

## OPTIMAL DISCRETE RIESZ ENERGY AND DISCREPANCY

JOHANN S. BRAUCHART

ABSTRACT. The Riesz  $s$ -energy of an  $N$ -point configuration in the Euclidean space  $\mathbb{R}^p$  is defined as the sum of reciprocal  $s$ -powers of all mutual distances in this system. In the limit  $s \rightarrow 0$  the Riesz  $s$ -potential  $1/r^s$  ( $r$  the Euclidean distance) governing the point interaction is replaced with the logarithmic potential  $\log(1/r)$ . In particular, we present a conjecture for the leading term of the asymptotic expansion of the optimal  $\mathbb{L}_2$ -discrepancy with respect to spherical caps on the unit sphere in  $\mathbb{R}^{d+1}$  which follows from Stolarsky's invariance principle [Proc. Amer. Math. Soc. 41 (1973)] and the fundamental conjecture for the first two terms of the asymptotic expansion of the optimal Riesz  $s$ -energy of  $N$  points as  $N \rightarrow \infty$ .

*Communicated by Oto Strauch*

### 1. The discrete Riesz $s$ -energy problem

The *Riesz  $s$ -energy* (real  $s \neq 0$ ) and the *logarithmic energy* ( $s = 0$ , by convention) of an  $N$ -point configuration  $X_N$  with points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  in the Euclidean space  $\mathbb{R}^p$  ( $p \geq 1$ ) are defined as

$$E_s(X_N) := \sum_{\substack{j=1 \\ j \neq k}}^N \sum_{k=1}^N \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|^s}, \quad E_0(X_N) := \sum_{\substack{j=1 \\ j \neq k}}^N \sum_{k=1}^N \log \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}.$$

The logarithmic energy can be understood as the limiting case  $s \rightarrow 0$ . For large  $s$  the nearest neighbor's interaction dominates and the other limiting case  $s \rightarrow \infty$  gives the *best-packing problem* (or *Tammes problem* [45]). Most deeply studied is the classical (*Newtonian*) case  $s = p - 2$  for the harmonic potential  $1/r^{p-2}$ ,

---

2000 Mathematics Subject Classification: Primary 11K38; Secondary 65D30, 31B15, 41A25.  
 Key words: Energy asymptotics, logarithmic energy, Riesz energy, spherical cap discrepancy, Stolarsky's invariance principle.  
 The author is recipient of an APART-fellowship of the Austrian Academy of Sciences conducted this research at UNSW (2010).

naturally with an abundance of literature in physics in the Coulomb case ( $p = 3$ ), where the Riesz  $s$ -energy essentially is the potential energy of an ensemble of (positive) unit point charges placed at the points of the configuration  $X_N$ .

For this note of interest are *sums of distances* (that is  $s = -1$ ) for points on the sphere  $\mathbb{S}^d$  because of the close connection to the spherical cap  $\mathbb{L}_2$ -discrepancy defined in Definition 3 by means of Stolarsky's invariance principle (Proposition 1) and to the worst-case error for equal weight quadrature formula for functions in the unit ball in a certain reproducing kernel Hilbert space over  $\mathbb{S}^d$  (cf. [11, 15]).

The  $N$ -point  $s$ -energy of an infinite compact set  $A \subseteq \mathbb{R}^p$  is defined as follows:

$$\begin{aligned} \mathcal{E}_s(A; N) &:= \sup \{E_s(\mathbf{x}_1, \dots, \mathbf{x}_N) : \mathbf{x}_1, \dots, \mathbf{x}_N \in A\} && \text{if } s < 0, \\ \mathcal{E}_s(A; N) &:= \inf \{E_s(\mathbf{x}_1, \dots, \mathbf{x}_N) : \mathbf{x}_1, \dots, \mathbf{x}_N \in A\} && \text{if } s \geq 0. \end{aligned}$$

It gives the optimal  $s$ -energy an  $N$ -point configuration  $X_N$  in  $A$  can assume; that is

$$\mathcal{E}_s(A; N) = E_s(X_N^{(s)}) \quad \text{for an optimal } s\text{-energy system } X_N^{(s)}.$$

Let  $d$  denote the Hausdorff dimension of  $A$ . When normalized appropriately (such that the total 'charge' of the  $N$ -point configuration is one) the quantity  $\mathcal{E}_s(A; N)/N^2$  remains finite (and has a limit as  $N \rightarrow \infty$ )<sup>1</sup> in the *potential-theoretical regime*  $s < d$  but grows beyond any bound in the *hypersingular case*  $s \geq d$ . In the regime  $s < d$  tools and result from classical potential theory (see, for example, Björck [7] ( $s < 0$ ), Saff and Totik [39] (logarithmic case) and Landkof [31]) are used to treat the limit  $N \rightarrow \infty$ . The limit distribution of optimal  $s$ -energy configurations is given by the (unique if  $-2 < s < d$ ) equilibrium (or extremal) measure  $\mu_A$  maximizing (if  $s < 0$ ) or minimizing (if  $s \geq 0$ ) the energy integral

$$\mathcal{I}_s[\mu] := \int \int k_s(\mathbf{x}, \mathbf{y}) \, d\mu(\mathbf{x}) \, d\mu(\mathbf{y}),$$

where  $k_s(\mathbf{x}, \mathbf{y}) := |\mathbf{x} - \mathbf{y}|^{-s}$  if  $s \neq 0$  and  $k_0(\mathbf{x}, \mathbf{y}) := -\log |\mathbf{x} - \mathbf{y}|$ , among all Borel probability measures  $\mu$  supported on  $A$ . The extremal quantity  $V_s(A) = \mathcal{I}_s[\mu_A]$  is called the  $s$ -energy of the set  $A$ .<sup>2</sup> If  $s \geq d$ , then  $\mathcal{I}_s[\mu] = +\infty$  for any measure  $\mu$  supported on  $A$ , that is  $V_s(A) = +\infty$ . In this case methods and results from geometrical measure theory are successfully used to gain more insight. One outcome is that other normalizations of the optimal  $s$ -energy would give a converging sequence for certain classes of compact sets (see, for example,

<sup>1</sup>Indeed, for example, for  $s > 0$  the sequence  $N(N-1)/\mathcal{E}_s(A; N)$  is monotone and bounded and converges to the 'generalized transfinite diameter of  $A$  of order  $s$ ' defined by Pólya and Szegő [37].

