ENERGY FUNCTIONALS, NUMERICAL INTEGRATION AND ASYMPTOTIC EQUIDISTRIBUTION ON THE SPHERE

STEVEN B. DAMELIN AND PETER J. GRABNER†

Abstract. In this paper, we study the numerical integration of continuous functions on d-dimensional spheres $S^d \subseteq \mathbb{R}^{d+1}$ by equally weighted quadrature rules based at $N \geq 1$ 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 $-\log\|x-y\|$. We deduce that extremal point configurations are asymptotically equidistributed on S^d as $N \to \infty$ and we present explicit rates of convergence for the special case $s = d$.

1. Introduction and Statement of Results

This paper deals with the subject of numerical integration of continuous functions on the d-dimensional unit spheres $S^d \in \mathbb{R}^{d+1}$. 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

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

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

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

Date: 15 February 2002.

2000 *Mathematics Subject Classification.* Primary: 41A55; Secondary: 11K38 65D30.

Key words and phrases. energy functionals, discrepancy, numerical integration.

†This author is supported by the START project Y96-MAT of the Austrian Science Fund.

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

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

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 in areas as diverse as spherical t-designs, discrepancy and combinatorics, Monte-Carlo and Quasi-Monte-Carlo methods, approximation theory, finite fields and complexity theory. We refer the reader to [3], [6], [9], [17], [16], [34] 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 [5], [3], [34], [11], [12], [13], [23], [25], [26], [32], [33], [38], [39], [40], [41], [42]. 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 balls and 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 [10]. 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 [19] and [15]. 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 [16] 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 [28] and [31] for $d \geq 4$ and estimates for the discrepancy were given in [11], [12], [13] for spheres of odd dimension. These latter estimates are based on Deligne's famous bound for the coefficients of cusp forms of integer weight [8]. In [25] and [26], 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 [17]. 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 points are $s \geq 0$ extremal configurations, i.e., 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 [23], [32], [33], [34],[38], [39], [40], [41], [42], have recently proved upper and lower bounds for (1.4) for $s > 0$ extremal configurations. Using these bounds, it is a consequence of Theorem 3 and Theorem 4 below, that the discrete distribution of $s > 0$ extremal configurations tends weakly to the normalized surface measure μ as $N \to \infty$ if $0 \le s \le d$. For $s > d$, nothing is known about the distribution of s extremal configurations, see Remark 4 below.

In what follows, for 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] [27]). For $d \ge 2$ we denote the Legendre polynomials corresponding to the d-dimensional sphere by $P_n^{(d)}(x)$, which are normalized by $P_n(1) = 1$. We will frequently omit the upper index, when the dimension is fixed. The following relation holds between Gegenbauer and Legendre polynomials

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

We are now able to introduce the following 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 $\forall n \ge 1$ and $0 < \delta \le \delta_0$ assume that $a_n(\delta) > 0$.

(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, $d \ge 2$ 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

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

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 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.

1.1. **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 [23], [32], [33], [38], [39], [40], [41], and 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

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

for the energy corresponding to the Riesz potential $\frac{1}{r^{2s}}$.

(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 [36]. By a general argument explained in [18], 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*

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

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, $m \geq 1$ 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

$$|R(f, Z_N)| \leq 12 C_f \frac{d}{m} + + \max_{1\leq k\leq m} \left(\frac{Z(d,k)}{\omega_d a_k(\delta)}\right)^{\frac{1}{2}} \|f\|_2 \left(\mathcal{E}(g, Z_N) + \frac{1}{N} g(1-\delta) - a_0(\delta)\right)^{\frac{1}{2}}. \tag{1.12}$$

We note that Theorems 1 and 2 are general results which hold for any choice of points Z_N on S^d. Related estimates are given in [21] and [4].

Remark 3. A set of points Z_N on S^d, is said to be *asymptotically equidistributed* if for every spherical cap $C \subseteq S^d$,

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

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, see for instance [38, 39].

