x}\,\phi(x)dx + O\Big(\frac{1}{L^{5/2}}\Big).$$

where

$$\phi(x) = \frac{\left(1-\frac{x}{e^x-1}\right)^2 e^x + \left(\frac{e^x x}{e^x-1}-1\right)^2}{e^x-1} - 1.$$

Integrating by parts,

$$\int_0^\infty x^{1/2}\phi(x)\,\mathrm{d}x = \left[x^{1/2}\left(-\frac{2+e^x(x-2)}{(e^x-1)^2}x\right)\right]_0^\infty + \frac{1}{2}\int_0^\infty x^{-1/2}\left(\frac{2+e^x(x-2)}{(e^x-1)^2}x\right)\mathrm{d}x.$$

The first term is equal to 0. The second can be obtained by integrating by parts again:

$$\begin{aligned}\int_0^\infty x^{-1/2}\left(\frac{2+e^x(x-2)}{(e^x-1)^2}x\right)\mathrm{d}x &= \left[x^{-1/2}\left(-\frac{x^2}{e^x-1}\right)\right]_0^\infty - \frac{1}{2}\int_0^\infty x^{-3/2}\frac{x^2}{e^x-1}\,\mathrm{d}x\\ &= -\frac{1}{2}\int_0^\infty \frac{x^{1/2}}{e^x-1}\,\mathrm{d}x.\end{aligned}$$

The last integral can be found in [GR07, 3.411 (1)]. Then we get

$$\begin{aligned}\mathbb{E}[\mathbb{D}_{2,\text{hem}}(X_N)^2] &= -\frac{1}{\pi}\frac{1}{2}\left(-\frac{1}{2}\right)\Gamma\left(\frac{3}{2}\right)\zeta\left(\frac{3}{2}\right)\frac{1}{N^{3/2}} + O\left(\frac{1}{N^{5/2}}\right)\\ &= \frac{1}{8\sqrt{\pi}}\zeta\left(\frac{3}{2}\right)\frac{1}{N^{3/2}} + o\left(\frac{1}{N^{3/2}}\right).\end{aligned}$$

□

3.4.2 L^∞ discrepancy on two-point homogeneous manifolds

Proof of Proposition 3.1.13. Since the process is invariant under the isometry group of $\mathbb{FP}^n$, the same is true for the variance of n_A. Therefore we can assume that $A = B(x_0, \theta_L)$, with x_0 a fixed point in $\mathbb{FP}^n$ and $\theta_L \in [0, \pi/2)$, and the result will not depend on x_0. We define $\alpha_L = L\theta_L$, which according to the hypothesis satisfies $\alpha_L = O(L)$ and $\alpha_L \to \infty$ when $L \to \infty$.

The variance can be computed with the following formula

$$\begin{aligned}\operatorname{Var}(n_A) &= \int_A \int_{A^c} |K_L^{(\alpha,\beta)}(x,y)|^2 \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\\ &= A^2_{\alpha,\beta,L} \int_A \int_{A^c} |P_L^{(\alpha+1,\beta)}(\cos(2\vartheta(x,y)))|^2 \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y),\end{aligned}$$

where $A_{\alpha,\beta,L} = \frac{(\alpha+\beta+2)_L}{(\beta+1)_L} \sim \frac{\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)} L^{\alpha+1}$ is the constant in (3.16).

We start by bounding the inner integral,

$$\begin{aligned}&\int_{A^c} |P_L^{(\alpha+1,\beta)}(\cos(2\vartheta(x,y)))|^2 \,\mathrm{d}\sigma(y)\\ &\le \int_{\mathbb{FP}^n \setminus B(x,\vartheta(x,\partial A))} |P_L^{(\alpha+1,\beta)}(\cos(2\vartheta(x,y)))|^2 \,\mathrm{d}\sigma(y)\\ &= \int_{\vartheta(x,\partial A)}^{\pi/2} |P_L^{(\alpha+1,\beta)}(\cos(2\theta))|^2 v(\theta)\,\mathrm{d}\theta,\end{aligned}$$

where in the equality we have applied (1.5) with

$$v(\theta) = \frac{1}{\gamma_{\alpha,\beta}} \sin^{2\alpha+1}(\kappa\theta)\cos^{2\beta+1}(\kappa\theta),$$

see (1.4). Then

$$\begin{aligned}&\operatorname{Var}(n_A)\\ &\lesssim A^2_{\alpha,\beta,L} \int_0^{\theta_L} v(\eta)\,\mathrm{d}\eta \int_{2(\theta_L-\eta)}^{\pi} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \sin^{2\alpha+1}\left(\frac{\theta}{2}\right)\cos^{2\beta+1}\left(\frac{\theta}{2}\right)\mathrm{d}\theta\\ &\lesssim A^2_{\alpha,\beta,L} \int_0^{\theta_L} \sin^{2\alpha+1}\eta \int_{2(\theta_L-\eta)}^{\pi} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \sin^{2\alpha+1}\left(\frac{\theta}{2}\right)\cos^{2\beta+1}\left(\frac{\theta}{2}\right)\mathrm{d}\theta\,\mathrm{d}\eta\\ &\le A^2_{\alpha,\beta,L} \int_0^{\theta_L} \eta^{2\alpha+1} \int_{2(\theta_L-\eta)}^{\pi} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \sin^{2\alpha+1}\left(\frac{\theta}{2}\right)\cos^{2\beta+1}\left(\frac{\theta}{2}\right)\mathrm{d}\theta\,\mathrm{d}\eta\\ &= \frac{A^2_{\alpha,\beta,L}}{L^{2\alpha+2}} \int_0^{\alpha_L} \eta^{2\alpha+1} \int_{\frac{2(\alpha_L-\eta)}{L}}^{\pi} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \sin^{2\alpha+1}\left(\frac{\theta}{2}\right)\cos^{2\beta+1}\left(\frac{\theta}{2}\right)\mathrm{d}\theta\,\mathrm{d}\eta.\end{aligned}$$

Here and all along the proof the constants in $\lesssim$ can depend on α and β. Since $A_{\alpha,\beta,L} \sim \frac{\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)} L^{\alpha+1}$,

$$\operatorname{Var}(n_A) \lesssim \int_0^{\alpha_L} \eta^{d-1} \int_{\frac{2(\alpha_L-\eta)}{L}}^{\pi} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \sin^{2\alpha+1}\left(\frac{\theta}{2}\right)\cos^{2\beta+1}\left(\frac{\theta}{2}\right)\mathrm{d}\theta\,\mathrm{d}\eta.$$

Now, as done in the proof of [BMOC16, Proposition 2], we split the inner integral above in three summands corresponding to the regions

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

for some fixed $c > 0$.

To bound the integral over I, we will use the following classical estimate for Jacobi polynomials from [Sze39, Theorem 8.21.13]

$$P_L^{(\alpha,\beta)}(\cos\theta) = L^{-1/2} k(\theta) \left[\cos(B\theta + \gamma) + (L \sin\theta)^{-1} O(1) \right], \tag{3.22}$$

where $B = L + \frac{\alpha+\beta+1}{2}$, $\gamma = -\left(\alpha + \frac{1}{2}\right)\frac{\pi}{2}$ and

$$k(\theta) = \pi^{-1/2} \sin^{-\alpha-1/2}\left(\frac{\theta}{2}\right) \cos^{-\beta-1/2}\left(\frac{\theta}{2}\right).$$

Then

$$\begin{aligned} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 &\lesssim L^{-1} k^2(\theta) \\ &\simeq L^{-1} \sin^{-2\alpha-3}\left(\frac{\theta}{2}\right) \cos^{-2\beta-1}\left(\frac{\theta}{2}\right). \end{aligned}$$

Therefore, integrating over I,

$$\begin{aligned} \mathrm{Var}(n_A)_{\mathrm{I}} &\lesssim \frac{1}{L} \int_0^{\alpha_L} \eta^{d-1} \, \mathrm{d}\eta \int_{\frac{\max\{2(\alpha_L-\eta),c\}}{L}}^{\pi-c/L} \frac{1}{\sin^2\left(\frac{\theta}{2}\right)} \, \mathrm{d}\theta \\ &= \frac{2}{L} \int_0^{\alpha_L} \eta^{d-1} \, \mathrm{d}\eta \left(\cot\left(\frac{\max\{2(\alpha_L-\eta),c\}}{2L} \right) - \tan\left(\frac{c}{2L}\right) \right) \\ &= \frac{2}{L} \Bigg[\underbrace{\int_0^{\alpha_L} \eta^{d-1} \cot\left(\frac{\max\{2(\alpha_L-\eta),c\}}{2L} \right) \mathrm{d}\eta}_{\mathrm{I}_1} - \underbrace{\frac{\alpha_L^d}{d} \tan\left(\frac{c}{2L}\right)}_{\text{order } L^{-1}\alpha_L^d} \Bigg]. \end{aligned}$$

After a change of variables, the integral I_1 can be expressed as

$$\mathrm{I}_1 = \underbrace{\int_{c/2}^{\alpha_L} (\alpha_L - \eta)^{d-1} \cot\left(\frac{\eta}{L}\right) \mathrm{d}\eta}_{\mathrm{I}_2} + \underbrace{\underbrace{\int_{\alpha_L - c/2}^{\alpha_L} \eta^{d-1} \, \mathrm{d}\eta}_{\text{order } \alpha_L^{d-1}} \cot\left(\frac{c}{2L}\right)}_{\text{order } L\alpha_L^{d-1}}.$$

To deal with I_2, we expand the polynomial in η and use that $x \cot x \leq 1$ for $x \in [0, \pi/2]$ to get

$$\begin{aligned} \mathrm{I}_2 &= \alpha_L^{d-1} \int_{c/2}^{\alpha_L} \cot\left(\frac{\eta}{L}\right) \mathrm{d}\eta + L\, O\left(\alpha_L^{d-1}\right) \\ &= L\alpha_L^{d-1} \log\left(\frac{\sin\left(\frac{\alpha_L}{L}\right)}{\sin\left(\frac{c}{2L}\right)} \right) + L\, O\left(\alpha_L^{d-1}\right) \\ &\leq L\alpha_L^{d-1} \log\left(\frac{4\alpha_L}{c} \right) + L\, O\left(\alpha_L^{d-1}\right) \\ &= L\alpha_L^{d-1} \log \alpha_L + L\, O\left(\alpha_L^{d-1}\right), \end{aligned}$$

where in the third line we have used that log is an increasing function and $\sin x \le x$, $\sin x \ge x/2$ for $x \in [0, \pi/2]$. Therefore,

$$\mathrm{Var}(n_A)_{\mathrm{I}} \lesssim \alpha_L^{d-1} \log \alpha_L + O\left(L^{d-1}\right).$$

Now we study the contribution of II. With the trivial bound $\sin x \le 1$, we have

$$\mathrm{Var}(n_A)_{\mathrm{II}} \lesssim \int_0^{\alpha_L} \eta^{d-1}\, \mathrm{d}\eta \int_{\pi - c/L}^{\pi} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \cos^{2\beta+1}\left(\frac{\theta}{2}\right) \mathrm{d}\theta.$$

The inner integral can be rewritten as

$$\begin{aligned}\int_{\pi-\frac{c}{L}}^{\pi} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \cos^{2\beta+1}\left(\frac{\theta}{2}\right) \mathrm{d}\theta &= \int_0^{c/L} |P_L^{(\alpha+1,\beta)}(\cos(\pi-\theta))|^2 \cos^{2\beta+1}\left(\frac{\pi-\theta}{2}\right) \mathrm{d}\theta \\ &= \int_0^{c/L} |P_L^{(\alpha+1,\beta)}(-\cos\theta)|^2 \sin^{2\beta+1}\left(\frac{\theta}{2}\right) \mathrm{d}\theta \\ &\lesssim \int_0^{c/L} |P_L^{(\alpha+1,\beta)}(-\cos\theta)|^2 \theta^{2\beta+1}\, \mathrm{d}\theta.\end{aligned}$$

Since $P_L^{(\alpha,\beta)}(\cos\theta) = (-1)^L P_L^{(\beta,\alpha)}(-\cos\theta)$, we have

$$|P_L^{(\alpha+1,\beta)}(-\cos\theta)| = |P_L^{(\beta,\alpha+1)}(\cos\theta)|$$

and

$$\mathrm{Var}(n_A)_{\mathrm{II}} \lesssim \int_0^{\alpha_L} \eta^{d-1}\, \mathrm{d}\eta \int_0^{c/L} |P_L^{(\beta,\alpha+1)}(\cos\theta)|^2 \theta^{2\beta+1}\, \mathrm{d}\theta.$$

From [Sze39, Theorem 7.32.2], $P_L^{(\alpha,\beta)}(\cos\theta) = O\left(L^{\alpha}\right)$ for $0 \le \theta \le c/L$. Hence,

$$|P_L^{(\beta,\alpha+1)}(\cos\theta)|^2 = O\left(L^{2\beta}\right)$$

and

$$\mathrm{Var}(n_A)_{\mathrm{II}} \lesssim \alpha_L^d L^{2\beta} L^{-2\beta-2} = L^{-2}\alpha_L^d = O\left(L^{d-2}\right).$$

For the integral over III, observe that the inner integral is zero unless $\eta \in [\alpha_L - c/2, \alpha_L]$. Therefore, using that $\cos x \le 1$ and $\sin x \le x$,

$$\mathrm{Var}(n_A)_{\mathrm{III}} \lesssim \int_{\alpha_L - c/2}^{\alpha_L} \eta^{d-1}\, \mathrm{d}\eta \int_0^{c/L} |P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \theta^{2\alpha+1}\, \mathrm{d}\theta.$$

Again by [Sze39, Theorem 7.32.2],

$$|P_L^{(\alpha+1,\beta)}(\cos\theta)|^2 \lesssim L^{2\alpha+2}$$

and

$$\mathrm{Var}(n_A)_{\mathrm{III}} \lesssim L^{2\alpha+2} \int_{\alpha_L - c/2}^{\alpha_L} \eta^{d-1}\, \mathrm{d}\eta \int_0^{c/L} \theta^{2\alpha+1}\, \mathrm{d}\theta \lesssim \alpha_L^{d-1} = O\left(L^{d-1}\right).$$

Summing up,

$$\mathrm{Var}(n_A) \lesssim \alpha_L^{d-1} \log \alpha_L + O\left(L^{d-1}\right) \lesssim L^{d-1} \log L + O\left(L^{d-1}\right).$$

□

Chapter 4

Green energy in two-point homogeneous manifolds

In this chapter, we prove the sharpest known to date lower bounds for the minimal Green energy of the compact two-point homogeneous manifolds of any dimension. Moreover, we relate the Green energy of a configuration X_N to a Sobolev discrepancy from which it is possible to deduce an upper bound for the discrepancy of N-point minimizers of the Green energy.

Part of this chapter is based on [BdlTL22].

4.1 Introduction and main results

4.1.1 Minimal Green energy

Let $\mathcal{M}$ be any compact Riemannian manifold without boundary. From [Aub98, Section 4.2], the *Green function* is the unique function $G_{\mathcal{M}} : \mathcal{M} \times \mathcal{M} \to \mathbb{R} \cup \{\infty\}$ with the properties:

1. In the sense of distributions, $\Delta_y G_{\mathcal{M}} = \delta_x - 1$, where δ_x is Dirac's delta.

2. $G_{\mathcal{M}}$ is $\mathcal{C}^\infty$ on $\mathcal{M} \times \mathcal{M}$ minus the diagonal.

