ENERGY FUNCTIONALS, NUMERICAL INTEGRATION AND ASYMPTOTIC EQUIDISTRIBUTION ON THE SPHERE

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ABSTRACT. In this paper, we study the numerical integration of continuous functions on d-dimensional spheres $S^d \subset \mathbb{R}^{d+1}$ by equally weighted quadrature rules based at $N \geq 2$ points on S^d which minimize a generalized energy functional. Examples of such points are configurations, which minimize energies for the Riesz kernel $\|x-y\|^{-s}$, $0 < s \leq d$ and logarithmic kernel $-\log\|x-y\|$, $s=0$. We deduce that point configurations which are extremal for the Riesz energy are asymptotically equidistributed on S^d for $0 \leq s \leq d$ as $N \to \infty$ and we present explicit rates of convergence for the special case $s = d$, which had been open.

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1. Introduction and Statement of Results

This paper deals with the subject of numerical integration of continuous functions on d-dimensional unit spheres $S^d \subset \mathbb{R}^{d+1}$. More precisely, given $d \geq 2$, we let

$$S^d := \left\{x \in \mathbb{R}^{d+1} \mid \langle x, x\rangle = 1\right\}$$

denote the unit sphere in $\mathbb{R}^{d+1}$. Here and throughout, we will denote by $\langle\cdot,\cdot\rangle$ the usual inner product on $\mathbb{R}^{d+1}$. Throughout σ will denote Lebesgue measure on S^d and we shall put

$$\omega_d := \int_{S^d} d\sigma.$$

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Thus $\mu := \frac{\sigma}{\omega_d}$ has total mass 1. Given a collection

$$Z_N := \{x_1, \ldots, x_N\},\ N \geq 1$$

of N points on the sphere S^d and a continuous function $f : S^d \to \mathbb{R}$, the error in numerical integration is given by

$$R(f, Z_N) := \frac{1}{N}\sum_{k=1}^{N} f(x_k) - \int_{S^d} f(x)\, d\mu(x). \tag{1.1}$$

Numerical integration of continuous functions on spheres using equally and non equally weighted rules is a very active and popular area of research with many applications. Different areas as diverse as spherical t-designs, discrepancy and combinatorics, Monte-Carlo and Quasi-Monte-Carlo methods, approximation theory, finite fields and complexity theory are involved. We refer the reader to [3], [7], [10], [20], [21], [41] for a more detailed account of this vast subject. The closely related subject of distributing points on a sphere has also been the subject of many papers. See for instance [3], [5], [14], [15], [16], [30], [32], [33], [39], [40], [41], [45], [46], [47], [48], [49]. On the one hand it has some interest on its own to describe a "well distributed" point set of cardinality N and even to define suitable notions of what "well distributed" should mean. On the other hand numerical integration procedures on the sphere require node sets which are spread evenly all over the sphere and allow positive weights for the according quadrature rule. In this paper we will only focus on equal weight (Chebyshev) quadrature.

A natural measure for the quality of the distribution of a point set $Z_N = \{x_1, \ldots, x_N\}$ on the sphere S^d is the spherical cap discrepancy

$$D_N(Z_N) = \sup_{C \subseteq S^d} \left| \frac{1}{N}\sum_{k=1}^{N} \chi_C(x_k) - \mu(C) \right|, \tag{1.2}$$

where the supremum ranges over all spherical caps $C \subseteq S^d$ (intersections of half spaces with S^d) and where χ_C denotes the indicator function of C. The discrepancy simply measures the maximal deviation between the discrete point distribution $\{x_1, \ldots, x_N\}$ and the normalized surface measure. For more general notions of discrepancy and their properties we refer to [13]. Unfortunately, discrepancy is rather difficult to compute explicitly. In order to circumvent this, estimates for the discrepancy in terms of Weyl sums

$$\frac{1}{N}\sum_{n=1}^{N} K_{m,j}(x_n) \tag{1.3}$$

have been given in [24] and [19]. Here $K_{m,j}$ denotes an orthogonal basis of the spherical harmonics of order m. For an account on several different notions of discrepancy and other measures for the quality of spherical point distributions we refer to [20] and [3].