<sup>2</sup>For negative  $s$  the maximization problem is one particular instance of an extremal problem in distance geometry. We refer the reader to Alexander and Stolarsky [1].

Kuijlaars and Saff [30] and Hardin and Saff [26]). These results are the building blocks for the fundamental conjecture below.

The discrete Riesz energy problem is concerned with investigating properties of sequences of optimal (and nearly optimal) Riesz  $s$ -energy configurations. Questions concern (i) explicit computations of optimal configurations, (ii) limit distribution, (iii) asymptotic expansion of the optimal energy (cf. Smale's Problem #7 [42]), (iv) geometric properties ('well-separation', 'mesh'-norm). We refer the interested reader to the survey articles Saff and Kuijlaars [38] and Hardin and Saff [25].

Let  $\mathbb{S}^d$  denote the unit sphere in  $\mathbb{R}^{d+1}$ . The following long-standing open fundamental conjecture for the asymptotic expansion of the optimal Riesz  $s$ -energy is known. (In the upcoming paper [13] this conjecture and its history will be discussed in more detail.) Let  $\mathcal{H}_d$  denote the  $d$ -dimensional Hausdorff measure (normalized so that the  $d$ -dimensional unit cube in  $\mathbb{R}^p$  has measure 1).

**CONJECTURE 1** (Fundamental Conjecture). *Let  $d \geq 2$  and  $-2 < s < d + 2$  ( $s \neq 0, d$ ).<sup>3</sup> Then*

$$\mathcal{E}_s(\mathbb{S}^d; N) = V_s(\mathbb{S}^d) N^2 + \frac{C_{s,d}}{[\mathcal{H}_d(\mathbb{S}^d)]^{s/d}} N^{1+s/d} + \mathcal{R}_s(\mathbb{S}^d; N),$$

where  $\mathcal{R}_s(\mathbb{S}^d; N)/N^{1+s/d-\varepsilon} \rightarrow 0$  as  $N \rightarrow \infty$  for some  $\varepsilon > 0$  possibly depending on  $d$  and  $s$ .

This conjecture combines known results on the basis of the *principle of analytic continuation*:

- In the potential-theoretical regime  $-2 < s < d$  ( $s \neq 0$ ) the dominant term grows like  $N^2$  and the coefficient is given by the  $s$ -energy of the unit sphere

$$V_s(\mathbb{S}^d) = 2^{d-s-1} \frac{\Gamma((d+1)/2) \Gamma((d-s)/2)}{\sqrt{\pi} \Gamma(d-s/2)}, \quad -2 < s < d (s \neq 0). \quad (1)$$

For other values of  $s$  it is understood to be the analytic continuation of the right-hand side above to the complex  $s$ -plane except at the simple poles at  $s = d, d+2, \dots, 2d-2$  (finitely many) if  $d$  is even and at  $s = d, d+2, d+4, \dots$  (infinitely many) if  $d$  is odd.

- In the hyper-singular case  $s > d$  the leading term behaves like  $N^{1+s/d}$  and it is shown by Kuijlaars and Saff [30] that the limit  $\mathcal{E}_s(\mathbb{S}^d; N)/N^{1+s/d}$  exists.<sup>4</sup> It is believed that the constant  $C_{s,d}$  can be analytically continued

<sup>3</sup>For  $s < -2$  the extremal distribution is concentrated in no more than  $d+1$  points on  $\mathbb{S}^d$  ([7]).

<sup>4</sup>The existence of this limit is proven for the class of rectifiable  $d$ -dimensional manifolds in [26] and for weighted Riesz  $s$ -energy for rectifiable  $d$ -dimensional sets in [8].

to the  $s$ -plane, which is supported by the conjecture for its value in case of  $d = 2$  also provided in [30].

- In the boundary case  $s = d$  [30] gives that ( $\mathbb{B}^d$  denotes the unit ball in  $\mathbb{R}^d$ )

$$\mathcal{E}_d(\mathbb{S}^d; N) \sim \frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)} N^2 \log N \quad \text{as } N \rightarrow \infty,$$

which can be also understood by means of a limit process  $s \rightarrow d$  assuming that the poles of  $V_s(\mathbb{S}^d)$  and  $C_{s,d}$  at  $s = d$  cancel each other. (Obviously, one can also consider limit processes  $s \rightarrow s'$ , where  $s'$  is a pole of  $V_s$ . In such a case one would gain information about the singularity at  $s = s'$  of the coefficient of the corresponding term in the asymptotic expansion of the optimal  $s$ -energy ( $s$  near  $s'$ ) provided this lesser-order term exists. The limit process  $s \rightarrow 0$  connects the asymptotic expansion of the optimal logarithmic energy and optimal  $s$ -energy for  $s$  near 0.)