3. Symmetry: $G_{\mathcal{M}}(x, y) = G_{\mathcal{M}}(y, x)$.

4. The mean of $G_{\mathcal{M}}(x, \cdot)$ is zero for all $x \in \mathcal{M}$, i.e., $\int_{y\in\mathcal{M}} G_{\mathcal{M}}(x, y)\,\mathrm{d}\sigma(y) = 0$, where σ is the normalized uniform measure on $\mathcal{M}$.

For an N-point configuration $X_N = \{x_1, \ldots, x_N\} \subset \mathcal{M}$, the *discrete Green energy of X_N* is defined by

$$E_{\mathcal{M}}(X_N) = \sum_{i\neq j} G_{\mathcal{M}}(x_i, x_j).$$

Since $G_{\mathcal{M}}$ is lower semicontinuous, the *minimal discrete Green energy* is achieved by some N-point configuration $X_N^* \subset \mathcal{M}$ and we denote it by

$$\mathcal{E}_G(\mathcal{M}, N) = \min_{X_N \subset \mathcal{M}} E_{\mathcal{M}}(X_N).$$

The search for minimizers of the Green energy is an interesting and difficult mathematical problem. If $\mathcal{M} = \mathbb{S}^2$ is the 2–sphere, we have

$$G_{\mathbb{S}^2}(x, y) = 2 \log \frac{1}{\|x - y\|} - 1 + 2 \log 2, \tag{4.1}$$

where log denotes the natural logarithm. Hence, the search for minimizers of the Green energy in $\mathbb{S}^2$ is closely related to Smale's 7th problem [Sma00].

In a general compact Riemannian manifold, if $x_1, \ldots, x_N$ are minimizers of the Green energy for increasing values of N, then they are asymptotically uniformly distributed, i.e., the associated counting probability measure converges in the weak sense to the uniform probability measure in $\mathcal{M}$, see [BCCdR19]. More quantitatively, in [Ste21] it is shown that the Wasserstein 2–distance between these two measures is of order $N^{-1/d}$, which is the best possible for dimension greater than or equal to 3. For a general compact Riemannian manifold, Steinerberger also proved in [Ste21, p. 4, Corollary] that

$$\mathcal{E}_G(\mathcal{M}, N) \geq \begin{cases} -c_{\mathcal{M}} N \log N & d = 2, \\ -c_{\mathcal{M}} N^{2-2/d} & d \geq 3, \end{cases} \tag{4.2}$$

where $c_{\mathcal{M}} > 0$ is a constant depending on the manifold $\mathcal{M}$. Here and all along the chapter, $d = d_{\mathcal{M}} = \dim(\mathcal{M})$ stands for the real dimension of the manifold $\mathcal{M}$.

Our goal is to improve these lower bounds for two-point homogeneous manifolds. We start by recalling some previous results.

Minimal value of the Green energy in spheres

Upper and lower bounds for the least possible Green energy have been investigated by several authors. The most studied case is that of $\mathbb{S}^2$, where we find again the elliptic Fekete points. As explained in Section 2.4, after [Wag89, RSZ94, Bra08, BS18, Ste22] it is known that

$$\min_{x_1,\ldots,x_N \in \mathbb{S}^2} \sum_{i \neq j} \log \frac{1}{\|x_i - x_j\|} = \left(\frac{1}{2} - \log 2 \right) N^2 - \frac{1}{2} N \log N + C_{\log} N + o(N),$$

where $C_{\log}$ is a constant whose value is not known. From [BS18] we have

$$C_{\log} \leq C_{BHS} = 2 \log 2 + \frac{1}{2} \log \frac{2}{3} + 3 \log \frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.0556 \ldots$$

This upper bound has been conjectured to be an equality using several different approaches [BHS12, BS18, Ste22]; see also [BHS19] for context and history of these results.

The best currently known lower bound [Lau21] has the same form but for a slightly different constant $\log 2 - \frac{3}{4} = -0.0568\ldots$ instead of $C_{\log}$. These bounds can be written in terms of the Green energy using (4.1),

$$-\frac{N}{2} + o(N) \leq \mathcal{E}_G(\mathbb{S}^2, N) + N\log N \leq \\ (2C_{BHS} + 1 - 2\log 2)\, N + o(N) \approx -0.49750N + o(N). \quad (4.3)$$

It has been proved in [BL22] that, if $\mathcal{M} = \mathbb{S}^d$, $d > 2$, the argument in [Lau21, Appendix B] (see also [LN75, SM76]) can be extended to get a seemingly almost sharp lower bound

$$\mathcal{E}_G(\mathbb{S}^d, N) \geq -\frac{d^{1+2/d}}{d^2-4}\left(\frac{V_{\mathbb{S}^d}}{V_{\mathbb{S}^{d-1}}}\right)^{2/d} N^{2-2/d} + o(N^{2-2/d}), \quad (4.4)$$

where the notation has been adapted, since the authors in [BL22] do not normalize the volume form on $\mathcal{M}$.

Minimal value of the Green energy in two-point homogeneous manifolds

Recall from Section 1.1 that the compact connected two-point homogeneous manifolds are the sphere $\mathbb{S}^d$, the real, complex and quaternionic projective spaces $\mathbb{RP}^n, \mathbb{CP}^n, \mathbb{HP}^n$ and the Cayley plane $\mathbb{OP}^2$. These spaces satisfy that if we have $x_1, y_1, x_2, y_2 \in \mathcal{M}$ with $\vartheta(x_1, y_1) = \vartheta(x_2, y_2)$, where ϑ denotes the geodesic distance, then there exists an isometry of $\mathcal{M}$ taking x_1 to x_2 and y_1 to y_2. This fact implies that many geometric properties (including minimal energy computations) can be described in a simpler manner than for general manifolds. For each two-point homogeneous manifold, we associate parameters α, β, κ defined in Table 4.1. We denote by $d = d_{\mathcal{M}} = \dim_{\mathbb{R}}(\mathcal{M})$ the real dimension of $\mathcal{M}$, whose value is d for the sphere $\mathbb{S}^d$ and $d = n \cdot \dim_{\mathbb{R}}(\mathbb{F})$ for a projective space $\mathbb{FP}^n$.

	$\mathbb{S}^d$	$\mathbb{FP}^n$
α	$\frac{d}{2} - 1$	
β	α	$\frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1$
κ	$1/2$	1
d	d	$n \cdot \dim_{\mathbb{R}}(\mathbb{F})$

Table 4.1: Parameters α, β, κ associated to each two-point homogeneous manifold, along with its real dimension $d = d_{\mathcal{M}} = \dim(\mathcal{M})$.

The case $\mathcal{M} = \mathbb{RP}^2$ is particularly simple since, as noted in [BELG23], $E_{\mathbb{RP}^2}(x_1, \ldots, x_N)$ can be written in terms of $E_{\mathbb{S}^2}(x_1, \ldots, x_N, -x_1, \ldots, -x_N)$ and the lower bound on the latter implies a lower bound on the former,

$$\mathcal{E}_G(\mathbb{RP}^2, N) \geq -\frac{1}{2}N\log N + \frac{1}{2}\left(\frac{1}{2} - \log 2\right) N + o(N). \quad (4.5)$$

$\mathbb{FP}^n$	$C^{\mathrm{AD}}_{\mathbb{FP}^n}$	$C^{\mathrm{BL}}_{\mathbb{FP}^n}$
$\mathbb{RP}^n$	$\frac{n}{4(n-2)}\left(\frac{\sqrt{\pi}}{\Gamma\left(\frac{n+1}{2}\right)}\right)^{2/n}$	$\frac{n}{n^2-4}\left(\frac{\Gamma\left(\frac{n}{2}+1\right)\sqrt{\pi}}{\Gamma\left(\frac{n+1}{2}\right)}\right)^{2/n}$
$\mathbb{CP}^n$	$\frac{n}{4(n-1)n!^{1/n}}$	$\frac{n}{2(n^2-1)}$
$\mathbb{HP}^n$	$\frac{n}{2(2n-1)\Gamma(2n+2)^{1/2n}}$	$\frac{n}{(2n-1)(2n+1)^{1+1/2n}}$
$\mathbb{OP}^2$	$\frac{2}{7}\sqrt[8]{\frac{6}{11!}}$	$\frac{4}{63\sqrt[8]{165}}$

Table 4.2: Absolute value of the dominant coefficients in the lower bounds for $\mathcal{E}_G(\mathbb{FP}^n, N)$ in (4.7) and (4.9).

Moreover, $\mathbb{CP}^1$ is isometric to the Riemann sphere, that is, the sphere of radius 1/2 centered at $(0, 0, 1/2)$, and hence $E_{\mathbb{CP}^1}(x_1, \dots, x_N) = \frac{1}{4}E_{\mathbb{S}^2}(\hat{x}_1, \dots, \hat{x}_N)$, where $\hat{x}_i$ is the result of combining the aforementioned isometry with a transformation sending the Riemann sphere to $\mathbb{S}^2$. This implies from (4.3),

$$\mathcal{E}_G(\mathbb{CP}^1, N) \geq -\frac{1}{4}N\log N - \frac{1}{8}N + o(N). \tag{4.6}$$

These are the sharpest known lower bounds for the two-point homogeneous manifolds of real dimension 2. The higher–dimensional case has been studied in [BE18] for the complex projective space and in [ADG+22] for general projective spaces. This last paper contains the sharpest lower bounds for the Green energy known to date. In terms of α, β and the dimension d, the lower bounds are

$$\mathcal{E}_G(\mathbb{FP}^n, N) \geq -C^{\mathrm{AD}}_{\mathbb{FP}^n}N^{2-2/d} + o(N^{2-2/d}), \tag{4.7}$$

with

$$C^{\mathrm{AD}}_{\mathbb{FP}^n} = \frac{d}{4(d-2)}\left(\frac{\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}\right)^{2/d}, \tag{4.8}$$

where $n = 2$ if $\mathbb{F} = \mathbb{O}$. In Table 4.2 we summarize the dominant coefficient in each case.

The main goal of this chapter is to show that the argument in [Lau21, BL22] can indeed be extended quite straightforwardly to all the two-point homogeneous manifolds of any dimension, sharpening the lower bounds for the minimal Green energy.

Theorem 4.1.1. *Let $\mathcal{M}$ be a compact connected two-point homogeneous manifold with $d = \dim(\mathcal{M}) > 2$. Then*

$$\mathcal{E}_G(\mathcal{M}, N) \geq -C^{BL}_{\mathcal{M}}N^{2-2/d} + o(N^{2-2/d}), \tag{4.9}$$

where

$$C^{BL}_{\mathcal{M}} = \frac{d}{d^2-4}\kappa^{-2}\left(\frac{\Gamma(\alpha+2)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}\right)^{2/d} \tag{4.10}$$

with α, β, κ given in Table 4.1. Our method applies equally to $\mathbb{S}^2$, $\mathbb{RP}^2$ and $\mathbb{CP}^1$, which yields the same lower bounds as in (4.3), (4.5) *and* (4.6), *respectively.*

For the sphere $\mathbb{S}^d$, the result coincides with (4.4). For the projective spaces, we show in Table 4.2 the coefficient of the dominant term in each case. We can compare our bounds with the ones of [ADG+22] mentioned above, and in all the cases our bounds are better. Indeed, since $\kappa = 1$ for projective spaces, $C^{\mathrm{BL}}_{\mathbb{FP}^n} < C^{\mathrm{AD}}_{\mathbb{FP}^n}$ is equivalent to see

$$4\left[\Gamma\left(\frac{d}{2}+1\right)\right]^{2/d} < d+2.$$

Writing $x = d/2$, this reduces to check

$$2\frac{[\Gamma(x+1)]^{1/x}}{x+1} < 1 \tag{4.11}$$

for $x \geq 3/2$. From [LC07, Theorem 1],

$$2\frac{[\Gamma(x+1)]^{1/x}}{x+1} < \underbrace{\frac{2}{e}(x+1)^{\frac{1}{2x}}}_{g(x)}$$

and the right-hand side function g is decreasing with $g(3/2) \approx 0.9986 < 1$. Thus, (4.11) holds for $x \geq 3/2$ and $C^{\mathrm{BL}}_{\mathbb{FP}^n} < C^{\mathrm{AD}}_{\mathbb{FP}^n}$. In Figures 4.1, 4.2 and 4.3 we plot $C^{\mathrm{BL}}_{\mathbb{FP}^n}$, $C^{\mathrm{AD}}_{\mathbb{FP}^n}$ for the comparison in the real, complex and quaternionic projective cases. For the Cayley plane, observe that

$$C^{\mathrm{BL}}_{\mathbb{OP}^2} = \frac{4}{63\sqrt[8]{165}} = 0.0335\ldots < 0.0400\ldots = \frac{2}{7}\sqrt[8]{\frac{6}{11!}} = C^{\mathrm{AD}}_{\mathbb{OP}^2}.$$

The paper [ADG+22] also provides upper bounds on the minimal energies for the projective spaces, though only for some values of N. These bounds follow from the computation of the expected energies of the corresponding harmonic ensemble in $\mathbb{FP}^n$, introduced in Section 1.3.3. In fact, the work studies first the expected s-Riesz energies, which are given by the *chordal Riesz s-kernel*

$$K_s(x,y) = \frac{1}{\rho(x,y)^s} = \frac{1}{\sin(\kappa\vartheta(x,y))^s}, \qquad s > 0,$$

where $\rho(x,y) = \sin(\kappa\vartheta(x,y))$ is the *chordal metric*. Observe that for the sphere, since $\rho(x,y)$ is the Euclidean distance $\frac{1}{2}|x-y|$, the previous kernel is up to a constant the usual Riesz s-kernel. The expected Green energies (and thus the mentioned upper bounds) follow then from the relation between the Green energy and the Riesz energy with exponent $s = d-2$, that will be reviewed in (4.37). The upper bounds obtained in [ADG+22] are, in terms of α, β and $d > 2$,

$$\mathcal{E}_G(\mathbb{FP}^n, N) \leq -\frac{(\alpha+1)^2}{4\alpha(2\alpha+1)}\left(\frac{\Gamma(\beta+1)}{\Gamma(\alpha+2)\Gamma(\alpha+\beta+2)}\right)^{2/d} N^{2-2/d} + o\left(N^{2-2/d}\right)$$

and only hold for

$$N = \pi_L^{(\alpha,\beta)} = \frac{(\alpha+\beta+2)_L(\alpha+2)_L}{(\beta+1)_L L!} \sim \frac{\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)\Gamma(\alpha+2)} L^{2\alpha+2}, \tag{4.12}$$

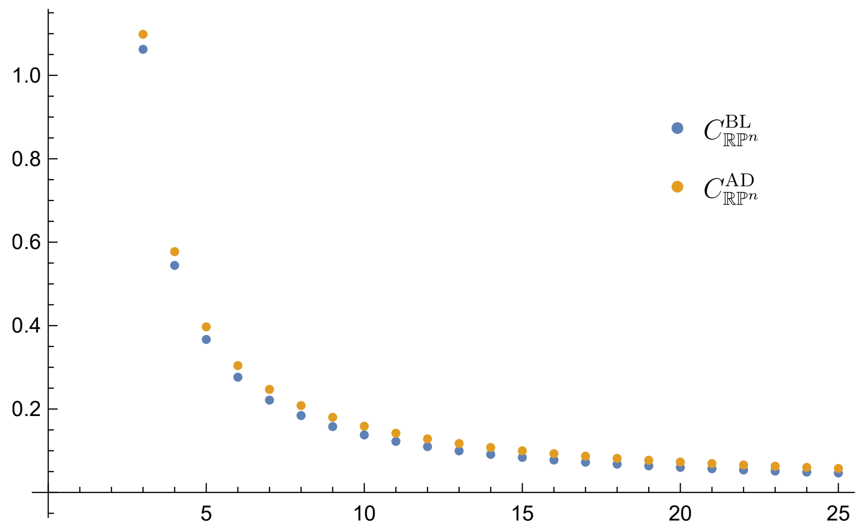

Figure 4.1: The absolute value of the dominant coefficients in the lower bound for $\mathcal{E}_G(\mathbb{RP}^n, N)$ for increasing values of n. Blue dots are our constants in Theorem 4.1.1 and yellow dots are those of [ADG+22].

that is, the number of points sampled by the harmonic ensemble in $\mathbb{FP}^n$ induced by the kernel $K_L^{(\alpha,\beta)}$, see Section 1.3.3 for a review.

