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The Diamond ensemble: A constructive set of spherical points with small logarithmic energy[☆,☆☆]

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ABSTRACT

We define a family of random sets of points, the Diamond ensemble, on the sphere $\mathbb{S}^2$ depending on several parameters. Its most important property is that, for some of these parameters, the asymptotic expected value of the logarithmic energy of the points can be computed rigorously and shown to attain very small values, quite close to the conjectured minimal value.

1. Introduction and main results

Sets of points on the sphere $\mathbb{S}^2$ that are well-distributed in some sense conform an interesting object of study, see for example [6] for an interesting survey with different approaches to well-distributed points and [4] for a complete monography. One usually seeks for points with small *cap discrepancy* or maximal *separation distance* or, as we do in this paper, minimal *potential energy*.

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1.1. Riesz and logarithmic energy

Given $s \in (0, \infty)$, the Riesz potential or s–energy of a set on points $\omega_N = \{x_1, \ldots, x_N\}$ on the sphere $\mathbb{S}^2$ is

$$\mathcal{E}_s(\omega_N) = \sum_{i \neq j} \frac{1}{\|x_i - x_j\|^s}. \tag{1}$$

This energy has a physical interpretation for some particular values of s, i.e. for $s = 1$ the Riesz energy is the Coulomb potential and in the special case $s = 0$ the energy is defined by

$$\mathcal{E}_{\log}(\omega_N) = \left.\frac{d}{ds}\right|_{s=0} \mathcal{E}_s(\omega_N) = \sum_{i \neq j} \log \|x_i - x_j\|^{-1}$$

and is related to the transfinite diameter and the capacity of the set by classical potential theory, see for example [15].

1.2. Smale's 7th problem

Shub and Smale [20] found a relation between the condition number (a quantity measuring the sensitivity of zero finding) of polynomials and the logarithmic energy of associated spherical points. Inspired by this relation, they proposed a problem that is nowadays known as Smale's 7th problem [21]: find a constructive (and fast) way to produce N points with quasioptimal logarithmic energy. More exactly, on input N, one must produce a set of N points ω_N on the unit sphere such that

$$\mathcal{E}_{\log}(\omega_N) - m_N \leq c \log N,$$

where c is some universal constant and m_N is the minimum possible value of $\mathcal{E}_{\log}$ among all collections of N spherical points.

1.3. The value of m_N

A major difficulty in Smale's 7th problem is that the value of m_N is not even known up to precision $\log N$. A series of papers [5,9,18,22] gave upper and lower bounds for the value of m_N. The last word has been given in [3] where this value is related to the minimum renormalized energy introduced in [19] proving the existence of an $O(N)$ term. The current knowledge is:

$$m_N = W_{\log}(\mathbb{S}^2) N^2 - \frac{1}{2} N \log N + C_{\log} N + o(N), \tag{2}$$

where

$$W_{\log}(\mathbb{S}^2) = \frac{1}{(4\pi)^2} \int_{x,y \in \mathbb{S}^2} \log \|x - y\|^{-1} \, dxdy = \frac{1}{2} - \log 2 \tag{3}$$

is the continuous energy and $C_{\log}$ is a constant. Here, as usual, $o(N)$ is a function of N with the property that $\lim_{N\to\infty} o(N)/N = 0$. Combining [9] with [3] it is known that

$$-0.223282\ldots \leq C_{\log} \leq 2\log 2 + \frac{1}{2} \log \frac{2}{3} + 3 \log \frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.055605\ldots,$$

and indeed the upper bound for $C_{\log}$ has been conjectured to be an equality using two different approaches [3,8]. This conjecture on the value of $C_{\log}$ was recently proved to be equivalent to two other well-known conjectures in potential theory: the Vortices Conjecture and the Cohn–Kumar Conjecture for the $2d$ Coulomb potential, see [17].

1.4. Explicit constructions toward Smale's 7th problem

Several point sequences that seem to have low logarithmic energy have been proposed. In [11] we find a number of families of points (some of them are random and some of them are not) together with numerical evidence of their properties for values as high as $N = 50.000$ spherical points. However, obtaining theoretical results for the properties of these sequences has proved a very hard task. Of course one can just run a generic optimization algorithm starting on those sequences and get seemingly optimal collections of points but theoretical results about the asymptotical properties of the output of such methods are quite out of reach.

Theoretical computations of the energy of constructively feasible families of points have only been done in a few cases.

Points coming from the spherical ensemble (that can be seen after a stereographic projection as the eigenvalues of $A^{-1}B$ where A and B are random Gaussian matrices, see [14]) have been proved in [1] to have average logarithmic energy

$$W_{\log}(\mathbb{S}^2)\,N^2 - \frac{1}{2}\,N\log N + c_1\,N + o(N),$$

where $c_1 = \log 2 - \gamma/2 = 0.404539\ldots$ (here, γ is the Euler–Mascheroni constant).

On the other hand, points obtained (after the stereographic projection) as zeros of certain random polynomials have been studied in [2] proving that the expected value of the logarithmic energy in this case is

$$W_{\log}(\mathbb{S}^2)\,N^2 - \frac{1}{2}\,N\log N + c_2\,N + o(N),$$

where $c_2 = -W_{\log}(\mathbb{S}^2) = 0.193147\ldots$

Both c_1 and c_2 are quite far from the known upper bound for $C_{\log}$ and thus these methods are far from providing an answer to Smale's problem.

1.5. Main result: the Diamond ensemble

In this paper, we define a collection of random points, the *Diamond ensemble* $\diamond(N)$, depending on several parameters. For appropriate choices of the parameters, our construction produces families of points that very much resemble some already known families for which the asymptotic expansion of the logarithmic energy is unknown, such as the octahedral points or the zonal equal area nodes, see [11,12,18]. Indeed our paper can be seen as a follow up of [18, Theorem 3.2].

A quasioptimal choice of these parameters is described in Section 4.3, we call the resulting set the *quasioptimal Diamond ensemble*, and its main interest is that we can prove the following bound.

Theorem 1.1. *The expected value of the logarithmic energy of the quasioptimal Diamond ensemble described in Section 4.3 is*

$$W_{\log}(\mathbb{S}^2)\,N^2 - \frac{1}{2}\,N\log N + c_\diamond\,N + o(N),$$

where $c_\diamond = -0.049222\ldots$ *satisfies*

$$\begin{aligned}14340\,c_\diamond &= 19120\log 239 - 2270\log 227 - 1460\log 73 - 265\log 53 - 1935\log 43\\ &-930\log 31 - 1710\log 19 - 1938\log 17 + 19825\log 13 + 1750\log 7\\ &-4250\log 5 - 131307\log 3 + 56586\log 2 - 7170.\end{aligned}$$

The value of the constant is thus approximately 0.0058 far from the value conjectured in [3,8]. The Diamond ensemble is fully constructive: once a set of parameters is chosen, one just has to choose some uniform random numbers $\theta_1, \ldots, \theta_p \in [0, 2\pi]$ and then the N points are simply given by the direct formulas shown in Section 4.3. It is thus extremely easy to generate these sequences of points.

As one can guess from the expression of $c_\diamond$, obtaining the exact value for that constant requires the computation of a huge number of elementary integrals and derivatives and has been done using the computer algebra package Maxima [16]. Our proof of Theorem 1.1 is thus, in some sense, a computer aided proof. A more simple example (with more simple parameters) that can actually be done by hand is presented in Section 4.1.

1.6. Structure of the paper

In Section 2 we present a formula for computing the energy of the roots of unity of some parallels. In Section 3 we define the Diamond ensemble and through the formula of Section 2 we compute its associated logarithmic energy. In Section 4 we present some concrete examples of the Diamond ensemble. In particular a simple model that can be made by hand, a more elaborated example and the quasioptimal Diamond ensemble in terms of minimizing logarithmic energy. In that section we also give the asymptotic expansion of the logarithmic energy associated to every single example. Section 5 is devoted to proofs and Appendix contains some bounds for the error of the trapezoidal rule.