The constant  $\mathcal{H}_d(\mathbb{B}^d)/\mathcal{H}_d(\mathbb{S}^d)$  is the ratio of the volume of the unit ball  $\mathbb{B}^d$  in  $\mathbb{R}^d$  and the surface area of  $\mathbb{S}^d$  (denoted by  $\omega_d$ ) and can be expressed in terms of a ratio of surface areas or a ratio of gamma functions

$$\frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)} = \frac{1}{d} \frac{\omega_{d-1}}{\omega_d} = \frac{1}{d} \frac{\Gamma((d+1)/2)}{\sqrt{\pi} \Gamma(d/2)} \sim \frac{1}{\sqrt{2\pi}} d^{-1/2} \quad (\text{as } d \rightarrow \infty). \quad (2)$$

It is a long-standing open problem what the precise value of the constant

$$C_{s,d} = \lim_{N \rightarrow \infty} \mathcal{E}_s([0, 1]^d; N) / N^{1+s/d} \quad (3)$$

is for  $d \geq 2$ . (In the case  $d = 1$  Martínez-Finkelshtein et al. showed that  $C_{s,1} = 2\zeta(s)$ , where  $\zeta(s)$  is the Riemann zeta function.) The significance of the constant  $C_{s,d}$  follows from the fact that the limit  $\lim_{s \rightarrow \infty} [C_{s,d}]^{1/s}$  can be expressed in terms of the 'largest sphere packing density' in  $\mathbb{R}^d$ , which is only known in three cases:  $d = 1, 2$  and  $d = 3$  (Kepler conjecture, rather recently proved by Hales [24]). For  $d = 2$  Kuijlaars and Saff [30] obtained the estimate

$$\limsup_{N \rightarrow \infty} \frac{\mathcal{E}_s(\mathbb{S}^2; N)}{N^{1+s/2}} \leq \frac{(\sqrt{3}/2)^{s/2} \zeta_\Lambda(s)}{(4\pi)^{s/2}}, \quad s > 2,$$

and they conjecture that equality holds above; that is:

**CONJECTURE 2** (Kuijlaars and Saff [30]). *For  $s > 2$ ,  $C_{s,2} = (\sqrt{3}/2)^{s/2} \zeta_\Lambda(s)$ .*

The function  $\zeta_\Lambda(s)$  is the zeta function of the hexagonal lattice

$$\Lambda := \{m(1, 0) + n(1/2, \sqrt{3}/2) : m, n \in \mathbb{Z}\},$$

which was used in [30] to locally approximate a minimal  $s$ -energy configuration on the sphere in the hypersingular case  $s > 2$ . For  $\operatorname{Re} s > 2$  it is defined as

$$\zeta_\Lambda(s) = \sum_{\mathbf{0} \neq \mathbf{a} \in \Lambda} \frac{1}{|\mathbf{a}|^s} = \sum_{(m,n) \in \mathbb{Z}^2 \setminus \{(0,0)\}} \frac{1}{(m^2 + mn + n^2)^{s/2}}$$

and it is understood that  $\zeta_\Lambda(s)$  is the meromorphic extension to  $\mathbb{C}$  of the right-hand side above. The function  $\zeta_\Lambda(s)$  admits a factorization (cf., for example, [16, Chapter X, Section 7])

$$\zeta_\Lambda(s) = 6 \zeta(s/2) L_{-3}(s/2), \quad \operatorname{Re} s > 2, \tag{4}$$

into a product of the Riemann zeta function  $\zeta$  and the first negative primitive Dirichlet L-Series

$$L_{-3}(s) := 1 - \frac{1}{2^s} + \frac{1}{4^s} - \frac{1}{5^s} + \frac{1}{7^s} - \dots, \quad \operatorname{Re} s > 1. \tag{5}$$

Interestingly, it is assumed in physics that a hexagonal configuration has lowest potential energy but there seems to be no mathematical proof for this. However, it is known that the hexagonal lattice is (even universal) optimal among all lattices in  $\mathbb{R}^2$ , see Montgomery [34] and Cohn and Kumar [17].

## 2. Uniform Distribution and Discrepancy

Let  $\sigma_d$  denotes the normalized surface area measure on  $\mathbb{S}^d$ .

**DEFINITION 1.** A sequence  $\{X_N\}$  is *asymptotically uniformly distributed on  $\mathbb{S}^d$*  if

$$\lim_{N \rightarrow \infty} \frac{\#\{k : \mathbf{x}_{k,N} \in B\}}{N} = \sigma_d(B)$$

for every  $\sigma_d$ -measurable clopen set  $B$  in  $\mathbb{S}^d$ .

Informally speaking: a reasonable test set gets a fair share of points as  $N$  becomes large.

The quality of a sequence  $\{X_N\}$  of  $N$ -point systems can be quantified using the discrepancy

$$D(\mathcal{F}; \mathbf{x}_1, \dots, \mathbf{x}_N) := \sup_{B \in \mathcal{F}} \left| \frac{\#\{k : \mathbf{x}_k \in B\}}{N} - \sigma_d(B) \right|$$

measuring the maximum deviation between the uniform measure (limit distribution of optimal configurations) and empirical point distribution with respect to a family  $\mathcal{F}$  of test sets (for example spherical caps). The *spherical cap discrepancy* of an  $N$ -point configuration  $X_N$  will be denoted by  $D_C(X_N)$ .

A different approach to uniform distribution makes use of numerical integration and function spaces. Let

$$I[f] := \int_{\mathbb{S}^d} f \, d\sigma_d, \quad Q_N[f] := \frac{1}{N} \sum_{k=1}^N f(\mathbf{x}_k).$$

**DEFINITION 2.**  $\{X_N\}$  is *equi-distributed with respect to every function in the space of continuous functions* if <sup>5</sup>

$$\lim_{N \rightarrow \infty} Q_N[f] = I[f] \quad \text{for every } f \in C(\mathbb{S}^d).$$

As it is well-known both Definitions 1 and 2 are equivalent.