A similar upper bound can be obtained by applying the same method, in this case using the expected Riesz energy from [BMOC16]. In this way we get the following upper bound for all two-point homogeneous manifolds.

Theorem 4.1.2. *Let $\mathcal{M}$ be a two-point homogeneous manifold with parameters α, β and κ and real dimension $d > 2$. Then*

$$\mathcal{E}_G(\mathcal{M}, N) \leq -\frac{(\alpha+1)^2}{4\kappa^2\alpha(2\alpha+1)} \left(\frac{\Gamma(\beta+1)}{\Gamma(\alpha+2)\Gamma(\alpha+\beta+2)}\right)^{2/d} N^{2-2/d} + o\left(N^{2-2/d}\right),$$

for values of N as in (4.12).

The previous result only gives upper bounds of the minimal energy for some values of N. In order to prove our results (in particular Theorem 4.1.7) we are going to need the following upper bound, which is valid for all N.

Proposition 4.1.3. *For each two-point homogeneous manifold $\mathcal{M}$ with $d > 2$, there exists a constant $C_{\mathcal{M}} > 0$ such that for $N \in \mathbb{N}$ sufficiently large,*

$$\mathcal{E}_G(\mathcal{M}, N) \leq -C_{\mathcal{M}} N^{2-2/d}. \tag{4.13}$$

Although this approach does not provide explicit values for the constant, it is enough for our purpose. For projective spaces the result is proved in [ADG+22, Corollary 4.3]. The sphere case follows the same strategy. For completeness we include a proof in Section 4.4.1.

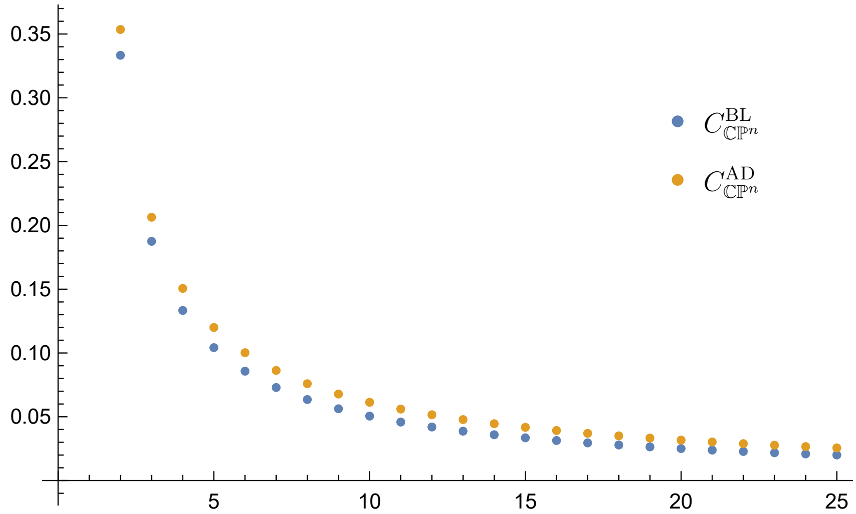

Figure 4.2: The absolute value of the dominant coefficients in the lower bound for $\mathcal{E}_G(\mathbb{CP}^n, N)$ for increasing values of n. Blue dots are our constants in Theorem 4.1.1 and yellow dots are those of [ADG+22].

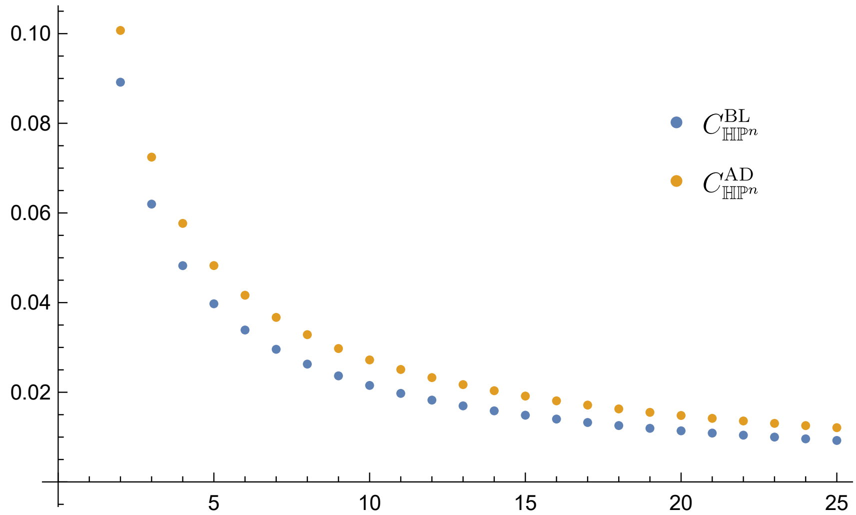

Figure 4.3: The absolute value of the dominant coefficients in the lower bound for $\mathcal{E}_G(\mathbb{HP}^n, N)$ for increasing values of n. Blue dots are our constants in Theorem 4.1.1 and yellow dots are those of [ADG+22].

4.1.2 Discrepancy of minimal Green energy points

Although finding N-point sets of minimal energy is a very hard problem that becomes unfeasible as N grows, it is possible to study some properties about their distribution. In his thesis [CdR18], Criado del Rey proved that the minimizers $X_N = \{x_1, \ldots, x_N\} \subset \mathcal{M}$ of the Green energy are well-separated for two-point homogeneous manifolds,

$$\min_{i \neq j} \vartheta(x_i, x_j) \geq \mathrm{sep}_{\mathcal{M}} N^{-1/d} \tag{4.14}$$

for some constant $\mathrm{sep}_{\mathcal{M}} > 0$ depending on the manifold $\mathcal{M}$. The constant is given in [CdR19, Theorem 1.2], and in terms of our parameters it reads

$$\mathrm{sep}_{\mathcal{M}} = \kappa^{-1} \left(\frac{\Gamma(\alpha+2)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)} \right)^{\frac{1}{d}}. \tag{4.15}$$

He also proved, together with Beltrán and Corral [BCCdR19], that any sequence of minimizers (X_N) of the Green energy are asymptotically uniformly distributed,

$$\lim_{N \to +\infty} \frac{1}{N} \sum_{i=1}^{N} f(x_i) = \int_{\mathcal{M}} f(x) \, \mathrm{d}\sigma(x), \quad \text{for } f \in \mathcal{C}(\mathcal{M}),$$

that is, the normalized uniform measure σ on $\mathcal{M}$ is the weak* limit of the sequence of normalized counting measures of the sets X_N, $\nu(X_N) = \frac{1}{N} \sum_{x \in X_N} \delta_x$. This property is known to hold if and only if the cap discrepancy converges to zero,

$$\lim_{N \to +\infty} \mathbb{D}_\infty(X_N) = 0,$$

where

$$\mathbb{D}_\infty(X_N) = \sup_{x \in \mathcal{M}, r > 0} \left| \frac{|X_N \cap B(x,r)|}{N} - \sigma(B(x,r)) \right|, \tag{4.16}$$

see [BHS19, Section 6.1]. Here we call *caps* the balls in any two-point homogeneous manifold by analogy with the sphere case. The speed of this convergence can be seen as a measure of how well distributed are the N-point sets of minimizers.

We will obtain an upper bound for the cap discrepancy of minimizers of the Green energy. We follow the ideas by Wolff in an unpublished manuscript, where he studied the logarithmic energy on the sphere $\mathbb{S}^2$. He proved the upper bound $O(N^{-1/3})$ for the spherical cap discrepancy of the minimizers of the logarithmic energy, which are also minimizers of the Green energy in $\mathbb{S}^2$ by (4.1). We observe that Wolff's 1985 result is, in fact, better than the upper bound of order $O(N^{-1/4})$ derived by Brauchart in 2008, [Bra08]. His method was later generalized to spheres of any dimension in [MM21] to work with minimizers of Riesz s-energies.

In our main result, we study the discrepancy of the minimizers of the Green energy for any two-point homogeneous space. Since the sphere $\mathbb{S}^2$ case corresponds to Wolff's work and the Green energies on $\mathbb{RP}^2$ and $\mathbb{CP}^1$ can be written in terms of $\mathbb{S}^2$, as detailed in the previous section, we do not need to consider manifolds of dimension 2.

Theorem 4.1.4. *Let $\mathcal{M}$ be a compact connected two-point homogeneous manifold of dimension $d > 2$. Let $X_N = \{x_1, \ldots, x_N\} \subset \mathcal{M}$ be an N-point set of minimizers of the Green energy. Then*

$$\mathbb{D}_\infty(X_N) \lesssim N^{-\frac{2}{3d}},$$

with the constant depending only on $\mathcal{M}$.

Remark 4.1.5. The same bound holds if the supremum in (4.16) is considered over the so-called K-regular sets, a more general family of sets including the balls $B(x, r)$ but also rectifiable curves. One only needs to adapt the functions $f_\epsilon^\pm$ in the proof of Proposition 4.4.4.

Recall from formula (3.9) that

$$cN^{-\frac{d+1}{2d}} \le \inf_{\substack{X_N \subset \mathcal{M}, \\ |X_N| = N}} \mathbb{D}_\infty(X_N) \le CN^{-\frac{d+1}{2d}} \sqrt{\log N}$$

for any two-point homogeneous manifold. Our result is far from the optimal cap discrepancy regardless of the logarithmic term. A possible reason could be the fact that, as pointed out in the remark, our proof is not specific for caps and works for more general sets such as the K-regular. For this family of sets, by combining ideas from [DG04], Korevaar's conjecture [Kor96] (proved by Götz [Göt00]) and the close relationship between the Green energy and the Riesz energy $s = d - 2$ (4.37), it is reasonable to think that the right order is $N^{-1/d}$. Our result, although it is not optimal, is closer to this order of magnitude.

Observe that Theorem 4.1.4 gives a quantitative proof of the asymptotic equidistribution of the energy minimizers mentioned above.

Following Wolff's approach, we will prove Theorem 4.1.4 through a sharp estimate of another discrepancy given in terms of Sobolev norms.

Sobolev discrepancy

In this subsection, we extend the setting in [MM21] to a general two-point homogeneous space.

The framework has already been introduced in Section 1.1.1. Recall that for each $\ell \geq 0$, V_ℓ denotes the vector space of eigenfunctions of eigenvalue $\lambda_\ell = 4\kappa^2 \ell(\ell + \alpha + \beta + 1)$ of the Laplace-Beltrami operator on $\mathcal{M}$. The multiplicity of the eigenvalue λ_ℓ is

$$m_\ell = \frac{2\ell + \alpha + \beta + 1}{\alpha + \beta + 1} \frac{(\alpha + \beta + 1)_\ell}{\ell!(\beta + 1)_\ell}.$$

As in the spherical setting, for the Hilbert space $L^2(\mathcal{M}) = L^2(\mathcal{M}, \sigma)$ of square integrable functions on the two-point homogeneous space $\mathcal{M}$ with inner product

$$\langle f, g \rangle = \int_{\mathcal{M}} f(x) g(x) \, \mathrm{d}\sigma(x)$$

the decomposition $L^2(\mathcal{M}) = \bigoplus_{\ell\geq 0} V_\ell$ holds. Then, if $\{Y_{\ell,k}\}_{k=1}^{m_\ell}$ is a real orthonormal basis of V_ℓ, given a function $f \in L^2(\mathcal{M})$ we have the Fourier representation

$$f = \sum_{\ell,k} f_{\ell,k} Y_{\ell,k}, \qquad f_{\ell,k} = \langle f, Y_{\ell,k}\rangle.$$

We consider the $L^2(\mathcal{M})$-based Sobolev Hilbert space defined in terms of the Fourier coefficients, that is,

$$\mathbb{H}^1(\mathcal{M}) = \left\{ f \in L^2(\mathcal{M}) : \sum_{\ell=0}^{\infty} \sum_{k=1}^{m_\ell} (1+\ell^2)|f_{\ell,k}|^2 < +\infty \right\},$$

with the norm

$$\|f\|_{\mathbb{H}^1(\mathcal{M})} = \left(\sum_{\ell=0}^{\infty} \sum_{k=1}^{m_\ell} (1+\ell^2)|f_{\ell,k}|^2 \right)^{1/2}.$$

This norm satisfies the equivalence

$$\|f\|^2_{\mathbb{H}^1(\mathcal{M})} \approx \|f\|^2_{L^2(\mathcal{M})} + \|\nabla f\|^2_{L^2(\mathcal{M})}. \tag{4.17}$$

Indeed, as done in [MM21, Section 2.4], from the first Green's identity and (1.6) we have

$$\int_{\mathcal{M}} |\nabla Y_{\ell,k}|^2 \, \mathrm{d}\sigma = \int_{\mathcal{M}} Y_{\ell,k} \, \Delta Y_{\ell,k} \; \mathrm{d}\sigma = 4\kappa^2 \ell(\ell+\alpha+\beta+1) \approx \ell^2.$$

Moreover, by the orthogonality of the eigenfunctions $\{Y_{\ell,k}\}_{k=1,\ell\geq 0}^{m_\ell}$,

$$\int_{\mathcal{M}} Y_{\ell,k} \, \Delta^j Y_{\ell',k'} \, \mathrm{d}\sigma = 0$$

for $j \in \{0,1\}$ whenever $(\ell,k) \neq (\ell',k')$. Then

$$\begin{aligned}
\|f\|^2_{\mathbb{H}^1(\mathcal{M})} &= \sum_{\ell=0}^{\infty} \sum_{k=1}^{m_\ell} (1+\ell^2)|f_{\ell,k}|^2 = \|f\|^2_{L^2(\mathcal{M})} + \sum_{\ell=1}^{\infty} \sum_{k=1}^{m_\ell} \ell^2 |f_{\ell,k}|^2 \\
&\approx \|f\|^2_{L^2(\mathcal{M})} + \sum_{\ell=1}^{\infty} \sum_{k=1}^{m_\ell} \int_{\mathcal{M}} Y_{\ell,k} \, \Delta Y_{\ell,k} \; \mathrm{d}\sigma \, |f_{\ell,k}|^2 \\
&= \|f\|^2_{L^2(\mathcal{M})} + \int_{\mathcal{M}} f \, \Delta f \, \mathrm{d}\sigma = \|f\|^2_{L^2(\mathcal{M})} + \int_{\mathcal{M}} |\nabla f|^2 \, \mathrm{d}\sigma,
\end{aligned}$$

where in the last equality we have applied the first Green's identity.

For any Borel measure μ on $\mathcal{M}$, we consider a "dual" Sobolev norm given by

$$\|\mu\|_{\mathbb{H}^{-1}(\mathcal{M})} = \sup \left\{ \int_{\mathcal{M}} \psi \, \mathrm{d}\mu : \psi \in \mathcal{C}^\infty(\mathcal{M}), \ \|\psi\|_{\mathbb{H}^1(\mathcal{M})} = 1 \right\}.$$

If the measure μ is of the form $\mu = h\sigma$ for some $h \in L^2(\mathcal{M})$, we write $\|h\|_{\mathbb{H}^{-1}(\mathcal{M})}$.

