Distributing many points on spheres: minimal energy and designs

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Abstract

This survey is devoted to the discussion of recent developments in the context of spherical designs and minimal energy point configurations on spheres. The recent solution of the long standing problem of the existence of spherical t-designs on $\mathbb{S}^d$ with $\mathcal{O}(t^d)$ number of points by A. Bondarenko, D. Radchenko, and M. Viazovska attracted new interest to this subject. Secondly, D. P. Hardin and E. B. Saff could prove that point sets minimising the discrete Riesz energy on $\mathbb{S}^d$ in the hypersingular case are asymptotically uniformly distributed. Both results are of great relevance to the problem of describing the quality of point distributions on $\mathbb{S}^d$, as well as finding point sets, which exhibit good distribution behaviour with respect to various quality measures.

Dedicated to Edward B. Saff on the occasion of his 70$^{\text{th}}$ birthday

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1. Introduction

Distributing a large number N of points *evenly* on the unit sphere

$$\mathbb{S}^d := \left\{\mathbf{x} \in \mathbb{R}^{d+1} \mid \|\mathbf{x}\| = 1\right\}$$

is a problem that occurs in several applications. The most prominent applications are in numerical integration, approximation, interpolation, and sampling.

Numerical computation of integrals over multidimensional domains is usually done by weighted sums of point evaluations of the function f to be integrated. Since the sphere is a domain with very high symmetry, it is preferable to use equal weight integration methods

$$\int_{\mathbb{S}^d} f(\mathbf{x})\,\mathrm{d}\sigma_d(\mathbf{x}) \approx \frac{1}{N}\sum_{j=1}^{N} f(\mathbf{x}_j).$$

Here, and throughout the paper, we denote by σ_d the *normalised* surface area measure on $\mathbb{S}^d$. For non-random collections of integration nodes using the right-hand side as approximation for the integral is known as *Quasi-Monte Carlo (QMC) method*. In order to obtain a good approximation of the integral by the sum, the point set $X_N = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ should be *well distributed* over the whole sphere $\mathbb{S}^d$. The notion of good distribution of a point set is described in an intrinsic way in this context: the distribution is *good*, if the error is small for a certain set of functions. Necessarily, a sequence of node sets will be asymptotically uniformly distributed. (Roughly speaking, each reasonable subset of the sphere eventually gets a fair share of points.)

Placing as many points as possible on the sphere so that the least distance (or equivalently, the smallest angle) between two points is maximised is qualitatively different from covering the sphere with the least number of equal-sized spherical caps so that each point on the sphere is in at least one spherical cap. Each approach requires a different notion of *well distribution*. The former is the problem of best packing which has attracted attention for a long time in and outside of mathematics. For instance, the best packing problem on the sphere is attributed to P. M. L. Tammes [122], a botanist, who searched for an explanation of the surface structure of pollen grains. The latter is the problem of best covering which is the realm of facility location problems where the farthest distance from a point on the sphere to the nearest covering point (service distance) is minimised. That

means that the largest cap, which does not contain a sample point, should be as small as possible. Its radius, called the *covering radius*, is also known as *mesh norm* or *fill radius*.

Sampling function values on the sphere (e.g., for approximation or interpolation by splines or radial basis functions) or exploring spatial directions in an efficient way requires again *well distributed* (but not necessary uniformly distributed) point sets on $\mathbb{S}^d$. The notion of quality of a point set is different in this context: distributing sample points requires these points to be *dense* in a quantifiable way. As the mesh norm arises in the error of approximation and good separation is generally associated with the "stability" of an approximation or interpolation method, one would prefer a *quasi-uniform* sequence of point sets with uniformly bounded *mesh-separation ratio*. The mesh-separation ratio can be regarded as the "condition number" for the point set. Quasi-uniformity is a crucial property for a number of methods (cf. [62, 92, 115]).

The present survey on point distributions on the sphere is motivated by two rather recent important contributions, which both shed new light on the subject. The first was D. P. Hardin's and E. B. Saff's [74] proof that minimal energy point configurations on the sphere provide asymptotically uniformly distributed point sets for hyper-singular Riesz potentials. (In the follow up paper [76], D. P. Hardin, E. B. Saff and J. T. Whitehouse showed that quasi-uniform sequences of point sets with a prescribed positive continuous limit distribution can be obtained using a certain weighted Riesz s-energy). This will be one subject of Section 3. The second breakthrough was A. V. Bondarenko's, D. Radchenko's, and M. S. Viazovska's [17] proof that spherical t-designs with $\mathcal{O}(t^d)$ number of points exist on $\mathbb{S}^d$. The definition of spherical designs, their properties, relevance, and occurrence in different contexts will be the subject of Section 2.

2. Spherical Designs

Spherical designs were initially defined in [57] in the context of algebraic combinatorics on spheres. For a survey on further developments in this context, we refer to [10].

In the meantime, spherical designs have gained interest in different areas of mathematics, ranging from number theory, geometry, algebraic and geometric combinatorics to numerical analysis. We will give an account of these aspects in this section.