On the sphere one has no satisfactory analogue to the celebrated Koksma-Hlawka inequality in the unit cube. Cui and Freeden [18] introduced the concept of *generalized discrepancy on  $\mathbb{S}^2$*  based on pseudo-differential operators. For a particular choice  $\mathbf{D}$  they obtained a *Koksma-Hlawka* like inequality

$$|Q_N[f] - I[f]| \leq \sqrt{6} D_{\text{CF}}(X_N) \|f\|_{\mathbb{H}^{3/2}(\mathbb{S}^2)},$$

where  $f$  is from a certain Sobolev space  $\mathbb{H}^{3/2}(\mathbb{S}^2)$  whose reproducing kernel is defined using  $\mathbf{D}$ . In this context, a sequence  $\{X_N\}$  of  $N$ -point systems is called  *$\mathbf{D}$ -equidistributed with respect to all functions in  $\mathbb{H}^{3/2}(\mathbb{S}^2)$*  if  $\lim_{N \rightarrow \infty} D_{\text{CF}}(X_N) = 0$ . Moreover, the generalized discrepancy associated with  $\mathbf{D}$  has a closed form expressible in terms of elementary functions

$$4\pi [D_{\text{CF}}(X_N)]^2 = 1 - \frac{1}{N^2} \sum_{j,k=1}^N \log(1 + |\mathbf{x}_j - \mathbf{x}_k|/2)^2.$$

(Sloan and Womersley [41] showed that  $[D_{\text{CF}}(X_N)]^2$  has a natural interpretation as the worst-case error for  $Q_N$  for function from the unit ball in  $\mathbb{H}^{3/2}(\mathbb{S}^2)$  provided with a norm which is equivalent to the one used by Cui and Freeden.) This approach is followed further in [15] leading to the generalized discrepancy

$$[D(X_N)]^2 = \frac{4}{3} - \frac{1}{N^2} \sum_{k,\ell=1}^N |\mathbf{x}_\ell - \mathbf{x}_k| \tag{6}$$

associated with the Sobolev space  $\mathbb{H}^{3/2}(\mathbb{S}^2)$  with the reproducing kernel

$$K(\mathbf{x}, \mathbf{y}) = (8/3) - |\mathbf{x} - \mathbf{y}|.$$

---

<sup>5</sup> That is, the discrete probability measure associated with  $X_N$  tends to  $\sigma_d$  as  $N \rightarrow \infty$  (in the weak-\* limit).

### 3. The spherical cap $\mathbb{L}_2$ -discrepancy on $\mathbb{S}^d$

A spherical cap on  $\mathbb{S}^d$  centered at  $\mathbf{x} \in \mathbb{S}^d$  is the set

$$C(\mathbf{x}; t) := \{ \mathbf{y} \in \mathbb{S}^d : \langle \mathbf{x}, \mathbf{y} \rangle \geq t \},$$

where  $\langle \cdot, \cdot \rangle$  denotes the usual inner product. The family of all spherical caps on  $\mathbb{S}^d$  forms a *discrepancy system* (see [21]) giving rise to the notion of *asymptotic uniform distribution*

**DEFINITION 3.** The *spherical cap  $\mathbb{L}_2$ -discrepancy* of an  $N$ -point configuration  $X_N$  on  $\mathbb{S}^d$  is given by

$$D_C^{\mathbb{L}_2}(X_N) := \left[ \int_{-1}^1 \int_{\mathbb{S}^d} \left| \frac{|X_N \cap C(\mathbf{x}, t)|}{N} - \sigma_d(C(\mathbf{x}, t)) \right|^2 d\sigma_d(\mathbf{x}) dt \right]^{1/2}.$$

The *optimal  $\mathbb{L}_2$ -discrepancy* of  $N$ -point configurations on  $\mathbb{S}^d$  is denoted by

$$D_C^{\mathbb{L}_2}(\mathbb{S}^d; N) := \inf \left\{ D_C^{\mathbb{L}_2}(X_N) : X_N \subseteq \mathbb{S}^d \right\}.$$

An obvious upper bound of the  $\mathbb{L}_2$ -discrepancy is in terms of the spherical cap discrepancy:

$$D_C^{\mathbb{L}_2}(X_N) \leq \sqrt{2} D_C(X_N), \quad X_N \subseteq \mathbb{S}^d.$$

The next result connects the sum of distances, the  $\mathbb{L}_2$ -discrepancy and the distance integral.

**PROPOSITION 1** (Stolarsky's invariance principle [43]). <sup>6</sup> *Let  $d \geq 2$ . Then for any  $N$ -point configuration  $X_N$  on  $\mathbb{S}^d$ :*

$$\frac{1}{N^2} \sum_{j,k=1}^N |\mathbf{x}_j - \mathbf{x}_k| + \frac{\mathcal{H}_d(\mathbb{S}^d)}{\mathcal{H}_d(\mathbb{B}^d)} \left[ D_C^{\mathbb{L}_2}(X_N) \right]^2 = \int \int |\mathbf{x} - \mathbf{x}'| d\sigma_d(\mathbf{x}) d\sigma_d(\mathbf{x}').$$

Clearly, reduction of the  $\mathbb{L}_2$ -discrepancy means increase of the sum of distances and vice versa.

Stolarsky's invariance principle provides a simple way to compute the  $\mathbb{L}_2$ -discrepancy of a given  $N$ -point configuration on  $\mathbb{S}^d$ . In the language of the discrete energy problem we have

$$\begin{aligned} \frac{\mathcal{H}_d(\mathbb{S}^d)}{\mathcal{H}_d(\mathbb{B}^d)} \left[ D_C^{\mathbb{L}_2}(X_N) \right]^2 &= V_{-1}(\mathbb{S}^d) - \frac{1}{N^2} \sum_{j,k=1}^N |\mathbf{x}_j - \mathbf{x}_k| \\ &= - [E_{-1}(X_N) - V_{-1}(\mathbb{S}^d) N^2] / N^2. \end{aligned} \tag{7}$$

---

<sup>6</sup>The given version is a special case of the result in [43] which is extended in [9].