Next we define a Sobolev discrepancy in the same way than Wolff [Wol], see also [MM21].

Definition 4.1.6. Let $X_N = \{x_1, \ldots, x_N\}$ be an N-point configuration on $\mathcal{M}$ and let $\epsilon > 0$. We define the *Sobolev discrepancy of* X_N by

$$D^{\epsilon}_{\mathcal{M}}(X_N) = \|h_{X_N,\epsilon}\|_{\mathbb{H}^{-1}(\mathcal{M})}, \tag{4.18}$$

where

$$h_{X_N,\epsilon} = \frac{1}{N}\sum_{j=1}^{N} \frac{1}{\sigma(D_j)}\chi_{D_j} - 1$$

and $D_j = B(x_j, \epsilon N^{-1/d})$.

Observe that we choose the radius of the balls so that the order coincides with that of the optimal separation distance (4.14).

We prove the following sharp estimate of the Sobolev discrepancy of minimizers.

Theorem 4.1.7. *Let $X_N = \{x_1, \ldots, x_N\} \subset \mathcal{M}$ be an N-point set of minimizers of the Green energy of $\mathcal{M}$. Then for every $\epsilon > 0$ small enough depending only on the manifold $\mathcal{M}$,*

$$N^{-1/d} \lesssim D^{\epsilon}_{\mathcal{M}}(X_N) \lesssim N^{-1/d},$$

where the constants depend on $\mathcal{M}$ and ϵ.

4.2 Technical results

4.2.1 Basic definitions and notation

Two-point homogeneous manifolds, introduced in Section 1.1, are the most symmetric manifolds that one can conceive. According to [Wan52], there are just five examples of compact connected two-point homogeneous manifolds (up to dimension choices): the sphere $\mathbb{S}^d$, the real, complex and quaternionic projective spaces $\mathbb{RP}^n, \mathbb{CP}^n, \mathbb{HP}^n$ and the Cayley plane $\mathbb{OP}^2$.

Let G denote the isometry group of the manifold $\mathcal{M}$. We recall that each two-point homogeneous space is equipped with its corresponding G-invariant volume form $\tilde{\sigma}$ and geodesic distance ϑ, normalized to take values in $[0, D]$, where $D = \frac{\pi}{2\kappa}$ is the diameter, that is, the maximum distance between two points in $\mathcal{M}$. Here we will consider the normalized uniform measure $\sigma = \tilde{\sigma}/V$, where V stands for the total volume of $\mathcal{M}$, i.e., $V = V_{\mathcal{M}} = \tilde{\sigma}(\mathcal{M})$. From (1.2),

$$V = V_{\mathbb{S}^{d-1}}\kappa^{-d}\gamma_{\alpha,\beta},$$

where

$$\gamma_{\alpha,\beta} = \frac{\mathrm{B}(\alpha+1, \beta+1)}{2}$$

and

$$V_{\mathbb{S}^d} = \frac{2\pi^{\frac{d+1}{2}}}{\Gamma\left(\frac{d+1}{2}\right)}.$$

We recall from Section 1.1 that given a sphere $S(x,a) = \{y \in \mathcal{M} : \vartheta(x,y) = a\}$ centered at x of radius a, its normalized surface measure is

$$v(a) = \frac{\kappa}{\gamma_{\alpha,\beta}} \sin^{2\alpha+1}(\kappa a) \cos^{2\beta+1}(\kappa a). \tag{4.19}$$

Thus, the normalized volume of the ball $B(x,a)$, $V(a) = V_{\mathcal{M}}(a) = \sigma(B(x,a))$, is

$$V(a) = \int_0^a v(r)\,\mathrm{d}r.$$

More generally, for any integrable function $F : \mathcal{M} \to \mathbb{R}$ such that $F(x) = f(\vartheta(x,x_0))$ for some point $x_0 \in \mathcal{M}$, the formula

$$\int_{\mathcal{M}} F(x)\,\mathrm{d}\sigma(x) = \int_0^D f(r)v(r)\,\mathrm{d}r \tag{4.20}$$

holds.

Finally, we define two functions that will be useful in our analysis:

$$K(\mathcal{M},a) = \frac{1}{V(a)} \int_0^a v(r) \int_0^r \frac{V(u)}{v(u)}\,\mathrm{d}u\,\mathrm{d}r, \tag{4.21}$$

$$\Theta(\mathcal{M},a) = \frac{1}{V(a)} \int_{y\in B(x_0,a)} G_{\mathcal{M}}(x_0,y)\,\mathrm{d}\sigma(y). \tag{4.22}$$

Note that due to the symmetry of two-point homogeneous manifolds, the second quantity does not depend on $x_0 \in \mathcal{M}$. In Appendix A, we provide closed-form expressions for these functions in the cases of $\mathcal{M} = \mathbb{CP}^n, \mathbb{HP}^n, \mathbb{OP}^2$, although we do not use them in our proofs. The term $K(\mathcal{M},a)$ appears in the next lemma.

4.2.2 Expected value of the Green function in a ball

The following closed formula for the expected value of the Green function in a ball will prove useful in our computations in this chapter.

Lemma 4.2.1. *Let $\mathcal{M}$ be a two-point homogeneous manifold.Then, for any $x_0, x \in \mathcal{M}$,*

- *If $\vartheta(x_0,x) \geq a$, then*

$$\frac{1}{V(a)} \int_{y\in B(x_0,a)} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(y) = G_{\mathcal{M}}(x,x_0) + K(\mathcal{M},a).$$

- *If $\vartheta(x_0,x) < a$, then*

$$\frac{1}{V(a)} \int_{y\in B(x_0,a)} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(y) = G_{\mathcal{M}}(x,x_0) + K(\mathcal{M},a) - \frac{1}{V(a)} \int_{\vartheta(x_0,x)}^a v(r) \int_{\vartheta(x_0,x)}^r \frac{\mathrm{d}u}{v(u)}\,\mathrm{d}r.$$

In particular, for any $x_0, x \in \mathcal{M}$,

$$\frac{1}{V(a)} \int_{y \in B(x_0,a)} G_{\mathcal{M}}(x,y)\, \mathrm{d}\sigma(y) \leq G_{\mathcal{M}}(x,x_0) + K(\mathcal{M},a).$$

Proof. We sketch a proof for completeness. For the first identity, multiplying by $V(a)$ and computing the derivative with respect to a, it suffices to check that

$$\frac{1}{v(a)} \int_{y \in S(x_0,a)} G_{\mathcal{M}}(x,y)\ \mathrm{d}S_a(y) = G_{\mathcal{M}}(x,x_0) + \int_0^a \frac{V(u)}{v(u)}\, \mathrm{d}u, \quad a < \vartheta(x_0,x), \tag{4.23}$$

where S_a is the Riemannian measure induced on $S(x_0,a)$ by σ, that satisfies $S_a(S(x_0,a)) = v(a)$.

It is clear that both sides of (4.23) are equal as $a \to 0$. We check that their derivatives also coincide. Call $F(a)$ the left–hand term in (4.23). Writing it down in normal coordinates with basepoint x_0, we find that the derivative of the left–hand side equals

$$F'(a) = \frac{1}{v(a)} \int_{y \in S(x_0,a)} \nabla_{N(y)} G_{\mathcal{M}}(x,y)\ \mathrm{d}S_a(y),$$

where $N(y)$ is the unit vector orthogonal to $S(x_0,a)$ at y and ∇ is the covariant derivative. From Green's second identity, we get

$$F'(a) = -\frac{1}{v(a)} \int_{B(x_0,a)} \Delta G_{\mathcal{M}}(x,y)\, \mathrm{d}\sigma(y) = \frac{V(a)}{v(a)}.$$

Hence, the derivatives at both sides of (4.23) are equal, proving (4.23) and the first claim of the lemma in the case that $\vartheta(x_0,x) < a$. The case $\vartheta(x_0,x) = a$ follows from the continuity of both sides of the equality. Finally, if $\vartheta(x_0,x) = t < a$ we can still compute the derivative using Green's second identity, now to the other open set delimited by $S(x_0,a)$ and using $-N(y)$:

$$F'(a) = \frac{1}{v(a)} \int_{\mathcal{M} \setminus B(x_0,a)} \Delta G_{\mathcal{M}}(x,y)\, \mathrm{d}\sigma(y) = -\frac{1}{v(a)}(1 - V(a)), \quad a > t.$$

All in one, we have proved

$$\begin{aligned} F(a) &= F(t) + \int_t^a \frac{V(u)-1}{v(u)}\, \mathrm{d}u \\ &= F(0) + \int_0^t \frac{V(u)}{v(u)}\, \mathrm{d}u + \int_t^a \frac{V(u)-1}{v(u)}\, \mathrm{d}u \\ &= G_{\mathcal{M}}(x,x_0) + \int_0^a \frac{V(u)}{v(u)}\, \mathrm{d}u - \int_t^a \frac{1}{v(u)}\, \mathrm{d}u. \end{aligned}$$

The second claim in the lemma now follows, since

$$\int_{y \in B(x_0,a)} G_{\mathcal{M}}(x,y)\, \mathrm{d}\sigma(y) = \int_0^a v(r) F(r)\, \mathrm{d}r.$$

□

4.2.3 Energy of a function

Given a function $f \in L^\infty(\mathcal{M})$, we define its Green transform by

$$G_{\mathcal{M}} f(x) := \int_{\mathcal{M}} G_{\mathcal{M}}(x,y) f(y)\, \mathrm{d}\sigma(y).$$

Our first result, which relates the energy of a smooth function with its Laplace-Fourier coefficients, is the Green version of [MM21, Proposition 2.2]. All results are stated for a two-point homogeneous manifold $\mathcal{M}$ of dimension $d > 2$.

Proposition 4.2.2. *Let $\{Y_{\ell,k}\}_{k=1,\ell\geq 0}^{m_\ell}$ be an orthonormal basis of eigenfunctions of the Laplace-Beltrami operator in $L^2(\mathcal{M})$. Given a $\mathcal{C}^\infty$ function $f = \sum_{\ell,k} f_{\ell,k} Y_{\ell,k} \in L^2(\mathcal{M})$, where $f_{\ell,k} = \int_{\mathcal{M}} f\, Y_{\ell,k}\, \mathrm{d}\sigma$, then $G_{\mathcal{M}} f$ is also smooth and*

$$G_{\mathcal{M}} f = \sum_{\ell \geq 1, k} \frac{1}{\lambda_\ell} f_{\ell,k} Y_{\ell,k}$$

in the $L^2(\mathcal{M})$ sense. In particular, $\|G_{\mathcal{M}} f\|_2 \leq \|f\|_2$.

Proof. From [Aub98, Theorem 4.13], there exists a constant $k_{\mathcal{M}}$ such that

$$|G_{\mathcal{M}}(x,y)| \leq k_{\mathcal{M}} \vartheta(x,y)^{2-d}. \tag{4.24}$$

Then

$$\begin{aligned}
|G_{\mathcal{M}} f(x)| &\leq \int_{\mathcal{M}} |G_{\mathcal{M}}(x,y)||f(y)|\, \mathrm{d}\sigma(y) \\
&\leq k_{\mathcal{M}} \|f\|_\infty \int_{\mathcal{M}} \vartheta(x,y)^{2-d}\, \mathrm{d}\sigma(y) \\
&\overset{(4.20)}{=} k_{\mathcal{M}} \|f\|_\infty \int_0^D r^{2-d} v(r)\, \mathrm{d}r \\
&\leq k'_{\mathcal{M}} \|f\|_\infty \int_0^D r^{2-d} r^{d-1}\, \mathrm{d}r \\
&= k'_{\mathcal{M}} \|f\|_\infty D^2/2 < \infty
\end{aligned} \tag{4.25}$$

and $\|G_{\mathcal{M}} f\|_\infty \leq k''_{\mathcal{M}} \|f\|_\infty$. Thus, $G_{\mathcal{M}} f \in L^\infty(\mathcal{M}) \subset L^2(\mathcal{M})$. We compute its Fourier-Laplace coefficients:

$$\begin{aligned}
\langle G_{\mathcal{M}} f, Y_{\ell,k} \rangle &= \int_{\mathcal{M}} \int_{\mathcal{M}} G_{\mathcal{M}}(x,y) f(y)\, \mathrm{d}\sigma(y) Y_{\ell,k}(x)\, \mathrm{d}\sigma(x) \\
&= \int_{\mathcal{M}} \int_{\mathcal{M}} G_{\mathcal{M}}(x,y) Y_{\ell,k}(x)\, \mathrm{d}\sigma(x) f(y)\, \mathrm{d}\sigma(y),
\end{aligned} \tag{4.26}$$

where the order of integration can be exchanged by Fubini's theorem. Indeed, from the well known fact that $\|Y_{\ell,k}\|_\infty$ grows as a power of λ_ℓ and the previous bound $\|G_{\mathcal{M}} f\|_\infty \leq k''_{\mathcal{M}} \|f\|_\infty$,

$$\int_{\mathcal{M}} \int_{\mathcal{M}} |G_{\mathcal{M}}(x,y) f(y) Y_{\ell,k}(x)|\, \mathrm{d}\sigma(y)\, \mathrm{d}\sigma(x) \leq k_{\mathcal{M},\ell} \|f\|_\infty < \infty.$$

To compute the inner integral in (4.26), we use the integral representation

$$G_{\mathcal{M}}(x,y) = \int_0^\infty (p_t(x,y) - 1)\,\mathrm{d}t$$

from [GZ19, Proposition 4.5], where

$$p_t(x,y) = \sum_{\ell=0}^{\infty} e^{-\lambda_\ell t} \sum_{k=1}^{m_\ell} Y_{\ell,k}(x) Y_{\ell,k}(y) \tag{4.27}$$

is the heat kernel of the Laplace-Beltrami operator on $\mathcal{M}$. The virtue of this kernel is that, in contrast with the formal expansion

$$G_{\mathcal{M}}(x,y) = \sum_{\ell=1}^{\infty} \frac{1}{\lambda_\ell} \sum_{k=1}^{m_\ell} Y_{\ell,k}(x) Y_{\ell,k}(y), \tag{4.28}$$

its series expansion converges uniformly in $x, y \in \mathcal{M}$ for every fixed $t > 0$. Then

$$\begin{aligned} \int_{\mathcal{M}} G_{\mathcal{M}}(x,y) Y_{\ell,k}(x)\,\mathrm{d}\sigma(x) &= \int_{\mathcal{M}} \int_0^\infty (p_t(x,y) - 1)\,\mathrm{d}t\; Y_{\ell,k}(x)\,\mathrm{d}\sigma(x) \\ &= \int_0^\infty \int_{\mathcal{M}} (p_t(x,y) - 1)\, Y_{\ell,k}(x)\,\mathrm{d}\sigma(x)\,\mathrm{d}t, \end{aligned}$$

where the application of Fubini's theorem is justified by the uniform bound of $|Y_{\ell,k}|$ in terms of a power of λ_ℓ and the global integrability

$$\int_0^\infty \int_{\mathcal{M}} |p_t(x,y) - 1|\,\mathrm{d}\sigma(x)\,\mathrm{d}t,$$

see [GZ19, Lemma 4.8]. Using the uniformly convergent expansion (4.27),

$$\begin{aligned} \int_{\mathcal{M}} G_{\mathcal{M}}(x,y) Y_{\ell,k}(x)\,\mathrm{d}\sigma(x) &= \int_0^\infty \int_{\mathcal{M}} \sum_{\ell'=1}^{\infty} e^{-\lambda_{\ell'} t} \sum_{k'=1}^{m_{\ell'}} Y_{\ell',k'}(x) Y_{\ell',k'}(y) Y_{\ell,k}(x)\,\mathrm{d}\sigma(x)\,\mathrm{d}t \\ &= \int_0^\infty \sum_{\ell'=1}^{\infty} e^{-\lambda_{\ell'} t} \sum_{k'=1}^{m_{\ell'}} Y_{\ell',k'}(y) \int_{\mathcal{M}} Y_{\ell',k'}(x) Y_{\ell,k}(x)\,\mathrm{d}\sigma(x)\,\mathrm{d}t \\ &= \int_0^\infty e^{-\lambda_\ell t}\,\mathrm{d}t\, Y_{\ell,k}(y) \\ &= \frac{1}{\lambda_\ell} Y_{\ell,k}(y) \end{aligned}$$

provided that $\ell \geq 1$. If $\ell = 0$, the integral vanishes. Therefore, going back to (4.26),

$$\begin{aligned} \langle G_{\mathcal{M}} f, Y_{\ell,k} \rangle &= \int_{\mathcal{M}} \int_{\mathcal{M}} G_{\mathcal{M}}(x,y) Y_{\ell,k}(x)\,\mathrm{d}\sigma(x) f(y)\,\mathrm{d}\sigma(y) \\ &= \int_{\mathcal{M}} \frac{1}{\lambda_\ell} Y_{\ell,k}(y) f(y)\,\mathrm{d}\sigma(y) = \frac{1}{\lambda_\ell} f_{\ell,k} \end{aligned}$$

for $\ell \geq 1$ and $\langle G_{\mathcal{M}} f, Y_{0,1}\rangle = 0$. Then the Fourier representation is $G_{\mathcal{M}} f = \sum_{\ell\geq 1,k} \frac{1}{\lambda_\ell} f_{\ell,k} Y_{\ell,k}$ in $L^2(\mathcal{M})$. From this expression it is easy to show that, since $f_{\ell,k}$ decays faster than any power when f is smooth, $G_{\mathcal{M}} f$ is a smooth function.

