



# Approximation to uniform distribution in SO(3)

Carlos Beltrán<sup>1</sup> · Damir Ferizović<sup>2</sup>

Received: 30 January 2019 / Revised: 11 December 2019 / Accepted: 12 March 2020 © Springer Science+Business Media, LLC, part of Springer Nature 2020

### Abstract

Using the theory of determinantal point processes we give upper bounds for the Green and Riesz energies for the rotation group SO(3), with Riesz parameter up to 3. The Green function is computed explicitly, and a lower bound for the Green energy is established, enabling comparison of uniform point constructions on SO(3). The variance of rotation matrices sampled by a certain determinantal point process is estimated, and formulas for the  $L^2$ -norm of Gegenbauer polynomials with index 2 are deduced, which might be of independent interest.

**Keywords** Rotation group  $\cdot$  Point arrangements  $\cdot$  Green energy  $\cdot$  Determinantal point processes

**Mathematics Subject Classification** Primary: 74G65 · 52C35; Secondary: 31B15 · 60G55

## 1 Introduction and results

In this paper we study properties of a finite collection of randomly generated points in SO(3), the rotation group of 3-dimensional Euclidean space, sampled by a certain

 Carlos Beltrán carlos.beltran@unican.es
 Damir Ferizović

damir.ferizovic@tugraz.at

- <sup>1</sup> Universidad de Cantabria, Santander, Spain
- <sup>2</sup> Graz University of Technology, Graz, Austria

This is a post-peer-review, pre-copyedit version of an article published in Constructive Approximation. The final authenticated version is available online at: https://doi.org/10.1007/s00365-020-09506-1

Communicated by Edward B. Saff.

Carlos Beltrán was supported by the Spanish "Ministerio de Economía y Competitividad" under projects MTM2017-83816-P and MTM2017-90682-REDT (Red ALAMA), as well as by the Banco Santander and Universidad de Cantabria under project 21.SI01.64658. Damir Ferizović thankfully acknowledges support by the Austrian Science Fund (FWF): F5503 "Quasi-Monte Carlo Methods" and FWF: W1230 "Doctoral School Discrete Mathematics".

*determinantal point process* (dpp). It turns out that these points tend to be well distributed, a property that is important for discretization, integration and approximation. Our goal is not to compute actual collections of evenly distributed rotation matrices, but rather to provide a comparison tool that allows one to decide the effectiveness of any given method.

If one is given an algorithm to generate finite (but arbitrarily large) collections of matrices, common methods to measure how well distributed these are include either calculating some discrete energy of them or looking at the speed of convergence of the counting measure towards uniform measure. Most work in this direction has been done on spheres of various dimensions, see the monography [8] for a very complete survey of the state of the art of this question; the particular question of finding collections of spherical points with small energy was posed by Shub and Smale in [21] and is nowadays known as Smale's 7th problem [22].

In order to extend part of the work done on spheres to the context of rotation matrices, we will obtain bounds on various energies for points generated through a certain dpp (technically speaking, a dpp is a counting measure where one identifies the measure with its set of atoms). Briefly, such a process is obtained by taking a Hilbert space  $\mathcal{H}(X)$  (usually  $\mathcal{H}(X) = L^2(X)$ ) of an underlying measure space  $(X, \mu)$  and an *N*-dimensional subspace  $H \subset \mathcal{H}(X)$ , with projection kernel  $\mathcal{K}$  onto H. Then, under mild conditions on *X*, one is guaranteed almost surely the existence of such a process with *N* distinct points in *X* associated to  $\mathcal{K}$ .

The theory of those processes has been summarized in [7]; there one also finds a pseudo-code which samples points from any given dpp. A main feature of the underlying points is that they tend to repel each other, and hence have become the theoretical basis of construction of well-distributed points on various symmetric spaces, see for instance [2,5,6,19].

Since one can sometimes compute the expected value of the energy of points coming from these processes with high precision, they have been used as a tool to understand the asymptotic properties of the discrete energy in that context; and in particular, for even dimensional spheres, with the exception of the usual 2-sphere, the best known bounds for some energies have been proved using this approach.

We will employ the same method for SO(3), considering first the (discrete) *Riesz s*-energy for  $A = \{\alpha_1, \ldots, \alpha_N\} \subset$  SO(3):

$$E_R^s(A) := \sum_{j \neq k} \frac{1}{\|\alpha_j - \alpha_k\|_F^s},$$

with  $\alpha_j$  being thought of as rotation matrices,  $\|\cdot\|_F$  being the Frobenius or  $L^2$ -norm, and  $s \in (0, \infty)$ . In contrast to this, the *continuous Riesz s-energy* is given by replacing the double sum by the double integral over SO(3). We further set

$$\mathcal{E}_R^s(N) = \inf_{|A|=N} E_R^s(A).$$

The investigation of these sums is very popular and results usually describe the behavior of the first leading terms. This seems particularly interesting in case *s* equals the dimension, where we have following result.

**Theorem 1.1** If 
$$N = \binom{2L+3}{3}$$
 for  $L \in \mathbb{N}$ , then the Riesz 3-energy satisfies

$$12\sqrt{2}\pi \ \mathcal{E}_R^3(N) \ \le \ N^2 \log(N) + \left(3\gamma + \log(8^2 \cdot 6) - \frac{21}{4}\right)N^2 + O(N^{5/3}\log(N)),$$

where  $\gamma$  is the Euler–Mascheroni constant.

The right-hand side is the expected value of the Riesz 3-energy with underlying points generated by a certain dpp. Now, given any particular method of generating finite point sets in SO(3), one can numerically compute their 3-energy and compare it to the value above to decide if the points are evenly distributed. This comparison would clearly rise in significance at the presence of lower bounds on the 3-energy. From [8, Th. 9.5.4] we have

$$\lim_{N \to \infty} \frac{\mathcal{E}_R^3(N)}{N^2 \log N} = \frac{\beta_3}{Vol(\mathrm{SO}(3))} = \frac{\frac{4\pi}{3}}{16\sqrt{2}\pi^2} = \frac{1}{12\sqrt{2}\pi}.$$

Here  $\beta_3$  is the volume of the unit ball in  $\mathbb{R}^3$  and Vol(SO(3)) is the volume, i.e., the Haursdoff measure, of SO(3) as a subset of  $\mathbb{R}^{3\times3} \equiv \mathbb{R}^9$ ; see [15] for a computation of that volume. We can thus see that random points from our dpp give the correct order of the asymptotic. The first order asymptotics for other *s*-energies are also understood (see the Poppy Seed Bagel Theorem [8, Th. 8.5.2] for s > 3 and the Fundamental Theorem [8, Th. 4.2.2] for s < 3). However, we have not found estimates on the next order term for the minimal 3–energy on SO(3), which leads to the following open question.

**Open Problem 1.2** Find bounds on the second term asymptotics for  $\mathcal{E}_R^3(N)$  or more generally for  $\mathcal{E}_R^s(N)$ .

We now turn our attention to the Green energy, where we obtain bounds with the continuous Green energy as coefficient of the factor  $N^2$  (zero in this case), and narrow the domain of the leading coefficient of the second term.

To recap, a Green function  $\mathcal{G}_L$  for a linear differential operator L is an integral kernel to produce solutions for inhomogeneous differential equations and is unique modulo Ker(L). In our case, we deal with the Laplace–Beltrami operator  $\Delta_g$ , and note that Ker( $\Delta_g$ ) is the set of harmonic functions—which are just constants on a compact Riemannian manifold (M, g). We will construct  $\mathcal{G} = \mathcal{G}_{\Delta_g}$  in such a way that it integrates to zero and speak of *the* Green function.

The (discrete) *Green energy* for  $A = \{\alpha_1, ..., \alpha_N\} \subset SO(3)$  will be given by

$$E_{\mathcal{G}}(A) := \sum_{i \neq j} \mathcal{G}(\alpha_i, \alpha_j),$$

and we let

$$\mathcal{E}_{\mathcal{G}}(N) = \inf_{|A|=N} E_{\mathcal{G}}(A).$$

It is noteworthy that  $\mathcal{G}(\alpha, \beta)d(\alpha, \beta) \approx 1$  for  $\alpha$  close to  $\beta$  in geodesic distance  $d(\cdot, \cdot)$ , and a set of points with small Green energy is hence expected to be well-distributed, which is indeed the main result in [4]. We know that if  $\{\alpha_1, \ldots, \alpha_N\}$  attains the minimal possible energy, then the associated discrete measure approaches the uniform distribution in SO(3) as  $N \to \infty$ . A set of points with small Green energy is also expected to be well-separated, see [9].

Now,  $\mathcal{G}(\cdot, \beta)$  is for any  $\beta \in SO(3)$  a zero mean function by definition, and if  $\{\alpha_1, \ldots, \alpha_N\}$  were simply chosen uniformly and independently in SO(3), then the expected value of the Green energy would equal 0, so in particular we have  $\mathcal{E}_{\mathcal{G}}(N) \leq 0$ . In this note we prove the following much stronger result.

**Theorem 1.3** If  $N = \binom{2L+3}{3}$  for  $L \in \mathbb{N}$ , then

$$-3\sqrt[3]{\pi}N^{4/3} + O(N) \le \mathcal{E}_{\mathcal{G}}(N) \le -4\left(\frac{3}{4}\right)^{4/3}N^{4/3} + O(N).$$

The right-hand side is the expected value of the Green energy with underlying points generated by a dpp, and that is where we have the restriction for N, as the process is related to subspaces H that we can project onto. The lower bound is valid for all N.

As mentioned above, another classical measure of the distribution properties of  $\{\alpha_1, \ldots, \alpha_N\}$  is the speed of convergence to uniform measure, which can be understood by choosing some range sets  $\{A_j\}_{j \in I}$  measurable with respect to the Haar measure  $\mu$  and investigating the behavior of

$$\sup_{j\in I} \left| \#\{k : \alpha_k \in A_j\} - N\mu(A_j) \right|$$

as N grows large. We will tackle this problem probabilistically, where we turn the count of points in  $A_i$  into a random variable.

In analogy to spherical caps on spheres, the range sets for SO(3) will be the balls  $B(\alpha, 2\varepsilon) := \{\beta \in SO(3) : \omega(\alpha^{-1}\beta) < 2\varepsilon\}$  for  $\varepsilon \in (0, \frac{\pi}{2})$  and  $\omega(\cdot)$  being the rotation angle distance introduced in the following sections. For given random points  $\{\alpha_1, \ldots, \alpha_N\}$  and fixed  $\alpha \in SO(3)$ , we define random variables via characteristic functions

$$X_{\alpha,\varepsilon}^k = \chi_{B(\alpha,2\varepsilon)}(\alpha_k)$$
 and  $\eta_{\alpha,\varepsilon} = \sum_{k=1}^N X_{\alpha,\varepsilon}^k$ .

Now, for a collection of random uniform points chosen independently in SO(3), denoting by 1 the identity matrix in SO(3), we have

$$\mathbb{E}[\eta_{\alpha,\varepsilon}] = N\mu(B(\alpha, 2\varepsilon)) = N\mu(B(\mathbb{1}, 2\varepsilon)),$$

🖄 Springer

and the variance can also be computed from the independence of the points:

$$\operatorname{Var}[\eta_{\alpha,\varepsilon}] = \mathbb{E}[\eta_{\alpha,\varepsilon}^2] - \mathbb{E}[\eta_{\alpha,\varepsilon}]^2 = N\left(\mu(B(\mathbb{1}, 2\varepsilon)) - \mu(B(\mathbb{1}, 2\varepsilon))^2\right).$$

We are able to bound the variance of this quantity for our dpp, proving that it is much smaller than in the previous case.