Evidently, the square of the optimal  $\mathbb{L}_2$ -discrepancy is closely related to the second term of the asymptotic expansion of the optimal Riesz  $(-1)$ -energy, cf. Conjecture 1. This connection between the spherical cap ( $\mathbb{L}_2$ -)discrepancy and the second term in the asymptotic expansion of the  $s$ -energy is exploited in [10], Grabner and Damelin [19].

The  $\mathbb{L}_2$ -discrepancy of an  $N$ -point configuration  $X_N$  is minimal if and only if the sum of distances of  $X_N$  is maximal. Thus, optimal  $\mathbb{L}_2$ -discrepancy configurations are, in fact, maximal sum-of-distance configurations or, equivalently, maximal Riesz  $(-1)$ -energy configurations. Such configurations can be generated using numerical optimization which is a highly non-linear process.

Stolarsky used his invariance principle and discrepancy results of Schmidt [40] on the discrepancy of spherical caps to estimate the difference

$$\int \int |\mathbf{x} - \mathbf{x}'| \, d\sigma_d(\mathbf{x}) \, d\sigma_d(\mathbf{x}') - \frac{\mathcal{E}_{-1}(\mathbb{S}^d; N)}{N^2}$$

and obtained the correct order of  $N$  for the upper bound. Harman [27] improved the lower bound (for the general invariance principle) and, finally, Beck [4] obtained the correct order of  $N$  for the Euclidean metric. By means of the invariance principle these bound for the energy difference translate into bounds for the spherical cap  $\mathbb{L}_2$ -discrepancy.

**PROPOSITION 2.** *Let  $d \geq 2$ . There exist constants  $c', C' > 0$  such that for sufficiently large  $N$*

$$c' N^{-1/2-1/(2d)} \leq D_C^{\mathbb{L}_2}(\mathbb{S}^d; N) \leq C' N^{-1/2-1/(2d)}.$$

*Remark.* By Proposition 2 the correct order of the decay of the optimal  $\mathbb{L}_2$ -discrepancy on  $\mathbb{S}^d$  in terms of powers of the number of points  $N$  is  $N^{-1/2-1/(2d)}$  which is the same rate (apart from the  $\sqrt{\log N}$  term in the upper bound) as for the optimal spherical discrepancy on  $\mathbb{S}^d$ .

Proposition 2 rises the question if  $D_C^{\mathbb{L}_2}(\mathbb{S}^d; N) N^{1/2+1/(2d)}$  has a limit as  $N \rightarrow \infty$ . By employing the connection to the discrete Riesz  $s$ -energy problem, where one has conjectures regarding the asymptotic expansion of the optimal  $s$ -energy, we derive the following conjectures for the leading term in the asymptotic expansion of the optimal  $\mathbb{L}_2$ -discrepancy.

**CONJECTURE 3.** *Let  $d \geq 2$ . If Conjecture 1 holds, then*

$$D_C^{\mathbb{L}_2}(\mathbb{S}^d; N) \sim A_d N^{-1/2-1/(2d)} + \dots \quad \text{as } N \rightarrow \infty,$$

where

$$A_d := \sqrt{\frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)} \frac{-C_{-1,d}}{[\mathcal{H}_d(\mathbb{S}^d)]^{-1/d}}}. \tag{8}$$

Justification. By Stolarsky's invariance principle (Prop. 1 and Eq. (7))

$$\frac{\mathcal{H}_d(\mathbb{S}^d)}{\mathcal{H}_d(\mathbb{B}^d)} \left[ D_C^{\mathbb{L}^2}(\mathbb{S}^d; N) \right]^2 = - \left[ \mathcal{E}_{-1}(\mathbb{S}^d; N) - V_{-1}(\mathbb{S}^d) N^2 \right] / N^2.$$

Application of the fundamental Conjecture 1 yields

$$\frac{\mathcal{H}_d(\mathbb{S}^d)}{\mathcal{H}_d(\mathbb{B}^d)} \left[ D_C^{\mathbb{L}^2}(\mathbb{S}^d; N) \right]^2 = \frac{-C_{-1,d}}{[\mathcal{H}_d(\mathbb{S}^d)]^{-1/d}} N^{-1-1/d} - \mathcal{R}_{-1}(\mathbb{S}^d; N) / N^2.$$

The conjecture follows. □

For the unit sphere  $\mathbb{S}^2$  one can make the conjecture more precise.

**CONJECTURE 4.** *If Conjectures 1 and 2 hold, then*

$$D_C^{\mathbb{L}^2}(\mathbb{S}^2; N) \sim A_2 N^{-1/2-1/(2d)} + \dots \quad \text{as } N \rightarrow \infty,$$

where

$$A_2 = \sqrt{\frac{3}{2} \left( \frac{8\pi}{\sqrt{3}} \right)^{1/2} [-\zeta(-1/2)] L_{-3}(-1/2)} = 0.44679728350408 \dots$$