2.1. Definition

A spherical t-design is a finite set of points $X \subset \mathbb{S}^d$, such that

$$\frac{1}{\#X} \sum_{\mathbf{x} \in X} f(\mathbf{x}) = \int_{\mathbb{S}^d} f(\mathbf{x}) \, \mathrm{d}\sigma_d(\mathbf{x}) \tag{2.1}$$

holds for all polynomials $f \in \mathbb{R}[x_1, \ldots, x_{d+1}]$ of total degree $\leq t$.This definition is equivalent to

$$\sum_{(\mathbf{x},\mathbf{y}) \in X \times X} P_k^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle) = 0 \tag{2.2}$$

for $k = 1, \dots, t$; here $P_k^{(d)}$ denotes the Legendre polynomial for the sphere $\mathbb{S}^d$ (cf. [101]). These polynomials are multiples of Gegenbauer polynomials C_k^α with $\alpha = \frac{d-1}{2}$, normalised so that $P_k^{(d)}(1) = 1$. The equivalence of (2.2) and (2.1) is then an immediate consequence of the fact that the restrictions of polynomials to $\mathbb{S}^d$ are spanned by the harmonic polynomials and the addition theorem for spherical harmonics (cf. [101])

$$\sum_{k=1}^{Z(d,\ell)} Y_{\ell,k}(\mathbf{x}) Y_{\ell,k}(\mathbf{y}) = Z(d,\ell)\, P_\ell^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle); \tag{2.3}$$

here $Y_{\ell,k}$ $(k = 1, \dots, Z(d,\ell) = \frac{2\ell+d-1}{d-1}\binom{\ell+d-2}{d-2})$ is a real orthonormal basis of the space of spherical harmonics of total degree $\le \ell$ with respect to the scalar product $\langle f, g \rangle := \int_{\mathbb{S}^d} f(\mathbf{x}) g(\mathbf{x})\, \mathrm{d}\sigma_d(\mathbf{x})$. Condition (2.2) is then obtained by considering condition (2.1) for $f = Y_{\ell,k}$, squaring it, summing over k, and using (2.3).

There are two further equivalent definitions of spherical t-designs, which show the connection of this concept to other areas of mathematics. It was observed in [95] that a spherical $2t$-design X with N points gives an isometric embedding of ℓ_2^{d+1} into ℓ_{2t}^N, which comes from the identity

$$\frac{1}{\#X} \sum_{\mathbf{x} \in X} \langle \mathbf{x}, \mathbf{a} \rangle^{2t} = \frac{1 \cdot 3 \cdot 5 \cdots (2t-1)}{(d+1)(d+2)\cdots(d+2t-1)} \langle \mathbf{a}, \mathbf{a} \rangle^t, \tag{2.4}$$

which is valid for all $\mathbf{a} \in \mathbb{R}^{d+1}$. This identity is an immediate consequence of (2.2) and the expansion of x^{2t} as a sum of Legendre polynomials.

A spherical t-design $X = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ is called *rigid* (cf. [9]), if there exists an $\varepsilon > 0$, such that for all t-designs $X' = \{\mathbf{x}'_1, \mathbf{x}'_2, \dots, \mathbf{x}'_N\}$ with $\|\mathbf{x}_i - \mathbf{x}'_i\| < \varepsilon$ (for $i = 1, \dots, N$) there exists a rotation $\sigma \in \mathrm{SO}(d+1)$ such that $X' = \sigma X$.

It was observed in [68] in passing and later rediscovered in [119] that X is a t-design, if and only if

$$E_p(X) := \sum_{(\mathbf{x},\mathbf{y}) \in X \times X} p(\langle \mathbf{x}, \mathbf{y} \rangle) = 0, \tag{2.5}$$

where p is a polynomial of degree t given by

$$p(z) = \sum_{k=1}^{t} a_k P_k^{(d)}(z) \quad \text{with } a_k > 0 \text{ for } k = 1, \dots, t.$$

Furthermore, since the sum (2.5) is non-negative for all X, designs are minimisers of this sum. This was used in [119] to characterise designs as stationary points of the "energy functional" $E_p(X)$.

In order to explain the connection to other questions of algebraic and geometric combinatorics on $\mathbb{S}^d$, we need one further notion. For a finite subset X of $\mathbb{S}^d$, we define

$$A(X) := \{\langle \mathbf{x}, \mathbf{y} \rangle \mid \mathbf{x}, \mathbf{y} \in X, \mathbf{x} \neq \mathbf{y}\}, \tag{2.6}$$

the set of mutual inner products. For a given $A \subset [-1,1)$, X is called an A-code, if $A(X) \subset A$. Then, for instance, the problem of best packing of N points on $\mathbb{S}^d$ can be formulated as finding the minimal β, such that there exists an A-code with $A = [-1,\beta]$. In particular, the determination of the *kissing number*, this is the maximum number of non-overlapping unit spheres, that can touch another given unit sphere, is equivalent to finding the maximal cardinality of an A-code for $A = [-1, \frac{1}{2}]$ (cf. [102]).