**Theorem 1.4** Let  $N = \binom{2L+3}{3}$  for  $L \in \mathbb{N}$ , and  $\varepsilon \in (0, \frac{\pi}{2})$  be fixed. Then the points generated by the dpp given in Lemma 2.3 satisfy

$$\mathbb{E}[\eta_{\alpha,\varepsilon}] = N\mu(B(\alpha, 2\varepsilon)) = N\mu(B(\mathbb{1}, 2\varepsilon)),$$

and moreover

$$\operatorname{Var}(\eta_{\alpha,\varepsilon}) = O\left(\frac{\varepsilon^2}{\cos(\varepsilon)}\right) N^{2/3} \log(N).$$

From Theorem 1.4 and for any fixed  $\varepsilon$ , we then have by Chebyshev's inequality

$$\sup_{\alpha \in \mathrm{SO}(3)} \mathbb{P}\Big( \Big| \eta_{\alpha,\varepsilon} - N\mu(B(\mathbb{1}, 2\varepsilon)) \Big| \ge T \Big) \le \mathrm{Var}(\eta_{\alpha,\varepsilon})T^{-2};$$

for example, letting  $T = N^{1/3} \log(N)$  and with some little arithmetic we obtain

$$\sup_{\alpha \in \mathrm{SO}(3)} \mathbb{P}\Big( \Big| \frac{1}{N} \eta_{\alpha,\varepsilon} - \mu(B(\mathbb{1}, 2\varepsilon)) \Big| \ge \frac{\log(N)}{N^{2/3}} \Big) = O\Big( \frac{1}{\log(N)} \Big).$$

In other words, for large N the counting and Haar measures are very similar with high probability.

### **2 Introductory Concepts**

In this section we collect some definitions and previous results that we will use and that are intended to make this manuscript reasonably self-contained. Definitions of Chebyshev polynomials and alike are postponed to Sect. 2.4.

### 2.1 Structure, distances and integration in SO(3)

The special orthogonal group SO(3) is the compact Lie group of 3 by 3 orthogonal matrices over  $\mathbb{R}$  that represent rotations in  $\mathbb{R}^3$ ; i.e., with determinant equal to one. It is a 3 dimensional manifold and since it is naturally included in  $\mathbb{R}^9$  it is customary to let it inherit its Riemannian submanifold structure.

Following [14], using Euler angles  $(\varphi_1, \theta, \varphi_2) \in [0, 2\pi) \times [0, \pi] \times [0, 2\pi)$ , every element  $R \in SO(3)$  can be decomposed as  $R = s_z(\varphi_1)s_x(\theta)s_z(\varphi_2)$  where

$$s_z(\varphi_1) := \begin{pmatrix} \cos(\varphi_1) - \sin(\varphi_1) & 0\\ \sin(\varphi_1) & \cos(\varphi_1) & 0\\ 0 & 0 & 1 \end{pmatrix}, \ s_x(\theta) := \begin{pmatrix} 1 & 0 & 0\\ 0 & \cos(\theta) - \sin(\theta)\\ 0 & \sin(\theta) & \cos(\theta) \end{pmatrix}$$

are rotations around the *z*-axis and *x*-axis respectively. The normalized Haar measure (i.e., the unique left and right invariant probability measure in SO(3)) is given by  $d\mu(R) = \frac{1}{8\pi^2} \sin(\theta) d\varphi_1 d\theta d\varphi_2$ , and it corresponds to the inherited Riemannian submanifold structure of SO(3) up to the normalizing constant.

The Riemannian distance associated to the structure of SO(3) is certainly a natural and useful concept, but for us it will be more convenient to use the so called *rotation* angle distance defined as follows: for  $\alpha$ ,  $\beta \in$  SO(3),

$$\omega(\alpha^{-1}\beta) = \arccos\left(\frac{\operatorname{Trace}(\alpha^{-1}\beta) - 1}{2}\right) \in [0, \pi].$$

Its convenience stems from the following fact, see for example, [14, page 173]: Given a function  $f \in L^1(SO(3))$  such that we can find  $\tilde{f} \in L^1([0, \pi])$  with  $f(x) = \tilde{f}(\omega(x))$ , then

$$\int_{SO(3)} f(x) \, \mathrm{d}\mu(x) = \frac{2}{\pi} \int_0^{\pi} \tilde{f}(t) \sin^2\left(\frac{t}{2}\right) \mathrm{d}t. \tag{1}$$

By the monotone convergence theorem (1) is also valid if f,  $\tilde{f}$  are just assumed to be non-negative and measurable.

#### 2.2 Laplace–Beltrami operator and Green function in SO(3)

The Laplace–Beltrami operator  $\Delta_g$  is defined on any Riemannian manifold (M, g) in terms of the Levi-Civita connection. Following [10], if  $\gamma_1(t), \ldots, \gamma_n(t)$  is a set of geodesics in an *n*-dimensional manifold such that  $\gamma_j(0) = p \in M$  for all  $1 \le j \le n$ , and such that  $\{\dot{\gamma}_j(0)\}$  form an orthonormal basis of the tangent space  $T_pM$  (geodesic normal coordinates), then the action of  $\Delta_g$  on  $C^2$ -functions f at p is given by

$$\Delta_g f(p) = -\sum_{j=1}^n \frac{\mathrm{d}^2}{\mathrm{d}t^2}\Big|_{t=0} f(\gamma_j(t)).$$

Note the convention given by the minus sign in front of the sum, which sometimes leads to confusion given the Laplacian in  $\mathbb{R}^n$ . The convention we use here is widely accepted, see for example [17]. A Green function  $\mathcal{G} = \mathcal{G}_{\Delta_g}$  is a distributional solution to

$$\Delta_g \mathcal{G}(\cdot, y) = \delta(\cdot, y) - \frac{1}{\mu_{dV}(\mathbf{M})},$$

where  $\mu_{dV}(M)$  is the Riemannian volume form in M. Defined this way it is unique modulo Ker $(\Delta_g)$  and it is common practice to add a constant in such a way that for all  $y \in M$  the function  $\mathcal{G}(\cdot, y)$  has zero mean, see [3]. We use this convention and simply refer to  $\mathcal{G}$  as *the* Green function.

It further follows from classical Fredholm theory that

$$\mathcal{G}_{\Delta_g}(x, y) = \sum_{j=1}^{\infty} \frac{\phi_j(x)\bar{\phi}_j(y)}{\lambda_j},\tag{2}$$

where  $0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \cdots$  is the sequence of eigenvalues for  $\Delta_g$  and  $\{\phi_j\}$ ,  $j \ge 1$  is a complete orthonormal set of associated eigenfunctions. Hence, this is true locally on any smooth manifold.

In the case M = SO(3), we obtain a Green function which is independent of any particular chart, thus valid globally. The eigenvalues and eigenfunctions of  $\Delta_g$  are known from the classical theory of continuous groups and have been intensively studied, see [14,16], [25, §15]:

**Lemma 2.1** The eigenvalues of  $\Delta_g$  in SO(3) are  $\lambda_{\ell} = \ell(\ell + 1)$  for  $\ell \geq 0$ . Moreover, if  $H_{\ell}$  is the eigenspace associated to  $\lambda_{\ell}$ , then the dimension of  $H_{\ell}$  is  $(2\ell + 1)^2$  and an orthonormal basis of  $H_{\ell}$  is given by  $\sqrt{2\ell + 1}\mathcal{D}_{m,n}^{\ell}$  where  $-\ell \leq m, n \leq \ell$  and  $\mathcal{D}_{m,n}^{\ell}$  are Wigner's  $\mathcal{D}$ -functions.

The actual form of the Wigner  $\mathcal{D}$ -functions will not be important for us, since we will only use the fact that they constitute an orthogonal basis and the following summation formula:

$$\sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \mathcal{D}_{m,n}^{\ell}(\alpha) \overline{\mathcal{D}_{m,n}^{\ell}(\beta)} = \mathcal{U}_{2\ell} \Big( \cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) \Big); \tag{3}$$

where  $U_{2\ell}(x)$  is the Chebyshev polynomial of second kind and degree  $2\ell$ , which will be briefly introduced in Sect. 2.4. For more on formula (3) see [16, Eq. 4.65] or [24, pp. 40–41] for a nice summary. The following simple form for the Green function is derived in Sect. 2.4, and to the best of our knowledge, this is the first time it has been formulated.

**Lemma 2.2** *The Green function for the Laplace–Beltrami operator on* SO(3) *can be written in terms of the metric*  $\omega$ *, i.e., for*  $\alpha$ *,*  $\beta \in$  SO(3) *with*  $\alpha \neq \beta$ *:* 

$$\mathcal{G}(\alpha,\beta) = \left(\pi - \omega(\alpha^{-1}\beta)\right) \cot\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) - 1.$$

#### 2.3 Determinantal point processes

We point the reader to the excellent monograph [7] for an introduction to point processes, and we briefly summarize part of this material below. As in [5,6], we will use only a fraction of the theory. A *simple point process* on a locally compact Polish space  $\Lambda$  with reference measure  $\mu$  is a random, integer-valued positive Radon measure  $\eta$ , that almost surely assigns at most measure 1 to singletons—we shall think of it as a counting measure

$$\eta = \sum_{j} \delta_{x_j},$$

with  $x_j \neq x_s$  for  $j \neq s$ . One usually identifies  $\eta$  with a discrete subset of  $\Lambda$ .

The *joint intensities* of  $\eta$  with respect to  $\mu$ , if they exist, are functions  $\rho_k : \Lambda^k \to [0, \infty)$  for k > 0, such that for pairwise disjoint sets  $\{D_s\}_{s=1}^k \subset \Lambda$ , the expected value of the product of number of points falling into  $D_s$  is given by

$$\mathbb{E}\bigg[\prod_{s=1}^k \eta(D_s)\bigg] = \int_{D_1 \times \ldots \times D_k} \rho_k(y_1, \ldots, y_k) \, \mathrm{d}\mu(y_1) \ldots \, \mathrm{d}\mu(y_k),$$

and  $\rho_k(y_1, \ldots, y_k) = 0$  in case  $y_j = y_s$  for some  $j \neq s$ .