2. A general construction and a formula for its average logarithmic energy

Fix $z \in (-1, 1)$. The parallel of height z in the sphere $\mathbb{S}^2 \subset \mathbb{R}^3$ is simply the set of points $x \in \mathbb{S}^2$ such that $\langle x, (0, 0, 1)\rangle = z$, where $\langle \cdot, \cdot \rangle$ is the euclidean inner product. A general construction of points can then be done as follows:

(1) Choose a positive integer p and $z_1, \ldots, z_p \in (-1, 1)$. Consider the p parallels with heights $z_1, \ldots, z_p$.
(2) For each j, $1 \le j \le p$, choose a number r_j of points to be allocated on parallel j.
(3) Allocate r_j points in parallel j (which is a circumference) by projecting the r_j roots of unity onto the circumference and rotating them by random phase $\theta_j \in [0, 2\pi]$.
(4) To the already constructed collection of points, add the North and South pole $(0, 0, 1)$ and $(0, 0, -1)$.

We will denote this random set by $\Omega(p, \{r_j\}, \{z_j\})$. Explicit formulas for this construction are easily produced: points in parallel of height z_j are of the form

$$x = \left(\sqrt{1 - z_j^2}\cos\theta, \sqrt{1 - z_j^2}\sin\theta, z_j\right) \tag{4}$$

for some $\theta \in [0, 2\pi]$ and thus the set we have described agrees with the following definition.

Definition 2.1. Let $\Omega(p, \{r_j\}, \{z_j\})$ be the following set of points

$$\Omega(p, \{r_j\}, \{z_j\}) = \begin{cases} \mathcal{N} = (0, 0, 1) \\ x_j^i = \left(\sqrt{1 - z_j^2}\cos\left(\frac{2\pi i}{r_j} + \theta_j\right), \sqrt{1 - z_j^2}\sin\left(\frac{2\pi i}{r_j} + \theta_j\right), z_j\right) \\ \mathcal{S} = (0, 0, -1) \end{cases} \tag{5}$$

where r_j is the number of roots of unity that we consider in the parallel j, $1 \le j \le p$ is the number of parallels, $1 \le i \le r_j$ and $0 \le \theta_j \le 2\pi$ is a random angle rotation in the parallel j.

The following proposition is easy to prove.

Proposition 2.2. *Let x be chosen uniformly and randomly in the parallel of height z_i and let y be chosen uniformly and randomly in the parallel of height z_j. The average value of $-\log\|x - y\|$ is*

$$-\frac{\log\left(1 - z_i z_j + |z_i - z_j|\right)}{2}.$$

The following result follows directly from Proposition 2.2.

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Corollary 2.3. *Let x_j^i be as in Definition 2.1. Then, for $j \neq k$,*

$$E_{\theta_j,\theta_k}\left[-\sum_{l=1}^{r_k}\sum_{i=1}^{r_j}\log\left(\|x_j^i - x_k^l\|\right)\right] = -r_j r_k \frac{\log\left(1 - z_j z_k + |z_j - z_k|\right)}{2},$$

where θ_j, θ_k are uniformly distributed in $[0, 2\pi]$.

From Corollary 2.3 we will prove the following result which gives us an expression for the expected logarithmic energy of the set $\Omega(p, \{r_j\}, \{z_j\})$.

Proposition 2.4. *The average logarithmic energy of points drawn from $\Omega(p, \{r_j\}, \{z_j\})$ is*

$$\begin{aligned}
&E_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathscr{E}_{\log}(\Omega(p, \{r_j\}, \{z_j\}))\right] = \\
&-2\log(2) - \sum_{j=1}^{p} r_j\left[\log(4) + \frac{1}{2}\log(1 - z_j^2) + \log r_j\right] \\
&- \sum_{j,k=1}^{p} r_j r_k \frac{\log\left(1 - z_j z_k + |z_j - z_k|\right)}{2}.
\end{aligned}$$

It turns out that, for any fixed choice of $r_1, \ldots, r_p$, one can compute exactly the optimal choice of the heights $z_1, \ldots, z_p$.

Proposition 2.5. *Given $\{r_1, \ldots, r_p\}$ such that $r_i \in \mathbb{N}$, there exists a unique set of heights $\{z_1, \ldots, z_p\}$ such that $z_1 > \cdots > z_p$ and $E_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathscr{E}_{\log}(\Omega(p, \{r_j\}, \{z_j\}))\right]$ is minimized. The heights are:*

$$z_l = \frac{\sum_{j=l+1}^{p} r_j - \sum_{j=1}^{l-1} r_j}{1 + \sum_{j=1}^{p} r_j} = 1 - \frac{1 + r_l + 2\sum_{j=1}^{l-1} r_j}{N - 1},$$

where $N = 2 + \sum_{j=1}^{p} r_j$ is the total number of points.

From now on we will denote by $\Omega(p, \{r_j\})$ the set $\Omega(p, \{r_j\}, \{z_j\})$ where the z_j are chosen as in Proposition 2.5. With this choice of z_j we have the main result of this section:

Theorem 2.6. *Let $p = 2M - 1$ be an odd integer. If $r_j = r_{p+1-j}$ and z_j are chosen as in Proposition 2.5 we then have*

$$\begin{aligned}
&E_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathscr{E}_{\log}(\Omega(p, \{r_j\}))\right] \\
&= -(N-1)\log(4) - \sum_{j=1}^{p} r_j \log r_j - (N-1)\sum_{j=1}^{p} r_j(1 - z_j)\log(1 - z_j) \\
&= -(N-1)\log(4) + r_M \log r_M - 2\sum_{j=1}^{M} r_j \log r_j \\
&- (N-1)\sum_{j=1}^{M} r_j(1 - z_j)\log(1 - z_j) - (N-1)\sum_{j=1}^{M} r_j(1 + z_j)\log(1 + z_j).
\end{aligned}$$

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3. The Diamond ensemble

We are now ready to define the construction that leads to Theorem 1.1. It amounts to choose some $r_1, \dots, r_p$ such that the energy bound computed in Theorem 2.6 is as low as possible and can be computed up to order $o(N)$. Our construction is based in the following heuristic argument.

3.1. A heuristic argument

Let us choose $z_1, \dots, z_p$ in such a way that they define p equidistant parallels on the sphere. In other words,

$$z_j = \cos \frac{j\pi}{p+1}$$

The distance between two consecutive parallels is $2\sin(\pi/(2(p+1)))$. We would like to choose r_j in such a way that the distance between two consecutive points of the same parallel is approximately equal to some constant times this distance. Since parallel of height z_j is a circumference of radius $\sin(j\pi/(p+1))$, this goal is attained by setting for example

$$r_j = \frac{K_0\pi \sin\left(\frac{j\pi}{p+1}\right)}{\sin\left(\frac{\pi}{2(p+1)}\right)}, \text{ for some constant } K_0 > 0. \tag{6}$$

Let us forget for a moment that this gives an impossible construction (since the r_j will not be integer numbers). One can then plug in Proposition 2.4 these values of z_j and r_j. After a considerable amount of work the right-hand term in Proposition 2.4 can be proved to have the asymptotic expansion

$$W_{\log}(\mathbb{S}^2)N^2 - \frac{1}{2}N\log(N) + \left(\frac{K_0\pi}{6} - \frac{1}{2}\log K_0 - \frac{\log\pi}{2}\right)N + o(N), \tag{7}$$

where $N = 2 + r_1 + \cdots + r_p$ is the total number of points in the sphere. The optimal value of K_0 is $K_0 = 3/\pi$, yielding the asymptotic

$$W_{\log}(\mathbb{S}^2)N^2 - \frac{1}{2}N\log(N) + \frac{1-\log(3)}{2}N + o(N),$$

where $\frac{1-\log(3)}{2} = -0.049306\dots$

Unfortunately, this reasoning does not actually produce collections of points since as pointed out above the number of points in each parallel must be an integer number. The computation of the formula (7) is done with techniques similar to the ones used below but we do not include it since we actually only use it as an inspiration of our true construction below.

3.2. An actual construction

Inspired on the heuristic argument above, we will try to search for sets of the form $\Omega(p, \{r_j\})$ such that the r_j are integer numbers close to $\frac{3\sin\left(\frac{j\pi}{p+1}\right)}{\sin\left(\frac{\pi}{2(p+1)}\right)}$. We will then choose the optimal values for the z_j given by Proposition 2.5. Our approach is to consider different piecewise linear approximations to the formula (6) with $K_0 = 3/\pi$.