2.2. Relation to lattices

Designs have a very interesting connection to the theory of lattices that we want to explain here. A lattice in $\mathbb{R}^d$ is a $\mathbb{Z}$-module

$$\Lambda := \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2 \oplus \cdots \oplus \mathbb{Z}\mathbf{v}_d, \tag{2.7}$$

where $\mathbf{v}_1, \ldots, \mathbf{v}_d$ is a basis of $\mathbb{R}^d$. For more detailed information on lattices, we refer to the book [52]. A lattice Λ is called *even*, if all the squared norms $\|\mathbf{v}\|^2$ for $\mathbf{v} \in \Lambda$ are even. Even lattices can only exist, if d is divisible by 8.

For any lattice Λ, the dual lattice is defined by

$$\Lambda^{\#} := \{\mathbf{x} \in \mathbb{R}^d \mid \forall \mathbf{v} \in \Lambda : \langle \mathbf{v}, \mathbf{x}\rangle \in \mathbb{Z}\}. \tag{2.8}$$

The set $\Lambda^{\#}$ is again a lattice. A lattice Λ is called *unimodular*, if $\Lambda^{\#} = \Lambda$. For an even unimodular lattice Λ, the θ-series

$$\theta_\Lambda(\tau) = \sum_{\mathbf{v}\in\Lambda} e^{\pi i \tau \|\mathbf{v}\|^2}, \qquad \Im\tau > 0, \tag{2.9}$$

is a modular form of weight $d/2$; *i.e.*, the transformation formula

$$\theta_\Lambda(-1/\tau) = \tau^{-d/2}\, \theta_\Lambda(\tau)$$

holds for all τ with $\Im\tau > 0$. This follows from application of Poisson's summation formula.

It follows from the theory of modular forms (cf. [6]) that for a form f of weight $d/2$, given by

$$f(\tau) = \sum_{n=0}^{\infty} a_n\, e^{2\pi i n \tau},$$

at least one of the coefficients a_n for $n = 1, \ldots, 2 + 2\lfloor \frac{d}{24} \rfloor$ has to be non-zero. This implies that every even unimodular lattice Λ contains a non-zero vector $\mathbf{v}$ with $\|\mathbf{v}\| \le 2 + 2\lfloor \frac{d}{24} \rfloor$. If the shortest non-zero vector $\mathbf{v}$ in Λ satisfies $\|\mathbf{v}\|^2 = 2 + 2\lfloor \frac{d}{24} \rfloor$, then the lattice is called *extremal*.

For a homogeneous polynomial p of degree $j \ge 1$, which is also harmonic ($\triangle p = 0$), and an even unimodular lattice Λ the series

$$\theta_{\Lambda,p}(\tau) = \sum_{\mathbf{v}\in\Lambda} p(\mathbf{v})\, e^{\pi i \tau \|\mathbf{v}\|^2}, \qquad \Im\tau > 0, \tag{2.10}$$

is a modular form of weight $d/2 + j$. It is immediate from the symmetry of Λ and the homogeneity of p that $\theta_{\Lambda,p} = 0$, if j is odd. Also, the series $\theta_{\Lambda,p}$ is a cusp form; *i.e.*,

$$\lim_{\Im\tau\to\infty} \theta_{\Lambda,p}(\tau) = 0,$$

since $p(\mathbf{0}) = 0$.

From the theory of modular forms (cf. [6]) it is known that there is a unique cusp form $\Delta(\tau)$ of weight 12 having an expansion of the form

$$\Delta(\tau) = e^{2\pi i\tau} + \sum_{n=2}^{\infty} a_n\, e^{2\pi i n\tau}.$$

It follows from degree considerations that for an even, unimodular, extremal lattice Λ and a homogeneous, harmonic polynomial p of degree $j \geq 1$,

$$\theta_{\Lambda,p}(\tau) = \Delta(\tau)^{1+\lfloor \frac{d}{24} \rfloor} f(\tau), \tag{2.11}$$

where $f(\tau)$ is a modular form of weight

$$\frac{d}{2} - 12 \left\lfloor \frac{d}{24} \right\rfloor + j - 12.$$

If this weight is negative, then f has to vanish identically, since there are no modular forms of negative weight. Consider $d = 24m + k$ with $k \in \{0, 8, 16\}$ and insert this into the above equation. This yields $k/2 + j - 12$ for the weight of f. For $k = 0$, 8 and 16, this yields negative weights for $j \leq 11$, 7 and 3, respectively, which shows that for all shells of the corresponding lattices the sum

$$\sum_{\|\mathbf{v}\|=n} p(\mathbf{v}) = \|\mathbf{v}\|^j \sum_{\|\mathbf{v}\|=n} p\left(\mathbf{v}/\|\mathbf{v}\|\right) = 0 \tag{2.12}$$

vanishes for all homogeneous harmonic polynomials of degree $j \leq 11, 7, 3$, respectively. Summing up, we have proved the following theorem.