Numerous constructions of 'well-distributed' point sets have been given in the literature. These range from constructions of so called low-discrepancy point sets in the unit cube, which can be transformed via standard parametrizations, to constructions given by integer solutions of the equation

$$x_1^2 + \cdots + x_{d+1}^2 = N$$

for $N \geq 1$ projected onto the sphere. Uniform distribution of these integer point sets were proved in [35] and [38] for $d \geq 4$ and estimates for the discrepancy were given in [14], [15], [16] for spheres of odd dimension. These latter estimates are based on Deligne's famous bound for the coefficients of cusp forms of integer weight [9]. In [32] and [33], the parametrization of $SO(3)$ by quaternions and again Deligne's estimate is used to construct a free subgroup of $SO(3)$ with 3 generators. The rotations in this subgroup applied to a point on the sphere are used to form a point set of small discrepancy on S^2. Spherical t-designs have been shown to be uniformly distributed as $t \to \infty$ in [21]. Estimates for the discrepancy in terms of the integration error for polynomials have been given in [4]. Furthermore, a construction of point sets based on finite field solutions of $x_1^2 + \cdots + x_{d+1}^2 = 1$ has been investigated in [5].

In this paper, we study numerical integration of continuous functions on S^d using equal weighted quadrature rules based at $N \geq 1$ points on S^d which minimize a generalized energy functional, see Definition 2 below. Important examples of such point sets are points which minimize energies for the Riesz kernel $\|x-y\|^{-s}$, $0 < s \leq d$ and logarithmic kernel $-\log\|x-y\|$, $s = 0$. In the case $s > 0$, the energy functionals above take the form of

$$\sum_{\substack{i,j=1 \\ i \neq j}}^{N} \|x_i - x_j\|^{-s} \tag{1.4}$$

where $\|.\|$ denotes the Euclidean metric on $\mathbb{R}^{d+1}$. The motivation for introducing such functionals comes from potential theory and will be explained carefully in Remark 1 below. In a series of papers Kuijlaars, Wagner, Rakhmanov, Saff, and Zhou, see [30], [39], [40], [41],[45], [46], [47], [48], [49], have recently proved upper and lower bounds for (1.4) for extremal configurations with respect to the Riesz kernel with $s \geq 0$. (See also the papers [26], [11] and [12]). Using these bounds, it is a consequence of Theorem 3 and Theorem 4 below, that the discrete distribution of extremal configurations tends weakly to the normalized surface measure μ as $N \to \infty$ if $0 \leq s \leq d$. For $s > d$, nothing is known about the distribution of extremal configurations, see Remark 6 below.

In what follows, for a parameter $\alpha > -1$, we denote by $C_n^\alpha(x)$ the n-th Gegenbauer polynomial of index α. The sequence of Gegenbauer polynomials is orthogonal with respect to the weight function $(1-x^2)^{\alpha-\frac{1}{2}}$ (see for instance [2], [34]). For $d \geq 2$ we denote the ultraspherical (or Legendre, cf. [36]) polynomials corresponding to the d-dimensional sphere by $P_n^{(d)}(x)$, which are normalized by $P_n^{(d)}(1) = 1$. We will frequently omit the upper index, when the dimension is fixed. The following relation holds between Gegenbauer and ultraspherical polynomials

$$C_n^{\frac{d-1}{2}}(x) = \binom{n+d-2}{n} P_n^{(d)}(x).$$

We are now able to introduce a class of functions which will be *admissible* in the following sense:

Definition 1. Let $\delta_0 > 0$ and $g : [-1-\delta_0, 1) \to \mathbb{R}$ be a continuous function satisfying the following conditions:

(a) g is strictly increasing with

$$\lim_{t \to 1-} g(t) = \infty.$$

(b) Let $g(t-\delta)$ be given by its ultraspherical expansion

$$\sum_{n=0}^{\infty} a_n(\delta) P_n^{(d)}(t).$$

Then $\forall n \geq 1$ and $0 < \delta \leq \delta_0$ assume that $a_n(\delta) > 0$. This expansion is valid for $t \in [-1, 1]$.