Justification. Since  $\mathcal{H}_d(\mathbb{S}^d) = \omega_2 = 4\pi$  and (by (2))

$$\left. \frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)} \right|_{d=2} = \frac{1}{2} \frac{\Gamma(3/2)}{\sqrt{\pi} \Gamma(1)} = \frac{1}{4},$$

one obtains (using Conjecture 2 and relations (4) and (8))

$$\begin{aligned} A_2 &= \sqrt{\frac{1}{4} \frac{-C_{-1,2}}{(4\pi)^{-1/2}}} = \sqrt{\frac{1}{4} \left( \sqrt{3}/2 \right)^{-1/2} \frac{-6 \zeta(-1/2) L_{-3}(-1/2)}{(4\pi)^{-1/2}}} \\ &= \sqrt{\frac{3}{2} \left( \frac{8\pi}{\sqrt{3}} \right)^{1/2} [-\zeta(-1/2)] L_{-3}(-1/2)} = 0.44679728350408 \dots \end{aligned}$$

□

**The case  $d = 1$**

Stolarsky' invariance principle also holds for  $d = 1$  as one can see from the proof given in [11]. In this case one has (cf. Eq.s (1) and (2))

$$\frac{1}{N^2} \sum_{j,k=1}^N |\mathbf{x}_j - \mathbf{x}_k| + \frac{1}{\pi} \left[ D_C^{\mathbb{L}^2}(X_N) \right]^2 = \frac{4}{\pi}, \quad X_N \subseteq \mathbb{S}^1.$$

On the other hand (in joint work with Hardin and Saff) [14] we obtained a complete asymptotic expansion of the Riesz  $s$ -energy  $\mathcal{L}_s(N)$  of the  $N$ th roots

of unity which represent optimal  $N$ -point configurations for  $s > -2$ . In general, for  $s \in \mathbb{C}$  with  $s \neq 0, 1, 3, \dots$

$$\begin{aligned} \mathcal{L}_s(N) &= V_s(\mathbb{S}) N^2 + \frac{2\zeta(s)}{(2\pi)^s} N^{1+s} + \frac{2}{(2\pi)^s} \sum_{n=1}^p \alpha_n(s) \zeta(s-2n) N^{1+s-2n} \\ &\quad + \mathcal{O}(N^{-1+\operatorname{Re} s-2p}). \end{aligned}$$

The coefficients  $\alpha_n(s)$ ,  $n \geq 0$ , satisfy the generating function relation

$$\left( \frac{\sin \pi z}{\pi z} \right)^{-s} = \sum_{n=0}^{\infty} \alpha_n(s) z^{2n}, \quad |z| < 1, \quad s \in \mathbb{C}.$$

It follows that

$$\begin{aligned} \frac{1}{\pi} \left[ D_C^{\mathbb{L}^2}(X_N) \right]^2 &= \frac{2[-\zeta(-1)]}{(2\pi)^{-1}} N^{-2} + \frac{2}{(2\pi)^{-1}} \sum_{n=1}^{p-1} \alpha_n(-1) \zeta(-1-2n) N^{-2-2n} \\ &\quad + \mathcal{O}(N^{-2-2p}), \end{aligned}$$

where  $(B_0 = 1, B_1 = -1/2, \dots)$  are *Bernoulli numbers* and  $(-1)^{n+1} B_{2n} > 0$ )

$$\alpha_n(-1) \zeta(-1-2n) = \frac{(-1)^{n+1} B_{2(n+1)}}{(2(n+1))!} \pi^{2n} < 0, \quad n \geq 1.$$

In the last step it was used that the Riemann zeta function at negative integers can be expressed in terms of Bernoulli numbers.

## Numeric Results

Recently, in joint work with Josef Dick we investigated the properties of so-called digital nets (see Niederreiter [36] and Dick and Pillichshammer [20]) lifted to the sphere by means of an area preserving map. Numerical experiments for Sobol' Sequences lifted to  $\mathbb{S}^2$  in [12] suggest that the order of  $N$  is optimal but the constant seems to be too large (in the range  $[0.50, 0.59]$  for  $N = 2^m$ ,  $m = 1, \dots, 20$ ). (Optimal  $(-1)$ -energy configurations are more difficult to come by and the number of points for which numerical optimization is feasible and the result could be trusted to be the global maximum is very limited. Cf. [3, 5, 6] and references cited therein. Recently, Hou and Shao [28] showed by means of a computer-assisted proof the conjecture that a 5-point configuration forming a double pyramid has optimal  $(-1)$ -energy using interval methods and related techniques.)

#### 4. Estimating the spherical cap discrepancy

The classical *Erdős-Turán type inequality* (cf. Grabner [23], also cf. Li and Vaaler [33]) estimate the spherical cap discrepancy in terms of Weyl sums. Recently, by generalizing LeVeques result for the unit circle [32], Narcowich et al. [35] obtained *LeVeque type inequalities* on the sphere:

$$c_1 \left[ \sum_{\ell=1}^{\infty} a_{\ell} \sum_{m=1}^{Z(d,\ell)} \left| \frac{1}{N} \sum_{j=0}^{N-1} Y_{\ell,m}(\mathbf{x}_j) \right|^2 \right]^{1/2} \leq D_C(X_N) \\ \leq c_2 \left[ \sum_{\ell=1}^{\infty} b_{\ell} \sum_{m=1}^{Z(d,\ell)} \left| \frac{1}{N} \sum_{j=0}^{N-1} Y_{\ell,m}(\mathbf{x}_j) \right|^2 \right]^{1/(d+2)},$$

where  $a_{\ell} := \Gamma(\ell - 1/2)/\Gamma(\ell + d + 1/2) \asymp 1/\ell^{d+1} =: b_{\ell}$  for some positive constant  $c_1$  and  $c_2$  and  $Z(d, n)$  denotes the number of linearly independent real spherical harmonics  $Y_{\ell,m}$  of degree  $\ell$ . In Sun and Chen [44] 'spherical basis functions' (as a counter part to radial basis function on spheres utilized in [35]) are used to investigate uniform distribution on spheres.