Definition 3.1. Let p, M be two positive integers with $p = 2M - 1$ odd and let $r_j = r(j)$ where $r : [0, 2M] \to \mathbb{R}$ is a continuous piecewise linear function satisfying $r(x) = r(2M - x)$ and

$$r(x) = \begin{cases} \alpha_1 + \beta_1 x & \text{if } 0 = t_0 \le x \le t_1, \\ \vdots & \vdots \\ \alpha_n + \beta_n x & \text{if } t_{n-1} \le x \le t_n = M. \end{cases}$$

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Here, $[t_0, t_1, \ldots, t_n]$ is some partition of $[0, M]$ and all the $t_\ell, \alpha_\ell, \beta_\ell$ are assumed to be integer numbers.

We assume that $\alpha_1 = 0$, $\alpha_\ell, \beta_\ell \geq 0$ and $\beta_1 > 0$. We will later let M vary but we assume that there exists a constant $A \geq 2$ not depending on M such that $n \leq A$, $\alpha_\ell \leq AM$, $\beta_\ell \leq A$ and $t_1 \geq M/A$ (although some of these bounds can be refined without affecting the proof). Note that in particular this implies the following bounds for the total number of points N:

$$N - 1 \geq \sum_{j=1}^{t_1} \beta_1 j \geq \frac{t_1(t_1+1)}{2} \geq \frac{M^2}{2A^2}, \quad N \leq 2 + 2\sum_{j=1}^{M}(AM + Aj) \leq 5AM^2. \tag{8}$$

Let z_j be as defined in Proposition 2.5. We call the set of points defined this way the *Diamond ensemble* and we denote it by $\diamond(N)$, omitting in the notation the dependence on all the parameters $n, t_1, \ldots, t_n, \alpha_1, \ldots, \alpha_n, \beta_1, \ldots, \beta_n$. Note that the total number of points is

$$N = 2 - (\alpha_n + \beta_n M) + 2\sum_{\ell=1}^{n} \sum_{j=t_{\ell-1}+1}^{t_\ell} (\alpha_\ell + \beta_\ell j).$$

We also denote by N_ℓ the total number of points in up to $t_{\ell-1}$ (without the North Pole), that is

$$N_\ell = \sum_{j=1}^{t_{\ell-1}-1} r_j.$$

Note that if $j \in [t_{\ell-1}, t_\ell]$ then

$$\begin{aligned} z_j &= 1 - \frac{1 + r_j + 2\sum_{k=1}^{j-1} r_k}{N-1} = 1 - \frac{1 + 2N_l - r_j + 2\sum_{k=t_{\ell-1}}^{j}(\alpha_\ell + \beta_\ell k)}{N-1} \\ &= 1 - \frac{1 + 2N_l - (\alpha_\ell + \beta_\ell j) + 2\alpha_\ell(j - t_{\ell-1} + 1) + \beta_\ell(j + t_{\ell-1})(j - t_{\ell-1} + 1)}{N-1}. \end{aligned} \tag{9}$$

We thus consider the function $z : [0, 2M] \to \mathbb{R}$, piecewise defined in each interval $[t_{\ell-1}, t_\ell] \subseteq [0, M]$ by the degree 2 polynomial

$$z_\ell(x) = 1 - \frac{1 + 2N_l - (\alpha_\ell + \beta_\ell x) + 2\alpha_\ell(x - t_{\ell-1} + 1) + \beta_\ell(x + t_{\ell-1})(x - t_{\ell-1} + 1)}{N-1} \tag{10}$$

and given in $[M, 2M]$ by $z(x) = -z(2M - x)$. Note that we have $z_j = z(j)$.

3.3. An exact formula for the expected logarithmic energy of the Diamond ensemble

From Theorem 2.6, the expected value of the log-energy of $\diamond(N)$ is given by

$$\begin{aligned} &\mathrm{E}_{\theta_1,\ldots,\theta_p \in [0,2\pi]^p}\left[\mathscr{E}_{\log}(\diamond(N))\right] \\ &= -(N-1)\log(4) + r(M)\log r(M) - 2\sum_{j=1}^{M} r(j)\log r(j) \\ &- (N-1)\sum_{j=1}^{M} r(j)(1 - z(j))\log(1 - z(j)) - (N-1)\sum_{j=1}^{M} r(j)(1 + z(j))\log(1 + z(j)). \end{aligned}$$

We write the sums as instances of a trapezoidal composite rule. Recall that for a function $f : [a, b] \to \mathbb{R}$ with $a < b$ integers, the composite trapezoidal rule is

$$T_{[a,b]}(f) = \frac{f(a) + f(b)}{2} + \sum_{j=a+1}^{b-1} f(j). \tag{11}$$

We then have

Corollary 3.2. *The expected logarithmic energy of points drawn from the Diamond ensemble equals*

$$E_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathcal{E}_{\log}(\diamond(N))\right] = -(N-1)\log(4) - 2\sum_{\ell=1}^{n} T_{[t_{\ell-1},t_\ell]}(f_\ell)$$
$$-(N-1)\sum_{\ell=1}^{n} T_{[t_{\ell-1},t_\ell]}(g_\ell) - (N-1)\sum_{\ell=1}^{n} T_{[t_{\ell-1},t_\ell]}(h_\ell),$$

where for $1\le \ell\le n$ *the functions* f_ℓ, g_ℓ, h_ℓ *are defined in the interval* $[t_{\ell-1}, t_\ell]$ *and satisfy*

$$\begin{aligned} f_\ell(x) =&(\alpha_\ell+\beta_\ell x)\log(\alpha_\ell+\beta_\ell x),\\ g_\ell(x) =&(\alpha_\ell+\beta_\ell x)(1-z_\ell(x))\log(1-z_\ell(x)),\\ h_\ell(x) =&(\alpha_\ell+\beta_\ell x)\,(1+z_\ell(x))\log(1+z_\ell(x)).\end{aligned}$$

3.4. An asymptotic formula for the expected logarithmic energy of the Diamond ensemble

Since f_ℓ is a continuous function for $1\le\ell\le n$, the trapezoidal rule $T_{[t_{\ell-1},t_\ell]}(f_\ell)$ approaches the integral of f_ℓ. Moreover,

Lemma 3.3. *For* $1\le\ell\le n$ *we have*

$$\left|T_{[t_{\ell-1},t_\ell]}(f_\ell) - \int_{t_{\ell-1}}^{t_\ell} f_\ell(x)\,dx\right| \le (t_\ell - t_{\ell-1})3A\log(2AM) \le 3AM\log(2AM).$$

Proof. Let S be the quantity in the lemma and note that

$$S \le \sum_{j=t_{\ell-1}+1}^{t_\ell} \int_{j-1}^{j}\left|f_\ell(x) - \frac{f_\ell(j-1)+f_\ell(j)}{2}\right| dx.$$

Now, for $x\in[j-1,j]$ we have

$$|f_\ell(x) - f_\ell(j-1)| \le \int_{j-1}^{j} |f_\ell'(t)|\,dt \le A + A\log(AM+AM) \le 2A\log(2AM).$$

We thus have

$$\left|f_\ell(x) - \frac{f_\ell(j-1)+f_\ell(j)}{2}\right| \le$$
$$|f_\ell(x)-f_\ell(j-1)| + \left|\frac{f_\ell(j-1)-f_\ell(j)}{2}\right| \le 3A\log(2AM).$$

The lemma follows. □

We can use the classical Euler–Maclaurin formula (see Lemma A.2) for estimating the difference between the composite trapezoidal rule and the integral in the cases of g_ℓ and h_ℓ. Indeed we have