A simple point process is *determinantal* with kernel  $\mathcal{K}$  if and only if for every  $k \in \mathbb{N}$  and all  $y_i$ 's

$$\rho_k(y_1,\ldots,y_k) = \det\left(\mathcal{K}(y_j,y_s)\right)_{1 \le j,s \le k}$$

Let (M, g) be a compact Riemannian manifold with measure  $d\mu = \mu_{dV}$ . Let  $H \subseteq L^2(M)$  be any *N*-dimensional subspace in the set of square-integrable functions. It follows from the Macchi-Soshnikov theorem [7, Thm. 4.5.5] that a simple point process with *N* points exists in M associated to H. An important property of that dpp is given by [7, Form. (1.2.2)]: For any measurable function  $f : M \times M \rightarrow [0, \infty]$ ,

$$\mathbb{E}\bigg[\sum_{i\neq j} f(x_i, x_j)\bigg] = \iint_{\mathcal{M}} f(x, y) \Big(\mathcal{K}_{\mathcal{H}}(x, x)\mathcal{K}_{\mathcal{H}}(y, y) - |\mathcal{K}_{\mathcal{H}}(x, y)|^2\Big) \,\mathrm{d}\mu(x, y);$$
(4)

where we write  $d\mu(x, y)$  as an abbreviation for  $d\mu(x) d\mu(y)$  and

- $\mathbb{E}[g(x_1, \ldots, x_N)]$  means expected value of some function defined from  $M \times \cdots \times M$  (*N* copies of M) to  $[0, \infty]$ , when  $x_1, \ldots, x_N$  are chosen from the point process associated to H;
- $\mathcal{K}_{\mathrm{H}}(x, y)$  is the (orthogonal) projection kernel on H, namely for any  $f \in L^{2}(\mathrm{M})$  the orthogonal projection of f onto H can be computed via:

$$\Pi_{\mathrm{H}}(f)(x) = \int_{y \in \mathrm{M}} f(y) \mathcal{K}_{\mathrm{H}}(x, y) \, \mathrm{d}\mu(y) \in L^{2}(\mathrm{H}).$$

Note that if  $\varphi_1, \ldots, \varphi_N$  is an orthonormal basis of H, then we can write

$$\mathcal{K}_{\mathrm{H}}(x, y) = \sum_{j=1}^{N} \varphi_j(x) \overline{\varphi_j(y)}, \qquad (5)$$

🖄 Springer

and clearly

$$\int_{\mathrm{SO}(3)} \mathcal{K}_{\mathrm{H}}(x, x) \, \mathrm{d}\mu(x) = N.$$

Coming back to the case of interest and following ideas in [6], we choose as subspace H the span of the first eigenspaces of  $\Delta_g$ . Recall the definition of classical Gegenbauer polynomials  $C_n^{(\lambda)}(t)$ ,  $\lambda > -1/2$ , a sequence of degree *n* polynomials orthogonal with respect to the weight  $(1 - t^2)^{\lambda - 1/2}$  in [-1, 1], normalized in such a way that

$$\mathcal{C}_n^{(\lambda)}(1) = \binom{2\lambda + n - 1}{2\lambda - 1}.$$

An equivalent definition of these polynomials is given by the formal power series

$$(1 - 2t\alpha + \alpha^2)^{-\lambda} = \sum_{n=0}^{\infty} \mathcal{C}_n^{(\lambda)}(t) \alpha^n.$$

**Lemma 2.3** Let  $L \ge 0$  and  $H_L \subseteq L^2(SO(3))$  be the span of the union of eigenspaces for eigenvalues  $\lambda_0, \ldots, \lambda_L$  of  $\Delta_g$ . Then, we define

$$N := \dim(\mathbf{H}_L) = \binom{2L+3}{3} = \mathcal{C}_{2L}^{(2)}(1) = \frac{4}{3}L^3 + O(L^2).$$

Moreover, the projection kernel is:

$$\mathcal{K}_L(\alpha,\beta) := \mathcal{K}_{\mathrm{H}_L}(\alpha,\beta) = \mathcal{C}_{2L}^{(2)} \Big( \cos \Big( \frac{\omega(\alpha^{-1}\beta)}{2} \Big) \Big).$$

We then consider the dpp associated to  $H_L$ .

#### 2.4 Proofs of the basic lemmas

The degree n + 1 Chebyshev polynomials of first and second kind satisfy the recurrence relation

$$P_{n+1}(x) = 2x P_n(x) - P_{n-1}(x),$$
(6)

with  $T_0 \equiv 1$ ,  $T_1(x) = x$  and  $U_{-1} \equiv 0$ ,  $U_0(x) \equiv 1$  in their respective notation. With this said, using (2), (3), and (5), we obtain

$$\mathcal{K}_{L}(\alpha,\beta) = \sum_{\ell=0}^{L} (2\ell+1) \,\mathcal{U}_{2\ell}\Big(\cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right)\Big);\tag{7}$$

$$\mathcal{G}(\alpha,\beta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \mathcal{U}_{2\ell}\left(\cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right)\right).$$
(8)

Further we list some equations for later reference and the reader's convenience.

$$2\mathcal{T}_{2\ell+1}(x) = \mathcal{U}_{2\ell+1}(x) - \mathcal{U}_{2\ell-1}(x) [1, \text{ Eq. } 22.5.8],$$
  

$$\mathcal{T}_n(1) = 1 \qquad [13, \text{ Eq. } 8.944.1],$$
  

$$\frac{d}{dx}\mathcal{T}_{2\ell+1}(x) = (2\ell+1)\mathcal{U}_{2\ell}(x) \qquad [13, \text{ Eq. } 8.949.1],$$
  

$$\frac{d}{dx}\mathcal{U}_{2L+1}(x) = 2\mathcal{C}_{2L}^{(2)}(x) \qquad [13, \text{ Eq. } 8.949.4],$$
  

$$\mathcal{C}_n^{(\lambda)}(1) = \binom{2\lambda+n-1}{2\lambda-1} \qquad [13, \text{ Eq. } 8.937.4].$$
(9)

**Proof of Lemma 2.3** Let  $y := \cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right)$ , then by (7) and (9)

$$\mathcal{K}_L(\alpha,\beta) = \frac{\mathrm{d}}{\mathrm{d}x} \sum_{\ell=0}^L \mathcal{T}_{2\ell+1}(x) \Big|_y = \frac{\mathrm{d}}{\mathrm{d}x} \frac{1}{2} \mathcal{U}_{2L+1}(x) \Big|_y = \mathcal{C}_{2L}^{(2)}(y).$$

The formula for the dimension of  $H_L$  can be proved as follows. The eigenspace associated to  $\lambda_{\ell} = \ell(\ell + 1)$  has dimension  $(2\ell + 1)^2$  since this is the number of elements of its basis  $D_{m,n}^{\ell}$ . Thus dim $(H_L)$  is given by  $\sum_{\ell=0}^{L} (2\ell + 1)^2 = \binom{2L+3}{3}$ .  $\Box$ 

*Proof of Lemma 2.2* In (8) we apply the equality

$$\mathcal{U}_{2\ell}(\cos(t)) = \frac{\sin\left((2\ell+1)t\right)}{\sin(t)} \quad [13, \text{ Eq. 8.940.1}],$$

and argue, under the assumption  $w := \omega(\alpha^{-1}\beta) \in (0, \pi]$ , as follows

$$\begin{aligned} \mathcal{G}(\alpha,\beta) &= \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \frac{\sin\left((2\ell+1)\frac{w}{2}\right)}{\sin\left(\frac{w}{2}\right)} \\ &= \frac{1}{\sin\left(\frac{w}{2}\right)} \sum_{\ell=1}^{\infty} \left(\frac{\sin\left((2\ell+1)\frac{w}{2}\right)}{\ell+1} + \frac{\sin\left((2\ell+1)\frac{w}{2}\right)}{\ell}\right) \\ &= \frac{1}{i} \left(-\log\left(1-e^{iw}\right) + \log\left(1-e^{-iw}\right)\right) \cot\left(\frac{w}{2}\right) - 1; \end{aligned}$$

where we used the well known fact that the power series for log(1 - x) at 1 converges at the boundary of its disc of convergence (except for x = 1) and equals the logarithm at these values:

$$\sum_{\ell=1}^{\infty} \frac{\sin\left((2\ell+1)\frac{w}{2}\right)}{\ell+1} = \frac{1}{2i} \sum_{\ell=1}^{\infty} \frac{e^{i\frac{w}{2}(2\ell+1)} - e^{-i\frac{w}{2}(2\ell+1)}}{\ell+1}$$
$$= \frac{e^{-i\frac{w}{2}}}{2i} \sum_{\ell=1}^{\infty} \frac{e^{iw(\ell+1)}}{\ell+1} - \frac{e^{i\frac{w}{2}}}{2i} \sum_{\ell=1}^{\infty} \frac{e^{-iw(\ell+1)}}{\ell+1}$$
$$= \frac{-e^{-i\frac{w}{2}}}{2i} \left(\log\left(1-e^{iw}\right) + e^{iw}\right) + \frac{e^{i\frac{w}{2}}}{2i} \left(\log\left(1-e^{-iw}\right) + e^{-iw}\right)$$

🖄 Springer

$$= \frac{-e^{-i\frac{w}{2}}}{2i} \log(1 - e^{iw}) + \frac{e^{i\frac{w}{2}}}{2i} \log(1 - e^{-iw}) - \sin(\frac{w}{2}),$$

and similarly

$$\sum_{\ell=1}^{\infty} \frac{\sin\left((2\ell+1)\frac{w}{2}\right)}{\ell} = \frac{-e^{i\frac{w}{2}}}{2i}\log\left(1-e^{iw}\right) + \frac{e^{-i\frac{w}{2}}}{2i}\log\left(1-e^{-iw}\right).$$

Further, by  $1 - e^{-iw} = 2ie^{-i\frac{w}{2}}\sin(\frac{w}{2})$ , we conclude

$$\log(1 - e^{-iw}) - \log(1 - e^{iw}) = \log(2ie^{-i\frac{w}{2}}\sin(\frac{w}{2})) - \log(-2ie^{i\frac{w}{2}}\sin(\frac{w}{2}))$$
$$= \log(2e^{i\frac{-w+\pi}{2}}\sin(\frac{w}{2})) - \log(2e^{i\frac{w-\pi}{2}}\sin(\frac{w}{2}))$$
$$= (-w + \pi)\frac{i}{2} - (w - \pi)\frac{i}{2} = i(\pi - w),$$

where we used a property of the principal branch of the complex logarithm:  $\log(re^{i\varphi}) = \log(r) + i\varphi$ .

#### 3 Riesz s-energy: Proof of Theorem 1.1

Recall that if A is a real matrix, we have  $||A||_F^2 := \text{Trace}(A^t A)$ . We set throughout  $N = N(L) = C_{2L}^{(2)}(1)$  for  $L \in \mathbb{N}$ .

**Lemma 3.1** For  $\alpha, \beta \in SO(3)$ , we have  $\|\alpha - \beta\|_F = \sqrt{8} \sin\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right)$ .

**Proof** We abbreviate  $w = \omega(\alpha^{-1}\beta)$ , and use the half-angle formula for sine:

$$\|\alpha - \beta\|_F^2 = \operatorname{Trace}\left[(\alpha - \beta)^t (\alpha - \beta)\right] = 6 - 2\operatorname{Trace}(\alpha^{-1}\beta)$$
$$= 8\frac{2 - \left(\operatorname{Trace}(\alpha^{-1}\beta) - 1\right)}{4} = 8\frac{1 - \cos(w)}{2} = 8\sin^2\left(\frac{w}{2}\right).$$

Recall the definition of Euler's Beta function  $\mathcal{B}(a, b) := \int_0^1 t^{a-1}(1-t)^{b-1} dt$  for a, b > 0. We are now ready to state our first proposition.