Since

$$\|G_{\mathcal{M}} f\|_2^2 = \sum_{\ell\geq 1,k} \frac{1}{\lambda_\ell^2} |f_{\ell,k}|^2$$

and $\lambda_\ell \geq \ell^2 \geq 1$ for $\ell \geq 1$, we have

$$\|G_{\mathcal{M}} f\|_2^2 \leq \sum_{\ell\geq 1,k} |f_{\ell,k}|^2 \leq \|f\|_2^2$$

and the last result holds. □

The previous Proposition allows us to extend the definition of the operator $G_{\mathcal{M}}$ to $L^2(\mathcal{M})$. Indeed, since $\mathcal{C}^\infty(\mathcal{M})$ is dense in $L^2(\mathcal{M})$, given a function $f \in L^2(\mathcal{M})$ we can define

$$G_{\mathcal{M}} f := \lim_{j\to\infty} G_{\mathcal{M}} f_j \quad \text{in } L^2(\mathcal{M}),$$

where $\{f_j\} \subset \mathcal{C}^\infty(\mathcal{M})$ is a sequence of smooth functions such that $f_j \to f$ in $L^2(\mathcal{M})$. It is immediate to check that the operator is well defined and that the properties

$$G_{\mathcal{M}} f = \sum_{\ell\geq 1,k} \frac{1}{\lambda_\ell} f_{\ell,k} Y_{\ell,k} \tag{4.29}$$

and $\|G_{\mathcal{M}} f\|_2 \leq \|f\|_2$ are preserved.

Given a function $f \in L^2(\mathcal{M})$, we define its Green energy by

$$E_{\mathcal{M}}(f) := \int_{\mathcal{M}} f(x) G_{\mathcal{M}} f(x) \, \mathrm{d}\sigma(x).$$

If $f = \sum_{\ell,k} f_{\ell,k} Y_{\ell,k} \in L^2(\mathcal{M})$, from (4.29) we get

$$E_{\mathcal{M}}(f) = \langle G_{\mathcal{M}} f, f\rangle = \sum_{\ell\geq 1,k} \frac{1}{\lambda_j} |f_{\ell,k}|^2.$$

In particular, since $\lambda_\ell \approx \ell^2$, we get the equivalence

$$E_{\mathcal{M}}(f) \approx \sum_{\ell\geq 1,k} \frac{1}{\ell^2} |f_{\ell,k}|^2. \tag{4.30}$$

Now we show that the Sobolev discrepancy defined in (4.18) is equivalent to the energy of the function $h_{X_N,\epsilon}$.

Lemma 4.2.3. *There exists a constant $C_{\mathcal{M}} > 0$ depending on the manifold $\mathcal{M}$ such that for every $h \in L^2(\mathcal{M})$ with $\int_{\mathcal{M}} h \, \mathrm{d}\sigma = 0$,*

$$C_{\mathcal{M}}^{-1} \|h\|_{\mathbb{H}^{-1}(\mathcal{M})}^2 \leq E_{\mathcal{M}}(h) \leq C_{\mathcal{M}} \|h\|_{\mathbb{H}^{-1}(\mathcal{M})}^2. \tag{4.31}$$

In particular,

$$D_{\mathcal{M}}^\epsilon(X_N)^2 \approx E_{\mathcal{M}}(h_{X_N,\epsilon}). \tag{4.32}$$

Proof. We first prove the result for a smooth function h. We have seen in (4.30) that if $h = \sum_{\ell,k} h_{\ell,k} Y_{\ell,k}$ then

$$E_{\mathcal{M}}(h) \approx \sum_{\ell \geq 1,k} \frac{1}{\ell^2} |h_{\ell,k}|^2.$$

Writing $\psi \in \mathcal{C}^\infty(\mathcal{M})$ as $\psi = \sum_{\ell,k} \psi_{\ell,k} Y_{\ell,k}$ and applying Cauchy-Schwarz inequality, we have

$$\begin{aligned}\left| \int_{\mathcal{M}} \psi h \, \mathrm{d}\sigma \right|^2 &= \left| \sum_{\ell,k} \psi_{\ell,k} h_{\ell,k} \right|^2 = \left| \sum_{\ell \geq 1,k} \psi_{\ell,k} h_{\ell,k} \right|^2 \\ &\leq \sum_{\ell \geq 1,k} \frac{1}{\ell^2} |h_{\ell,k}|^2 \sum_{\ell \geq 1,k} \ell^2 |\psi_{\ell,k}|^2 \\ &\lesssim E_{\mathcal{M}}(h) \|\psi\|^2_{\mathbb{H}^1(\mathcal{M})},\end{aligned}$$

and taking the supremum on $\psi \in \mathcal{C}^\infty(\mathcal{M})$ we obtain the first inequality.

Now we prove the second inequality. Since we are assuming that h is smooth, by the previous Proposition $G_{\mathcal{M}} h$ is also smooth. From (4.29), we have

$$G_{\mathcal{M}} h = \sum_{\ell \geq 1,k} \frac{1}{\lambda_\ell} h_{\ell,k} Y_{\ell,k}.$$

Then

$$\begin{aligned}E_{\mathcal{M}}(h) &= \int_{\mathcal{M}} h \, G_{\mathcal{M}} h \, \mathrm{d}\sigma \leq \|h\|_{\mathbb{H}^{-1}(\mathcal{M})} \|G_{\mathcal{M}} h\|_{\mathbb{H}^1(\mathcal{M})} \\ &= \|h\|_{\mathbb{H}^{-1}(\mathcal{M})} \left(\sum_{\ell \geq 1,k} (1+\ell^2) \left| \frac{h_{\ell,k}}{\lambda_\ell} \right|^2 \right)^{1/2} \\ &\approx \|h\|_{\mathbb{H}^{-1}(\mathcal{M})} \left(\sum_{\ell \geq 1,k} \frac{1}{\ell^2} |h_{\ell,k}|^2 \right)^{1/2} \approx \|h\|_{\mathbb{H}^{-1}(\mathcal{M})} E_{\mathcal{M}}(h)^{1/2}\end{aligned}$$

and we are done.

Now we extend the result to a function $h \in L^2(\mathcal{M})$. From [Gri09, Theorem 2.16], by convolving h with a mollifier we can obtain a sequence of smooth functions h_j that, besides converging to h in $L^2(\mathcal{M})$, also converges in $\mathbb{H}^{-1}(\mathcal{M})$. Then, since (4.31) holds for each h_j and $\|h_j\|_{\mathbb{H}^{-1}(\mathcal{M})} \to \|h\|_{\mathbb{H}^{-1}(\mathcal{M})}$ and

$$E_{\mathcal{M}}(h_j) = \langle G_{\mathcal{M}} h_j, h_j \rangle \to \langle G_{\mathcal{M}} h, h \rangle = E_{\mathcal{M}}(h)$$

as $j \to \infty$, the double inequality (4.31) holds for h.

Finally, since $\int_{\mathcal{M}} h_{X_N,\epsilon} \, \mathrm{d}\sigma = 0$, applying the result for $h_{X_N,\epsilon} \in L^2(\mathcal{M})$ gives the equivalence (4.32). □

4.2.4 The Green function in two-point homogeneous manifolds

The Green function is in general impossible to compute in terms of elementary functions. However, for two-point homogeneous manifold it only depends on the distance between x and y, i.e.,

$$G_{\mathcal{M}}(x, y) = g(\vartheta(x, y)),$$

g being the solution of a simple ODE, see [BCCdR19, Theorem A.10]. Alternatively, the eigenfunction expansion (4.28) is used in [ADG$^+$22] to derive a general expression for the Green function on the projective spaces,

$$g(\vartheta) = \frac{1}{4(\alpha+\beta+1)} \left(\sum_{k=1}^{\infty} \frac{(\alpha+\beta+1)_k}{k(\beta+1)_k} \cos^{2k}\vartheta - \gamma - \psi(\alpha+\beta+2) \right), \tag{4.33}$$

on which the authors work to obtain closed form expressions of the Green function, [ADG$^+$22, Proposition 2.10].

The same approach can be used for the sphere just by considering its corresponding eigenvalues (1.6) and addition formula (1.9). Thus, for a general two-point homogeneous space, we have

$$\begin{aligned} g(\vartheta) &= \frac{1}{4\kappa^2(\alpha+\beta+1)} \left(\sum_{k=1}^{\infty} \frac{(\alpha+\beta+1)_k}{k(\beta+1)_k} \cos^{2k}(\kappa\vartheta) - \gamma - \psi(\alpha+\beta+2) \right) \\ &= \frac{\cos^2(\kappa\vartheta)}{4\kappa^2(\beta+1)}\, {}_3\mathrm{F}_2\left(\left. \begin{matrix} 1, 1, \alpha+\beta+2 \\ 2, \beta+2 \end{matrix} \right| \cos^2(\kappa\vartheta) \right) \\ &\quad - \frac{1}{4\kappa^2(\alpha+\beta+1)} \left(\gamma - \psi(\alpha+\beta+2)\right). \end{aligned} \tag{4.34}$$

It is easy to see that for the sphere the function coincides with that of [BL22, Proposition 3.1].

From this general expression, we can deduce the constant $\mathcal{B}_{\mathcal{M}}$ in the asymptotic expression of the Green function,

$$g(\vartheta) = \frac{\mathcal{B}_{\mathcal{M}}}{\vartheta^{d-2}} + O\left(\frac{1}{\vartheta^{d-3}}\right), \qquad \vartheta \to 0, \tag{4.35}$$

in the case $d > 2$. Indeed, we have to compute the limit

$$\begin{aligned} \mathcal{B}_{\mathcal{M}} &= \lim_{\vartheta\to 0} \vartheta^{d-2} g(\vartheta) = \frac{1}{4\kappa^2(\beta+1)} \lim_{\vartheta\to 0} \vartheta^{d-2}\, {}_3\mathrm{F}_2\left(\left. \begin{matrix} 1, 1, \alpha+\beta+2 \\ 2, \beta+2 \end{matrix} \right| \cos^2(\kappa\vartheta) \right) \\ &= \frac{1}{4\kappa^2(\beta+1)} \frac{1}{\kappa^{d-2}} \lim_{\vartheta\to 0} \left(\frac{\kappa\vartheta}{\sin(\kappa\vartheta)} \right)^{d-2} \left(\sin^2(\kappa\vartheta)\right)^{\frac{d-2}{2}}\, {}_3\mathrm{F}_2\left(\left. \begin{matrix} 1, 1, \alpha+\beta+2 \\ 2, \beta+2 \end{matrix} \right| \cos^2(\kappa\vartheta) \right) \\ &= \frac{1}{4\kappa^d(\beta+1)} \lim_{x\to 1} (1-x)^{\alpha}\, {}_3\mathrm{F}_2\left(\left. \begin{matrix} 1, 1, \alpha+\beta+2 \\ 2, \beta+2 \end{matrix} \right| x \right). \end{aligned}$$

To perform this limit, we need the asymptotics of the generalized hypergeometric function around $x = 1$. From [Büh87], it turns out that

$${}_3\mathrm{F}_2\left(\left. \begin{matrix} a, b, c \\ e, f \end{matrix} \right| x \right) \sim (1-x)^s \frac{\Gamma(e)\Gamma(f)\Gamma(-s)}{\Gamma(a)\Gamma(b)\Gamma(c)}, \qquad x \to 1,$$

where $s = e + f - (a+b+c)$, if $s < 0$. In our case, $s = -\alpha < 0$ and thus

$$\begin{aligned} \mathcal{B}_{\mathcal{M}} &= \frac{1}{4\kappa^d(\beta+1)} \frac{\Gamma(\beta+2)\Gamma(\alpha)}{\Gamma(\alpha+\beta+2)} \\ &= \frac{\Gamma(\alpha)\Gamma(\beta+1)}{4\kappa^d\Gamma(\alpha+\beta+2)}. \end{aligned} \tag{4.36}$$

The knowledge of this dominant term will be enough to carry on our analysis.

As a final observation, (4.35) also can be expressed in terms of the chordal distance:

$$g(\vartheta) = \mathcal{B}_{\mathcal{M}} \kappa^{d-2} \frac{1}{\sin(\kappa\vartheta)^{d-2}} + O\left(\frac{1}{\sin(\kappa\vartheta)^{d-3}}\right), \qquad \vartheta \to 0, \tag{4.37}$$

coinciding with [ADG+22, eq. (2.9)] for projective spaces, i.e., $\kappa = 1$.

4.3 Energy decomposition

In this section we will deduce a connection between the discrete Green energy of an N-point configuration X_N and the Green energy of an associated function $f \in L^2(\mathcal{M})$ by generalizing to two-point homogeneous manifolds an idea sketched in [LN75, SM76]. This argument is described in detail in [Lau21, Appendix B] for a bounded region in the plane.