Lemma 3.4. *The following inequality holds for* $1\le\ell\le n$*:*

$$\left|T_{[t_{\ell-1},t_\ell]}(g_\ell) - \int_{t_{\ell-1}}^{t_\ell} g_\ell(x)\,dx - \frac{g_\ell'(t_\ell)-g_\ell'(t_{\ell-1})}{12}\right| \le \frac{C\log M}{M}$$

for some constant $C>0$*, that depends only on* A*.*

Proof. From Lemma A.2 it suffices to prove that $|g_\ell'''(x)|\,dx \le \frac{C\log M}{M^2}$ for some constant C. Now, $g_\ell = u(x)v(x)w(x)$ where u is a linear mapping, v is a quadratic polynomial and $w=\log v$. The Leibniz rule for the derivative of the product gives

$$g_\ell''' = uvw''' + 6u'v'w' + 3u'v''w + 3uv''w' + 3u'vw'' + 3uv'w''.$$

If $\ell = 1$ then g_ℓ''' has a simple expression and it is easily verified that

$$|g_1'''| \le \frac{C \log M}{M^2}$$

for some constant $C > 0$. For $\ell > 1$ note now that $u(x) = \alpha_\ell + \beta_\ell x$ satisfies

$$|u| \le CM, \quad |u'| \le C$$

where C is some constant. Moreover, $v(x) = 1 - z_\ell(x)$ in $[t_{\ell-1}, t_\ell]$ satisfies

$$\frac{1}{C} \le |v| \le 1, \quad |v'| \le \frac{C}{M}, \quad |v''| \le \frac{C}{M^2}$$

for some positive constant C, not depending on M. To see this, just note that since $\ell > 1$ we have $[t_{\ell-1}, t_\ell] \subseteq [t_1, M] \subseteq [M/A, M]$. Then,

$$|v| \ge |v_1(M/A)| \ge \frac{1 + \beta_1 M^2/A^2}{N-1} \overset{(8)}{\ge} \frac{1}{C},$$
$$|v'| = \left| \frac{2\beta_\ell x + 2\alpha_\ell}{N-1} \right| \overset{(8)}{\le} \left| \frac{2AM + 2AM}{M^2/2A^2} \right| \le \frac{C}{M},$$
$$|v''| = \left| \frac{2\beta_\ell}{N-1} \right| \le \left| \frac{2A}{M^2/2A^2} \right| \le \frac{C}{M^2},$$

where C is a constant depending on A whose value is not important for us. A similar, yet more lengthy computation shows that $w = \log v$ satisfies

$$|w| \le C, \quad |w'| \le \frac{C}{M}, \quad |w''| \le \frac{C}{M^2} \quad |w'''| \le \frac{C}{M^3}.$$

The lemma follows. □

Lemma 3.5. *The following inequality holds for $1 \le \ell \le n$:*

$$\left| T_{[t_{\ell-1}, t_\ell]}(h_\ell) - \int_{t_{\ell-1}}^{t_\ell} h_\ell(x)\, dx - \frac{h_\ell'(t_\ell) - h_\ell'(t_{\ell-1})}{12} \right| \le \frac{C}{M}$$

for some constant $C > 0$.

Proof. The proof is almost identical to that of Lemma 3.4, so we leave it to the reader. □

We have proved the following.

Theorem 3.6. *For the Diamond ensemble we have*

$$E_{\theta_1,\dots,\theta_p \in [0,2\pi]^p} \left[\mathcal{E}_{\log}(\diamond(N)) \right] = -(N-1)\log(4) - 2 \sum_{\ell=1}^{n} \int_{t_{\ell-1}}^{t_\ell} f_\ell(x)\, dx$$
$$- (N-1) \sum_{\ell=1}^{n} \left(\int_{t_{\ell-1}}^{t_\ell} g_\ell(x)\, dx + \frac{g_\ell'(t_\ell) - g_\ell'(t_{\ell-1})}{12} \right)$$
$$- (N-1) \sum_{\ell=1}^{n} \left(\int_{t_{\ell-1}}^{t_\ell} h_\ell(x)\, dx + \frac{h_\ell'(t_\ell) - h_\ell'(t_{\ell-1})}{12} \right) + O(M \log M),$$

where as before for $1 \le \ell \le n$ the functions f_ℓ, g_ℓ, h_ℓ are as in Corollary 3.2 and the constant hidden in the $O(M \log M)$ term depends only on A. Note that from (8), the term $O(M \log M)$ is $o(N)$.

3.4.1. Zonal equal area nodes

In [18] Rakhmanov et al. define a diameter bounded, equal area partition of $\mathbb{S}^2$ consisting on two spherical caps on the South and the North pole and rectilinear cells located on rings of parallels. The

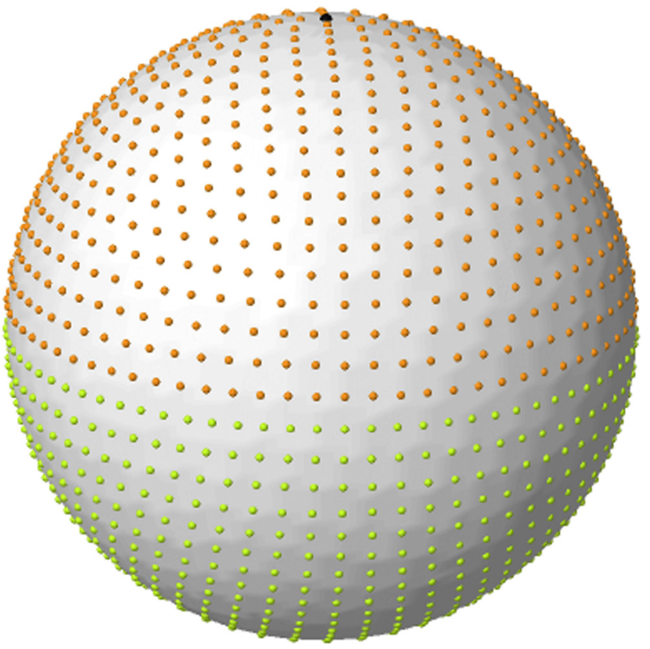

Fig. 1. A realization of a simple example with $K = 4$ and $N = 1602$. Different colors for points correspond to different linear pieces defining $r(x)$.

resemblance between our model and this model is remarkable, and even if the constructions are different, the points obtained seem to be really close. Actually, both the authors in [18] and ourselves try to approximate r_j as in Eq. (6) by an integer number. The theoretical bounds we obtain here for the logarithmic energy are slightly better than the numerical bounds obtained in [11] for the zonal equal area nodes.

An interesting fact is that among all the algorithmically generated point sets, the generalized spiral and zonal equal area points perform the best with respect to the logarithmic energy. [11, Proposition 2.3.] claims that the sequence of zonal equal area configurations is equidistributed and quasi-uniform. The same kind of result can probably be stated for the Diamond ensemble.

4. Concrete examples of the Diamond ensemble

Throughout this section we are going to explore three different examples of the Diamond ensemble. Each of them is illustrated with two kinds of figures: a concrete example of points following the model on $\mathbb{S}^2$ (Figs. 1–3) and a comparative between the r_j that define the model and the r_j in Eq. (6) with $K_0 = 3/\pi$, given in Fig. 4. In Figs. 1–3 we have used different colors for points obtained from the different linear pieces defining $r(x)$.

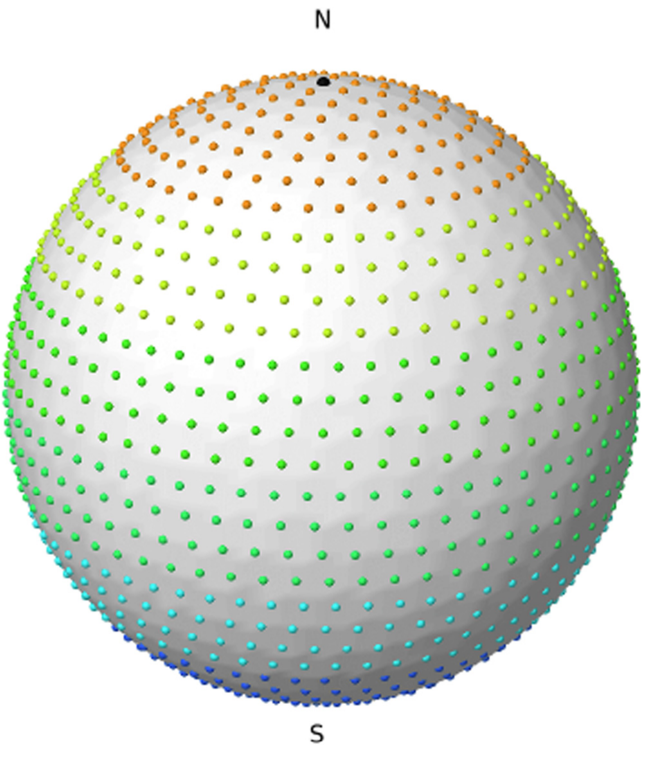

Fig. 2. A realization of a more elaborated example with $N = 1314$. Different colors for points correspond to different linear pieces defining $r(x)$.