(c) The integral

$$\int_{-1}^{1} g(t)(1-t^2)^{\frac{d}{2}-1} dt$$

exists.

For any admissible g, we have:

Definition 2. Let g be admissible, $d \geq 2$ and a collection Z_N on S^d be given. Then we define the corresponding energy functional associated to the point set Z_N and the function g by

$$E(g, Z_N) = \frac{1}{N^2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} g(\langle x_i, x_j \rangle). \tag{1.5}$$

Furthermore, we define

$$\mathcal{E}(g, N) = \min_{Z_N} E(g, Z_N). \tag{1.6}$$

A point set, for which the minimal energy $\mathcal{E}(g, N)$ is attained, is called a *g-minimal energy point set*. It is clear that any rotation of a point set of minimal energy again gives a point set of minimal energy; thus such point sets are not unique.

Why Energy Functionals? We now motivate the use of energy functionals in numerical integration by way of a series of remarks below. The first is contained in:

Remark 1. The study of energy functionals is motivated by the fact that for admissible g, the energy integral

$$\int_{S^d} \int_{S^d} g(\langle x, y \rangle)\, d\nu(x)\, d\nu(y) \tag{1.7}$$

is minimized by the normalized surface measure μ on S^d amongst all Borel probability measures ν. This is the content of Lemma 1 below. Thus heuristics expects that a point distribution Z_N of minimal energy gives a discrete approximation to the surface measure in the sense that the integral with respect to the surface measure is approximated by a discrete sum over the points of Z_N. For the circle, S^1, it is easy to see that minimal energy point sets correspond to the vertices of a regular N-gon and are thus the best points to use for numerical integration for equally weighted quadrature rules.

Remark 2. (a) It is easy to check that the classical energy functionals as studied in [30], [39], [40], [45], [46], [47], [48] correspond to the following choices for the admissible function g.

$$g_L^0(t) := \frac{1}{2} \log \frac{1}{1-t} - \frac{1}{2} \log 2, \; s = 0 \tag{1.8}$$

for the *logarithmic energy* and

$$g_R^s(t) := \frac{1}{2^{\frac{s}{2}} (1-t)^{\frac{s}{2}}}, \; s > 0 \tag{1.9}$$

for the energy corresponding to the *Riesz potential* $\frac{1}{r^s}$.

(b) Since our final purpose will be to make the energy $E(g, Z_N)$ as small as possible, and we want to have small energy to correspond to reasonable dispersion of the point set Z_N, it is natural to assume g to be strictly increasing.

(c) The condition (b) of Definition 1 is nothing else than positive definiteness of the functions $g(t-\delta)-a_0(\delta)$ in the sense of Schoenberg [43]. By a general argument explained in [23], under our assumptions continuity of g at $1-\delta$ implies continuity of g in $[-1-\delta, 1-\delta]$.

We will also assume throughout that δ_0 is fixed and small enough so that (b) in Definition 1 holds for all sufficiently small and positive δ. We are now in a position to state our main results.

Theorem 1. *Let g be admissible, $d \geq 2$, Z_N a collection of N points on S^d, f a polynomial of degree at most $n \geq 1$ on S^d and $0 < \delta \leq \delta_0$. Then*

$$|R(f, Z_N)| \leq \leq \max_{1\leq k\leq n} \left(\frac{Z(d,k)}{\omega_d a_k(\delta)}\right)^{\frac{1}{2}} \|f\|_2 \left(E(g, Z_N) + \frac{1}{N} g(1-\delta) - a_0(\delta)\right)^{\frac{1}{2}} \tag{1.10}$$

with $Z(d,k) = \frac{2k+d-1}{k+d-1}\binom{k+d-1}{d-1}$.