**Proposition 3.2** For  $s \in (0, 3)$  and  $N = N(L) = \binom{2L+3}{3}$ , we have

$$\mathcal{E}_{R}^{s}(N) \leq \frac{2}{8^{s/2}\pi} \mathcal{B}\left(\frac{3-s}{2}, \frac{1}{2}\right) N^{2} + O(N^{1+s/3}).$$

If  $s \in \{1, 2\}$ , we have more information on the term  $O(N^{1+s/3})$ : It is respectively

$$-\frac{\sqrt{2}}{\pi} \left(\frac{3}{4}\right)^{4/3} N^{4/3} + O(N) \quad and \quad -\frac{4}{15} \left(\frac{3}{4}\right)^{5/3} N^{5/3} + O(N^{4/3}).$$

🖄 Springer

Proof We use (4), Lemmas 2.3, 3.1, invariance of Haar measure, and (1):

$$\begin{split} &\iint_{\mathrm{SO}(3)} \frac{\mathcal{K}_{L}(\alpha, \alpha)^{2} - \mathcal{K}_{L}(\alpha, \beta)^{2}}{\|\alpha - \beta\|_{F}^{s}} \, \mathrm{d}\mu(\alpha, \beta) \\ &= \iint_{\mathrm{SO}(3)} \frac{\left[\mathcal{C}_{2L}^{(2)}(1)\right]^{2} - \left[\mathcal{C}_{2L}^{(2)}\left(\cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right)\right)\right]^{2}}{8^{\frac{s}{2}}\sin^{s}\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right)} \, \mathrm{d}\mu(\alpha, \beta) \\ &= \frac{2}{8^{\frac{s}{2}}\pi} \int_{0}^{\pi} \left(N^{2} - \left[\mathcal{C}_{2L}^{(2)}\left(\cos\left(\frac{t}{2}\right)\right)\right]^{2}\right) \sin^{2-s}\left(\frac{t}{2}\right) \, \mathrm{d}t \\ &= \frac{4}{8^{\frac{s}{2}}\pi} N^{2} \int_{0}^{\pi/2} \sin^{2-s}(t) \, \mathrm{d}t - \frac{4}{8^{\frac{s}{2}}\pi} \int_{0}^{1} \left[\mathcal{C}_{2L}^{(2)}(t)\right]^{2} (1 - t^{2})^{\frac{1-s}{2}} \, \mathrm{d}t \end{split}$$

The next line is, apart from the factor  $\frac{4}{8^{s/2}\pi}$ , the continuous Riesz *s*-energy:

$$\int_0^{\pi/2} \sin^{2-s}(t) \, \mathrm{d}t = \int_0^1 \frac{t^{1-s}t}{\sqrt{1-t^2}} \, \mathrm{d}t = \frac{1}{2} \int_0^1 t^{\frac{1-s}{2}} (1-t)^{-1/2} \, \mathrm{d}t = \frac{1}{2} \mathcal{B}\left(\frac{3-s}{2}, \frac{1}{2}\right).$$

On the other hand, for 0 < s < 3 we have

$$\begin{split} \int_0^1 & \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 (1-t^2)^{\frac{1-s}{2}} \, \mathrm{d}t = \int_0^{\pi/2} \left[ \mathcal{C}_{2L}^{(2)}(\cos(t)) \right]^2 \sin^{2-s}(t) \, \mathrm{d}t \\ & \lesssim \int_0^{1/L} \left[ \mathcal{C}_{2L}^{(2)}(\cos(t)) \right]^2 t^{2-s} \, \mathrm{d}t + \int_{1/L}^{\pi/2} \left[ \mathcal{C}_{2L}^{(2)}(\cos(t)) \right]^2 t^{2-s} \, \mathrm{d}t \\ & \le \left[ \mathcal{C}_{2L}^{(2)}(1) \right]^2 \frac{t^{3-s}}{3-s} \Big|_0^{1/L} - \frac{\mathcal{C}L^2}{1+s} \frac{1}{t^{1+s}} \Big|_{1/L}^{\pi/2} = \mathcal{O}(L^{3+s}); \end{split}$$

where we have used that  $|C_{2L}^{(2)}(t)| \le |C_{2L}^{(2)}(1)|$  for all  $t \in [-1, 1]$  and [23, Eq. 7.33.6], i.e., for every c > 0 there is  $C \ge 0$  such that

$$|C_{2L}^{(2)}(\cos(\theta))| \le \frac{CL}{\theta^2}, \quad \frac{c}{L} \le \theta \le \frac{\pi}{2}.$$

The case s = 1 is Lemma 6.2; the case s = 2 follows from Lemma 6.4:

$$\int_0^1 \frac{\left[\mathcal{C}_{2L}^{(2)}(t)\right]^2}{\sqrt{1-t^2}} \, \mathrm{d}t = \int_0^{\pi/2} \left[\mathcal{C}_{2L}^{(2)}(\cos(t))\right]^2 \, \mathrm{d}t = \frac{\pi}{2} \sum_{u=0}^{2L} c_{u,u} = \frac{8\pi}{15} L^5 + O(L^4),$$

where  $c_{u,u} = c_{u,u}^{(2)}(2L)$  with notation as in Lemma 6.4.

In the next proof we use (1) and the digamma function  $\psi$ , see Sect. 6.

**Proof of Theorem 1.1** We proceed as in the previous proof and use Lemma 6.4. In particular, we use the notation of that lemma for  $c_{j,k} = c_{j,k}^{(2)}(2L)$ :

$$\int_{0}^{\pi/2} \frac{\left[\mathcal{C}_{2L}^{(2)}(1)\right]^{2} - \left[\mathcal{C}_{2L}^{(2)}\left(\cos(t)\right)\right]^{2}}{\sin(t)} dt$$

$$= 2 \sum_{r=1}^{2L} \int_{0}^{\pi/2} \frac{1 - \cos(2rt)}{\sin(t)} dt \sum_{u=0}^{2L-r} c_{r+u,u}$$

$$= 4 \sum_{r=1}^{2L} \int_{0}^{\pi/2} \left[\mathcal{U}_{r-1}\left(\cos(t)\right)\right]^{2} \sin(t) dt \sum_{u=0}^{2L-r} c_{r+u,u}$$

$$= 4 \sum_{r=1}^{2L} \int_{0}^{1} \left[\mathcal{U}_{r-1}(t)\right]^{2} dt \sum_{u=0}^{2L-r} c_{r+u,u} = (\star).$$

We use (14) and obtain

$$(\star) = 2(\gamma + \log(4)) \sum_{r=1}^{2L} \sum_{u=0}^{2L-r} c_{r+u,u} + 2 \sum_{r=1}^{2L} \psi(r + \frac{1}{2}) \sum_{u=0}^{2L-r} c_{r+u,u} =: S_1 + S_2.$$

By  $c_{r+u,u} = c_{r+u,u}^{(2)}(2L) = (r+u+1)(2L-r-u+1)(u+1)(2L-u+1)$ , we have

$$\sum_{u=0}^{2L-r} c_{r+u,u} = \frac{16}{15}L^5 + \frac{2}{3}L^2r^3 - \frac{4}{3}L^3r^2 - \frac{r^5}{30} + O_{a+b<5}(L^ar^b),$$

and hence, by well known formulas for the sum of powers of integers:

$$S_{1} = 2(\gamma + \log(4)) \left( \frac{16}{15}L^{5}2L + \frac{2}{3}L^{2}4L^{4} - \frac{4}{3}L^{3}\frac{8}{3}L^{3} - \frac{1}{30}\frac{32}{3}L^{6} \right) + O(L^{5})$$
  
=  $\frac{16}{9}(\gamma + \log(4))L^{6} + O(L^{5}).$ 

Invoking Lemma 3.3 yields

$$\frac{1}{2}S_2 = \frac{16}{15}L^5 \left(2L \psi(2L) - 2L\right) + \frac{2}{3}L^2 \left(\frac{(2L)^4}{4}\psi(2L) - \frac{(2L)^4}{4^2}\right) - \frac{4}{3}L^3 \left(\frac{(2L)^3}{3}\psi(2L) - \frac{(2L)^3}{3^2}\right) - \frac{1}{30} \left(\frac{(2L)^6}{6}\psi(2L) - \frac{(2L)^6}{6^2}\right) + O(L^5 \log(L)) = \frac{8}{9}L^6 \psi(2L) - \frac{14}{9}L^6 + O(L^5 \log(L)).$$

Since  $N^2 = C_{2L}^{(2)}(1)^2 = \frac{16}{9}L^6(1 + O(L^{-1}))$ , and  $(\frac{3}{4}N)^{1/3} = L(1 + O(L^{-1}))^{1/6}$  we see

$$\frac{1}{3}\log\left(\frac{3}{4}N\right) = \log(L) + O(L^{-1});$$

and using harmonic numbers  $H_n := \sum_{k=1}^n \frac{1}{k} = \log(n) + \gamma + O(n^{-1})$  which satisfy  $\psi(2L) = H_{2L-1} - \gamma$ , see [1, Eq. 6.3.2]:

$$\begin{aligned} (\star) &= \frac{16}{9} L^6 \Big( \psi(2L) + \gamma + \log(4) \Big) - \frac{7}{4} \frac{16}{9} L^6 + O(L^5 \log(L)) \\ &= N^2 \Big( \log \big( 2(3N/4)^{1/3} - 1 \big) + \gamma + \log(4) \Big) - \frac{7}{4} N^2 + O(N^{5/3} \log(N)) \\ &= \frac{1}{3} N^2 \log(N) + \frac{1}{3} \Big( 3\gamma + \log \big( 8^3 \frac{3}{4} \big) - \frac{21}{4} \Big) N^2 + O(N^{5/3} \log(N)); \end{aligned}$$

proving the claim when multiplied by  $\frac{4}{8^{3/2}\pi}$ .

**Lemma 3.3** Let  $\psi(t)$  be the digamma function and  $m \ge 0$ , then

$$\sum_{k=1}^{n} k^{m} \psi\left(k + \frac{1}{2}\right) = \frac{n^{m+1}}{m+1} \psi(n) - \frac{n^{m+1}}{(m+1)^{2}} + O(n^{m} \log(n)).$$

**Proof** Since  $\psi(t) = \log(t) + O(\frac{1}{t})$  for t > 2, we have

$$\sum_{k=1}^{n} k^{m} \psi \left( k + \frac{1}{2} \right) = \int_{1}^{n} t^{m} \log(t) \, \mathrm{d}t + O(n^{m} \log(n));$$

as the sum can be bounded from above and below by the same integral, apart from integration boundaries, where we obtain the error term. We finish by integrating:  $\left(\frac{t^{m+1}}{m+1}\log(t) - \frac{t^{m+1}}{(m+1)^2}\right)\Big|_{1}^{n}$ .

#### 4 Green energy: Proof of Theorem 1.3

We prove the lower and upper bound separately in the following two sections.

#### 4.1 Estimate of the Green energy: lower bound

We follow an exposition due to N. Elkies, found in [18, Lem. 5.2 pp. 149–154]. The results in [18] are stated in detail for Riemann surfaces, i.e., one–dimensional complex manifolds, although it is mentioned that the argument can be extended to more general manifolds. Here we work out the details for SO(3).

The idea is to find a function with nice properties smaller than  $\mathcal{G}$ , and to bound its energy from below. For  $\alpha$ ,  $\beta \in SO(3)$  and t > 0, we define:

$$\mathcal{G}_t(\alpha,\beta) = \sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)t} \frac{2\ell+1}{\ell(\ell+1)} \mathcal{U}_{2\ell}\Big(\cos\big(\frac{\omega(\alpha^{-1}\beta)}{2}\big)\Big).$$

Quantitative estimates depend on asymptotics for this function. The following is the version of Elkies' result for SO(3).