G. Wagner obtained ground-breaking results concerning estimates of the Riesz  $s$ -energy and explored connections between  $s$ -energy and discrepancy (see [46, 47, 48]). In fact, the proofs of both the Erdős-Turán type inequality and the LeVeque type inequality can be modified yielding estimates of the spherical cap discrepancy in terms of  $s$ -energy. A different approach exploits the connection between the error of numerical integration for polynomials (cf. Damelin and Grabner [19]) and, by utilizing a result of Andrievskii, Blatt and Götz [2] (see this author [10]).

We close this note by recalling that optimal Riesz  $s$ -energy configurations may not have optimal spherical cap discrepancy (essentially of order  $\mathcal{O}(N^{-1/2-1/(2d)})$ , see Beck [4]) which is reflected in Korevaar's conjecture [29] claiming for the harmonic case  $s = d - 1$  that the spherical cap discrepancy is of order  $\mathcal{O}(N^{-1/d})$ . This was essentially proved by Götz [22]. He also showed that the bound is sharp for  $d = 2$ . The conjecture is still open for other values of  $s$  and  $d$ .

**Acknowledgement:** The author is grateful to the School of Mathematics and Statistics at UNSW for their support.

## REFERENCES

- [1] R. ALEXANDER AND K. B. STOLARSKY: *Extremal problems of distance geometry related to energy integrals*, Trans. Amer. Math. Soc. **193** (1974), pages 1–31.
- [2] V. V. ANDRIEVSKII, H.-P. BLATT, AND M. GÖTZ: *Discrepancy estimates on the sphere*, Monatsh. Math. **128** (1999), no. 3, pages 179–188.
- [3] B. BALLINGER, G. BLEKHERMAN, H. COHN, N. GIANIRACUSA, E. KELLY, AND A. SCHÜRMAN: *Experimental study of energy-minimizing point configurations on spheres*, Experiment. Math. **18** (2009), no. 3, pages 257–283.
- [4] J. BECK: *Sums of distances between points on a sphere—an application of the theory of irregularities of distribution to discrete geometry*, Mathematika **31** (1984), no. 1, pages 33–41.
- [5] E. BENDITO, A. CARMONA, A. M. ENCINAS, J. M. GESTO, A. GÓMEZ, C. MOURIÑO, AND M. T. SÁNCHEZ: *Computational cost of the Fekete problem. I. The forces method on the 2-sphere*, J. Comput. Phys. **228** (2009), no. 9, pages 3288–3306.
- [6] M. K. BERKENBUSCH, I. CLAUS, C. DUNN, L. P. KADANOFF, M. NICEWICZ, AND S. C. VENKATARAMANI: *Discrete charges on a two dimensional conductor*, J. Statist. Phys. **116** (2004), pages 1301–1358.
- [7] G. BJÖRCK: *Distributions of positive mass, which maximize a certain generalized energy integral*, Ark. Mat. **3** (1956), pages 255–269.
- [8] S. V. BORODACHOV, D. P. HARDIN, AND E. B. SAFF: *Asymptotics for discrete weighted minimal Riesz energy problems on rectifiable sets*, Trans. Amer. Math. Soc. **360** (2008), no. 3, pages 1559–1580.
- [9] J. S. BRAUCHART: *Note on a generalized invariance principle and its relevance for cap discrepancy and energy*, in Modern developments in multivariate approximation, vol. 145 of Internat. Ser. Numer. Math., Birkhäuser, Basel, 2003, pages 41–55.
- [10] J. S. BRAUCHART: *Optimal logarithmic energy points on the unit sphere*, Math. Comp. **77** (2008), no. 263, pages 1599–1613.
- [11] J. S. BRAUCHART AND J. DICK: *A simple Proof of Stolarsky’s Invariance Principle*. arXiv:1101.4448v1 [math.NA]; accepted by Proc. Amer. Math. Soc., 2011.
- [12] J. S. BRAUCHART AND J. DICK: *Quasi-Monte Carlo rules for numerical integration over the unit sphere  $S^2$* . arXiv:1101.5450v1 [math.NA]; accepted by Numerische Mathematik, 2011.
- [13] J. S. BRAUCHART, D. P. HARDIN, AND E. B. SAFF: *The next-order term for optimal logarithmic and Riesz energy on the unit sphere*. Manuscript: 35 pages.
- [14] J. S. BRAUCHART, D. P. HARDIN, AND E. B. SAFF: *The Riesz energy of the  $N$ th roots of unity: an asymptotic expansion for large  $N$* , Bull. Lond. Math. Soc. **41** (2009), no. 4, pages 621–633.
- [15] J. S. BRAUCHART AND R. S. WOMERSLEY: *Numerical integration over the unit sphere,  $L_2$ -discrepancy and sum of distances*. Manuscript: 27 pages.
- [16] H. COHN: *Advanced number theory*, Dover Publications Inc., New York, 1980. Reprint of *A second course in number theory*, 1962, Dover Books on Advanced Mathematics.
- [17] H. COHN AND A. KUMAR: *Universally optimal distribution of points on spheres*, J. Amer. Math. Soc. **20** (2007), no. 1, pages 99–148.
- [18] J. CUI AND W. FREEDEN: *Equidistribution on the sphere*, SIAM J. Sci. Comput. **18** (1997), no. 2, pages 595–609.