Theorem 2. *Let g be admissible, $d \geq 2$, Z_N a collection of N points on S^d, $n \geq 1$ and $0 < \delta \leq \delta_0$. Let f be a continuous function of S^d satisfying:*

$$|f(x) - f(y)| \leq C_f \arccos(\langle x, y\rangle),\ x, y \in S^d. \tag{1.11}$$

Then

$$|R(f, Z_N)| \leq 12 C_f \frac{d}{n} + + \max_{1\leq k\leq n} \left(\frac{Z(d,k)}{\omega_d a_k(\delta)}\right)^{\frac{1}{2}} \|f\|_\infty \left(E(g, Z_N) + \frac{1}{N} g(1-\delta) - a_0(\delta)\right)^{\frac{1}{2}}. \tag{1.12}$$

We note that Theorems 1 and 2 are general results which hold for any choice of points Z_N on S^d.

Remark 3. Part (c) in the definition of admissibility is not necessary for the validity of Theorems 1 and 2. Nevertheless, the proof of Theorem 4 will show that the right hand side of the inequality does only tend to zero for special choices of the function g. See also Remark 7.

Remark 4. A sequence of point sets Z_N on S^d, is said to be *asymptotically equidistributed* if for every spherical cap $C \subseteq S^d$,

$$\lim_{N\to\infty} \frac{\#\{1 \le j \le N : x_j \in C\}}{N} = \mu(C). \tag{1.13}$$

i.e., each intersection of the sphere and half space gets an equal portion of points. By duality, it follows that (1.13) is equivalent to

$$\lim_{N\to\infty} R(f, Z_N) = 0 \tag{1.14}$$

for every continuous function f on S^d.

The following theorem is well known; for instance, it follows from the estimates given in [45, 46].

Theorem 3. *Let $d \ge 2$ and $0 \le s < d$. Then g_R^s-minimal energy point sets are asymptotically equidistributed.*

We remark that Theorem 3 may also be proved using Theorems 1 and 2 and the Cramer-Wold theorem which says that a probability measure on Euclidean space is uniquely determined by its values it takes on half spaces, see [8]. For $0 < s < d$, this is mainly because the energy integral given by (1.7) is finite with value

$$\frac{\Gamma((d+1)/2)\Gamma(d-s)}{\Gamma(d-s/2)\Gamma((d-s+1)/2)}.$$

For $s \ge d$, (1.7) diverges for every measure ν which means that the nearest neighbor interactions in (1.4) are dominating. For $s = d$, we are able to present:

Theorem 4. *Let $d \ge 2$ and Z_N a collection of g_R^d-minimal energy points on S^d and $N \ge (\log N + d/2)^{2d}$. Then for every continuous function f on S^d satisfying (1.11) we have*

$$|R(f, Z_N)| \le \frac{C_f^*}{\sqrt{\log N}} \tag{1.15}$$

where $C_f^* := \sqrt{C_d}\|f\|_\infty + 12dC_f$, where C_d could be chosen as

$$C_d = \frac{ed\Gamma\left(\frac{d+1}{2}\right)^2}{4\pi^{\frac{d+2}{2}}\Gamma\left(\frac{d}{2}\right)}(2\log\pi - 3\log 2 + 2\gamma) + \frac{d\Gamma\left(\frac{d+1}{2}\right)}{(2\pi)^{\frac{d+1}{2}}}$$

with

$$\psi(x) = \frac{\Gamma'(x)}{\Gamma(x)} \text{ and } \gamma = -\psi(1).$$

Moreover,

$$D_N(Z_N) \leq \mathcal{O}\left(\frac{1}{\sqrt{\log N}}\right). \tag{1.16}$$

Remark 5. It is quite probable that the estimates for the integration error and the discrepancy given in Theorem 4 are not sharp. Indeed, for $s = d - 1$, a conjecture of Korevaar in [27], which was essentially proved by Götz in [17] says that the error bound for the discrepancy is $O(N^{-1/d})$. Moreover, in light of [30], we expect that the order of magnitude of the discrepancy should be the same as for all g_R^s-minimal points with $s < d$.

In particular, g_R^d-minimal points are asymptotically equidistributed with rate $\frac{1}{\sqrt{\log N}}$. We note that the asymptotic equidistribution of g_R^d-minimal points (without rate of convergence) was recently shown in an indirect way by Götz and Saff in [18].