4.1. A simple example

We choose $n = 1$, $r_j = Kj$ with K a positive integer for $1 \leq j \leq M$. Then, for $l \in \{1, \dots, M\}$ we have

$$z_l = 1 - \frac{1 + Kl^2}{N - 1}.$$

The number of parallels is $2M - 1$ and the number of points of the Diamond ensemble is

$$N = 2 + \sum_{j=1}^{p} r_j = 2 - KM + 2\sum_{j=1}^{M} Kj = 2 + KM^2.$$

One can then write down the functions in Corollary 3.2 getting

$$\begin{aligned} f(x) =& Kx \log(Kx), \\ g(x) =& Kx \frac{1 + Kx^2}{N - 1} \log\left(\frac{1 + Kx^2}{N - 1}\right), \\ h(x) =& Kx \left(2 - \frac{1 + Kx^2}{N - 1}\right) \log\left(2 - \frac{1 + Kx^2}{N - 1}\right). \end{aligned}$$

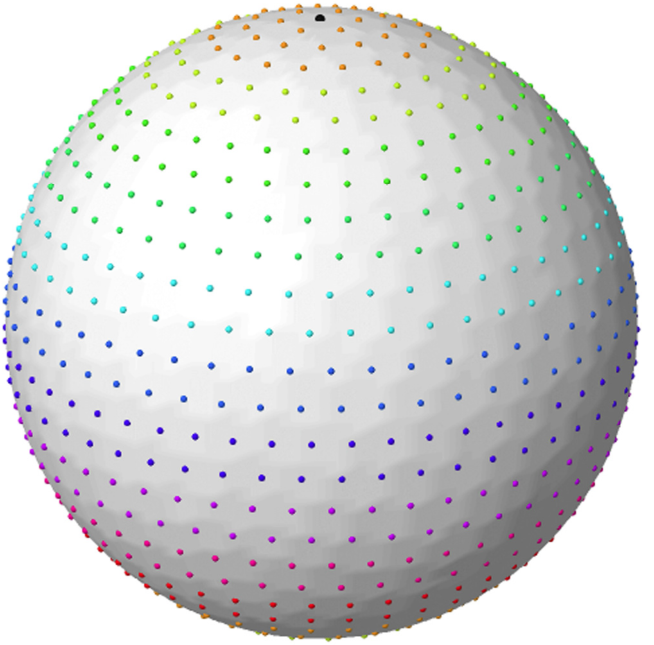

Fig. 3. A realization of a quasioptimal example with $N = 958$. Different colors for points correspond to different linear pieces defining $r(x)$.

Then, the formula in Theorem 3.6 reads

$$\mathrm{E}_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathscr{E}_{\log}(\diamond(N))\right] = -(N-1)\log(4) - 2\int_0^M f(x)\,dx$$
$$-(N-1)\left(\int_0^M (g(x)+h(x))\,dx + \frac{g'(M)-g(0)}{12} + \frac{h'(M)-h'(0)}{12}\right) + o(M^2).$$

All these integrals and derivatives can be computed, obtaining the following result.

Theorem 4.1. *The expected value of the logarithmic energy of the Diamond ensemble in this section is*

$$E_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathscr{E}_{\log}(\diamond(N))\right] = W_{\log}(\mathbb{S}^2)N^2 - \frac{1}{2}N\log N$$
$$+N\left(\frac{\log 2}{6}K - \frac{1}{2} + \log 2 - \frac{\log K}{2}\right) + o(N).$$

In particular, if $K = 4$ we have

$$E_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathscr{E}_{\log}(\diamond(N))\right] = W_{\log}(\mathbb{S}^2) - \frac{1}{2}N\log N + N\left(\frac{2\log 2}{3} - \frac{1}{2}\right) + o(N).$$

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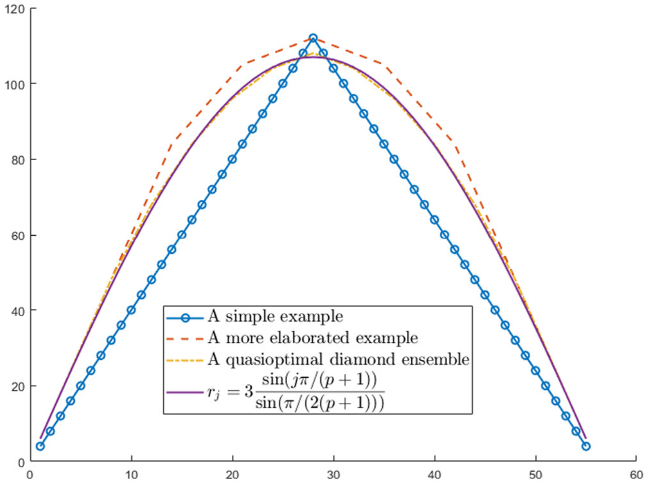

Fig. 4. Comparison of the number of points in each parallel for the different models for $p = 55$ parallels.

Note that $\frac{2\log 2}{3} - \frac{1}{2} = -0.037901\ldots$ Using this simple example we are thus approximately 0.0177 far from the valued conjectured in [3,8].

4.1.1. *Octahedral configurations of points*

In [12] an area preserving map from the unit sphere to the regular octahedron is defined. Considering some hierarchical triangular grids on the facets of the octahedron a grid can be mapped into the sphere obtaining two different sets of points: those coming from the vertex of the grid Ω_N and the centers of the triangles Λ_N.

The set Ω_N consists on $4M^2+2$ points in the sphere that very much resemble our simple example. In the paper, the authors give some numerical simulations for the logarithmic energy of this set of points that are confirmed by Theorem 4.1. Also in [11, Figure 2.2] new numerical simulations for the same set are done obtaining a bound which is very similar to the one we prove here.

4.2. *A more elaborated example*

The following choice of r_j produces much better results. Let $p = 2M - 1$ where $M = 4m$ with m a positive integer. Let $n = 3$ and let $r_j = r(j)$ where

$$r(x) = \begin{cases} 6x & 0 \le x \le 2m \\ 6m + 3x & 2m \le x \le 3m \\ 12m + x & 3m \le x \le 4m \\ 20m - x & 4m \le x \le 5m \\ 30m - 3x & 5m \le x \le 6m \\ 48m - 6x & 6m \le x \le 8m \end{cases}$$

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that satisfies $r(x) = r(p+1-x) = r(8m-x)$. Let $z_j = z(j)$ where $z(x)$ is defined by (10), that is,

$$z(x) = \begin{cases} \frac{82m^2-6x^2}{82m^2+1} & 0 \le x \le 2m \\ \frac{94m^2-12mx-3x^2}{82m^2+1} & 2m \le x \le 3m \\ \frac{112m^2-24mx-x^2}{82m^2+1} & 3m \le x \le 4m \\ \frac{144m^2-40mx+x^2}{82m^2+1} & 4m \le x \le 5m \\ \frac{194m^2-60mx+3x^2}{82m^2+1} & 5m \le x \le 6m \\ \frac{302m^2-96mx+6x^2}{82m^2+1} & 6m \le x \le 8m \end{cases}$$

We moreover have $N = 82m^2 + 2$. Again, all the integrals and derivatives in Theorem 3.6 can be computed, although this time the computer algebra package `Maxima` has been used, getting the following result.

Theorem 4.2. *The expected value of the logarithmic energy of the Diamond ensemble in this section is*

$$E_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathcal{E}_{\log}(\diamond(N))\right] = W_{\log}(\mathbb{S}^2)N^2 - \frac{N}{2}\log N + cN + o(N),$$

where $c = -0.048033\ldots$ *satisfies*

$$\begin{aligned} 492c = & -113\log 113 - 982\log 82 - 210\log 70 - 51\log 51 \\ & +1638\log 41 + 900\log 15 - 36\log 12 - 1536\log 8 \\ & +144\log 6 - 492\log 4 + 1968\log 2 - 246. \end{aligned}$$

Using this more elaborated example we are thus approximately 0.0076 far from the value conjectured in [3,8].