Theorem 2.1 ([126]). *Let Λ be an extremal even unimodular lattice in $\mathbb{R}^d$ with $d = 24m + k$ ($k = 0, 8, 16$). Then any non-empty shell of Λ defines a j-design $\{\mathbf{v}/\sqrt{n} \in \Lambda \mid \|\mathbf{v}\|^2 = n\}$ for $j = 11 - k/2$.*

For further developments in the context of designs, lattices, modular forms, and algebraic codes, we refer to [7, 8, 10, 54, 103, 104].

2.3. Lower bounds

Another interesting question is to find the minimal cardinality of $A(X)$ for sets X with N points. In [57] a linear programming method is developed, which allows to give answers to such questions. This method has also been applied for proving lower bounds for the minimal cardinality of spherical t-designs.

We give a short explanation of this powerful method, that has been applied with great success to several problems of discrete geometry, the most prominent being the solution of Kepler's conjecture by T. Hales [72]. We restrict to the description of the method used for application on the sphere. Let $f : [-1, 1] \to \mathbb{R}^+$ be a continuous positive function given by its expansion in terms of Legendre polynomials; i.e.,

$$f(x) = \sum_{n=0}^{\infty} \widehat{f}(n)\, Z(d, n)\, P_n^{(d)}(x). \tag{2.13}$$

If the coefficients $\widehat{f}(n)$ are non-positive for $n > t$, then any t-design X has to have cardinality $\geq f(1)/\widehat{f}(0)$. The proof of this fact is given by the relations

$$\begin{aligned} f(1)\,(\#X) &\leq \sum_{(\mathbf{x},\mathbf{y})\in X\times X} f(\langle \mathbf{x}, \mathbf{y}\rangle) \\ &= \widehat{f}(0)\,(\#X)^2 + \sum_{n>t} \widehat{f}(n)\, Z(d, n) \sum_{(\mathbf{x},\mathbf{y})\in X\times X} P_n^{(d)}(\langle \mathbf{x}, \mathbf{y}\rangle) \\ &\leq \widehat{f}(0)\,(\#X)^2 . \end{aligned}$$

The first inequality is a consequence of the positivity of f, the equality uses the characterisation of t-designs by (2.2), and the second inequality uses that $\widehat{f}(n) \leq 0$ for $n > t$ and the non-negativity of the double sums $\sum_{(\mathbf{x},\mathbf{y})\in X\times X} P_n^{(d)}(\langle \mathbf{x}, \mathbf{y}\rangle)$. Equality can only occur, if $f(t) = 0$ for all $t \in A(X)$ and $\widehat{f}(n) = 0$ for $n > t$; *i.e.*, f is a polynomial of degree $\leq t$.

In [57] a polynomial p_t of degree t was constructed, which gives the lower bound

$$\#X \geq \begin{cases} \binom{d+t/2}{d} + \binom{d+t/2-1}{d} & \text{for } t \text{ even}, \\ 2\binom{d+(t-1)/2}{d} & \text{for } t \text{ odd}. \end{cases} \tag{2.14}$$

This polynomial is actually providing the best possible lower bound that can be obtained by polynomial functions f. Designs attaining this lower bound are called *tight*. It was shown in [11, 12] that tight designs only exist for $d = 1$ and all t or finitely many values of t, if $d \geq 2$. The proof uses the fact that for a tight spherical t-design X the corresponding set $A(X)$ has to consist exactly of the zeros of the polynomial p_t constructed in [57]. Galois theory is then used to derive a contradiction, if t is large enough. The same fact about $A(X)$ also shows that tight designs are rigid (cf. [9]). Notice that the bound is of order t^d. Later V. A. Yudin [129] constructed a new linear programming function f. The bounds for spherical designs he could give are again of order t^d, but they are larger by a factor depending on d. This factor is growing exponentially in d. For $d = 2$ the gain is asymptotically about 7%.

We give a short description of Yudin's construction. The function f is obtained as the spherical convolution of two positive functions F and G, which ensures the positivity of f. The spherical convolution of two functions F and G is given by

$$F \star G(\langle \mathbf{x}, \mathbf{y}\rangle) := \int_{\mathbb{S}^d} F(\langle \mathbf{x}, \mathbf{z}\rangle) G(\langle \mathbf{z}, \mathbf{y}\rangle)\, \mathrm{d}\sigma_d(\mathbf{z}).$$

In order to obtain the required sign change of the Laplace-Fourier coefficients of f, the function G is chosen as

$$G(x) = (1-x^2)^{1-\frac{d}{2}} \left((1-x^2)^{\frac{d}{2}} F'(x) \right)' + (t+1)(t+d)F(x),$$

which is motivated by the fact that the Legendre polynomials are eigenfunctions of the differential operator

$$LF(x) := (1-x^2)^{1-\frac{d}{2}} \left((1-x^2)^{\frac{d}{2}} F'(x) \right)'.$$

If F is expressed in terms of its Laplace-Fourier expansion

$$F(x) = \sum_{n=0}^{\infty} \widehat{F}(n)\, Z(d,n)\, P_n^{(d)}(x),$$

then the function G is given by

$$G(x) = \sum_{n=0}^{\infty} (t+1-n)\,(n+t+d)\, \widehat{F}(n)\, Z(d,n)\, P_n^{(d)}(x).$$