For a fixed $a > 0$, consider the following terms:

$$\begin{aligned}
U_{BB} &= N^2 \int_{x,y\in\mathcal{M}} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) = 0,\\
U_{ij} &= G_{\mathcal{M}}(x_i, x_j),\\
\widehat{U}_i &= -\frac{2N}{V(a)} \int_{B(x_i,a)} \int_{\mathcal{M}} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) = 0,\\
\widehat{U}_{ij} &= \frac{1}{V(a)^2} \int_{B(x_i,a)} \int_{B(x_j,a)} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y).
\end{aligned}$$

Define $\alpha(\mathcal{M},a)$, $\gamma(\mathcal{M},a)$ and $\delta(\mathcal{M},a)$ by

$$E_{\mathcal{M}}(x_1,\ldots,x_N) = \underbrace{U_{BB} + \sum_{i=1}^{N} \widehat{U}_i + \sum_{i,j} \widehat{U}_{ij}}_{\alpha(\mathcal{M},a)} \underbrace{- \sum_{i=1}^{N} \widehat{U}_{ii}}_{\gamma(\mathcal{M},a)} + \underbrace{\sum_{i\neq j} (U_{ij} - \widehat{U}_{ij})}_{\delta(\mathcal{M},a)}.$$

Observe that

$$\begin{aligned}
\alpha(\mathcal{M},a) &= N^2 \int_{x,y\in\mathcal{M}} G_{\mathcal{M}}(x,y) h_{X_N}^{(a)}(x) h_{X_N}^{(a)}(y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\\
&= N^2 E_{\mathcal{M}}\left(h_{X_N}^{(a)}\right),
\end{aligned} \tag{4.38}$$

with

$$h_{X_N}^{(a)}(x) := \frac{1}{N} \sum_{i=1}^{N} \frac{1}{V(a)} \chi_{B(x_i,a)}(x) - 1.$$

Thus,

$$E_{\mathcal{M}}(x_1,\ldots,x_N) = N^2 E_{\mathcal{M}}\left(h_{X_N}^{(a)}\right) + \gamma(\mathcal{M},a) + \delta(\mathcal{M},a). \tag{4.39}$$

This decomposition of the Green energy is valid for any radius a. In particular, since the order of the optimal separation is $N^{-1/d}$, a natural choice for the radius is $a = \epsilon N^{-1/d}$. In that case, $h_{X_N}^{(\epsilon N^{-1/d})}$ is the function $h_{X_N,\epsilon}$ from the definition (4.18) and (4.39) becomes

$$E_{\mathcal{M}}(x_1,\ldots,x_N) = N^2 E_{\mathcal{M}}\left(h_{X_N,\epsilon}\right) + \gamma(\mathcal{M},\epsilon N^{-1/d}) + \delta(\mathcal{M},\epsilon N^{-1/d}). \tag{4.40}$$

Since $E_{\mathcal{M}}\left(h_{X_N,\epsilon}\right) \approx D_{\mathcal{M}}^{\epsilon}(X_N)^2$, we have found a relationship between the discrete Green energy and the Sobolev discrepancy.

In the next sections, we will perform our analysis by considering a radius $a \to 0$. Finally, we will specialize the obtained results to $a = \epsilon N^{-1/d}$ to derive a lower bound for $\mathcal{E}(\mathcal{M},N)$ and, using the aforementioned connection with the discrete energy, an upper bound for $D_{\mathcal{M}}^{\epsilon}(X_N)$.

4.3.1 Lower bound for the discrete Green energy

The decomposition in (4.39) readily yields a lower bound for the discrete Green energy. Indeed, since the energy of a function is nonnegative, we have $E_{\mathcal{M}}(h_{X_N}^{(a)}) \geq 0$ for any $a > 0$ and then

$$E_{\mathcal{M}}(x_1,\ldots,x_N) \geq \gamma(\mathcal{M},a) + \delta(\mathcal{M},a).$$

We now need to find lower bounds for $\gamma(\mathcal{M},a)$ and $\delta(\mathcal{M},a)$. From Lemma 4.2.1, we immediately have

$$\begin{aligned}
\delta(\mathcal{M},a) &= \sum_{i\neq j}\left(G_{\mathcal{M}}(x_i,x_j) - \frac{1}{V(a)^2}\int_{B(x_i,a)}\int_{B(x_j,a)} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(y)\,\mathrm{d}\sigma(x)\right)\\
&\geq \sum_{i\neq j}\left(G_{\mathcal{M}}(x_i,x_j) - \frac{1}{V(a)}\int_{B(x_i,a)} \left(G_{\mathcal{M}}(x,x_j) + K(\mathcal{M},a)\right)\mathrm{d}\sigma(x)\right)\\
&\geq \sum_{i\neq j}\left(G_{\mathcal{M}}(x_i,x_j) - \left(G_{\mathcal{M}}(x_i,x_j) + 2K(\mathcal{M},a)\right)\right)\\
&= -2N(N-1)K(\mathcal{M},a),
\end{aligned} \tag{4.41}$$

(and moreover, although we do not use it in the proof, if $B(x_i,a)\cap B(x_j,a) = \emptyset$ then the inequalities above are equalities).

On the other hand, an elementary symmetry argument shows that

$$\gamma(\mathcal{M},a) = -\frac{N}{V(a)^2}\int_{B(x_0,a)}\int_{B(x_0,a)} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y),$$

where x_0 is any point in $\mathcal{M}$. We obtain a simpler formula for γ using the fact that the integral in $\mathcal{M}$ of $G_{\mathcal{M}}(x,\cdot)$ is zero:

$$\begin{aligned}
\gamma(\mathcal{M},a) &= -\frac{N}{V(a)^2}\int_{x\in B(x_0,a)}\left[\int_{y\in\mathcal{M}} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(y) - \int_{y\notin B(x_0,a)} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(y)\right]\mathrm{d}\sigma(x)\\
&= \frac{N}{V(a)^2}\int_{x\in B(x_0,a)}\int_{y\notin B(x_0,a)} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(y)\,\mathrm{d}\sigma(x)\\
&= \frac{N}{V(a)^2}\int_{y\notin B(x_0,a)}\int_{x\in B(x_0,a)} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y).
\end{aligned}$$

Again from Lemma 4.2.1, we conclude

$$\begin{aligned}\gamma(\mathcal{M},a) &= \frac{N}{V(a)}\int_{y\notin B(x_0,a)} (G_{\mathcal{M}}(x_0,y)+K(\mathcal{M},a))\,\mathrm{d}\sigma(y)\\ &= N\left(\frac{1-V(a)}{V(a)}K(\mathcal{M},a)-\frac{1}{V(a)}\int_{y\in B(x_0,a)} G_{\mathcal{M}}(x_0,y)\,\mathrm{d}\sigma(y)\right)\\ &= N\left(\frac{1-V(a)}{V(a)}K(\mathcal{M},a)-\Theta(\mathcal{M},a)\right).\end{aligned} \tag{4.42}$$

Putting all together, we have proved that for any collection of N points $x_1,\dots,x_N\in\mathcal{M}$,

$$\begin{aligned}E_{\mathcal{M}}(x_1,\dots,x_N) &\geq \gamma(\mathcal{M},a)+\delta(\mathcal{M},a)\\ &\geq N\left\{\left(1-2N+\frac{1}{V(a)}\right)K(\mathcal{M},a)-\Theta(\mathcal{M},a)\right\}.\end{aligned} \tag{4.43}$$

4.3.2 Upper bound for the Green energy of $h^{(a)}_{X_N}$

Let $X_N=\{x_1,\dots,x_N\}\subset\mathcal{M}$ be a collection of N points minimizing the discrete Green energy. From (4.39),

$$E_{\mathcal{M}}\left(h^{(a)}_{X_N}\right)=\frac{1}{N^2}\left(\mathcal{E}_G(\mathcal{M},N)-(\gamma(\mathcal{M},a)+\delta(\mathcal{M},a))\right).$$

Thus, combining Proposition 4.1.3 and the second inequality (4.43), we obtain that for $N\in\mathbb{N}$ sufficiently large,

$$E_{\mathcal{M}}\left(h^{(a)}_{X_N}\right)\leq\frac{1}{N^2}\left(-C_{\mathcal{M}}N^{2-2/d}-N\left\{\left(1-2N+\frac{1}{V(a)}\right)K(\mathcal{M},a)-\Theta(\mathcal{M},a)\right\}\right). \tag{4.44}$$

4.3.3 Upper bound for the Green energy of $h^{(a)}_{X_N}$

From (4.38) and the definition of $\alpha(\mathcal{M},a)$,

$$\begin{aligned}E_{\mathcal{M}}\left(h^{(a)}_{X_N}\right)=\frac{1}{N^2}\Bigg(&\sum_{i\neq j}\frac{1}{V(a)^2}\int_{B(x_i,a)}\int_{B(x_j,a)} G_{\mathcal{M}}(x,y)\ \mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\\ &+\sum_{i=1}^{N}\frac{1}{V(a)^2}\int_{B(x_i,a)}\int_{B(x_i,a)} G_{\mathcal{M}}(x,y)\ \mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)\Bigg).\end{aligned} \tag{4.45}$$

The second term corresponds to $-\gamma(\mathcal{M},a)$ in (4.39). The first term in (4.45) can be bounded from below by the minimal Green energy. Indeed, since the measures $\frac{\chi_{B(x_i,a)}}{V(a)}\sigma$ are probability measures,

$$\begin{aligned}\mathcal{E}_G(\mathcal{M},N) &\leq \int_{B(x_1,a)}\cdots\int_{B(x_N,a)}\sum_{i\neq j}G_{\mathcal{M}}(x_i,x_j)\frac{\mathrm{d}\sigma(x_1)}{V(a)}\cdots\frac{\mathrm{d}\sigma(x_N)}{V(a)}\\ &= \sum_{i\neq j}\frac{1}{V(a)^2}\int_{B(x_i,a)}\int_{B(x_j,a)} G_{\mathcal{M}}(x_i,x_j)\,\mathrm{d}\sigma(x_i)\,\mathrm{d}\sigma(x_j).\end{aligned}$$

Combining this bound with (4.2), we get

$$E_{\mathcal{M}}\left(h_{X_N}^{(a)}\right) \geq \frac{1}{N^2}\left(-c_{\mathcal{M}}N^{2-2/d} - \gamma(\mathcal{M},a)\right). \tag{4.46}$$

4.4 Proofs

4.4.1 Upper bounds for the discrete Green energy

We start by proving Theorem 4.1.2 for the sphere $\mathbb{S}^d$ (recall that the projective cases were already proved in [ADG+22]).

Proof of Theorem 4.1.2. The expected Green energy for $\pi_L^{(\alpha,\beta)}$-point configurations sampled from the harmonic ensemble on a two-point homogeneous manifold $\mathcal{M}$ is

$$\mathbb{E}[E_{\mathcal{M}}(X_N)] = \int_{\mathcal{M}}\int_{\mathcal{M}} \left[K_L^{(\alpha,\beta)}(x,x)K_L^{(\alpha,\beta)}(y,y) - K_L^{(\alpha,\beta)}(x,y)^2\right] G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y).$$

Since $K_L^{(\alpha,\beta)}(x,x)$ is a constant (recall (1.24)) and $\int_{\mathcal{M}}\int_{\mathcal{M}} G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) = 0$ by definition of the Green function,

$$\mathbb{E}[E_{\mathcal{M}}(X_N)] = -\int_{\mathcal{M}}\int_{\mathcal{M}} K_L^{(\alpha,\beta)}(x,y)^2 G_{\mathcal{M}}(x,y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y).$$

From (4.37), we have that $G_{\mathcal{M}}(x,y) = g(\vartheta(x,y))$ with

$$g(\vartheta) = \mathcal{B}_{\mathcal{M}}\kappa^{d-2}\frac{1}{\sin(\kappa\vartheta)^{d-2}} + O\left(\frac{1}{\sin(\kappa\vartheta)^{d-3}}\right), \qquad \vartheta \to 0.$$

Thus, there exists a constant $D_{\mathcal{M}} > 0$ such that

$$\left|g(\vartheta) - \mathcal{B}_{\mathcal{M}}\kappa^{d-2}\frac{1}{\sin(\kappa\vartheta)^{d-2}}\right| \leq \frac{D_{\mathcal{M}}}{\sin(\kappa\vartheta)^{d-3}}$$

around $\vartheta = 0$. Since the Green function is $\mathcal{C}^\infty$ away from the diagonal and the manifold $\mathcal{M}$ is compact, the inequality above holds for any $\vartheta \leq D$ for some updated constant $D_{\mathcal{M}} > 0$.

Therefore,

$$\begin{aligned}
&\mathbb{E}[E_{\mathcal{M}}(X_N)] \\
&\quad = -\int_{\mathcal{M}}\int_{\mathcal{M}} K_L^{(\alpha,\beta)}(x,y)^2 g(\vartheta(x,y))\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) \\
&\quad = -\int_{\mathcal{M}}\int_{\mathcal{M}} K_L^{(\alpha,\beta)}(x,y)^2\left[g(\vartheta(x,y)) - \mathcal{B}_{\mathcal{M}}\kappa^{d-2}\frac{1}{\sin(\kappa\vartheta(x,y))^{d-2}}\right]\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) \\
&\qquad - \mathcal{B}_{\mathcal{M}}\kappa^{d-2}\int_{\mathcal{M}}\int_{\mathcal{M}} K_L^{(\alpha,\beta)}(x,y)^2\frac{1}{\sin(\kappa\vartheta(x,y))^{d-2}}\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) \\
&\quad \leq -D_{\mathcal{M}}\int_{\mathcal{M}}\int_{\mathcal{M}} K_L^{(\alpha,\beta)}(x,y)^2\frac{1}{\sin(\kappa\vartheta(x,y))^{d-3}}\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) \\
&\qquad - \mathcal{B}_{\mathcal{M}}\kappa^{d-2}\int_{\mathcal{M}}\int_{\mathcal{M}} K_L^{(\alpha,\beta)}(x,y)^2\frac{1}{\sin(\kappa\vartheta(x,y))^{d-2}}\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y).
\end{aligned} \tag{4.47}$$

Since the projective cases are already solved, we set $\mathcal{M} = \mathbb{S}^d$. Recall that the parameters are $\alpha = \beta = \lambda$, with $\lambda := d/2 - 1$, and $\kappa = 1/2$. Then

$$\frac{1}{\sin(\kappa\vartheta(x,y))^s} = \frac{1}{\sin\left(\frac{\vartheta(x,y)}{2}\right)^s} = \frac{2^s}{|x-y|^s},$$

where $|x-y|$ is the Euclidean distance, and we get

$$\begin{aligned}\mathbb{E}[E_{\mathbb{S}^d}(X_N)] \leq &- D_{\mathbb{S}^d} 2^{d-3} \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} K_L^{(\lambda,\lambda)}(x,y)^2 \frac{1}{|x-y|^{d-3}} \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) \\ &- \mathcal{B}_{\mathbb{S}^d} \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} K_L^{(\lambda,\lambda)}(x,y)^2 \frac{1}{|x-y|^{d-2}} \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y).\end{aligned} \tag{4.48}$$

Observe that the expected s-Riesz energy for sets X_N of $N = \pi_L^{(\lambda,\lambda)}$ points sampled from the harmonic ensemble on $\mathbb{S}^d$ is given by

$$\begin{aligned}\mathbb{E}[E_s(X_N)] &= \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} \left[K_L^{(\lambda,\lambda)}(x,x)^2 - K_L^{(\lambda,\lambda)}(x,y)^2\right] \frac{1}{|x-y|^s} \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) \\ &= V_s(\mathbb{S}^d) N^2 - \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} K_L^{(\lambda,\lambda)}(x,y)^2 \frac{1}{|x-y|^s} \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y),\end{aligned}$$

where recall from (1.14) that

$$V_s(\mathbb{S}^d) = \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} \frac{1}{|x-y|^s} \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) = 2^{d-s-1} \frac{\Gamma\left(\frac{d+1}{2}\right)\Gamma\left(\frac{d-s}{2}\right)}{\sqrt{\pi}\,\Gamma\left(d - \frac{s}{2}\right)} \tag{4.49}$$

for $0 < s < d$, so the integrals in (4.48) correspond to the second order term in the expected s-Riesz energy up to the constant 2^s. From [BMOC16], for $0 < s < d$,

$$\mathbb{E}[E_s(X_N)] = V_s(\mathbb{S}^d) N^2 - C_{s,d} N^{1+s/d} + o(N^{1+s/d}),$$

where

$$C_{s,d} = 2^{s - \frac{s}{d}} V_s(\mathbb{S}^d) (d!)^{-1+\frac{s}{d}} \frac{d\,\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(\frac{1+s}{2}\right)\Gamma\left(d-\frac{s}{2}\right)}{\sqrt{\pi}\Gamma\left(1+\frac{s}{2}\right)\Gamma\left(1+\frac{s+d}{2}\right)}. \tag{4.50}$$