Theorem 3. *Let $d \geq 2$ and $0 \leq s < d$. Then $0 \leq s < d$ extremal configurations are asymptotically equidistributed.*

We remark that Theorem 3 may also be proved using general principles from potential theory and the Cramer-Wold theorem, see [7], which says that a probability measure on Euclidean space is uniquely determined by its values it takes on half spaces, see [7]. This is mainly because the energy integral given by (1.7) is finite in this case with value

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

For $s \geq d$, (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 $d \geq 2$ and Z_N a collection of d extremal points on S^d. Then for every continuous function f on S^d satisfying* (1.11) *we have*

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

where $C_f^* := \max\{C_d' ||f||_2, 6dC_f\}$, where C_d' could be chosen as

$$C_d' = \frac{\Gamma(\frac{d+1}{2})}{\sqrt{\pi}\Gamma(\frac{d}{2})}\left(\log \pi + \psi\left(\frac{d}{2}\right) - 2\log 2 + \gamma\right) \text{ with } \psi(x) = \frac{\Gamma'(x)}{\Gamma(x)} \text{ and } \gamma = -\psi(1).$$

Moreover,

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

In particular, d extremal points are asymptotically equidistributed with rate $\frac{1}{\sqrt{\log N}}$. We note that the asymptotic equidistribution of d extremal points (without rate of convergence) was recently shown in an indirect way by Götz and Saff in [14].

We close this section with:

Remark 4. It seems intuitively clear that for $s > d$ extremal points should be asymptotically equidistributed as well. 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 [6]. 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 [24]. We provide a short independent proof.

Proof. From [36], it follows that (b) in Definition 1 implies that (1.7) is always nonnegative. Moreover, it follows from the orthogonality relations of the Legendre polynomials P_n and the positivity of the Fourier coefficients of g that for the surface measure μ the value of the energy is 0. Here we also use the basic rule, see [23]:

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

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

$$\gamma_d := \frac{\Gamma\left(\frac{d+1}{2}\right)}{\sqrt{\pi}\Gamma\left(\frac{d}{2}\right)}. \tag{2.2}$$

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

$$\int_{S^d}\int_{S^d} P_n(\langle x, y\rangle)d\nu(x)d\nu(y) = 0 \tag{2.3}$$

for all $n \geq 1$. We recall the Funk-Hecke addition formula for spherical harmonics, see [2, Section 9.8]:

$$\int_{S^d} P_n(\langle x, \eta\rangle)P_n(\langle y, \eta\rangle)d\mu(\eta) = \frac{1}{Z(d,n)}P_n(\langle x, y\rangle) \tag{2.4}$$

where

$$Z(d,n) := \frac{2n+d-1}{n+d-1}\binom{n+d-1}{d-1} \tag{2.5}$$

was defined in the statement of Theorem 1. Applying (2.3) and (2.4) gives

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

which implies that

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

vanishes μ-almost everywhere. As x is free, we may choose a finite index J set 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 [29]. 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 $0<\delta\le\delta_0$ then*

$$\frac{1}{N^2}\sum_{i,j=1}^{N} g(\langle x_i,x_j\rangle-\delta)\le E(g,Z_N)+\frac{1}{N}g(1-\delta). \tag{2.6}$$

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 (2.6). □

We are now ready for:

Proof of Theorem 1. We will make use of spherical harmonics and we refer the reader to [29] 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:

$$f(x)=\sum_{k=0}^{n} Y_k(x), \tag{2.7}$$

where

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

Observe that

$$\|f\|^2 = \sum_{k=0}^{n} \|Y_k\|^2 . \tag{2.8}$$

Then the error of integration can be written as

$$-R(f, Z_N) = \sum_{k=1}^{n} \frac{Z(d,k)}{\omega_d} \int_{S^d} Y_k(\eta) Q_k(\eta) d\sigma(\eta), \tag{2.9}$$

where $Q_n(\eta)$ is given by

$$Q_n(\eta) = Q_n(\eta, Z_N) = \frac{1}{N} \sum_{j=1}^{N} P_n^{(d)}(\langle \eta, x_j \rangle). \tag{2.10}$$