Then the spherical convolution is given as

$$f(x) = F \star G(x) = \sum_{n=0}^{\infty} (t+1-n)\,(n+t+d)\, \widehat{F}(n)^2\, Z(d,n)\, P_n^{(d)}(x),$$

which has the required sign-change in its Laplace-Fourier coefficients. The problem of maximising the quotient $f(1)/\widehat{f}(0) = f(1)/\widehat{F}(0)^2$ then turns out to be a variational problem for F:

$$\begin{aligned} f(1) &= \frac{\omega_{d-1}}{\omega_d} \int_{-1}^{1} F(x)G(x) \left(1-x^2\right)^{d/2-1} \mathrm{d}x \\ &= \frac{\omega_{d-1}}{\omega_d} \int_{-1}^{1} \Big(-\left(1-x^2\right) F'(x)^2 + (t+1)\,(t+d)\, F(x)^2 \Big) \left(1-x^2\right)^{d/2-1} \mathrm{d}x \end{aligned}$$

has to be maximised subject to the condition

$$\widehat{F}(0) = \frac{\omega_{d-1}}{\omega_d} \int_{-1}^{1} F(x) \left(1-x^2\right)^{d/2-1} \mathrm{d}x = c.$$

Here we used the Funk-Hecke formula (2.25) (cf. [101]). The symbol ω_d denotes the surface area of $\mathbb{S}^d$ and it satisfies

$$\int_{-1}^{1} \left(1-x^2\right)^{d/2-1} \mathrm{d}x = \frac{\omega_d}{\omega_{d-1}} = \frac{\sqrt{\pi}\,\Gamma(d/2)}{\Gamma((d+1)/2)}.$$

Furthermore, f has to be non-negative on $[-1,1]$. This is achieved by assuming that F and G are both non-negative. The solution of this variational problem with the additional condition on the sign of F is then given by

$$F(x) = \begin{cases} P_{t+1}^{(d)}(x) - P_{t+1}^{(d)}(\alpha_t) & \text{for } \alpha_t \le x \le 1, \\ 0 & \text{for } -1 \le x \le \alpha_t, \end{cases}$$

where α_t is the largest zero of $\frac{d}{dx} P_{t+1}^{(d)}(x)$. In this case G is a piecewise constant function. Putting everything together yields the lower bound

$$\#X \ge \frac{\int_{-1}^{1} (1-x^2)^{d/2-1} \, \mathrm{d}x}{\int_{\alpha_t}^{1} (1-x^2)^{d/2-1} \, \mathrm{d}x} = \frac{1}{\sigma_d(\{\mathbf{y} \in \mathbb{S}^d \mid \langle \mathbf{y}, \mathbf{x} \rangle \ge \alpha_t\})} \gg_d t^d \tag{2.15}$$

for a t-design X. For a more detailed exposition, we refer to [129]. Even if the obtained function f gives a better value for the lower bound than the polynomial given in [57], the technical requirement of non-negativity of F seems to leave room for further improvement.

A rather similar construction for a linear programming function is used in [48] to obtain bounds for the packing density of spheres in $\mathbb{R}^d$. The function obtained there has similar features; in particular, it is supported on a short interval. In [48, Section 5] it is mentioned that the function constructed by this convolution method does **not** produce optimal bounds (cf. [47]). The reason seems to be exactly the non-negativity requirement on the corresponding function F. Thus there is reason to believe that Yudin's lower bound for the cardinality of t-designs can still be improved.

2.4. Existence

On the other hand, the question of existence of spherical t-designs has been answered affirmatively. First a rather general result obtained in [117] shows that for given t and large enough N, there exists a t-design with N points. Actually, the result given in [117] is more general: given a path connected topological space Ω, and a finite measure μ that charges every non-empty open set, then for any finite set of continuous real valued functions $f_1, \ldots, f_t$ there exists an N, such that for every $n > N$ there exists a set $X \subset \Omega$ with $\#X = n$, such that

$$\frac{1}{\#X} \sum_{x \in X} f_j(x) = \frac{1}{\mu(\Omega)} \int_{\Omega} f_j(x) \, \mathrm{d}\mu(x)$$

for $j = 1, \ldots, t$. The result even gives a bound for the number of points needed in terms of geometric quantities defined in terms of Ω and the functions $f_1, \ldots, f_t$. But it turns out that these quantities are very difficult to compute even in the special case of the sphere.

In order to discuss the question of existence of spherical designs further, we introduce two quantities:

$$N(t,d) := \min\left\{n \mid \exists X \subset \mathbb{S}^d : \#X = n \wedge X \text{ is a } t\text{-design}\right\},$$
$$N^*(t,d) := \min\left\{n \mid \forall k \ge n : \exists X \subset \mathbb{S}^d : \#X = k \wedge X \text{ is a } t\text{-design}\right\}.$$

By definition it is clear that $N^*(t,d) \geq N(t,d)$.