Thus,

$$\int_{\mathbb{S}^d}\int_{\mathbb{S}^d} K_L^{(\lambda,\lambda)}(x,y)^2 \frac{1}{|x-y|^s} \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) = C_{s,d} N^{1+s/d} + o\left(N^{1+s/d}\right) \tag{4.51}$$

for $0 < s < d$. Moreover, since trivially $\mathbb{E}\left[\sum_{i\neq j} \frac{1}{|x-y|^0}\right] = N^2 - N$,

$$\int_{\mathbb{S}^d}\int_{\mathbb{S}^d} K_L^{(\lambda,\lambda)}(x,y)^2 \frac{1}{|x-y|^0} \,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) = N. \tag{4.52}$$

For $d > 3$, using (4.51) with $s = d-3$ and $s = d-2$ in (4.48), we have

$$\begin{aligned}\mathbb{E}[E_{\mathbb{S}^d}(X_N)] \leq &- D_{\mathbb{S}^d} 2^{d-3} \left(C_{d-3,d} N^{2-3/d} + o\left(N^{2-3/d}\right)\right) \\ &- \mathcal{B}_{\mathbb{S}^d} \left(C_{d-2,d} N^{2-2/d} + o\left(N^{2-2/d}\right)\right) \\ = &- \mathcal{B}_{\mathbb{S}^d} C_{d-2,d} N^{2-2/d} + o\left(N^{2-2/d}\right).\end{aligned}$$

For $d=3$, using (4.52) and (4.51) with $s=1$ in (4.48), we have

$$\begin{aligned}\mathbb{E}[E_{\mathbb{S}^3}(X_N)] \leq & - D_{\mathbb{S}^3}N - \mathcal{B}_{\mathbb{S}^3}\left(C_{1,3}N^{2-2/3} + o\left(N^{2-2/3}\right)\right) \\ = & - \mathcal{B}_{\mathbb{S}^3}C_{1,3}N^{2-2/3} + o\left(N^{2-2/3}\right).\end{aligned}$$

Therefore, for any $d \geq 3$,

$$\mathbb{E}[E_{\mathbb{S}^d}(X_N)] \leq -\mathcal{B}_{\mathbb{S}^d}C_{d-2,d}N^{2-2/d} + o\left(N^{2-2/d}\right).$$

To obtain the leading coefficient, from (4.50) we get

$$\begin{aligned}C_{d-2,d} &= 2^{d-2-\frac{d-2}{d}}V_{d-2}(\mathbb{S}^d)(d!)^{-1+\frac{d-2}{d}}\frac{d\,\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(d-\frac{d-2}{2}\right)}{\sqrt{\pi}\,\Gamma\left(1+\frac{d-2}{2}\right)\Gamma\left(1+\frac{2d-2}{2}\right)} \\ &= 2^{d-3+\frac{2}{d}}V_{d-2}(\mathbb{S}^d)(d!)^{-\frac{2}{d}}\frac{d\,\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(\frac{d}{2}+1\right)}{\sqrt{\pi}\,\Gamma\left(\frac{d}{2}\right)\Gamma\left(d\right)},\end{aligned}$$

with

$$V_{d-2}(\mathbb{S}^d) = 2\frac{\Gamma\left(\frac{d+1}{2}\right)}{\sqrt{\pi}\,\Gamma\left(\frac{d}{2}+1\right)},$$

see (4.49). Then

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

From (4.36),

$$\mathcal{B}_{\mathbb{S}^d} = \frac{\Gamma(\alpha)\Gamma(\beta+1)}{4\kappa^d\Gamma(\alpha+\beta+2)} = \frac{\Gamma\left(\frac{d}{2}-1\right)\Gamma\left(\frac{d}{2}\right)2^{d-2}}{\Gamma\left(d\right)}$$

and putting all together

$$\mathcal{B}_{\mathbb{S}^d}C_{d-2,d} = 2^{2d-4+\frac{2}{d}}(d!)^{-\frac{2}{d}}\frac{d\,\Gamma\left(1+\frac{d}{2}\right)\Gamma\left(\frac{d+1}{2}\right)\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(\frac{d}{2}-1\right)}{\pi\,\Gamma\left(d\right)^2}.$$

Applying the Legendre duplication formula,

$$\begin{aligned}\mathcal{B}_{\mathbb{S}^d}C_{d-2,d} &= 2^{2d-4+\frac{2}{d}}(d!)^{-\frac{2}{d}}\frac{d\,2^{1-(d+1)}\sqrt{\pi}\,\Gamma\left(d+1\right)2^{1-(d-2)}\sqrt{\pi}\,\Gamma\left(d-2\right)}{\pi\,\Gamma\left(d\right)^2} \\ &= 2^{-1+\frac{2}{d}}(d!)^{-\frac{2}{d}}\frac{d\,\Gamma\left(d+1\right)\Gamma\left(d-2\right)}{\Gamma\left(d\right)^2} \\ &= \frac{\left(\frac{d}{2}\right)^2}{\left(\frac{d}{2}-1\right)\left(d-1\right)}\left(\frac{1}{\frac{d}{2}\Gamma(d)}\right)^{2/d} \\ &= \frac{(\alpha+1)^2}{\alpha(2\alpha+1)}\left(\frac{\Gamma(\beta+1)}{\Gamma(\alpha+2)\Gamma(\alpha+\beta+2)}\right)^{2/d}.\end{aligned}$$

□

Proposition 4.1.3 is proved in [ADG+22, Corollary 4.3] for projective spaces by using the jittered sampling, a determinantal point process that distributes one point in each piece of a partition of $\mathcal{M}$. We reproduce the proof here including the sphere case. Its first ingredient is the existence of a partition of $\mathcal{M}$ with the following properties.

Proposition 4.4.1 ([GL17, Theorem 2])**.** *For each two-point homogeneous manifold $\mathcal{M}$, there exist positive constants c_1 and c_2 such that for all $N \in \mathbb{N}$ sufficiently large, there is a partition of $\mathcal{M}$ into N regions, each of measure $1/N$, contained in a geodesic ball of radius $c_1 N^{-1/d}$ and containing a geodesic ball of radius $c_2 N^{-1/d}$.*

We observe that in [GL17] this result is stated in a much more general setting which includes all Riemannian manifolds.

Proof of Proposition 4.1.3. For $N \in \mathbb{N}$ sufficiently large, from Proposition 4.4.1 we have a partition of $\mathcal{M}$ into N equal area regions $D_1, \ldots, D_N$ contained in geodesic balls of radius $c_1 N^{-1/d}$. Denoting $\mathrm{d}\sigma_j(x) = N\chi_{D_j}(x)\,\mathrm{d}\sigma(x)$, we have

$$
\begin{aligned}
\mathcal{E}_G(\mathcal{M}, N) &\leq \int_{\mathcal{M}} \cdots \int_{\mathcal{M}} \sum_{i \neq j} G_{\mathcal{M}}(x_i, x_j)\,\mathrm{d}\sigma_1(x_1) \cdots \mathrm{d}\sigma_N(x_N) \\
&= N^2 \sum_{i \neq j} \int_{D_i} \int_{D_j} G_{\mathcal{M}}(x_i, x_j)\,\mathrm{d}\sigma(x_i)\,\mathrm{d}\sigma(x_j) \\
&= N^2 \Bigg(\underbrace{\int_{\mathcal{M}} \int_{\mathcal{M}} G_{\mathcal{M}}(x, y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y)}_{=0} - \sum_{i=1}^{N} \int_{D_i} \int_{D_i} G_{\mathcal{M}}(x, y)\,\mathrm{d}\sigma(x)\,\mathrm{d}\sigma(y) \Bigg).
\end{aligned}
$$

From (4.24), there exists a constant $k_{\mathcal{M}} > 0$ such that

$$
G_{\mathcal{M}}(x, y) \leq \frac{k_{\mathcal{M}}}{\vartheta(x, y)^{d-2}}
$$

for $x, y \in D_i$. Therefore,

$$
\begin{aligned}
\mathcal{E}_G(\mathcal{M}, N) &\leq -N^2 \sum_{i=1}^{N} \frac{c_3}{\operatorname{diam}(D_i)^{d-2}} \sigma(D_i)^2 \\
&\leq -N \frac{c_3}{(2c_1)^{d-2} N^{-(d-2)/d}} \\
&= -\frac{c_3}{(2c_1)^{d-2}} N^{2-2/d}.
\end{aligned}
$$

□

4.4.2 Proofs of Theorem 4.1.1 and Theorem 4.1.7

Here we prove Theorem 4.1.1 and Theorem 4.1.7 by applying the bounds obtained in the previous sections for $a = \epsilon N^{-1/d}$.

We will need the following asymptotics.

Lemma 4.4.2. *For $a \to 0$, we have:*

$$\begin{aligned} V(a) &= \frac{\kappa^d}{\gamma_{\alpha,\beta}\, d} a^d + O\left(a^{d+1}\right), \\ v(a) &= \frac{\kappa^d}{\gamma_{\alpha,\beta}} a^{d-1} + O\left(a^d\right), \\ K(\mathcal{M}, a) &= \frac{1}{2(d+2)} a^2 + O\left(a^3\right), \\ \Theta(\mathcal{M}, a) &= \frac{d\mathcal{B}_{\mathcal{M}}}{2} a^{2-d} + O\left(a^{3-d}\right). \end{aligned}$$

The last of these equalities needs $d > 2$, but the rest of them hold in all cases.

Proof. By expanding (4.19) around $a = 0$,

$$v(a) = \frac{\kappa}{\gamma_{\alpha,\beta}} \kappa^{2\alpha+1} a^{2\alpha+1} + O\left(a^{2\alpha+2}\right) = \frac{\kappa^d}{\gamma_{\alpha,\beta}} a^{d-1} + O\left(a^d\right).$$

Since $V(a) = \int_0^a v(r)\,\mathrm{d}r$, integrating the previous expansion we get

$$V(a) = \frac{\kappa^d}{\gamma_{\alpha,\beta}\, d} a^d + O\left(a^{d+1}\right).$$

This yields the third formula of the lemma:

$$K(\mathcal{M}, a) = \frac{1}{a^d} \int_0^a r^{d-1} \int_0^r u \,\mathrm{d}u\,\mathrm{d}r + \text{l.o.t} = \frac{1}{2(d+2)} a^2 + O\left(a^3\right).$$

For the last asymptotic we reason in the same way:

$$\begin{aligned} \Theta(\mathcal{M}, a) &= \frac{1}{V(a)} \int_{y \in B(x_0, a)} G_{\mathcal{M}}(x_0, y)\,\mathrm{d}\sigma(y) \\ &\overset{(4.20)}{=} \frac{1}{V(a)} \int_0^a \phi(r) v(r)\,\mathrm{d}r \\ &\overset{(4.35)}{=} \frac{d}{a^d} \int_0^a \frac{\mathcal{B}_{\mathcal{M}}}{r^{d-2}} r^{d-1}\,\mathrm{d}r + \text{l.o.t} \\ &= \frac{d\mathcal{B}_{\mathcal{M}}}{2} a^{2-d} + \text{l.o.t.} \end{aligned}$$

□

Proof of Theorem 4.1.1. Combining Lemma 4.4.2 with the lower bound (4.43) we have

$$E_{\mathcal{M}}(x_1, \ldots, x_N) \geq N \left\{ \left(1 - 2N + \frac{\gamma_{\alpha,\beta}\, d\, \kappa^{-d}}{a^d}\right) \frac{a^2}{2(d+2)} - \frac{d\mathcal{B}_{\mathcal{M}}}{2} a^{2-d} \right\} + \text{l.o.t.}$$

Choosing a of the form $\epsilon N^{-1/d}$ with ϵ a constant, we conclude (up to l.o.t.):

$$E_{\mathcal{M}}(x_1, \ldots, x_N) \geq -\, N^{2-2/d} \left(\frac{\epsilon^2}{d+2} + \frac{d\,\epsilon^{2-d}}{2} \left(\underbrace{\mathcal{B}_{\mathcal{M}} - \frac{\gamma_{\alpha,\beta}\, \kappa^{-d}}{d+2}}_{\mathcal{A}_{\mathcal{M}}} \right) \right). \tag{4.53}$$

This last formula is maximized choosing

$$\epsilon = \left(\frac{d(d-2)(d+2)}{4}\mathcal{A}_{\mathcal{M}}\right)^{\frac{1}{d}}.$$

Observe that from (4.36) and the definition of $\gamma_{\alpha,\beta}$,

$$\begin{aligned}\mathcal{A}_{\mathcal{M}} &= \frac{\Gamma(\alpha)\Gamma(\beta+1)}{4\kappa^d\Gamma(\alpha+\beta+2)} - \frac{\Gamma(\alpha+1)\Gamma(\beta+1)}{2\kappa^d(d+2)\Gamma(\alpha+\beta+2)} \\ &= \frac{\Gamma(\alpha)\Gamma(\beta+1)}{4\kappa^d\Gamma(\alpha+\beta+2)}\left(1-\frac{2\alpha}{d+2}\right) \\ &= \frac{\Gamma(\alpha)\Gamma(\beta+1)}{\kappa^d(d+2)\Gamma(\alpha+\beta+2)}.\end{aligned} \tag{4.54}$$

Thus,

$$\begin{aligned}\epsilon &= \left(\frac{d(d-2)}{4}\frac{\Gamma(\alpha)\Gamma(\beta+1)}{\kappa^d\Gamma(\alpha+\beta+2)}\right)^{\frac{1}{d}} \\ &= \kappa^{-1}\left(\frac{\Gamma(\alpha+2)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}\right)^{\frac{1}{d}}\end{aligned}$$

and for that concrete value of ϵ:

$$E_{\mathcal{M}}(x_1,\ldots,x_N) \geq -\frac{d\,\epsilon^2 N^{2-2/d}}{d^2-4} + o\left(N^{2-2/d}\right),$$

which yields the claimed lower bound. □

Remark 4.4.3. The optimal radius ϵ turns out to be the constant $\operatorname{sep}_{\mathcal{M}}$ given by Criado del Rey in his lower bound for the separation distance (4.15). This means that if we apply our argument to a set X_N minimizing the Green energy, then the inequality in the estimate of $\delta(\mathcal{M},a)$ in (4.41) is indeed an equality when we take $a=\epsilon N^{-1/d}$. Thus, all the precision we lose comes from the term $\alpha\left(\mathcal{M},\epsilon N^{-1/d}\right)$ in (4.38) we throw away in the estimate (4.43). This discarded term, however, has the same order $N^{2-2/d}$ as the sum of $\gamma\left(\mathcal{M},\epsilon N^{-1/d}\right)$ and $\delta\left(\mathcal{M},\epsilon N^{-1/d}\right)$ as a consequence of Theorem 4.1.7 and the equivalence $D^{\epsilon}_{\mathcal{M}}(X_N)^2 \approx E_{\mathcal{M}}(h_{X_N,\epsilon})$. Therefore, the neglected term plays an important role in the energy and the improvement of our lower bound calls for a better estimation of the term $\alpha\left(\mathcal{M},\epsilon N^{-1/d}\right)$, since nothing is lost in the other two terms.