We now insert $b_k^{-1} b_k$ into (2.9) and apply the Cauchy-Schwarz inequality to obtain

(2.11)

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

It is a consequence of (2.4) that

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

Furthermore, we choose $b_k = (a_k(\delta) Z(d,k))^{\frac{1}{2}}$ $(k \geq 1)$, use (2.8) and a simple estimate for the first factor in (2.11) and extend the finite sum in the second factor in (2.11) to obtain

(2.12)

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

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 [30] and [17, Theorem 1]. For the given $m \geq 1$, let

$$K_m(t) := a_m \left(\frac{P_{m+1}^d(t)}{t - \alpha_{m+1}} \right)^2, \; t \in (-1, 1) \tag{2.13}$$

where α_{m+1} is the largest zero of P^d_{m+1} and a_m is chosen such that

$$\int_{S^d} K_m(\langle x, y\rangle)d\mu(x) = 1,\, y \in S^d. \tag{2.14}$$

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

$$f_m(x) := \int_{S^d} f(y)K_m(\langle x, y\rangle)d\mu(y),\, x \in S^d. \tag{2.15}$$

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

$$\begin{aligned}|R(f, Z_N)| \le \|f - f_m\|_\infty +\\ + \max_{1\le k\le 2m} \left(\frac{Z(d, k)}{\omega_d a_k(\delta)}\right)^{\frac{1}{2}} \|f_m\|_2 \left(\mathcal{E}(g, Z_N) + \frac{1}{N} g(1 - \delta) - a_0(\delta)\right)^{\frac{1}{2}}.\end{aligned} \tag{2.16}$$

Now we observe in view of (2.13) that $\|f_m\|_2 \le \|f\|_2$. Moreover, using the definitions (2.13), (2.14) and well known lower bounds for α_{m+1}, see [37, pg 331], gives that

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

These two later observations together with (2.16) give the theorem. □

3. Asymptotic equidistribution of s extremal configurations

In this section we present the proofs of Theorems 3 and 4. To this end, we will need to investigate the classical energy functionals as studied in [23]. We recall that these correspond to the following choices for the admissible function g:

$$g(t) = \frac{1}{2^\alpha(1 - t)^\alpha} \quad \text{for the energy corresponding to the potential } \frac{1}{r^{2\alpha}}.$$

First we will need to compute the Gegenbauer coefficients for the functions $g(t - \delta)$ in these cases. Throughout this section we will denote $\lambda = \frac{d-1}{2}$. 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 [27, pg 227]

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

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

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

with

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

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 $\alpha=\lambda+\frac{1}{2}=\frac{d}{2}$

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

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 Theorems 3 and 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 $g(t)=\frac{1}{(2-2t)^{\frac{d}{2}}}$. From [23] it is known that

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

with γ_d given by (2.2) (notice that our definition of energy is twice the energy defined in [23]). The best value for the constant C_d is still unknown. From the computations in [23] it follows that $C_d \leq \gamma_d \log \pi$.

From (3.4) and (3.5) we know that

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

and

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

We now assume that $N \geq (m+d/2)^d$. Inserting $\delta = N^{-\frac{2}{d}}$ into (1.12) yields

$$E(g, Z_N) + \frac{1}{N} g(1-\delta) - a_0(\delta) \leq C'_d \tag{3.6}$$

and therefore

$$|R(f, Z_N)| \leq \frac{12dC_f}{m} + C'_d \frac{\|f\|_2}{\sqrt{\frac{2}{d}\log N - 2\log(m+\frac{d}{2})}}$$

with $C'_d = C_d + \gamma_d(\psi(d/2) - 2\log 2 + \gamma)$. We now choose $m := [\sqrt{\log N}] + 1$ to obtain (1.15). Finally (1.16) follows using (1.10), (3.6) and [4, Theorem 1]. ☐

References

[1] G. D. Anderson, R. W. Barnard, K. C. Richards, M. K. Vamanamurthy, and M. Vuorinen, *Inequalities for zero-balanced hypergeometric functions*, Trans. Amer. Math. Soc. **347** (1995), 1713–1723.