Only very recently, the long standing problem of existence of spherical t-designs with $\mathcal{O}(t^d)$ points could be answered affirmatively by A. V. Bondarenko, D. Radchenko, and M. S. Viazovska [17]. They could prove that $N^*(t,d) = \mathcal{O}(t^d)$ with an explicit, but rather large implied constant. The proof reformulates the design property of a point set $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ as being the zero of a cleverly constructed continuous function $\Phi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$. Then an application of Brouwer's degree theory to Φ allows to conclude the existence of that zero, i.e., a spherical design. The auxiliary function Φ is constructed using the solution of a differential equation with initial values chosen in an equal area partition of the sphere with diameters controlled by the cardinality of the partition. A spherical version of the Marcinkiewicz-Zygmund inequality is used to prove the hypothesis of Brouwer's theorem.

In a forthcoming paper [18] the same authors could even show that there exist well separated t-designs with optimal growth order of the number of points:

Theorem 2.2. *Let $d \geq 2$. Then there exist positive constants C_d and λ_d such that for every $N \geq C_d t^d$ one has a t-design X with $\#X = N$ and*

$$\|\mathbf{x} - \mathbf{y}\| \geq \lambda_d \, N^{-1/d} \qquad \text{for all } \mathbf{x}, \mathbf{y} \in X \text{ with } \mathbf{x} \neq \mathbf{y}.$$

The proof is a refinement of their original proof keeping control on the distance of distinct points.

2.5. Numerical results

Besides the theoretical investigation on the existence of spherical designs, several attempts were made to compute lists of t-designs for moderately large values of t and small number of points. Since most of these computations have been done for $d = 2$, we will restrict to this case in this section.

A first list of t-designs for $t \leq 21$ was provided by R. H. Hardin and N. J. A. Sloane (cf. [77, 78, 79]). Their list is still available on the web [80]. These numerical computations, as well as those performed in [119], seem to suggest that $N(t,2)$ is close to $\frac{1}{2}(t+1)^2$. Furthermore, X. Chen and R. S. Womersley found spherical t-designs by numerical computations for $t \leq 100$ (cf.[44]). Their computations seem to indicate that there exist t-designs with less than $(t+1)^2$ points. Later X. Chen, A. Frommer and B. Lang [43] used interval arithmetic to prove that there exist spherical t-designs with $(t+1)^2$ points for $1 \leq t \leq 100$. Recently, M. Gräf and D. Potts [69] derived a new method based on fast Fourier transform, which allows to find t-designs numerically with high precision for values of t up to 1000. They also provide their results on the web [70]. Again these numerical results show that $N(t,2)$ is close to $\frac{1}{2}(t+1)^2$ for small values of t.

2.6. Designs and uniform distribution

It was observed independently in [68] and in [86] that spherical designs provide well-distributed point sets on the sphere.

Table 1: The lower bounds for the number of points of a t-design derived in [57] ($D(t)$) and in [129] ($Y(t)$) compared to the number of points of t-designs $N(t)$ obtained in [69] (as provided on the website [70]).

t	5	7	9	10	20	30	40	50	60	70	80	90	100	114	124
$D(t)$	12	20	30	36	121	256	441	676	961	1296	1681	2116	2601	3364	3969
$Y(t)$	12	20	31	37	127	271	470	723	1031	1394	1810	2282	2808	3635	4292
$N(t)$	12	24	48	60	216	480	840	1296	1860	2520	3276	4140	5100	6612	7812
$\lfloor\frac{(t+1)^2}{2}\rfloor$	18	32	50	60	220	480	840	1300	1860	2520	3280	4140	5100	6612	7812

The *spherical cap discrepancy* of a point set X_N of N points is given by

$$D(X_N) := \sup_{\substack{\mathbf{x}\in\mathbb{S}^d,\\ \varphi\in[0,\pi]}} \left| \frac{1}{N} \sum_{\mathbf{y}\in X_N} \mathbb{1}_{\mathbf{x}\in C(\mathbf{y},\varphi)} - \sigma_d(C(\mathbf{y},\varphi)) \right|; \tag{2.16}$$

the supremum is extended over all spherical caps

$$C(\mathbf{y},\varphi) = \left\{ \mathbf{x}\in\mathbb{S}^d \mid \langle \mathbf{x},\mathbf{y}\rangle > \cos(\varphi) \right\},$$

and measures the maximum deviation between the empirical distribution of the point set X_N from uniform distribution. In [66] the estimate

$$D(X_N) \le \frac{C_1(d)}{M} + \sum_{\ell=1}^{M} \frac{C_2(d)}{\ell} \sum_{k=1}^{Z(d,\ell)} \left| \frac{1}{N} \sum_{j=1}^{N} Y_{\ell,k}(\mathbf{x}_j) \right| \tag{2.17}$$

was proved; here M is an arbitrary positive integer, and $C_1(d)$ and $C_2(d)$ are explicit constants depending only on the dimension d. A similar inequality was later given in [94]. The inequality (2.17) resembles the classical Erdős-Turán-Koksma inequality estimating the Euclidean discrepancy of a point set in $[0,1]^d$ in terms of trigonometric sums (cf. [90]). In [88], N. M. Korobov introduced *good lattice points* $(g_1,\ldots,g_d)\in\mathbb{Z}^d$ by the requirement that the point set $\{(\{\frac{jg_1}{N}\},\ldots,\{\frac{jg_d}{N}\}) \mid j=0,\ldots,N-1\}$ has small discrepancy.