OPTIMAL DISCRETE RIESZ ENERGY AND DISCREPANCY

- [19] S. B. DAMELIN AND P. J. GRABNER: *Energy functionals, numerical integration and asymptotic equidistribution on the sphere*, J. Complexity **19** (2003), no. 3, pages 231–246. Numerical integration and its complexity (Oberwolfach, 2001).
- [20] J. DICK AND F. PILLICHSHAMMER: *Digital Nets and Sequences. Discrepancy Theory and Quasi-Monte Carlo Integration*, Cambridge University Press, Cambridge, 2010.
- [21] M. DRMOTA AND R. TICHY: *Sequences, discrepancies and applications*, vol. 1651 of Lecture Notes in Mathematics, Springer-Verlag, Berlin, 1997.
- [22] M. GÖTZ: *On the distribution of weighted extremal points on a surface in  $\mathbf{R}^d$ ,  $d \geq 3$* , Potential Anal. **13** (2000), no. 4, pages 345–359.
- [23] P. J. GRABNER: *Erdős-Turán type discrepancy bounds*, Monatsh. Math. **111** (1991), no. 2, pages 127–135.
- [24] T. C. HALES: *A proof of the Kepler conjecture*, Ann. of Math. (2) **162** (2005), no. 3, pages 1065–1185.
- [25] D. P. HARDIN AND E. B. SAFF: *Discretizing manifolds via minimum energy points*, Notices Amer. Math. Soc. **51** (2004), no. 10, pages 1186–1194.
- [26] D. P. HARDIN AND E. B. SAFF: *Minimal Riesz energy point configurations for rectifiable  $d$ -dimensional manifolds*, Adv. Math. **193** (2005), no. 1, pages 174–204.
- [27] G. HARMAN: *Sums of distances between points of a sphere*, Internat. J. Math. Math. Sci. **5** (1982), no. 4, pages 707–714.
- [28] X. HOU AND J. SHAO, *Spherical distribution of 5 points with maximal distance sum*, Discrete Comput. Geom. **46** (2011), no. 1, pp. 156–174.
- [29] J. KOREVAAR: *Fekete extreme points and related problems*, in Approximation theory and function series (Budapest, 1995), vol. 5 of Bolyai Soc. Math. Stud., János Bolyai Math. Soc., Budapest, 1996, pages 35–62.
- [30] A. B. J. KUIJLAARS AND E. B. SAFF: *Asymptotics for minimal discrete energy on the sphere*, Trans. Amer. Math. Soc. **350** (1998), no. 2, pages 523–538.
- [31] N. S. LANDKOF: *Foundations of modern potential theory*, Springer-Verlag, New York, 1972. Translated from the Russian by A. P. Doohovskoy, Die Grundlehren der mathematischen Wissenschaften, Band 180.
- [32] W. J. LEVEQUE: *An inequality connected with Weyl’s criterion for uniform distribution*, in Proc. Sympos. Pure Math., Vol. VIII, Amer. Math. Soc., Providence, R.I., 1965, pages 22–30.
- [33] X.-J. LI AND J. D. VAALER: *Some trigonometric extremal functions and the Erdős-Turán type inequalities*, Indiana Univ. Math. J. **48** (1999), no. 1, pages 183–236.
- [34] H. L. MONTGOMERY: *Minimal theta functions*, Glasgow Math. J. **30** (1988), no. 1, pages 75–85.
- [35] F. J. NARCOWICH, X. SUN, J. D. WARD, AND Z. WU: *Leveque type inequalities and discrepancy estimates for minimal energy configurations on spheres*, J. Approx. Theory **162** (2010), no. 6, pages 1256–1278.
- [36] H. NIEDERREITER: *Low-discrepancy and low-dispersion sequences*, J. Number Theory **30** (1988), no. 1, pages 51–70.
- [37] G. PÓLYA AND G. SZEGŐ: *Über den transfiniten Durchmesser (Kapazitätskonstante) von ebenen und räumlichen Punktmengen.*, J. Reine Angew. Math. **165** (1931), pages 4–49.
- [38] E. B. SAFF AND A. B. J. KUIJLAARS: *Distributing many points on a sphere*, Math. Intelligencer **19** (1997), no. 1, pages 5–11.

J. S. BRAUCHART

- [39] E. B. SAFF AND V. TOTIK: *Logarithmic potentials with external fields*, vol. 316 of Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences], Springer-Verlag, Berlin, 1997. Appendix B by Thomas Bloom.
- [40] W. M. SCHMIDT: *Irregularities of distribution. IV*, Invent. Math. **7** (1969), pages 55–82.
- [41] I. H. SLOAN AND R. S. WOMERSLEY: *Extremal systems of points and numerical integration on the sphere*, Adv. Comput. Math. **21** (2004), no. 1–2, pages 107–125.
- [42] S. SMALE: *Mathematical problems for the next century*, Math. Intelligencer **20** (1998), no. 2, pages 7–15.
- [43] K. B. STOLARSKY: *Sums of distances between points on a sphere. II*, Proc. Amer. Math. Soc. **41** (1973), pages 575–582.
- [44] X. SUN AND Z. CHEN: *Spherical basis functions and uniform distribution of points on spheres*, J. Approx. Theory **151** (2008), no. 2, pages 186–207.
- [45] P. M. L. TAMMES: *On the origin of number and arrangement of places of exit on the surface of pollen grains*, Recueil des Travaux Botanique Neerlandais **27** (1930), pages 1–84.
- [46] G. WAGNER: *On means of distances on the surface of a sphere (lower bounds)*, Pacific J. Math. **144** (1990), no. 2, pages 389–398.
- [47] G. WAGNER: *Erdős-Turán inequalities for distance functions on spheres*, Michigan Math. J. **39** (1992), no. 1, pages 17–34.
- [48] G. WAGNER: *On means of distances on the surface of a sphere. II. Upper bounds*, Pacific J. Math. **154** (1992), no. 2, pages 381–396.

Received February 15, 2011  
Accepted November 12, 2011

**Johann S. Brauchart**  
*School of Mathematics and Statistics,  
University of New South Wales,  
Sydney, NSW, 2052,  
Australia*  
*E-mail: j.brauchart@unsw.edu.au*