Proof of Theorem 4.1.7. From the equivalence $D^{\epsilon}_{\mathcal{M}}(X_N)^2 \approx E_{\mathcal{M}}(h_{X_N,\epsilon})$, all we have to see is

$$N^{-2/d} \lesssim E_{\mathcal{M}}(h_{X_N,\epsilon}) \lesssim N^{-2/d}.$$

The upper bound follows from (4.44). Taking $a=\epsilon N^{-1/d}$ as in the proof of Theorem 4.1.1, for $N\in\mathbb{N}$ large enough we have

$$\begin{aligned}E_{\mathcal{M}}\left(h_{X_N,\epsilon}\right) = E_{\mathcal{M}}\left(h_{X_N}^{(\epsilon N^{-1/d})}\right) &\leq \frac{1}{N^2}\left(-C_{\mathcal{M}}N^{2-2/d} + N^{2-2/d}\left(\frac{\epsilon^2}{d+2}+\frac{d\,\epsilon^{2-d}}{2}\mathcal{A}_{\mathcal{M}}\right)\right) \\ &= N^{-2/d}\left(\frac{\epsilon^2}{d+2}+\frac{d\,\epsilon^{2-d}}{2}\mathcal{A}_{\mathcal{M}} - C_{\mathcal{M}}\right).\end{aligned}$$

where $\mathcal{A}_{\mathcal{M}}$ has been defined in (4.53). Then we can choose a constant depending on $\mathcal{M}$ and ϵ such that the previous inequality holds for any $N \geq 2$.

For the lower bound we use (4.46). Combining (4.42) with the asymptotics in Lemma 4.4.2,

$$-\gamma(\mathcal{M}, a) = N\left(\frac{d\,\mathcal{A}_{\mathcal{M}}}{2}a^{2-d} + O\left(a^{3-d}\right)\right), \quad a \to 0.$$

Applying this expansion with $a = \epsilon N^{-1/d}$ for a fixed $N \in \mathbb{N}$ and $\epsilon \to 0$,

$$\begin{aligned}-\gamma(\mathcal{M}, \epsilon N^{-1/d}) &= N^{2-2/d}\epsilon^{2-d}\left(\frac{d\,\mathcal{A}_{\mathcal{M}}}{2} + o_{\epsilon\to 0}(1)\right)\\ &\geq N^{2-2/d}\epsilon^{2-d}\frac{d\,\mathcal{A}_{\mathcal{M}}}{4}\end{aligned}$$

for ϵ small enough, since the constant $\mathcal{A}_{\mathcal{M}}$ is positive, see (4.54).

Combining this bound with (4.46), for ϵ sufficiently small we obtain

$$E_{\mathcal{M}}\left(h_{X_N,\epsilon}\right) \geq N^{-2/d}\left(-c_{\mathcal{M}} + \epsilon^{2-d}\frac{d\,\mathcal{A}_{\mathcal{M}}}{4}\right).$$

Since we are assuming $d > 2$, this provides a non-trivial bound for ϵ small enough.

□

4.4.3 Theorem 4.1.4

The upper bound of Theorem 4.1.7 together with the following Proposition proves Theorem 4.1.4.

Proposition 4.4.4. *Given $\epsilon_0 > 0$ and $C_1 > 0$, there exists $C_2 > 0$ depending on $\mathcal{M}, \epsilon_0$ and C_1 such that, for every set $X_N = \{x_1, \ldots, x_N\} \subset \mathcal{M}$ with Sobolev discrepancy*

$$D_{\mathcal{M}}^{\epsilon_0}(X_N) \leq C_1 N^{-1/d}, \tag{4.55}$$

the discrepancy of X_N satisfies

$$\mathbb{D}_{\infty}(X_N) \leq C_2 N^{-\frac{2}{3d}}. \tag{4.56}$$

Proof. The proof is similar to that of [MM21, Proposition 5.2].

Let $B = B(z, r)$ with $z \in \mathcal{M}$ and $r > 0$. We can assume that $r < D/2$. Let ϕ be a smooth function on $\mathbb{R}$ such that $\chi_{(-\infty,0]} \leq \phi \leq \chi_{(-\infty,1)}$. Given $0 < \epsilon < r/2$, we define $f_\epsilon^+(x) = \phi\left(\epsilon^{-1}(\vartheta(x,z) - r - \epsilon)\right)$ and $f_\epsilon^-(x) = \phi\left(\epsilon^{-1}(\vartheta(x,z) - r + 2\epsilon)\right)$. These functions satisfy that $0 \leq f_\epsilon^{\pm} \leq 1$ and

$$f_\epsilon^+(x) = \begin{cases} 1 & \text{if } \vartheta(x,z) < r + \epsilon, \\ 0 & \text{if } \vartheta(x,z) > r + 2\epsilon, \end{cases} \qquad f_\epsilon^-(x) = \begin{cases} 1 & \text{if } \vartheta(x,z) < r - 2\epsilon, \\ 0 & \text{if } \vartheta(x,z) > r - \epsilon. \end{cases}$$

It is easy to check that there exists a constant $C > 0$ depending on $\mathcal{M}$ such that

$$\sigma(B) - C\epsilon \leq \int_{\mathcal{M}} f_\epsilon^-\,\mathrm{d}\sigma \leq \int_{\mathcal{M}} f_\epsilon^+\,\mathrm{d}\sigma \leq \sigma(B) + C\epsilon \tag{4.57}$$

and

$$\|f_\epsilon^\pm\|_{\mathbb{H}^1(\mathcal{M})} \le C\epsilon^{-1/2}. \tag{4.58}$$

In particular, to prove (4.58), it is clear that ϕ is Lipschitz continuous, i.e., there exists $C > 0$ such that $|\phi(t) - \phi(s)| \le C|t - s|$. Therefore,

$$|f_\epsilon^\pm(x) - f_\epsilon^\pm(y)| \le C|\epsilon^{-1}(\vartheta(x,z) - \vartheta(y,z))| \le C\epsilon^{-1}\vartheta(x,y),$$

and from [Gri09, p.296],

$$\|\nabla f_\epsilon^\pm\|_\infty \le \sup_{x,y\in\mathcal{M}} \frac{|f_\epsilon^\pm(x) - f_\epsilon^\pm(y)|}{\vartheta(x,y)} \le \frac{C}{\epsilon},$$

so

$$\int_{\mathcal{M}} |\nabla f_\epsilon^+|^2 \, \mathrm{d}\sigma \le \frac{C'}{\epsilon^2}\sigma\left(B(z, r+2\epsilon)\backslash B(z, r+\epsilon)\right) = \frac{O(\epsilon)}{\epsilon^2} = O\left(\epsilon^{-1}\right).$$

The same bound can be obtained for f_ϵ^-. Applying the equivalence (4.17), the fact that $0 \le f_\epsilon^\pm \le 1$ and the previous bound, we have

$$\|f_\epsilon^\pm\|^2_{\mathbb{H}^1(\mathcal{M})} \approx \|f_\epsilon^\pm\|^2_{L^2(\mathcal{M})} + \|\nabla f_\epsilon^\pm\|^2_{L^2(\mathcal{M})} \le C''\epsilon^{-1}.$$

Recall from (4.18) that

$$h_{X_N,\epsilon_0} = \frac{1}{N}\sum_{j=1}^{N} \frac{1}{\sigma(D_j)}\chi_{D_j} - 1, \qquad D_j = B(x_j, \epsilon_0 N^{-1/d}).$$

Observe that if $\epsilon > \epsilon_0 N^{-1/d}$ then $f_\epsilon^+ \equiv 1$ in D_j for all $x_j \in B$. Since $f_\epsilon^+ \ge 0$,

$$\frac{|X_N \cap B|}{N} \le \frac{1}{N}\sum_{j=1}^{N}\frac{1}{\sigma(D_j)}\int_{D_j} f_\epsilon^+ \, \mathrm{d}\sigma = \int_{\mathcal{M}} f_\epsilon^+ h_{X_N,\epsilon_0} \, \mathrm{d}\sigma + \int_{\mathcal{M}} f_\epsilon^+ \, \mathrm{d}\sigma.$$

In the same way, since $f_\epsilon^- \equiv 0$ in D_j for all $x_j \notin B$ and $f_\epsilon^- \le 1$,

$$\frac{|X_N \cap B|}{N} \ge \frac{1}{N}\sum_{i=1}^{N}\frac{1}{\sigma(D_j)}\int_{D_j} f_\epsilon^- \, \mathrm{d}\sigma = \int_{\mathcal{M}} f_\epsilon^- h_{X_N,\epsilon_0} \, \mathrm{d}\sigma + \int_{\mathcal{M}} f_\epsilon^- \, \mathrm{d}\sigma.$$

Combining these bounds with (4.57), we have

$$\int_{\mathcal{M}} f_\epsilon^- h_{X_N,\epsilon_0} \, \mathrm{d}\sigma - C\epsilon \le \frac{|X_N \cap B|}{N} - \sigma(B) \le \int_{\mathcal{M}} f_\epsilon^+ h_{X_N,\epsilon_0} \, \mathrm{d}\sigma + C\epsilon,$$

from which

$$\begin{aligned}\left|\frac{|X_N \cap B|}{N} - \sigma(B)\right| &\le \max\left\{\left|\int_{\mathcal{M}} f_\epsilon^+ h_{X_N,\epsilon_0} \, \mathrm{d}\sigma\right|, \left|\int_{\mathcal{M}} f_\epsilon^- h_{X_N,\epsilon_0} \, \mathrm{d}\sigma\right|\right\} + C\epsilon \\ &\le \max\left\{\|f_\epsilon^-\|_{\mathbb{H}^1(\mathcal{M})}, \|f_\epsilon^+\|_{\mathbb{H}^1(\mathcal{M})}\right\} \|h_{X_N,\epsilon_0}\|_{\mathbb{H}^{-1}(\mathcal{M})} + C\epsilon,\end{aligned}$$

by definition of $\|h\|_{\mathbb{H}^{-1}(\mathcal{M})}$. From (4.58) and the hypothesis (4.55),

$$\left|\frac{|X_N \cap B|}{N} - \sigma(B)\right| \leq C'\epsilon^{-1/2}N^{-1/d} + C\epsilon. \tag{4.59}$$

This inequality holds under the condition that $\epsilon > \epsilon_0 N^{-1/d}$. Then we can take

$$\epsilon = N^{-\frac{2}{3d}}$$

for all N big enough and (4.56) follows from (4.59). □

Appendix A

Closed formulas for $K(\mathcal{M}, a)$ and $\Theta(\mathcal{M}, a)$

Although we have not used them in our analysis or proofs above, in the cases $\mathcal{M} = \mathbb{CP}^n, \mathbb{HP}^n, \mathbb{OP}^2$ it is possible to produce exact formulas for these two functions. We summarize them in the following result.

Proposition A.0.1. *Denoting $S = \sin a$, we have:*

$$K(\mathbb{CP}^n, a) = \frac{1}{4nVS^{2n}}\left((1-S^{2n})\log(1-S^2) + \sum_{k=1}^{n}\frac{S^{2k}}{k}\right),$$

$$\Theta(\mathbb{CP}^n, a) = \frac{1}{2nV}\left(-H_{n-1} - \log S + \frac{n}{2}\sum_{k=1}^{n-1}\frac{1}{k(n-k)S^{2k}}\right),$$

$$\begin{aligned}K(\mathbb{HP}^n, a) =& \frac{1}{4(2n+1)(2n(1-S^2)+1)V} \\ &\times \left[\frac{1}{S^{4n}}\left(\sum_{k=1}^{2n+1}\frac{S^{2k}}{k} + \log(1-S^2)\right) - (2n(1-S^2)+1)\log(1-S^2)\right],\end{aligned}$$

$$\begin{aligned}\Theta(\mathbb{HP}^n, a) =& \frac{1}{V}\left(\frac{n}{2(2n(1-S^2)+1)}\sum_{k=1}^{2n-1}\frac{1}{k(k+1)(2n-k)S^{2k}}\right. \\ &\left. - \frac{H_{2n-1}}{2(2n+1)} - \frac{\log S}{2(2n+1)} - \frac{1+2(n-1)S^2}{4(2n+1)(2n(1-S^2)+1)}\right),\end{aligned}$$

$$\begin{aligned}K(\mathbb{OP}^2, a) = & \frac{1}{1219680VS^{16}(-120S^6+396S^4-440S^2+165)}\times \\ & \big[S^2(815640S^{20} - 1826748S^{18} + 1019480S^{16} + 3465S^{14} + 3960S^{12} \\ & + 4620S^{10} + 5544S^8 + 6930S^6 + 9240S^4 + 13860S^2 + 27720) \\ & + 27720(120S^{22} - 396S^{20} + 440S^{18} - 165S^{16} + 1)\log(1-S^2)\big],\end{aligned}$$

$$\Theta(\mathbb{OP}^2, a) = \frac{1}{V}\left[\frac{1}{9240S^{14}\left(-120S^6+396S^4-440S^2+165\right)}\Big(101420S^{20} - 353334S^{18} + 427500S^{16} - 190150S^{14} + 9900S^{12} + 2310S^{10} + 924S^8 + 495S^6 + 330S^4 + 275S^2 + 330\Big) - \frac{1}{22}\ln S\right].$$

Proof. These are all obtained directly from the definitions (4.21) and (4.22). Once computed, their correctness can be checked by automatic differentiation. □

Resum en català

Estudiem problemes de minimització d'energia discreta en varietats 2-punts homogènies. Com que trobar configuracions de N punts amb energia òptima és molt complicat, recentment s'ha explorat l'ús de processos de punts aleatoris amb baixa energia esperada com a mètode per obtenir bones configuracions de punts.

Al Capítol 2, calculem la segona intensitat conjunta del procés de punts aleatoris donat pels zeros de polinomis el·líptics, el que ens permet recuperar l'energia logarítmica esperada a la 2-esfera prèviament calculada per Armentano, Beltrán i Shub. A més, obtenim l'energia de Riesz esperada per a aquest procés, que és notablement propera a l'energia òptima conjecturada. L'energia esperada serveix com a fita per a l'energia extremal, millorant així les fites derivades de l'estudi d'Alishahi i Zamani del conjunt esfèric. Entre d'altres resultats addicionals, obtenim una expressió tancada per a la distància esperada de separació entre punts aleatoris donats pels zeros de polinomis el·líptics.

Al Capítol 3, explorem les discrepàncies mitjanes i els *worst-case errors* de configuracions aleatòries de punts a la d-esfera. Trobem que els punts extrets de l'anomenat conjunt esfèric i els zeros de polinomis el·líptics aconsegueixen discrepància L^2 òptima en mitjana. A més, proporcionem una cota superior de la discrepància L^∞ per a configuracions de N punts obtinguts del conjunt harmònic en qualsevol espai 2-punts homogeni, generalitzant així els resultats previs per a la d-esfera obtinguts per Beltrán, Marzo i Ortega-Cerdà. Introduïm una versió no determinista del Quasi Monte Carlo (QMC) *strength* per a successions aleatòries de punts i calculem el seu valor per al conjunt esfèric, els zeros de polinomis el·líptics i el conjunt harmònic. Finalment, comparem els nostres resultats amb els QMC *strengths* conjecturats per a certes distribucions deterministes associades amb aquests processos de punts aleatoris.

Al Capítol 4, desplacem el focus al problema de minimització de l'energia de Green. En primer lloc, ampliem el treball de Beltrán i Lizarte en esferes per establir una fita inferior propera a l'òptima per a l'energia de Green mínima en qualsevol varietat 2-punts homogènia, millorant els resultats existents en espais projectius. En segon lloc, mitjançant l'adaptació d'un mètode introduït per Wolff, deduïm una cota superior de la discrepància L^∞ per a conjunts de N punts que minimitzen l'energia de Green.

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