In [68] spherical t-designs were regarded as spherical analogues of good lattice points, in the sense that the estimate (2.17) becomes especially simple when applied to a t-design and choosing the parameter M to be t: then the estimate reduces to

$$D(X_N) \le \frac{C_1(d)}{t}.$$

Similarly, for a continuous function $f:\mathbb{S}^d\to\mathbb{R}$ satisfying $|f(\mathbf{x})-f(\mathbf{y})| \le C_f \arccos(\langle \mathbf{x},\mathbf{y}\rangle)$ (a Lipschitz-condition), the estimate

$$\left| \frac{1}{N} \sum_{\mathbf{x}\in X_N} f(\mathbf{x}) - \int_{\mathbb{S}^d} f(\mathbf{x})\,\mathrm{d}\sigma_d(\mathbf{x}) \right| \le C_f \left(6\frac{d}{M} + \pi \sum_{\ell=1}^{2M} \sum_{k=1}^{Z(d,\ell)} \left| \frac{1}{N} \sum_{\mathbf{x}\in X_N} Y_{\ell,k}(\mathbf{x}) \right| \right) \tag{2.18}$$

was shown. Again, taking X_N to be a $2t$-design and $M = t$ gives an estimate $6dC_f/t$ for the integration error.

J. Korevaar and J. L. H. Meyers [86] take a potential theoretic point of view. In their papers [86, 87] they state the conjecture that $N(t,d) = \mathcal{O}(t^d)$, which could finally be proved by Bondarenko, Radchenko, and Viazovska in [17]. Let $\mu_N := \frac{1}{N}\sum_{\mathbf{x}\in X_N}\delta_{\mathbf{x}}$ be the discrete equal weight distribution supported on $X_N \subset \mathbb{S}^d$. Then the deviation of μ_N and the equilibrium measure σ_d is measured by the deviation of the potential

$$U_{d-1}^{\mu_N}(\mathbf{x}) = \frac{1}{N}\sum_{\mathbf{y}\in X_N}\frac{1}{\|\mathbf{x}-\mathbf{y}\|^{d-1}} \tag{2.19}$$

from the equilibrium potential

$$U_{d-1}^{\sigma_d}(\mathbf{x}) = \int_{\mathbb{S}^d}\frac{1}{\|\mathbf{x}-\mathbf{y}\|^{d-1}}\,\mathrm{d}\sigma_d(\mathbf{y}) = 1$$

for $\|\mathbf{x}\| \le r < 1$.

Taking a spherical t-design X_N and using the identity (cf. [96])

$$\frac{1}{\|r\mathbf{x}-\mathbf{y}\|^{d-1}} = \sum_{n=0}^{\infty}\binom{n+d-2}{d-2}P_n^{(d)}(\langle\mathbf{x},\mathbf{y}\rangle)\,r^n,$$

we obtain

$$U_{d-1}^{\mu_N}(r\mathbf{x}) - 1 = \sum_{n=t+1}^{\infty}\binom{n+d-2}{d-2}r^n\frac{1}{N}\sum_{\mathbf{y}\in X_N}P_n^{(d)}(\langle\mathbf{x},\mathbf{y}\rangle). \tag{2.20}$$

Estimating the right hand side by $|P_n^{(d)}(\cdot)| \le 1$ we obtain

$$\left|U_{d-1}^{\mu_N}(r\mathbf{x}) - 1\right| \le \sum_{n=t+1}^{\infty}\binom{n+d-2}{d-2}r^n. \tag{2.21}$$

The sum on the right hand side can be expressed in closed form.

$$\begin{aligned}
&\sum_{n=t+1}^{\infty}\binom{n+d-2}{d-2}r^n \\
&\quad= (d-1)\binom{t+d-1}{d-1}\frac{1}{(1-r)^{d-1}}\int_0^r(1-\rho)^{d-2}\rho^t\,\mathrm{d}\rho \\
&\quad= \frac{r^{t+1}}{(1-r)^{d-1}}(d-1)\binom{t+d-1}{d-1}\sum_{\ell=0}^{d-2}\binom{d-2}{\ell}(-1)^\ell\frac{r^\ell}{t+\ell+1},
\end{aligned}$$

which can be proved by multiplying with $(1-r)^{d-1}$ and differentiating. Estimating the integral in the second line by $r^{t+1}/(t+1)$ we get the estimate

$$|U^{\mu_N}(r\mathbf{x}) - 1| \le \binom{t+d-1}{d-2}\frac{r^{t+1}}{(1-r)^{d-1}} \tag{2.22}$$

valid for any t-design X_N, $\mathbf{x} \in \mathbb{S}^d$, and $0 \le r < 1$. This together with the fact that $N(t,d) = \mathcal{O}(t^d)$ generalises [86, Theorem 2.2] to arbitrary dimension.