We close this section with:

Remark 6. Though intuitively clear it is still unknown, whether g_R^s-mimimal points are asymptotically equidistributed for $s > d$. To understand this, define

$$\delta(Z_N) := \inf_{i \neq j} \|x_i - x_j\|; \ \ \delta_N := \sup_{Z_N \subset S^d} \delta(Z_N).$$

The determination of δ_N is called *Tammes problem* or the *Spherical packing problem*, see [7], [22]. It asks to maximize the smallest distance amongst N points on S^d. Fixing N and allowing $s \to \infty$, the minimal energy problem $s > d$ reduces to the best packing problem.

The remainder of this paper is devoted to the proofs of Theorems 1, 2, and 4. These are contained in Sections 2 and 3 below.

2. Numerical integration

In this section, we present the proofs of Theorems 1 and 2. In what follows, for $x \in \mathbb{R}$ and $n \geq 1$,

$$(x)_n := \prod_{k=0}^{n-1}(x+k) = \frac{\Gamma(x+n)}{\Gamma(x)}, \quad (x)_0 = 1$$

will denote Pochhammer's shifted factorial.

We begin with Lemma 1 which is of independent interest.

Lemma 1. *The energy integral given by* (1.7) *is minimized uniquely by the normalized surface measure* μ.

The essential ideas behind Lemma 1 are well known, see [31]. We provide a short independent proof.

Proof. From [43], it follows that (b) in Definition 1 implies that (1.7) is always nonnegative. Moreover, it follows from the orthogonality relations of the ultraspherical polynomials $P_n^{(d)}$ that for the surface measure μ the value of the energy is a_0. Here we also use the basic rule, see [30]:

$$\int_{S^d} g(\langle x, x_0\rangle) d\mu(x) = \gamma_d \int_{-1}^{1} g(t)(1-t^2)^{d/2-1} dt \tag{2.1}$$

where $x_0 \in S^d$ is some fixed point and

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

Thus it remains to prove that the measure μ is unique. Assume that ν is a Borel probability measure that yields minimal energy. Then we have

$$\int_{S^d}\int_{S^d} P_n^{(d)}(\langle x, y\rangle) d\nu(x) d\nu(y) = 0 \tag{2.2}$$

for all $n \geq 1$ by the positivity of the Fourier coefficients and the fact that

$$\int_{S^d}\int_{S^d} P_n^{(d)}(\langle x, y\rangle) d\nu(x) d\nu(y) \geq 0$$

by the positive definiteness of $P_n^{(d)}$. We recall the Funk-Hecke addition formula for spherical harmonics, see [2, Section 9.8]:

$$\int_{S^d} P_n^{(d)}(\langle x, \eta\rangle) P_n^{(d)}(\langle y, \eta\rangle) d\mu(\eta) = \frac{1}{Z(d,n)} P_n^{(d)}(\langle x, y\rangle) \tag{2.3}$$

where

$$Z(d,n) := \frac{2n+d-1}{n+d-1}\binom{n+d-1}{d-1} \tag{2.4}$$

was defined in the statement of Theorem 1. Applying (2.2) and (2.3) gives

$$\int_{S^d}\left(\int_{S^d} P_n^{(d)}(\langle x, \eta\rangle) d\nu(\eta)\right)^2 d\mu(x) = 0$$

which implies that the polynomial

$$\int_{S^d} P_n^{(d)}(\langle x, \eta\rangle) d\nu(\eta)$$

vanishes identically. As x is free, we may choose a finite index set J and a collection of points $x_j \in S^d$, $j \in J$ such that $P_n^{(d)}(\langle x_j, \eta\rangle)$ form a basis of the spherical harmonics of order n, see [36]. A standard approximation argument using the Stone-Weierstraß theorem then shows that

$$\int_{S^d} f(x)d\nu(x) = \int_{S^d} f(x)d\mu(x)$$

for all $f \in C(S^d)$. This completes the proof of Lemma 1. □

Next we need:

Lemma 2. *Let g be admissible and $0 < \delta \leq \delta_0$ then*

$$\frac{1}{N^2}\sum_{i,j=1}^{N} g(\langle x_i, x_j\rangle - \delta) \leq E(g, Z_N) + \frac{1}{N} g(1-\delta). \tag{2.5}$$

Proof. This follows by using the fact that g is increasing and collecting the terms with $i = j$ into the second term on the right hand side of (2.5). □

We are now ready for:

Proof of Theorem 1. We will make use of spherical harmonics and we refer the reader to [36] for the details. Especially, we will make use of the fact that there are exactly $Z(d, n)$ linearly independent spherical harmonics of order n. Furthermore, we use the Funk-Hecke formula given by (2.3). Since f is a polynomial of degree at most n, we may represent it as a linear combination of spherical harmonics of order at most n:

$$f(x) = \sum_{k=0}^{n} Y_k(x), \tag{2.6}$$

where

$$Y_k(x) = \frac{Z(d,k)}{\omega_d}\int_{S^d} f(\eta) P_k^{(d)}(\langle x, \eta\rangle) d\sigma(\eta).$$

Observe that

$$\|f\|_2^2 = \sum_{k=0}^{n} \|Y_k\|_2^2 . \tag{2.7}$$

Then the error of integration can be written as

$$-R(f, Z_N) = \sum_{k=1}^{n} \frac{Z(d,k)}{\omega_d} \int_{S^d} Y_k(\eta) Q_k(\eta) d\sigma(\eta), \tag{2.8}$$

where $Q_n(\eta)$ is given by

$$Q_n(\eta) = Q_n(\eta, Z_N) = \frac{1}{N} \sum_{j=1}^{N} P_n^{(d)}(\langle \eta, x_j \rangle). \tag{2.9}$$

We now insert $b_k^{-1} b_k$ into (2.8) and apply the Cauchy-Schwarz inequality to obtain

(2.10)

$$|R(f, Z_N)|^2 \le \frac{1}{\omega_d^2} \int\limits_{S^d} \sum_{k=1}^{n} \frac{Z(d,k)^2}{b_k^2} |Y_k(\eta)|^2 \, d\sigma(\eta) \int\limits_{S^d} \sum_{k=1}^{n} b_k^2 \, |Q_k(\eta)|^2 \, d\sigma(\eta).$$

It is a consequence of (2.3) that

$$\int\limits_{S^d} |Q_k(\eta)|^2 \, d\sigma(\eta) = \frac{1}{N^2} \frac{\omega_d}{Z(d,k)} \sum_{i,j=1}^{N} P_k^{(d)}(\langle x_i, x_j \rangle).$$

Furthermore, we choose $b_k = (a_k(\delta) Z(d,k))^{\frac{1}{2}}$ $(k \ge 1)$, use (2.7) and a simple estimate for the first factor of the right hand side in (2.10) and extend the finite sum in the second factor of the right hand side in (2.10) to obtain

(2.11)

$$|R(f, Z_N)|^2 \le \frac{1}{\omega_d} \max_{1 \le k \le n} \frac{Z(d,k)}{a_k(\delta)} \|f\|_2^2 \left[\frac{1}{N^2} \sum_{i,j=1}^{N} g(\langle x_i, x_j \rangle - \delta) - a_0(\delta) \right].$$

By Lemma 2.2, we obtain the required estimate. □

Next we present:

Proof of Theorem 2. The key to the proof is an approximation kernel due to Newman and Shapiro, see [37] and [21, Theorem 1]. For the given $m \ge 1$, let

$$K_m(t) := c_m \left(\frac{P_{m+1}^{(d)}(t)}{t - \alpha_{m+1}} \right)^2, \; t \in (-1, 1) \tag{2.12}$$

where α_{m+1} is the largest zero of $P_{m+1}^{(d)}$ and c_m is chosen such that

$$\int_{S^d} K_m(\langle x, y \rangle) d\mu(x) = 1, \; y \in S^d. \tag{2.13}$$

Note that K_m is a polynomial of degree $2m$. Set

$$f_m(x) := \int_{S^d} f(y)K_m(\langle x, y\rangle)d\mu(y),\ x \in S^d. \tag{2.14}$$