**Lemma 4.1** *For all* t > 0 *and*  $\alpha \neq \beta$  *we have* 

$$\mathcal{G}(\alpha, \beta) \geq \mathcal{G}_t(\alpha, \beta) - t.$$

Proof Using uniform convergence, we differentiate term by term and define

$$h_t(\alpha,\beta) := -\partial_t \mathcal{G}_t(\alpha,\beta) = \sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)t} (2\ell+1) \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \mathcal{D}_{m,n}^{\ell}(\alpha) \overline{\mathcal{D}_{m,n}^{\ell}(\beta)}.$$

Given a smooth test function  $\phi$ , with uniformly converging representation as  $\sum_{\ell=0}^{\infty} \phi_{\ell}$ , where  $\phi_{\ell} = \sum_{m,n} \varphi_{m,n}^{\ell} \mathcal{D}_{m,n}^{\ell} \sqrt{2\ell+1}$ , we set

$$u(\alpha, t) := \int_{\mathrm{SO}(3)} h_t(\alpha, \beta) \phi(\beta) \, \mathrm{d}\mu(\beta) = \sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)t} \phi_\ell(\alpha),$$

where we interchanged integration and summation by uniform convergence and used that  $\{\mathcal{D}_{m,n}^{\ell}\sqrt{2\ell+1}\}$  is an orthonormal basis. Now we have uniformly

$$\lim_{t \to 0} u(\alpha, t) = \phi(\alpha) - \int_{\mathrm{SO}(3)} \phi(\beta) \, \mathrm{d}\mu(\beta) = \phi(\alpha) - \phi_0.$$

For t > 0 fixed, we can interchange differentiation and integration yielding

$$\Delta_g u(\alpha, t) + \partial_t u(\alpha, t) = 0.$$

By the strong maximum principle (Theorem A.2), we have for every t > 0:

$$\min_{\alpha \in \mathrm{SO}(3)} u(\alpha, t) \ge \min_{\alpha \in \mathrm{SO}(3)} u(\alpha, 0).$$

The same PDE and estimates hold for

$$v(\alpha, t) = u(\alpha, t) + \phi_0.$$

If  $\phi \ge 0$ , then so is  $v(\alpha, t)$  for all t > 0 by the maximum principle as  $v(\alpha, 0) = \phi(\alpha)$ . Hence

$$u(\alpha, t) = v(\alpha, t) - \phi_0 \ge -\phi_0 \quad \text{for } \phi \ge 0.$$

We further set

$$\mathbb{I}(\alpha, t) := \int_{\mathrm{SO}(3)} \mathcal{G}_t(\alpha, \beta) \phi(\beta) \, \mathrm{d}\mu(\beta) = \sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)t} \frac{\phi_\ell(\alpha)}{\ell(\ell+1)},$$

where we interchanged sum and integral again. Differentiating term-wise for t > 0 yields

$$\partial_t \mathbb{I}(\alpha, t) = -\sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)t} \phi_\ell(\alpha) = -u(\alpha, t) \le \phi_0 \quad \text{for } \phi \ge 0.$$

Finally, for fixed  $\alpha$  let  $t > \epsilon > 0$ , then by the fundamental theorem of calculus:

$$\mathbb{I}(\alpha, t) - \mathbb{I}(\alpha, \epsilon) = \int_{\epsilon}^{t} -u(\alpha, s) \, \mathrm{d}s \le \phi_0(t - \epsilon)$$

and thus, for all non-negative test functions  $\phi$ 

$$\int_{\mathrm{SO}(3)} \left( \mathcal{G}_t(\alpha,\beta) - \mathcal{G}_\epsilon(\alpha,\beta) - (t-\epsilon) \right) \phi(\beta) \, \mathrm{d}\mu(\beta) \le 0.$$

Since the integrand is continuous, this proves that for  $t > \epsilon$ 

$$\mathcal{G}_t(\alpha,\beta) - t \leq \mathcal{G}_\epsilon(\alpha,\beta) - \epsilon,$$

and for any fixed  $\alpha$ ,  $\beta$  with  $\alpha \neq \beta$  taking the limit as  $\epsilon \rightarrow 0$  proves the result.  $\Box$ 

Now by Lemma 4.1, we have for some t > 0 which will be determined later, and any collection of distinct points  $\{\alpha_1, \ldots, \alpha_N\} \subset SO(3)$ :

$$\begin{split} &\sum_{s \neq k}^{N} \mathcal{G}(\alpha_{s}, \alpha_{k}) + N(N-1)2t \geq \sum_{s \neq k}^{N} \mathcal{G}_{2t}(\alpha_{s}, \alpha_{k}) \\ &= \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \sum_{s \neq k}^{N} e^{-\ell(\ell+1)2t} \mathcal{D}_{m,n}^{\ell}(\alpha_{s}) \overline{\mathcal{D}_{m,n}^{\ell}(\alpha_{k})} \\ &= \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \left( \left| \sum_{k=1}^{N} e^{-\ell(\ell+1)t} \mathcal{D}_{m,n}^{\ell}(\alpha_{k}) \right|^{2} - \sum_{k=1}^{N} e^{-\ell(\ell+1)2t} \left| \mathcal{D}_{m,n}^{\ell}(\alpha_{k}) \right|^{2} \right) \\ &\geq -\sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \sum_{k=1}^{\ell} e^{-\ell(\ell+1)2t} \left| \mathcal{D}_{m,n}^{\ell}(\alpha_{k}) \right|^{2} = -N\mathcal{G}_{2t}(\alpha, \alpha). \end{split}$$

Thus our remaining task is to find an asymptotic for  $\mathcal{G}_t(\alpha, \alpha)$  in *t*. First we note that

$$\frac{e^{-\ell(\ell+1)t}}{\ell(\ell+1)} = 4\frac{e^{-\ell(\ell+1)t}}{(2\ell+1)^2} \left(1 + \frac{1}{4\ell(\ell+1)}\right) = 4\frac{e^{-\ell(\ell+1)t}}{(2\ell+1)^2} + O(l^{-4}).$$

For  $0 < t \ll 1$  we then obtain

$$\begin{aligned} \mathcal{G}_{t}(\alpha,\alpha) &= \sum_{\ell=1}^{\infty} e^{-\ell(\ell+1)t} \frac{(2\ell+1)^{2}}{\ell(\ell+1)} = \sum_{\ell=1}^{\infty} \left( 4e^{-\ell(\ell+1)t} + \frac{e^{-\ell(\ell+1)t}}{\ell(\ell+1)} \right) \\ &= 4e^{t/4} \int_{0}^{\infty} e^{-(2x+1)^{2}t/4} \, dx + O(1) \\ &= 2e^{t/4} \int_{1}^{\infty} e^{-x^{2}t/4} \, dx + O(1) \\ &= \frac{4e^{t/4}}{\sqrt{t}} \int_{\sqrt{t}/2}^{\infty} e^{-x^{2}} \, dx + O(1) \\ &= \frac{4e^{t/4}}{\sqrt{t}} \int_{0}^{\infty} e^{-x^{2}} \, dx + O(1) = 2\sqrt{\frac{\pi}{t}} + O(1). \end{aligned}$$

If we choose  $2t = \frac{\sqrt[3]{\pi}}{N^{2/3}}$ , then we conclude

$$\mathcal{G}_{2t}(\alpha, \alpha) = 2\sqrt[3]{\pi}N^{\frac{1}{3}} + O(1),$$

and hence

$$\sum_{s\neq k}^{N} \mathcal{G}(\alpha_s, \alpha_k) \geq -3\sqrt[3]{\pi} N^{\frac{4}{3}} + O(N),$$

proving the lower bound in Theorem 1.3.

### 4.2 Estimate of the Green energy: upper bound

According to (4), we have to estimate the integral

$$I = \iint_{\mathrm{SO}(3)} \mathcal{G}(\alpha, \beta) \left( \mathcal{K}_L(\alpha, \alpha)^2 - \mathcal{K}_L(\alpha, \beta)^2 \right) \, \mathrm{d}\mu(\alpha, \beta),$$

which by Lemmas 2.2 and 2.3 and by invariance of Haar measure equals

$$\int_{\mathrm{SO}(3)} \left( \left( \pi - \omega(\alpha) \right) \cot\left( \frac{\omega(\alpha)}{2} \right) - 1 \right) \left( \mathcal{C}_{2L}^{(2)}(1)^2 - \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left( \frac{\omega(\alpha)}{2} \right) \right) \right]^2 \right) \, \mathrm{d}\mu(\alpha).$$

The integrand is in  $L^1(SO(3))$  since the singularity of the cotangent is removed by the zero of the difference of Gegenbauer polynomials, thus being a continuous function

on a compact set. We can then apply (1) getting:

$$I = \frac{2}{\pi} \int_0^{\pi} \left( \left( \pi - t \right) \cot\left( \frac{t}{2} \right) - 1 \right) \left( \mathcal{C}_{2L}^{(2)}(1)^2 - \left[ \mathcal{C}_{2L}^{(2)}\left( \cos\left( \frac{t}{2} \right) \right) \right]^2 \right) \sin^2\left( \frac{t}{2} \right) dt$$

Since

$$\int_0^{\pi} \left( \left( \pi - t \right) \cot \left( \frac{t}{2} \right) - 1 \right) \sin^2 \left( \frac{t}{2} \right) dt = 0.$$

we indeed have

$$-I = \frac{2}{\pi} \int_0^{\pi} \left( (\pi - t) \cot\left(\frac{t}{2}\right) - 1 \right) \left[ \mathcal{C}_{2L}^{(2)} (\cos\left(\frac{t}{2}\right)) \right]^2 \sin^2\left(\frac{t}{2}\right) dt.$$

We simplify by noticing that

$$\int_0^{\pi} \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{t}{2}\right) \right) \right]^2 \sin^2\left(\frac{t}{2}\right) dt = 2 \int_0^1 \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \sqrt{1 - t^2} dt$$
$$= \int_{-1}^1 \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \sqrt{1 - t^2} dt$$
$$= \int_{-1}^1 \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \sqrt{1 - t^2} (1 + t) dt.$$

where we used that odd functions integrate to zero over symmetric intervals. But

$$\int_{-1}^{1} \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \sqrt{1 - t} (1 + t)^{3/2} \, \mathrm{d}t = \frac{\pi}{2} \binom{2L + 3}{2L},\tag{10}$$

by the following equality, valid for  $\nu > \frac{1}{2}$  and found in [13, Eq. 7.314]:

$$\int_{-1}^{1} (1-x)^{\nu-\frac{3}{2}} (1+x)^{\nu-\frac{1}{2}} \left| \mathcal{C}_n^{(\nu)}(x) \right|^2 \mathrm{d}x = \frac{\pi^{1/2} \Gamma(\nu-\frac{1}{2}) \Gamma(2\nu+n)}{n! \Gamma(\nu) \Gamma(2\nu)}.$$

We have then proved that

$$-I = \frac{2}{\pi} \int_0^{\pi} (\pi - t) \cot\left(\frac{t}{2}\right) \left[ \mathcal{C}_{2L}^{(2)}(\cos\left(\frac{t}{2}\right)) \right]^2 \sin^2\left(\frac{t}{2}\right) dt + O(L^3)$$
  
$$= \frac{4}{\pi} \int_0^1 (\pi - 2 \arccos(t)) t \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 dt + O(L^3)$$
  
$$= 4 \int_0^1 t \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 dt - \frac{4}{\pi} \int_0^1 2 \arccos(t) t \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 dt + O(L^3).$$

Next we use Lemmas 6.1 and 6.2 in

$$\int_0^1 t^2 \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \mathrm{d}t < \int_0^1 t \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \mathrm{d}t < \int_0^1 \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \mathrm{d}t,$$

and obtain

$$\int_0^1 t \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \mathrm{d}t = L^4 + O(L^3).$$

Finally we use

$$0 \le 2 \arccos(t) \le \pi \sqrt{1-t}, \quad \text{for } t \in [0, 1]$$

so that, by (10),

$$\begin{split} \int_0^1 2 \arccos(t) t \Big[ \mathcal{C}_{2L}^{(2)}(t) \Big]^2 \, \mathrm{d}t &< \int_0^1 \pi \sqrt{1-t} t \Big[ \mathcal{C}_{2L}^{(2)}(t) \Big]^2 \, \mathrm{d}t \\ &< \pi \int_{-1}^1 \Big[ \mathcal{C}_{2L}^{(2)}(t) \Big]^2 \sqrt{1-t} (1+t)^{3/2} \, \mathrm{d}t = O(L^3). \end{split}$$

Hence

$$I = -4L^4 + O(L^3),$$

and the upper bound in Theorem 1.3 follows from  $N = \frac{4}{3}L^3 + O(L^2)$ .