[2] G. Andrews, R. Askey, and R. Roy, *Special functions*, Encyclopedia of Mathematics and Its Applications, vol. 71, Cambridge University Press, 1999.

[3] V. V. Andrievskii and H.-P. Blatt, *Discrepancy of signed measures and polynomial approximation*, Springer-Verlag, New York, 2002.

[4] V. V. Andrievskii, H.-P. Blatt, and M. Götz, *Discrepancy estimates on the sphere*, Monatsh. Math. **128** (1999), 179–188.

[5] B. Bajnok, S. B. Damelin, J. Li, and G. Mullen, *A constructive finite field method for scattering points on the surface of a d-dimensional sphere*, Computing **?** (2002), ?–?, to appear.

[6] J. H. Conway and N. J. A. Sloane, *Sphere packings, lattices and groups*, Grundlehren d. math. Wiss., vol. 290, Springer, Berlin, New York, 1988.

[7] H. Cramer and H. Wold, *Some theorems on distribution functions*, J. London Math. Soc **11** (1936), 290–294.

[8] P. Deligne, *La conjecture de Weil*, Publ. Math. I.H.E.S. **43** (1974), 273–307.

[9] P. Delsarte, J. M. Goethals, and J. J. Seidel, *Spherical codes and designs*, Geometriae Dedicata **6** (1977), 363–388.

[10] M. Drmota and R. F. Tichy, *Sequences, discrepancies, and applications*, Lecture Notes in Math., vol. 1651, Springer, Berlin, New York, 1997.

[11] E. P. Golubeva and O. M. Fomenko, *Application of spherical functions to a problem of the theory of quadratic forms*, Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI) **144** (1985), no. Anal. Teor. Chisel i Teor. Funktsii. 6, 38–45, 173–174, translation in *J. Soviet Math., 1987, 38, 2054–2060*.

[12] E. P. Golubeva and O. M. Fomenko, *Asymptotic distribution of lattice points on the three-dimensional sphere*, Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI) **160** (1987), no. Anal. Teor. Chisel i Teor. Funktsii. 8, 54–71, 297, translation in *J. Soviet Math. 52 (1990), 3036–3048*.

[13] E. P. Golubeva and O. M. Fomenko, *A remark on the asymptotic distribution of lattice points on a large three-dimensional sphere*, Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI) **185** (1990), no. Anal. Teor. Chisel i Teor. Funktsii. 10, 22–28, 183, translation in *J. Soviet Math. 59 (1992), 1148–1152*.

[14] M. Götz and E. B. Saff, *Note on d-extremal configurations for the sphere in* $\mathbb{R}^{d+1}$, Recent Progress in Multivariate Approximation (W. Haussmann, K. Jetter, and M. Reimer, eds.), International Series of Numerical Mathematics, vol. 137, Birkhäuser Verlag, 2001, pp. 159–162.

[15] P. J. Grabner, *Erdős-Turán type discrepancy bounds*, Monatsh. Math. **111** (1991), 127–135.

[16] P. J. Grabner, B. Klinger, and R. F. Tichy, *Discrepancies of point sequences on the sphere and numerical integration*, Multivariate Approximation, Recent Trends and Results, Proc. of the 2nd International Conference on Multivariate Approximation Theory, Witten-Bommerholz (Berlin) (W. Haußmann, K. Jetter, and M. Reimer, eds.), Akademie Verlag, 1997, pp. 95–112.

[17] P. J. Grabner and R. F. Tichy, *Spherical designs, discrepancy and numerical integration*, Math. Comp. **60** (1993), 327–336.

[18] E. Hewitt and K.A. Ross, *Abtract harmonic analysis*, Springer, Berlin, 1970.

[19] E. Hlawka, *Gleichverteilung auf Produkten von Sphären*, J. reine angew. Math. **330** (1982), 1–43.

[20] E. Hlawka, *Beiträge zur Theorie der Gleichverteilung und ihren Anwendungen I–V*, Österr. Akad. Wiss. SB II **197** (1988), 1–154.