Then applying Theorem 1 with f_m and using the triangle inequality gives:

$$|R(f, Z_N)| \leq \|f - f_m\|_\infty + \\ + \max_{1\leq k\leq 2m} \left(\frac{Z(d,k)}{\omega_d a_k(\delta)}\right)^{\frac{1}{2}} \|f_m\|_2 \left(E(g, Z_N) + \frac{1}{N}g(1-\delta) - a_0(\delta)\right)^{\frac{1}{2}}. \tag{2.15}$$

Now we observe in view of (2.12) and (2.13) that $\|f_m\|_2 \leq \|f_m\|_\infty \leq \|f\|_\infty$. Moreover, using the definitions (2.12), (2.13) and well known lower bounds for α_{m+1}, see [44, pg 331], gives that

$$\|f - f_m\|_\infty \leq \frac{6dC_f}{m}.$$

These two later observations together with (2.15) give the theorem for even $n = 2m$. For odd $n > 1$ we choose $m = \frac{n-1}{2}$. □

3. Asymptotic equidistribution of g_R^s-mimimal configurations for $0 < s \leq d$

In this section we present the proof of Theorem 4. To this end, we will need to investigate the classical energy functionals as studied in [30]. We recall that these correspond to the following choice for the admissible function g:

$$g_R^{2\alpha}(t) = \frac{1}{2^\alpha(1-t)^\alpha},\ \alpha > 0$$

for the energy corresponding to the potential $\frac{1}{r^{2\alpha}}$. First we will need to compute the Gegenbauer coefficients for the functions $g(t-\delta)$ in these cases. Throughout this section we will set $\lambda = \frac{d-1}{2}$. We use

$$(1+\delta-t)^{-\alpha} = (1+\delta)^{-\alpha}\sum_{n=0}^{\infty}\binom{n+\alpha-1}{n}\frac{t^n}{(1+\delta)^n} \tag{3.1}$$

and [34, pg 227]

$$t^n = 2^{-n}n!\sum_{m=0}^{\lfloor\frac{n}{2}\rfloor}\frac{n+\lambda-2m}{m!(\lambda)_{n+1-m}}C_{n-2m}^{\lambda}(t). \tag{3.2}$$

Inserting (3.2) into (3.1) and changing the order of summation yields

$$
\begin{aligned}
(3.3)\qquad & 2^{-\alpha}(1+\delta-t)^{-\alpha} \\
&= (1+\delta)^{-\alpha}\sum_{k=0}^{\infty}\frac{(\alpha)_k}{(\lambda)_k 2^{k+\alpha}(1+\delta)^k}\times \\
&\times {}_2F_1\left(\frac{\alpha+k}{2},\frac{\alpha+k+1}{2};\lambda+k+1;\frac{1}{(1+\delta)^2}\right)C_k^{\lambda}(t) \\
&= \sum_{k=0}^{\infty} a_k^{\alpha}(\delta)P_k^{(d)}(t).
\end{aligned}
$$

Here

$$
\begin{aligned}
(3.4)\qquad a_k^{\alpha}(\delta) &= \frac{(\alpha)_k(d-1)_k}{(\frac{d-1}{2})_k k! 2^{k+\alpha}(1+\delta)^{k+\alpha}}\times \\
&\times {}_2F_1\left(\frac{\alpha+k}{2},\frac{\alpha+k+1}{2};\frac{d+1}{2}+k;\frac{1}{(1+\delta)^2}\right),
\end{aligned}
$$

where ${}_2F_1$ denotes the basic hypergeometric function. Alternatively, this expansion could be derived by computing the according Fourier integrals. The coefficients of $P_k^{(d)}$ in this expansion are positive and decreasing functions of δ.