#### 5 Variance: Proof of Theorem 1.4

Let  $A = B(1, 2\varepsilon) \subseteq SO(3)$  be as in the introduction, namely

$$A = \{\beta \in \mathrm{SO}(3) : \omega(\beta) < 2\varepsilon\} = \{\beta \in \mathrm{SO}(3) : \|\beta - \mathbb{1}\|_F < \sqrt{8}\sin(\varepsilon)\},\$$

where the equality follows from Lemma 3.1. Note that by rotation invariance it suffices to study the variance of the random variable

$$\eta_A = \sum_{k=1}^N \chi_A(\alpha_k),$$

where  $\{\alpha_1, \ldots, \alpha_N\}$  are generated by our dpp. The expected value of  $\eta_A$  satisfies  $\mathbb{E}[\eta_A] = \mu(A)N$ , and the variance of  $\eta_A$  is, by definition (using  $\chi_A(\alpha_k)^2 = \chi_A(\alpha_k)$ ),

$$\operatorname{Var}(\eta_A) = \mathbb{E}[\eta_A^2] - \mathbb{E}[\eta_A]^2 = \mathbb{E}\bigg[\sum_{i \neq j} \chi_A(\alpha_i)\chi_A(\alpha_j)\bigg] + \mu(A)N - \mu(A)^2N^2.$$

The expected value of the right-hand side equals, by (4), (with  $f(x, y) = \chi_A(x)\chi_A(y)$ )

$$\iint_{\alpha,\beta\in A} \left[ \mathcal{C}_{2L}^{(2)}(1) \right]^2 - \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) \right) \right]^2 \mathrm{d}\mu(\beta,\alpha)$$
$$= \mu(A)^2 N^2 - \iint_{\alpha,\beta\in A} \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) \right) \right]^2 \mathrm{d}\mu(\beta,\alpha).$$

In other words, we have

$$\operatorname{Var}(\eta_A) = \mu(A)N - \iint_{\alpha,\beta \in A} \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) \right) \right]^2 \mathrm{d}\mu(\beta,\alpha),$$

and therefore, using invariance of Haar measure, (1), and (10)

$$\operatorname{Var}(\eta_A) - \int_A \int_{A^c} \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) \right) \right]^2 d\mu(\beta) d\mu(\alpha)$$
  
=  $\mu(A)N - \int_{\operatorname{SO}(3)} \chi_A(\alpha) \int_{\operatorname{SO}(3)} \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{\omega(\beta)}{2}\right) \right) \right]^2 d\mu(\beta) d\mu(\alpha)$   
=  $\mu(A)N - \int_{\operatorname{SO}(3)} \chi_A(\alpha)N d\mu(\alpha) = 0.$ 

All in one we have proved the variance version of [20, Eq. 28]:

$$\operatorname{Var}(\eta_A) = \int_A \int_{A^c} \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) \right) \right]^2 \mathrm{d}\mu(\beta) \, \mathrm{d}\mu(\alpha).$$

Now, note that

$$A^{c} = \left\{ \beta \in \mathrm{SO}(3) : \|\beta - \mathbb{1}\|_{F} \ge \sqrt{8} \sin(\varepsilon) \right\},\$$

and by the triangle inequality  $\|\beta - \mathbb{1}\|_F \le \|\beta - \alpha\|_F + \|\mathbb{1} - \alpha\|_F$  for  $\alpha \in A$ , we see that

$$A^{c} \subset S_{\alpha} := \left\{ \beta \in \mathrm{SO}(3) : \omega(\alpha^{-1}\beta) \ge f(\omega(\alpha)) \right\},\$$

 $\underline{\textcircled{O}}$  Springer

where  $f(\omega(\alpha)) := 2 \arcsin\left(\sin(\varepsilon) - \sin\left(\frac{\omega(\alpha)}{2}\right)\right)$ . With the characteristic function  $\chi_{\alpha}$  of  $S_{\alpha}$ ,  $\chi_{\alpha}(\beta) = \chi_{[f(\omega(\alpha)),\pi]}(\omega(\alpha^{-1}\beta))$ , we integrate over SO(3) and use (1):

$$\int \chi_{\alpha}(\beta) \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right) \right) \right]^2 d\mu(\beta)$$

$$= \int \chi_{\alpha}(\alpha\beta) \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{\omega(\beta)}{2}\right) \right) \right]^2 d\mu(\beta)$$

$$= \frac{2}{\pi} \int_{f(\omega(\alpha))}^{\pi} \left[ \mathcal{C}_{2L}^{(2)} \left( \cos\left(\frac{t}{2}\right) \right) \right]^2 \sin^2\left(\frac{t}{2}\right) dt$$

$$= \frac{4}{\pi} \int_{\frac{f(\omega(\alpha))}{2}}^{\pi/2} \left[ \mathcal{C}_{2L}^{(2)} \left( \cos(t) \right) \right]^2 \sin^2(t) dt$$

$$= \frac{4}{\pi} \int_{0}^{\cos\left(\frac{f(\omega(\alpha))}{2}\right)} \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \sqrt{1 - t^2} dt.$$

Applying (1) one more time yields with  $\chi_A(\beta) = \chi_{[0,2\varepsilon)}(\omega(\beta))$ 

$$\begin{aligned} \operatorname{Var}(\eta_{A}) &\leq \int_{\operatorname{SO}(3)} \chi_{A}(\alpha) \int_{\operatorname{SO}(3)} \chi_{\alpha}(\beta) \mathcal{C}_{2L}^{(2)} \left(\cos\left(\frac{\omega(\alpha^{-1}\beta)}{2}\right)\right)^{2} d\mu(\beta) d\mu(\alpha) \\ &= \frac{4}{\pi} \int_{\operatorname{SO}(3)} \chi_{A}(\alpha) \int_{0}^{\cos\left(\frac{f(\omega(\alpha))}{2}\right)} \left[\mathcal{C}_{2L}^{(2)}(t)\right]^{2} \sqrt{1 - t^{2}} dt d\mu(\alpha) \\ &= \frac{16}{\pi^{2}} \int_{0}^{\varepsilon} \sin^{2}(x) \int_{0}^{\sqrt{1 - (\sin(\varepsilon) - \sin(x))^{2}}} \left[\mathcal{C}_{2L}^{(2)}(t)\right]^{2} \sqrt{1 - t^{2}} dt dx \\ &= \frac{16}{\pi^{2}} \int_{0}^{\varepsilon} \sin^{2}(x) \int_{\cos(\varepsilon)}^{\sqrt{1 - (\sin(\varepsilon) - \sin(x))^{2}}} \left[\mathcal{C}_{2L}^{(2)}(t)\right]^{2} \sqrt{1 - t^{2}} dt dx \\ &+ \frac{16}{\pi^{2}} \int_{0}^{\varepsilon} \sin^{2}(x) \int_{0}^{\cos(\varepsilon)} \left[\mathcal{C}_{2L}^{(2)}(t)\right]^{2} \sqrt{1 - t^{2}} dt dx =: I_{1} + I_{2}. \end{aligned}$$

Next we change the order of integration, thus for  $t \in [\cos(\varepsilon), 1]$ , we integrate over  $\{t\} \times [z(t), \varepsilon]$ , where  $z(t) := \arcsin(\sin(\varepsilon) - \sqrt{1-t^2})$ . We do this since  $x \in [z(t), \varepsilon]$  implies  $\sqrt{1 - (\sin(\varepsilon) - \sin(x))^2} \in [t, 1]$ . Thus

$$I_1 = \frac{16}{\pi^2} \int_{\cos(\varepsilon)}^1 \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \sqrt{1 - t^2} \int_{z(t)}^{\varepsilon} \sin^2(x) \, \mathrm{d}x \, \mathrm{d}t.$$

Further, by a standard estimate and the mean value theorem, we get

$$\begin{split} \int_{z(t)}^{\varepsilon} \sin^2(x) \, \mathrm{d}x &\leq \sin^2(\varepsilon) \Big( \arcsin\left(\sin(\varepsilon)\right) - \arcsin\left(\sin(\varepsilon) - \sqrt{1 - t^2}\right) \Big) \\ &\leq \sin^2(\varepsilon) \frac{\sqrt{1 - t^2}}{\cos(\varepsilon)}, \end{split}$$

and hence by Lemma 6.1

$$I_1 \leq \frac{16\sin^2(\varepsilon)}{\pi^2\cos(\varepsilon)} \int_0^1 \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 (1-t^2) \, \mathrm{d}t = \frac{\sin^2(\varepsilon)}{\cos(\varepsilon)} O(L^2\log(L)).$$

We now estimate  $I_2$ . Using  $\sin(\varepsilon) = \sqrt{1 - \cos^2(\varepsilon)} \le \sqrt{1 - t^2}$  for  $t \in [0, \cos(\varepsilon)]$ , Lemma 6.1, and  $\frac{\sin(x)}{\sin(\varepsilon)} \le 1$  yields

$$I_2 \le \frac{16}{\pi^2} \int_0^{\varepsilon} \sin^2(x) \int_0^{\cos(\varepsilon)} \left[ \mathcal{C}_{2L}^{(2)}(t) \right]^2 \sqrt{1 - t^2} \frac{\sqrt{1 - t^2}}{\sin(\varepsilon)} \, \mathrm{d}t \, \mathrm{d}x = \varepsilon^2 O(L^2 \log(L)).$$

Theorem 1.4 is now proved.

### 6 The L<sup>2</sup>-norm of Gegenbauer polynomials

First we recall the digamma function  $\psi(x) := \frac{d}{dx} \log (\Gamma(x))$  and its property:

$$\psi(n+\frac{1}{2}) = \sum_{k=1}^{n} \frac{2}{2k-1} - \gamma - \log(4), \text{ for } n \in \mathbb{N},$$
(11)

see [1, Eq. 6.3.4], where  $\gamma \approx 0.577$  is the Euler-Mascheroni constant.