4.3. A quasioptimal Diamond example

We have made a number of tries with different choices of the parameters for the Diamond ensemble. The best one (i.e. the one with minimal logarithmic energy) that we have found is the following one: let $M = 7m$ with m a positive integer, let $p = 2M - 1$ and let

$$r(x) = \begin{cases} 6x & 0 \le x \le 2m \\ 2m + 5x & 2m \le x \le 3m \\ 5m + 4x & 3m \le x \le 4m \\ 9m + 3x & 4m \le x \le 5m \\ 14m + 2x & 5m \le x \le 6m \\ 20m + x & 6m \le x \le 7m \\ 34m - x & 7m \le x \le 8m \\ 42m - 2x & 8m \le x \le 9m \\ 51m - 3x & 9m \le x \le 10m \\ 61m - 4x & 10m \le x \le 11m \\ 72m - 5x & 11m \le x \le 12m \\ 84m - 6x & 12m \le x \le 14m = p + 1 \end{cases}$$

that satisfies $r(x) = r(p+1-x) = r(14m-x)$. Let $z_j = z(j)$ where $z(x)$ is defined by (10), that is,

$$z(x) = \frac{1}{239m^2+1} \times \begin{cases} 239m^2 - 6x^2 & 0 \le x \le 2m \\ 243m^2 - 4mx - 5x^2 & 2m \le x \le 3m \\ 252m^2 - 10mx - 4x^2 & 3m \le x \le 4m \\ 268m^2 - 18mx - 3x^2 & 4m \le x \le 5m \\ 293m^2 - 28mx - 2x^2 & 5m \le x \le 6m \\ 329m^2 - 40mx - x^2 & 6m \le x \le 7m \\ 427m^2 - 68mx + x^2 & 7m \le x \le 8m \\ 491m^2 - 84mx + 2x^2 & 8m \le x \le 9m \\ 572m^2 - 102mx + 3x^2 & 9m \le x \le 10m \\ 672m^2 - 122mx + 4x^2 & 10m \le x \le 11m \\ 793m^2 - 144mx + 5x^2 & 11m \le x \le 12m \\ 937m^2 - 168mx + 6x^2 & 12m \le x \le 14m = p+1. \end{cases}$$

We moreover have $N = 239m^2 + 2$. Again, all the integrals and derivatives of Theorem 3.6 have been computed using the computer algebra package `Maxima`, obtaining Theorem 1.1.

5. Proofs of the main results

5.1. *Proof of Proposition 2.2*

In order to prove Proposition 2.2, we will need the following equality from [10, Formula 4.224], valid for $a \ge |b| > 0$:

$$\int_0^{\pi} \log(a + b\cos(\theta))d\theta = \pi \log\left(\frac{a+\sqrt{a^2-b^2}}{2}\right). \tag{12}$$

Note that

$$\|x-y\| = \left\|\left(\sqrt{1-z_i^2}\cos\theta_i, \sqrt{1-z_i^2}\sin\theta_i, z_i\right) - \left(\sqrt{1-z_j^2}\cos\theta_j, \sqrt{1-z_j^2}\sin\theta_j, z_j\right)\right\|$$
$$= \sqrt{2}\sqrt{1 - z_iz_j - \sqrt{1-z_i^2}\sqrt{1-z_j^2}\cos(\theta_i-\theta_j)}.$$

We compute then

$$\mathrm{E}_{\theta_i,\theta_j\in[0,2\pi]^2}\left[-\log\left(\|x-y\|\right)\right]$$
$$= \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} -\log\left(\sqrt{2}\sqrt{1 - z_iz_j - \sqrt{1-z_i^2}\sqrt{1-z_j^2}\cos(\theta_i-\theta_j)}\right)d\theta_i d\theta_j$$
$$= \frac{-\log(2)}{2} - \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}\log\left(1 - z_iz_j - \sqrt{1-z_i^2}\sqrt{1-z_j^2}\cos(\theta_i-\theta_j)\right)d\theta_i d\theta_j$$
$$= \frac{-\log(2)}{2} - \frac{1}{4\pi}\int_0^{2\pi}\log\left(1 - z_iz_j - \sqrt{1-z_i^2}\sqrt{1-z_j^2}\cos(\theta)\right)d\theta$$
$$= \frac{-\log(2)}{2} - \frac{1}{2\pi}\int_0^{\pi}\log\left(1 - z_iz_j - \sqrt{1-z_i^2}\sqrt{1-z_j^2}\cos(\theta)\right)d\theta.$$

From (12) with $a = 1 - z_i z_j$, $b = -\sqrt{1-z_i^2}\sqrt{1-z_j^2}$ and $z_i \neq z_j$ we have that

$$\begin{aligned}\mathrm{E}_{\theta_i,\theta_j\in[0,2\pi]^2}\left[-\log\left(\|x-y\|\right)\right] &= \frac{-\log(2)}{2} - \frac{1}{2\pi}\pi\log\left(\frac{1-z_iz_j+|z_i-z_j|}{2}\right)\\ &= \frac{-\log(2)}{2} - \frac{1}{2}\left[\log\left(1-z_iz_j+|z_i-z_j|\right)-\log(2)\right]\\ &= -\frac{\log\left(1-z_iz_j+|z_i-z_j|\right)}{2}. \quad \square\end{aligned}$$

5.2. Proof of Proposition 2.4

In order to compute the logarithmic energy associated to $\Omega(p,\{r_j\},\{z_j\})$, we have to sum the following quantities:

- $\mathscr{A}$: the sum of $2\log\|x_j^i - \mathscr{N}\|^{-1}$, $1 \le j \le p$ and $1 \le i \le r_j$ and the same expression but changing the North pole $\mathscr{N}$ to the South pole $\mathscr{S}$, plus $2\log\|\mathscr{N}-\mathscr{S}\|^{-1} = -2\log 2$.
- $\mathscr{B}$: the energy of the scaled roots of unity for every parallel $1 \le j \le p$.
- $\mathscr{C}$: the energy between the points of every pair of parallels, as in Corollary 2.3.

5.2.1. Computation of quantity $\mathscr{A}$

Note that

$$\begin{aligned}\|(0,0,1)-x_j^i\| &= \sqrt{2}\sqrt{1-z_j},\\ \|(0,0,-1)-x_j^i\| &= \sqrt{2}\sqrt{1+z_j}.\end{aligned}$$

Quantity $\mathscr{A}$ thus equals

$$\mathscr{A} = -2\log(2) - \sum_{j=1}^{p} r_j\left(\log(4)+\log\left(1-z_j^2\right)\right). \tag{13}$$

5.2.2. Computation of quantity $\mathscr{B}$

We will use the following result from [7, Pg. 3]: the logarithmic energy associated to N roots of unity in the unit circumference is $-N\log N$. As a trivial consequence, the logarithmic energy associated to N points which are equidistributed in a circumference of radius R is $-N\log N - N(N-1)\log R$.