[21] J. Korevaar and J. L. H. Meyers, *Spherical Faraday cage for the case of equal point charges and Chebyshev-type quadrature on the sphere*, Integral Transforms Spec. Funct. **1** (1993), 105–117.

[22] J. Korevaar and M. A. Monterie, *Approximation of the equilibrium distribution by distributions of equal point charges with minimal energy*, Trans. Amer. Math. Soc. **350** (1998), 2329–2348.

[23] A. B. J. Kuijlaars and E. B. Saff, *Asymptotics for minimal discrete energy on the sphere*, Trans. Amer. Math. Soc. **350** (1998), 523–538.

[24] N.S. Landkof, *Foundations of modern potential theory*, Grundlehren d. math. Wiss., vol. 180, Springer, Berlin, New York, 1972.

[25] A. Lubotzky, R. Phillips, and P. Sarnak, *Hecke operators and distributing points on the sphere I*, Comm. Pure App. Math. **39** (1986), S148–S186.

[26] A. Lubotzky, R. Phillips, and P. Sarna, *Hecke operators and distributing points on the sphere II*, Comm. Pure App. Math. **40** (1987), 401–420.

[27] W. Magnus, F. Oberhettinger, and R.P. Soni, *Formulas and theorems for the special functions of mathematical physics*, Springer, Berlin, New York, 1966.

[28] A. V. Malyshev, *The distribution of integer points on a four-dimensional sphere*, Dokl. Akad. Nauk SSSR (N.S.) **114** (1957), 25–28.
[29] C. Müller, *Spherical harmonics*, Lecture Notes in Mathematics, vol. 17, Springer, Berlin, New York, 1966.
[30] D. J. Newman and H. S. Shapiro, *Jackson's Theorem in Higher Dimensions*, Über Approximationstheorie (P.L. Butzer and J. Korevaar, eds.), Birkhäuser, 1964, pp. 209–219.
[31] C. Pommerenke, *Über die Gleichverteilung von Gitterpunkten auf m-dimensionalen Ellipsoiden*, Acta Arith. **5** (1959), 227–257.
[32] E. A. Rakhmanov, E. B. Saff, and Y. M. Zhou, *Minimal discrete energy on the sphere*, Math. Res. Lett. **1** (1994), 647–662.
[33] E. A. Rakhmanov, E. B. Saff, and Y. M. Zhou, *Electrons on the sphere*, Computational Methods in Function Theory, World Scientific Publishing, River Edge, NJ, 1995, pp. 293–309.
[34] E. B. Saff and A. B. J. Kuijlaars, *Distributing many points on a sphere*, Math. Intell. **19** (1997), 5–14.
[35] E.B. Saff and V. Totik, *Logarithmic potentials with external fields*, Grundlehren, vol. 316, Springer, Berlin, 1998.
[36] I. J. Schoenberg, *Positive definite functions on spheres*, Duke Math. J. **9** (1942), 96–108.
[37] G. Szegő, *Orthogonal polynomials*, Amer. Math. Soc. Colloq. Publ., vol. 23, American Mathematical Society, Providence RI, 1939.
[38] G. Wagner, *On the product of distances to a point on the sphere*, J. Austral. Math. Soc. (A) **47** (1989), 466–482.
[39] G. Wagner, *On the means of distances on the surface of a sphere (lower bounds)*, Pacific J. Math. **144** (1990), 389–398.
[40] G. Wagner, *On averaging sets*, Monatsh. Math. **111** (1991), 69–78.
[41] G. Wagner, *On the means of distances on the surface of a sphere II (upper bounds)*, Pacific J. Math. **154** (1992), 381–396.
[42] G. Wagner, *On a new method for constructing good point sets on spheres*, Discrete Comput. Geom. **9** (1993), 111–129.

Department of Mathematics and Computer Science,, Georgia Southern University,, Postoffice Box 8093,, Statesboro, Georgia, 30460-8093,, USA

E-mail address: damelin@gsu.cs.gasou.edu

Institut für Mathematik A, Technische Universität Graz, Steyrergasse 30, 8010 Graz, Austria

E-mail address: peter.grabner@tugraz.at