**Lemma 6.1** The Gegenbauer polynomials  $C_{n-2}^{(2)}(x)$  satisfy

$$\int_0^1 (x^2 - 1) \left[ \mathcal{C}_{n-2}^{(2)}(x) \right]^2 dx = -\frac{2n^2 - 1}{16} \left( \psi(n + \frac{1}{2}) + \gamma + \log(4) \right) + \frac{n^2}{8}.$$

**Lemma 6.2** The Gegenbauer polynomials  $C_{n-2}^{(2)}(x)$  satisfy

$$\int_0^1 \left[ \mathcal{C}_{n-2}^{(2)}(x) \right]^2 \mathrm{d}x = \frac{n^4}{16} + \frac{4n^2 - 1}{64} \left( \psi(n + \frac{1}{2}) + \gamma + \log(4) \right) - \frac{5}{32}n^2.$$

For the proofs, we need a result from [11], showing the following recursive formula for squares of Gegenbauer polynomials:

$$\left(\frac{n}{2\lambda}\right)^2 \left[\mathcal{C}_n^{(\lambda)}(x)\right]^2 = \sum_{k=0}^{n-1} \frac{\lambda+k}{\lambda} \left[\mathcal{C}_k^{(\lambda)}(x)\right]^2 - (1-x^2) \left[\mathcal{C}_{n-1}^{(\lambda+1)}(x)\right]^2,$$

which, for  $\lambda = 1$ , i.e., Chebyshev polynomials of 2nd kind [11, Corollary 6.2], is

$$\frac{(n+1)^2}{4} \left[ \mathcal{U}_{n+1}(x) \right]^2 - \sum_{k=0}^n (k+1) \left[ \mathcal{U}_k(x) \right]^2 = (x^2 - 1) \left[ \mathcal{C}_n^{(2)}(x) \right]^2.$$
(12)

**Proof of Lemma 6.1** We will use a well known identity for  $m \le n$ :

$$\mathcal{U}_m(x)\mathcal{U}_n(x) = \sum_{k=0}^m \mathcal{U}_{n-m+2k}(x),$$
(13)

which follows by induction on *m*, starting and re-applying the recurrence (6). Using (13) with m = n in (12) and integrating yields

$$\begin{split} &\int_{0}^{1} (x^{2} - 1) \left[ \mathcal{C}_{n}^{(2)}(x) \right]^{2} dx \\ &= \frac{(n+1)^{2}}{4} \sum_{k=0}^{n+1} \int_{0}^{1} \mathcal{U}_{2k}(x) dx - \sum_{k=0}^{n} (k+1) \sum_{s=0}^{k} \int_{0}^{1} \mathcal{U}_{2s}(x) dx \\ &= \frac{(n+1)^{2}}{4} \sum_{k=0}^{n+1} \frac{\mathcal{T}_{2k+1}(1) - \mathcal{T}_{2k+1}(0)}{2k+1} - \sum_{k=0}^{n} (k+1) \sum_{s=0}^{k} \frac{\mathcal{T}_{2s+1}(1) - \mathcal{T}_{2s+1}(0)}{2s+1} \\ &= \frac{(n+1)^{2}}{4} \sum_{k=0}^{n+1} \frac{1}{2k+1} - \sum_{k=0}^{n} \sum_{s=0}^{k} \frac{k+1}{2s+1}, \end{split}$$

where we used (9) and that  $T_{2n+1}(x)$  is odd. By (11), we state for later use:

$$\int_0^1 [\mathcal{U}_n(x)]^2 \, \mathrm{d}x = \sum_{k=0}^n \frac{1}{2k+1} = \frac{1}{2} \Big( \psi(n+\frac{3}{2}) + \gamma + \log(4) \Big), \text{ for } n \in \mathbb{N}_0.$$
(14)

We continue with

$$\int_{0}^{1} (x^{2} - 1) \left[ C_{n}^{(2)}(x) \right]^{2} dx$$

$$= \frac{(n+1)^{2}}{8} \left( \psi(n+\frac{5}{2}) + \gamma + \log(4) \right)$$

$$- \sum_{k=0}^{n} \frac{k+1}{2} \psi(k+\frac{3}{2}) - (\gamma + \log(4)) \frac{(n+2)(n+1)}{4}$$

$$= \frac{(n+1)^{2}}{8} \psi(n+\frac{5}{2})$$

$$- \sum_{k=1}^{n+1} \frac{k}{2} \psi(k+\frac{1}{2}) - \frac{(n+3)(n+1)}{8} (\gamma + \log(4)).$$

Also, we find by induction:

$$\sum_{k=1}^{n} \frac{k}{2} \psi(k+\frac{1}{2}) = \frac{1}{16} \left[ (2n+1)^2 \psi(n+\frac{3}{2}) - 2(n+1)^2 + \gamma + \log(4) \right],$$

where we used the recurrence  $\psi(z + 1) = \psi(z) + \frac{1}{z}$ , see [1, Eq. 6.3.5]. Thus

$$\int_0^1 (x^2 - 1) \left[ \mathcal{C}_{n-2}^{(2)}(x) \right]^2 dx$$
  
=  $\frac{2(n-1)^2 - (2n-1)^2}{16} \psi(n+\frac{1}{2}) + \frac{n^2}{8}$   
 $- \frac{2(n+1)(n-1) + 1}{16} (\gamma + \log(4))$   
=  $-\frac{2n^2 - 1}{16} \left( \psi(n+\frac{1}{2}) + \gamma + \log(4) \right) + \frac{n^2}{8}$ 

finishing the proof.

The proof of Lemma 6.2 first needs some preparation.

**Lemma 6.3** Let  $c_{j,k}$  for  $j, k \in \{0, ..., n\}$  be real numbers such that

(1)  $c_{j,k} = c_{j+r,k+r}$  for j + k = n - r with  $r \in \{1, ..., n\}$ , (2)  $c_{j,k} = c_{n-j,k}$  for  $j \ge k$ , (3)  $c_{j,k} = c_{k,j}$ .

Then for any function  $f : \mathbb{N}_0 \to \mathbb{R}$ , we have<sup>1</sup>

$$\sum_{j,k=0}^{n} c_{j,k} f(|j-k|) = \sum_{j,k=0}^{n} c_{j,k} f(|n-j-k|) = 2 \sum_{r=0}^{n'} f(r) \sum_{u=0}^{n-r} c_{r+u,u}.$$
 (15)

**Proof** We first fix some  $r \in \{1, ..., n\}$  and regard the second sum. Observe that for all tuples such that  $j_i + k_i = n - r$  and  $\hat{j}_i + \hat{k}_i = n + r$ , we also have  $|n - j_i - k_i| = |n - \hat{j}_i - \hat{k}_i| = r$ . These tuples are listed in the following table:

i	1	2	 n - r + 1
ji	0	1	n-r
$k_i$	n - r	n - r - 1	 0
Ĵi	r	r + 1	n
$\hat{k}_i$	n	n - 1	r

So for all  $r, (j_i, k_i) \mapsto (j_i + r, k_i + r) = (\hat{j}_i, \hat{k}_i)$  is a bijection with  $c_{j_i, k_i} = c_{\hat{j}_i, \hat{k}_i}$  and

$$\sum_{j,k=0}^{n} c_{j,k} f(|n-j-k|) = 2 \sum_{\substack{j,k=0\\j+k < n}}^{n} c_{j,k} f(n-j-k) + f(0) \sum_{u=0}^{n} c_{n-u,u}.$$

		-	

<sup>&</sup>lt;sup>1</sup> The apostrophe on the sum-symbol sigma means taking half the first term.

The first sum of (15) can be restricted to j > k when doubled, apart from the sum  $f(0) \sum_{u=0}^{n} c_{u,u}$ . Again, we list all tuples with  $j_i - k_i = r = n - \hat{j}_i - \hat{k}_i$ :

i	1	2		n - r + 1
ji	r	r + 1		п
$k_i$	0	1		n-r
$\hat{j}_i$	n-r	n - r - 1		0
$\hat{k}_i$	0	1		n-r

Similarly,  $(j_i, k_i) \mapsto (n - j_i, k_i) = (\hat{j}_i, \hat{k}_i)$  is a bijection with  $c_{j_i, k_i} = c_{\hat{j}_i, \hat{k}_i}$ , and

$$\sum_{i>k=0}^{n} c_{j,k} f(j-k) = \sum_{\substack{j,k=0\\j+k< n}}^{n} c_{j,k} f(n-j-k).$$

Rewriting the first sum above via j = r + u and k = u for some  $u \in \{0, ..., n - r\}$  and using that  $c_{n-u,u} = c_{u,u}$  finishes the argument.

Requirement 2. in Lemma 6.3 is valid for all j, k. To see this, let j < k, then

$$c_{j,k} \stackrel{2.+3.}{=} c_{j,n-k} \stackrel{1.}{=} c_{j+(k-j),n-k+(k-j)} = c_{k,n-j} \stackrel{3.}{=} c_{n-j,k}.$$

**Lemma 6.4** Let  $n \in \mathbb{N}$  and  $\lambda \in (-1/2, 0) \cup (0, \infty)$ . For  $j, k \in \{0, \ldots, n\}$  we define

$$c_{j,k}^{(\lambda)} = c_{j,k}^{(\lambda)}(n) = \frac{1}{[\Gamma(\lambda)]^4} \frac{\Gamma(\lambda+j)\Gamma(\lambda+n-j)}{j!(n-j)!} \frac{\Gamma(\lambda+k)\Gamma(\lambda+n-k)}{k!(n-k)!}.$$

Then

$$\left[\mathcal{C}_{n}^{(\lambda)}(\cos(t))\right]^{2} = \sum_{u=0}^{n} c_{u,u}^{(\lambda)} + 2\sum_{r=1}^{n} \cos(2rt) \sum_{u=0}^{n-r} c_{r+u,u}^{(\lambda)}.$$

In particular,

$$\int_0^{\pi/2} [C_n^{(\lambda)}(\cos\varphi)]^2 \, d\varphi = \frac{\pi}{2} \sum_{u=0}^n c_{u,u}^{(\lambda)}.$$

*Proof* We will use Lemma 6.3 with [13, Eq. 8.934]:

$$C_n^{(\lambda)}(\cos(\varphi)) = \sum_{\substack{k,\ell=0\\k+\ell=n}}^n \frac{\Gamma(\lambda+k)\Gamma(\lambda+\ell)}{k!\ell![\Gamma(\lambda)]^2} \cos((k-\ell)\varphi),$$

in conjunction with the angle-sum and half-angle formula for cosine and sine:

$$\begin{aligned} \left[\mathcal{C}_{n}^{(\lambda)}(1)\right]^{2} &- \left[\mathcal{C}_{n}^{(\lambda)}\left(\cos(t)\right)\right]^{2} = \sum_{j,k=0}^{n} c_{j,k}^{(\lambda)} \left(1 - \cos\left((n-2j)t\right)\cos\left((n-2k)t\right)\right) \\ &= \sum_{j,k=0}^{n} c_{j,k}^{(\lambda)} \frac{1}{2} \left(1 - \cos\left((j-k)2t\right) + 1 - \cos\left((n-j-k)2t\right)\right) \\ &= \sum_{j,k=0}^{n} c_{j,k}^{(\lambda)} \left(\sin^{2}\left((j-k)t\right) + \sin^{2}\left((n-j-k)t\right)\right) = 4\sum_{r=1}^{n} \sin^{2}(rt) \sum_{u=0}^{n-r} c_{r+u,u}^{(\lambda)} \end{aligned}$$

Hence, with  $\left[\mathcal{C}_{n}^{(\lambda)}\left(\cos(t)\right)\right]^{2} = \left[\mathcal{C}_{n}^{(\lambda)}(1)\right]^{2} - \left(\left[\mathcal{C}_{n}^{(\lambda)}(1)\right]^{2} - \left[\mathcal{C}_{n}^{(\lambda)}\left(\cos(t)\right)\right]^{2}\right)$ 

$$\begin{split} \left[ \mathcal{C}_n^{(\lambda)} \big( \cos(t) \big) \right]^2 &= 2 \sum_{r=0}^{n'} \sum_{u=0}^{n-r} c_{r+u,u}^{(\lambda)} - 4 \sum_{r=1}^{n} \sin^2(rt) \sum_{u=0}^{n-r} c_{r+u,u}^{(\lambda)} \\ &= \sum_{u=0}^{n} c_{u,u}^{(\lambda)} + 2 \sum_{r=1}^{n} \big( 1 - 2 \sin^2(rt) \big) \sum_{u=0}^{n-r} c_{r+u,u}^{(\lambda)}, \end{split}$$

and we finish using  $1 - 2\sin^2(rt) = \cos(2rt)$ .