We also need the following inequality for the hypergeometric function, which was derived in [1]. For $\alpha = \lambda + \frac{1}{2} = \frac{d}{2}$

$$
\begin{aligned}
(3.5)\ & {}_2F_1\left(\frac{\alpha+k}{2},\frac{\alpha+k+1}{2};\lambda+k+1;x\right) \geq \\
&\geq \frac{2^{\alpha+k-1}\Gamma(\alpha+k+\frac{1}{2})}{\sqrt{\pi}\Gamma(\alpha+k)}\left(\log\frac{1}{1-x}-2\psi(k+\alpha)+4\log 2-2\gamma\right) \geq \\
&\geq \frac{2^{\alpha+k-1}\Gamma(\alpha+k+\frac{1}{2})}{\sqrt{\pi}\Gamma(\alpha+k)}\log\frac{1}{(\alpha+k)^2(1-x)},
\end{aligned}
$$

where $\psi(x) = \frac{\Gamma'(x)}{\Gamma(x)}$ denotes the digamma function and $\gamma = -\psi(1)$ is the Euler-Mascheroni constant. Furthermore, we have used the estimate $\psi(x) \leq \log x$.

We are now able to present the

Proof of Theorem 4. We estimate the second term on the right hand side of (1.12) first. Let Z_N be a minimal energy point set for the g-energy with $g_R^d(t) = \frac{1}{(2-2t)^{\frac{d}{2}}}$. From [30] it is known that

$$
(3.6)\qquad E(g, Z_N) \leq \frac{1}{d}\gamma_d \log N + C_d
$$

where we recall that γ_d is given by

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

(Notice that our definition of energy is twice the energy defined in [30]). The best value for the constant C_d is still unknown. From the computations in [30] it follows that $C_d \leq \gamma_d \log \pi$.

¿From (3.4) and (3.5) we know that (using $1/(1-(1+\delta)^{-2}) \geq \frac{1}{2\delta}$)

$$a_k(\delta) \geq \gamma_d \frac{Z(d,k)}{(1+\delta)^{k+\frac{d}{2}}} \log \frac{1}{2(k+\frac{d}{2})^2\delta}$$

and

$$a_0(\delta) \geq \frac{\gamma_d}{2}\left(\log\frac{1}{2\delta} - 2\psi\left(\frac{d}{2}\right) + 4\log 2 - 2\gamma\right).$$

We now assume that $N \geq (m+d/2)^{2d}$. Inserting $\delta = N^{-\frac{2}{d}}$ into the right hand side of (1.12) and using (3.7) yields

$$\text{(3.7)}\quad E(g,Z_N) + \frac{1}{N}g(1-\delta) - a_0(\delta) \leq$$
$$\frac{1}{d}\gamma_d \log N + C_d + 2^{-\frac{d}{2}} - \frac{\gamma_d}{2}\left(\log N^{-\frac{2}{d}} - \log 2 - 2\psi\left(\frac{d}{2}\right) + 4\log 2 - 2\gamma\right) \leq$$
$$\gamma_d(\log \pi - \frac{3}{2}\log 2 + \gamma) + 2^{-\frac{d}{2}} =: C'_d.$$

Putting everything together yields

$$|R(f,Z_N)| \leq \frac{12dC_f}{m} + \sqrt{\frac{C'_d}{\omega_d}}\left(1+N^{-\frac{2}{d}}\right)^{\frac{m}{2}+\frac{d}{4}} \frac{\|f\|_\infty}{\sqrt{\frac{2}{d}\log N - 2\log(m+\frac{d}{2})}}.$$

We now choose $m := [\sqrt{\log N}]+1$ and observe that $\frac{2}{d}\log N - 2\log(m + d/2) \geq \frac{1}{d}\log N$ to obtain

$$|R(f,Z_N)| \leq \frac{12dC_f + \|f\|_\infty\sqrt{\frac{edC'_d}{\omega_d}}}{\sqrt{\log N}},$$

which is (1.15). Finally (1.16) follows using (1.10), (3.6) and [4, Theorem 1]. □

Remark 7. When trying to apply the same reasoning to g_R^s-energies with $s > d$ it turns out that the upper bounds for the minimal s-energy (cf. [30]) do not coincide with the bounds for the Fourier coefficients as

$\delta \to 0^+$ as is the case for $s = d$. This shows that the inequalities (1.10) and (1.12) give only trivial bounds for the integration error for $s > d$.

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