Since the parallel at height z_j is a circumference of radius $\sqrt{1-z_j^2}$, quantity $\mathscr{B}$ equals

$$\mathscr{B} = -\sum_{j=1}^{p} r_j\log r_j + \frac{r_j(r_j-1)}{2}\log(1-z_j^2). \tag{14}$$

5.2.3. Computation of quantity $\mathscr{C}$

This has been done in Corollary 2.3:

$$\mathscr{C} = \sum_{k,j=1;k\neq j}^{p} -r_jr_k\frac{\log\left(1-z_jz_k+|z_j-z_k|\right)}{2}. \tag{15}$$

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In order to compute the logarithmic energy associated to the set $\Omega(p, \{r_j\}, \{z_j\})$ it only rests to sum the quantities (13), (14) and (15).

$$\mathrm{E}_{\theta_1,\dots\theta_p\in[0,2\pi]^p}\left[\mathcal{E}_{\log}(\Omega(p,\{r_j\},\{z_j\}))\right] = -2\log(2) - \sum_{j=1}^{p} r_j\left(\log(4)+\log\left(1-z_j^2\right)\right)$$

$$-\sum_{j=1}^{p}\left(r_j\log r_j + \frac{r_j(r_j-1)}{2}\log(1-z_j^2)\right) - \sum_{j=1}^{p}\sum_{k\neq j} r_j r_k \frac{\log\left(1-z_jz_k+|z_j-z_k|\right)}{2}$$

$$= -2\log(2) - \sum_{j=1}^{p}\left[r_j\log(4) + r_j\log(1-z_j^2) + r_j\log r_j + \frac{r_j^2}{2}\log(1-z_j^2)\right.$$

$$\left. -\frac{r_j}{2}\log(1-z_j^2) + \sum_{k\neq j} r_j r_k\frac{\log\left(1-z_jz_k+|z_j-z_k|\right)}{2}\right],$$

and Proposition 2.4 follows. □

5.3. *Proof of Proposition 2.5*

We derivate the formula from Proposition 2.4 for z_l obtaining:

$$\frac{\partial \mathrm{E}_{\theta_1,\dots,\theta_p\in[0,2\pi]^p}\left[\mathcal{E}_{\log}(\Omega(p,\{r_j\},\{z_j\}))\right]}{\partial z_l}$$

$$= \frac{\partial}{\partial z_l}\left(-\sum_{j=1}^{p}\frac{r_j}{2}\log(1-z_j^2) - \sum_{j=1}^{p}\sum_{k=1}^{p} r_j r_k\frac{\log\left(1-z_jz_k+|z_j-z_k|\right)}{2}\right)$$

$$= \frac{z_l r_l}{1-z_l^2} + \frac{z_l r_l^2}{1-z_l^2} + \sum_{j=1}^{l-1} r_j r_l\frac{1+z_j}{(1-z_l)(1+z_j)} - \sum_{j=l+1}^{p} r_j r_l\frac{1-z_j}{(1+z_l)(1-z_j)}$$

$$= \frac{z_l r_l(1+r_l)}{1-z_l^2} + \sum_{j=1}^{l-1}\frac{r_j r_l}{1-z_l} - \sum_{j=l+1}^{p}\frac{r_j r_l}{1+z_l}$$

$$= \frac{r_l}{1-z_l^2}\left((1+r_l)z_l + (1+z_l)\sum_{j=1}^{l-1} r_j - (1-z_l)\sum_{j=l+1}^{p} r_j\right)$$

$$= \frac{r_l}{1-z_l^2}\left(z_l + \sum_{j=1}^{l-1} r_j - \sum_{j=l+1}^{p} r_j + z_l\sum_{j=1}^{p} r_j\right).$$

We have then

$$\frac{\partial \mathrm{E}_{\theta_1,\dots,\theta_p\in[0,2\pi]^p}\left[\mathcal{E}_{\log}(\Omega(p,\{r_j\},\{z_j\}))\right]}{\partial z_l} = 0 \iff z_l\left(1+\sum_{j=1}^{p} r_j\right) = \sum_{j=l+1}^{p} r_j - \sum_{j=1}^{l-1} r_j.$$

In other words,

$$z_l = \frac{\sum_{j=l+1}^{p} r_j - \sum_{j=1}^{l-1} r_j}{1+\sum_{j=1}^{p} r_j}. \quad \square$$

5.4. Proof of Theorem 2.6

To prove Theorem 2.6 the following lemma will be useful.

Lemma 5.1. *If $r_j = r_{p+1-j}$ and z_j are chosen as in Proposition 2.5 we then have*

$$\frac{1}{2}\sum_{j=1}^{p}\sum_{k=1}^{p} r_j r_k \log\left(1 - z_j z_k + |z_j - z_k|\right) = (N-1)\sum_{j=1}^{p} r_j(1-z_j)\log(1-z_j) - \sum_{j=1}^{p} r_j \log(1-z_j).$$

Proof. Let

$$a_{j,k} = r_j r_k \log\left(1 - z_j z_k + |z_j - z_k|\right), \quad b_{j,k} = r_j r_k \log\left(1 + z_j z_k + |z_j + z_k|\right)$$

and note that they satisfy:

$$a_{j,k} = a_{k,j}, \quad a_{j,p+1-k} = b_{j,k}, \quad a_{p+1-j,k} = b_{j,k}, \quad a_{p+1-j,p+1-k} = a_{j,k}, \quad a_{M,M} = 0.$$

We thus have

$$\sum_{j=1}^{p}\sum_{k=1}^{p} a_{j,k} = \sum_{j=1}^{p} a_{j,j} + \sum_{\substack{j,k=1\\ j\neq k}}^{p} a_{j,k} = 2\sum_{j=1}^{M-1} r_j^2 \log(1-z_j^2) + \sum_{\substack{j,k=1\\ j\neq k}}^{p} a_{j,k}.$$

Moreover, recalling that $p = 2M-1$,

$$\sum_{\substack{j,k=1\\ j\neq k}}^{p} a_{j,k} = \sum_{\substack{j,k=1\\ j\neq k}}^{M} a_{j,k} + \sum_{j=1}^{M}\sum_{k=M+1}^{2M-1} a_{j,k} + \sum_{j=M+1}^{2M-1}\sum_{k=1}^{M} a_{j,k} + \sum_{\substack{j,k=M+1\\ j\neq k}}^{2M-1} a_{j,k}. \tag{16}$$

The two sums in the middle of the right hand term in (16) can be rewritten as

$$\sum_{j=1}^{M}\sum_{k=1}^{M-1} b_{j,k} + \sum_{j=1}^{M-1}\sum_{k=1}^{M} b_{j,k} = 2\sum_{j=1}^{M}\sum_{k=1}^{M-1} b_{j,k},$$

and using that $z_j \geq 0$ for $1 \leq j \leq M$ this last equals

$$\begin{aligned} 2\sum_{j=1}^{M}\sum_{k=1}^{M-1} b_{j,k} =& 2\sum_{j=1}^{M}\sum_{k=1}^{M-1} r_j r_k \log(1+z_j) + 2\sum_{j=1}^{M}\sum_{k=1}^{M-1} r_j r_k \log(1+z_k) \\ =& 2\left(\sum_{k=1}^{M-1} r_k\right)\sum_{j=1}^{M} r_j \log(1+z_j) + 2\left(\sum_{j=1}^{M} r_j\right)\sum_{k=1}^{M-1} r_k \log(1+z_k) \\ =& 2\left(r_M + 2\sum_{j=1}^{M-1} r_j\right)\sum_{k=1}^{M-1} r_k \log(1+z_k), \end{aligned}$$

where in the last step we have used that $z_M = 0$. From (16) we then have proved that the sum in the lemma equals

$$\sum_{j=1}^{M-1} r_j^2 \log(1-z_j^2) + \left(r_M + 2\sum_{j=1}^{M-1} r_j\right)\sum_{k=1}^{M-1} r_k \log(1+z_k) + \frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{M} a_{j,k} + \frac{1}{2}\sum_{\substack{j,k=M+1\\ j\neq k}}^{2M-1} a_{j,k} =$$

$$\sum_{j=1}^{M-1} r_j^2 \log(1-z_j^2) + \left(r_M + 2\sum_{j=1}^{M-1} r_j \right) \sum_{k=1}^{M-1} r_k \log(1+z_k) + \frac{1}{2} \sum_{\substack{j,k=1\\ j\neq k}}^{M} a_{j,k} + \frac{1}{2} \sum_{\substack{j,k=1\\ j\neq k}}^{M-1} a_{j,k},$$

where we have used $a_{p+1-j,p+1-k} = a_{j,k}$. The two sums in the expression above have many common terms. We can rearrange them as follows:

$$\begin{aligned}\frac{1}{2} \sum_{\substack{j,k=1\\ j\neq k}}^{M} a_{j,k} + \frac{1}{2} \sum_{\substack{j,k=1\\ j\neq k}}^{M-1} a_{j,k} = \sum_{\substack{j,k=1\\ j\neq k}}^{M-1} a_{j,k} + \frac{1}{2}\sum_{k=1}^{M-1} a_{M,k} + \frac{1}{2}\sum_{j=1}^{M-1} a_{j,M} \\ =2\sum_{j=1}^{M-1}\sum_{k=1}^{j-1} a_{j,k} + \sum_{k=1}^{M-1} a_{M,k} \\ =2\sum_{j=1}^{M-1}\sum_{k=1}^{j-1} a_{j,k} + \sum_{k=1}^{M-1} r_M r_k \log\left(1+z_k\right),\end{aligned}$$

where again we are using $a_{j,k} = a_{k,j}$ and $z_M = 0$. All in one, we have proved that the sum in the lemma equals

$$\begin{aligned}\sum_{j=1}^{M-1} r_j^2 \log(1-z_j^2) + \left(r_M + 2\sum_{j=1}^{M-1} r_j \right) \sum_{k=1}^{M-1} r_k \log(1+z_k) \\ +2\sum_{j=1}^{M-1}\sum_{k=1}^{j-1} a_{j,k} + \sum_{k=1}^{M-1} r_M r_k \log\left(1+z_k\right).\end{aligned}$$