**Proof of Lemma 6.2** With the notation of Lemma 6.4, where  $c_{j,k} = c_{j,k}^{(2)}(n-2)$ :

$$\sum_{u=0}^{n-2-r} c_{r+u,u} = \sum_{u=1}^{n-1-r} (r+u)(n-u)u(n-r-u)$$
$$= \frac{4r^2 - 1}{120} \left( r \left( 5n^2 - \frac{1}{4} \right) - r^3 - 5n(n^2 - 1) \right) - \frac{2r}{64} (4n^2 - 1) + \binom{2n+2}{5} \frac{1}{8}$$

Further, we see by induction  $\sum_{r=1}^{n-2} \frac{1}{4r^2-1} = \frac{n-2}{2n-3}$ , and thus by Lemma 6.4

$$\int_{0}^{1} \left[ \mathcal{C}_{n-2}^{(2)}(x) \right]^{2} dx$$
  
=  $\sum_{u=0}^{n-2} c_{u,u} + 2 \sum_{r=1}^{n-2} \int_{0}^{\frac{\pi}{2}} \cos(2rt) \sin(t) dt \sum_{u=0}^{n-2-r} c_{r+u,u}$   
=  $\sum_{u=0}^{n-2} c_{u,u} - 2 \sum_{r=1}^{n-2} \frac{1}{4r^{2} - 1} \sum_{u=0}^{n-2-r} c_{r+u,u}$   
=  $\frac{n^{5} - n}{30} - \frac{1}{60} \sum_{r=1}^{n-2} \left( r \left( 5n^{2} - \frac{1}{4} \right) - r^{3} - 5n(n^{2} - 1) \right)$ 

$$+2\sum_{r=1}^{n-2} \frac{1}{4r^2 - 1} \left( \frac{2r}{64} (4n^2 - 1) - \binom{2n+2}{5} \frac{1}{8} \right)$$
$$= \frac{2n^4 - 5n^2}{32} + \sum_{r=0}^{n-1} \frac{1}{4r^2 - 1} \frac{2r - 1}{32} (4n^2 - 1),$$

as  $\left(\frac{4n^2-1}{32} - \binom{2n+2}{5}\frac{1}{4}\right)\frac{n-2}{2n-3}$  has a simple form. Equation (14) finishes the proof.  $\Box$ 

Acknowledgements Elkies' general argument for the lower bound of Green Energy (see Sect. 4.1) has been pointed out to the authors by E. Saff, and his help is thankfully acknowledged. We also thank the two anonymous referees for helpful comments.

#### Appendix A: The strong maximum principle on manifolds

We state the classical strong maximum principle Theorem A.1 for open, bounded, and connected subsets  $U \subset \mathbb{R}^n$ , and regard second order parabolic partial differential operators  $L + \frac{\partial}{\partial t}$  acting on functions  $C_1^2(U \times (0, T])$ , i.e., twice differentiable with respect to spatial variables and once with respect to time. T > 0. A special case of this is extended in Theorem A.2. We set for smooth coefficients:

$$Lu(x,t) = -\sum_{i,j}^{n} a_{ij}(x,t) \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} u(x,t) + \sum_{j}^{n} b_j(x,t) \frac{\partial}{\partial x_j} u(x,t), \quad (16)$$

and without loss of generality,  $a_{ij}(x, t) = a_{ji}(x, t)$ .

**Definition A.1** L +  $\frac{\partial}{\partial t}$  is said to be uniformly parabolic if there is a C > 0, such that

$$\sum_{i,j} a_{ij}(x,t)\xi_i\xi_j \ge C \|\xi\|_2^2, \quad \text{where } \xi \in \mathbb{R}^n, \ (x,t) \in U \times (0,T].$$
(17)

**Theorem A.1** (Thm. 11, page 396 of [12]) Let  $u \in C_1^2(U \times (0, T]) \cap C(\overline{U} \times [0, T])$  be such that

$$\mathcal{L}u + \frac{\partial}{\partial t}u = 0,$$

for  $U \subset \mathbb{R}^n$  as above,  $L + \frac{\partial}{\partial t}$  uniformly parabolic, and L as in (16). If the maximum or minimum of u is attained at a point  $(x_0, t_0) \in U \times (0, T]$ , then u equals this value everywhere in  $U \times [0, t_0]$ .

Given a manifold M with or without boundary, we set  $M^\circ = M \setminus \partial M$ , and for  $x \in M$ , define  $M_x$  as the connected component of M containing x. Now, the next theorem should be known, but we haven't found a reference.

**Theorem A.2** Let (M, g) be an n-dimensional (smooth) compact Riemannian manifold with or without boundary, not necessarily connected. Suppose  $u \in C_1^2(M^\circ \times (0, T]) \cap C(M \times [0, T])$  satisfies for  $(x, t) \in M^\circ \times (0, T]$ :

$$\Delta_g u(x,t) + \frac{\partial}{\partial t} u(x,t) = 0.$$

If the maximum or minimum of u is attained at a point  $(x_0, t_0) \in M^{\circ} \times (0, T]$ , then u equals this value everywhere in  $M_{x_0} \times [0, t_0]$ . In particular, the maximum and minimum of u are attained in  $(\partial M \times [0, T]) \cup (M^{\circ} \times \{0\})$ .

**Proof** For every  $\alpha \in M^{\circ}$ , there is an open neighborhood  $U_{\alpha} \subset M$  and a chart  $\mathbf{x}_{\alpha}$ :  $U_{\alpha} \to B_{\alpha} \subset \mathbb{R}^{n}$ , such that  $\mathbf{x}_{\alpha}(U_{\alpha})$  is an open ball  $B_{\alpha}$ , and the local representation of  $\Delta_{g}$  in  $U_{\alpha}$  is of type (16), and satisfies (17) for C = 1/2. This follows from the fact that the Laplace–Beltrami operator at a point  $\beta$  in the interior can be written as the usual Laplacian at  $\beta$ , and by continuity of the coefficients, there is an open set of  $\beta$  where the inequality (17) is true for C = 1/2.

Assume there were a  $t_0 > 0$  such that the maximum/minimum of u would be attained at  $(\alpha, t_0)$ . Writing  $\Delta_g$  with respect to the chart  $\mathbf{x}_{\alpha}$  as  $\Delta_{\alpha}$ , and regarding the equation

$$\Delta_{\alpha}u(\boldsymbol{x}_{\alpha}^{-1}(x),t) + \frac{\partial}{\partial t}u(\boldsymbol{x}_{\alpha}^{-1}(x),t) = 0,$$

in  $B_{\alpha} \times (0, T]$ , a neighborhood of  $(\mathbf{x}_{\alpha}(\alpha), t_0)$ , we deduce by Theorem A.1 that  $u(x, t) \equiv u(\alpha, t_0)$  for all  $(x, t) \in B_{\alpha} \times [0, t_0]$ .

Further,  $M_{\alpha}$  is covered by finitely many intersecting charts as above, and Theorem A.1 would yield that *u* is constant and equals  $u(\alpha, t_0)$  in all of  $M_{\alpha} \times [0, t_0]$ . The maximum/minimum is in particular attained at the boundary as claimed.

#### References

- Abramowitz, M., Stegun, I.A.: Handbook of Mathematical Functions With Formulas, Graphs, and Mathematical Tables. Department of Commerce (USA), National Bureau of Standards, Applied Mathematics Series 55 (1972)
- Alishashi, K., Zamani, M.S.: The spherical ensemble and uniform distribution of points on the sphere. Electron. J. Probab. 20(23), 27 (2015)
- Aubin, T.: Some Nonlinear Problems in Riemannian Geometry. Springer Monographs in Mathematics. Springer, Berlin (1998)
- Beltrán, C., Criado del Rey, J.G., Corral, N.: Discrete and continuous Green energy on compact manifolds. J. Approx. Theory 237, 160–185 (2019)
- Beltrán, C., Etayo, U.: The projective ensamble and distribution of points in odd-dimensional spheres. Constr. Approx. 48(1), 163–182 (2018)
- Beltrán, C., Marzo, J., Ortega-Cerdà, J.: Energy and discrepancy of rotationally invariant determinantal point processes in high dimensional spheres. J. Complex. 37, 76–109 (2016)
- Ben Hough, J., Krishnapur, M., Peres, Y., Virág, V.: Zeros of Gaussian Analytic Functions and Determinantal Point Processes. American Mathematical Society, Providence (2009)
- 8. Borodachov, S.V., Hardin, D.P., Saff, E.B.: Discrete Energy on Rectifiable Sets. Springer, Berlin (2019)
- Criado del Rey, J.G.: On the Separation Distance of Minimal Green Energy Points on Compact Riemannian Manifolds. arXiv:1901.00779v1 (2019)

- 10. do Carmo, M.P.: Riemannian Geometry. Birkhäuser, Boston (1992)
- Dette, H.: New identities for orthogonal polynomials on a compact interval. J. Math. Anal. Appl. 179, 547–573 (1993)
- 12. Evans, L.C.: Partial Differential Equations, 2nd edn. American Mathematical Society, Providence (2010)
- 13. Gradshteyn, I.S., Ryzhik, I.M., Jeffrey, A., Zwillinger, D.: Table of Integrals, Series, and Products, 6th edn. Academic Press, New York (2000)
- Hangelbroek, T., Schmid, D.: Surface spline approximation on SO(3). Appl. Comput. Harmon. Anal. 31(2), 169–184 (2011)
- Hua, L.K.: Harmonic analysis of functions of several complex variables in the classical domains (Translated from the Russian by L. Ebner and A. Korányi). American Mathematical Society, Providence (1963)
- Joshi, A.W.: Elements of Group Theory for Physicists. Wiley Eastern Private Limited, New Delhi (1973)
- 17. Jost, J.: Riemannian Geometry and Geometric Analysis, 6th edn. Springer, Heidelberg (2011)
- 18. Lang, S.: Introduction to Arakelov Theory. Springer, New York (1988)
- Marzo, J., Ortega-Cerdà, J.: Expected Riesz energy of some determinantal processes on flat tori. Constr. Approx. 47(1), 75–88 (2018)
- Rider, B., Virág, B.: Complex determinantal processes and H<sup>1</sup> noise. Electron. J. Probab. 12, 1238–57 (2007)
- Shub, M., Smale, S.: Complexity of Bezout's theorem II—Volumes and Probabilities. Computational Algebraic Geometry, Progr. Math., vol. 109, Birkhäuser Boston, Boston, MA, pp 267–285 (1993)
- 22. Smale, S.: Mathematical problems for the next century. Math. Intell. 20(2), 7–15 (1998)
- 23. Szegö, G.: Orthogonal Polynomials. Amer. Math. Soc (1939)
- Vollrath, A.: The Nonequispaced Fast SO(3) Fourier Transform, Generalisations and Applications (PhD-Thesis). University of Lübeck (2010)
- Wigner, E.P.: Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra. Academic Press, New York (1959)

**Publisher's Note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.