With little algebra we rewrite this expression as:

$$\begin{aligned}2\sum_{j=1}^{M-1}\sum_{k=1}^{j-1} r_j r_k \log(1-z_j) + 2\sum_{j=1}^{M-1}\sum_{k=1}^{j-1} r_j r_k \log(1+z_k), \\ + \sum_{j=1}^{M-1} r_j^2 \log(1-z_j^2) + 2\left(\sum_{j=1}^{M} r_j\right) \sum_{k=1}^{M-1} r_k \log(1+z_k).\end{aligned}$$

Changing the summation order and the name of the variables, the second term can be rewritten as

$$\begin{aligned}2\sum_{j=1}^{M-2} r_j \log(1+z_j) \sum_{k=j+1}^{M-1} r_k &= 2\sum_{j=1}^{M-2} r_j \log(1+z_j) \left(\sum_{k=1}^{M-1} r_k - r_j - \sum_{k=1}^{j-1} r_k \right) \\ &= 2\sum_{j=1}^{M-1} r_j \log(1+z_j) \left(\frac{N-r_M}{2} - 1 - r_j - \sum_{k=1}^{j-1} r_k \right)\end{aligned}$$

We have then proved that the sum of the lemma equals:

$$\begin{aligned}2\sum_{j=1}^{M-1} r_j \log(1-z_j) \left(\sum_{k=1}^{j-1} r_k\right) + 2\sum_{j=1}^{M-1} r_j \log(1+z_j) \left(\frac{N-r_M}{2} - 1 - r_j - \sum_{k=1}^{j-1} r_k \right) \\ + \sum_{j=1}^{M-1} r_j^2 \log(1-z_j^2) + (N-2+r_M) \sum_{j=1}^{M-1} r_j \log(1+z_j).\end{aligned}$$

After simplification, we get the more compact but equivalent expression

$$\sum_{j=1}^{M-1} r_j\left(r_j+2\sum_{k=1}^{j-1} r_k\right)\log(1-z_j)-\sum_{j=1}^{M-1} r_j\left(r_j+2\sum_{k=1}^{j-1} r_k\right)\log(1+z_j)$$
$$+(2N-4)\sum_{j=1}^{M-1} r_j\log(1+z_j).$$

Now we look at the first two terms recalling that

$$z_j=1-\frac{1+r_j+2\sum_{k=1}^{j-1}r_k}{N-1}\Longrightarrow r_j+2\sum_{k=1}^{j-1} r_k=(N-1)(1-z_j)-1,$$

and hence the sum in the lemma equals

$$(N-1)\sum_{j=1}^{M-1} r_j(1-z_j)\log(1-z_j)-\sum_{j=1}^{M-1} r_j\log(1-z_j)$$
$$-\ (N-1)\sum_{j=1}^{M-1} r_j(1-z_j)\log(1+z_j)+\sum_{j=1}^{M-1} r_j\log(1+z_j)$$
$$+\ (2N-4)\sum_{j=1}^{M-1} r_j\log(1+z_j),$$

that is

$$(N-1)\sum_{j=1}^{M-1} r_j(1-z_j)\log(1-z_j)-\sum_{j=1}^{M-1} r_j\log(1-z_j)$$
$$+\ (N-1)\sum_{j=1}^{M-1} r_j(1+z_j)\log(1+z_j)-\sum_{j=1}^{M-1} r_j\log(1+z_j).$$

The symmetries $r_j=r_{p+1-j}$ and $z_j=-z_{p+1-j}$ imply that the last expression equals

$$(N-1)\sum_{j=1}^{M-1} r_j(1-z_j)\log(1-z_j)-\sum_{j=1}^{M-1} r_j\log(1-z_j)$$
$$+\ (N-1)\sum_{j=M+1}^{p} r_j(1-z_j)\log(1-z_j)-\sum_{j=M+1}^{p} r_j\log(1-z_j).$$

We thus have proved (using $z_M=0$) that the sum of the lemma equals

$$(N-1)\sum_{j=1}^{p} r_j(1-z_j)\log(1-z_j)-\sum_{j=1}^{p} r_j\log(1-z_j).\quad\square$$

We now finally prove Theorem 2.6. From Proposition 2.4 and Lemma 5.1 we have

$$\mathrm{E}_{\theta_1,\ldots,\theta_p\in[0,2\pi]^p}\left[\mathcal{E}_{\log}(\Omega(p,\{r_j\}))\right]=-2\log(2)-(N-2)\log(4)-\frac{1}{2}\sum_{j=1}^{p} r_j\log(1-z_j^2)$$
$$-\sum_{j=1}^{p} r_j\log r_j-(N-1)\sum_{j=1}^{p} r_j(1-z_j)\log(1-z_j)+\sum_{j=1}^{p} r_j\log(1-z_j).$$

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Now, using $r_j = r_{p+1-j}$ and $z_j = -z_{p+1-j}$ we have

$$\frac{1}{2}\sum_{j=1}^{p} r_j \log(1-z_j^2) = \frac{1}{2}\sum_{j=1}^{p} r_j \log(1-z_j) + \frac{1}{2}\sum_{j=1}^{p} r_j \log(1+z_j)$$
$$= \frac{1}{2}\sum_{j=1}^{p} r_j \log(1-z_j) + \frac{1}{2}\sum_{j=1}^{p} r_j \log(1-z_j) = \sum_{j=1}^{p} r_j \log(1-z_j).$$

The theorem follows. □

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Appendix. The error in the composite trapezoidal rule

The following result is a well known fact in Fourier analysis.

Lemma A.1. *Let $f : [n, n+1] \to \mathbb{R}$ be a C^1 function with $n \in \mathbb{Z}$. Let $C > 0$ be such that $|f'| \le C$. Then, for all $k \ge 1$,*

$$\left| \int_n^{n+1} \cos(2\pi kx) f(x)\, dx \right| \le \frac{C}{2\pi k}.$$

Proof. Integrate by parts. □

Lemma A.2. *Let $f : [a, b] \to \mathbb{R}$ be a C^2 function with $a < b$ integers and assume that f is C^3 in the open interval with $|f'''| \le C$. Then,*

$$\left| T_{[a,b]}(f) - \int_a^b f(x)\, dx - \frac{f'(b) - f'(a)}{12} \right| \le C(b-a)\frac{\zeta(3)}{4\pi^3},$$

where $\zeta(3) = 1.202056\ldots$ is Apéry's constant

Proof. Let S be the quantity in the lemma. From the Euler–Maclaurin identity (see the version in [13, Theorem 9.26]),

$$S \le \sum_{k=1}^{\infty} \frac{1}{2\pi^2 k^2} \left| \int_a^b \cos(2\pi k(x-a)) f''(x)\, dx \right| \le$$
$$\sum_{k=1}^{\infty} \frac{1}{2\pi^2 k^2} \sum_{n=a}^{b-1} \left| \int_n^{n+1} \cos(2\pi k(x-a)) f''(x)\, dx \right|.$$

From Lemma A.1, the integral inside is at most $\frac{C}{2\pi k}$. Then,

$$S \le \sum_{k=1}^{\infty} \frac{b-a}{2\pi^2 k^2} \frac{C}{2\pi k} = C(b-a)\frac{\zeta(3)}{4\pi^3},$$

as claimed. □

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