2.7. Applications to numerical integration on $\mathbb{S}^d$

Equal weight quadrature formulas like spherical design QMC methods are especially useful for integrating functions taken from suitably defined Sobolev spaces on $\mathbb{S}^d$. These spaces are *reproducing kernel Hilbert spaces*, which makes the study of the worst case error in integration especially simple and transparent (cf. [106]).

In order to describe the results on numerical integration in more detail, we give a precise definition of the function spaces. The negative Laplace-Beltrami operator $-\Delta_d^*$ on $\mathbb{S}^d$ has the eigenvalues $\lambda_\ell := \ell(\ell+d-1)$, $\ell \in \mathbb{N}_0$. The space of eigenfunctions for the eigenvalue λ_ℓ is spanned by the spherical harmonics $Y_{\ell,k}$ for $k = 1, \ldots, Z(d,\ell)$. Since the eigenfunctions of $-\Delta_d^*$ form a complete function system, every function $f \in L^2(\mathbb{S}^d)$ can be represented by its Laplace-Fourier series expansion

$$f(\mathbf{x}) = \sum_{\ell=0}^{\infty} \sum_{k=1}^{Z(d,\ell)} \widehat{f}_{\ell,k}\, Y_{\ell,k}(\mathbf{x}), \tag{2.23}$$

where the Laplace-Fourier coefficients are given by

$$\widehat{f}_{\ell,k} = \int_{\mathbb{S}^d} f(\mathbf{x})\, Y_{\ell,k}(\mathbf{x})\, \mathrm{d}\sigma_d(\mathbf{x}).$$

The series (2.23) has to be interpreted in L^2-sense. Furthermore, Parseval's identity

$$\sum_{\ell=0}^{\infty} \sum_{k=1}^{Z(d,\ell)} \left|\widehat{f}_{\ell,k}\right|^2 = \int_{\mathbb{S}^d} |f(\mathbf{x})|^2 \, \mathrm{d}\sigma_d(\mathbf{x}) = \|f\|_2^2 \tag{2.24}$$

and the Funk-Hecke formula

$$\sum_{k=1}^{Z(d,\ell)} \widehat{f}_{\ell,k}\, Y_{\ell,k}(\mathbf{x}) = Z(d,\ell) \int_{\mathbb{S}^d} f(\mathbf{y})\, P_\ell^{(d)}\big(\langle \mathbf{x}, \mathbf{y}\rangle\big)\, \mathrm{d}\sigma_d(\mathbf{y}) \tag{2.25}$$

hold. For more details on the harmonic analysis on $\mathbb{S}^d$, we refer to [101].

In the following we adopt the notation in [40]. For $s \geq 0$, we define the space

$$H^s(\mathbb{S}^d) := \left\{ f \in L^2(\mathbb{S}^d) \;\middle|\; \sum_{\ell=0}^{\infty} (1+\ell)^{2s} \sum_{k=1}^{Z(d,\ell)} \left|\widehat{f}_{\ell,k}\right|^2 < \infty \right\}. \tag{2.26}$$

From this definition, it is clear that the "weight sequence" $((1+\ell)^{2s})_\ell$ can be replaced by any other sequence $(w_\ell)_\ell$ of the same order of magnitude, in the sense of

$$\exists C_1, C_2 > 0 : \forall \ell \in \mathbb{N}_0 : C_1(1+\ell)^{2s} \leq w_\ell \leq C_2(1+\ell)^{2s}.$$

We define a norm on $H^s(\mathbb{S}^d)$ by

$$\|f\|_{H^s} := \left(\sum_{\ell=0}^{\infty} (1+\ell)^{2s} \sum_{k=1}^{Z(d,\ell)} \left|\widehat{f}_{\ell,k}\right|^2 \right)^{1/2}. \tag{2.27}$$

From the definition it is clear that the spaces $H^s(\mathbb{S}^d)$ are getting smaller as the smoothness index s increases. Furthermore, the Sobolev embedding theorem ensures that $H^s(\mathbb{S}^d)$ embeds continuously into $C^k(\mathbb{S}^d)$, if $s > k + d/2$; especially, $H^s(\mathbb{S}^d)$ embeds continuously into $C(\mathbb{S}^d)$, if $s > d/2$.

As a consequence of the embedding of $H^s(\mathbb{S}^d)$ into $C(\mathbb{S}^d)$ for $s > d/2$, point evaluation of a function is a continuous functional, which can be represented as a scalar product by the Riesz representation theorem. This ensures the existence of a reproducing kernel given by

$$K^{(s)}\big(\langle \mathbf{x}, \mathbf{y}\rangle\big) := \sum_{\ell=0}^{\infty} (1+\ell)^{-2s}\, Z(d,\ell)\, P_\ell^{(d)}\big(\langle \mathbf{x}, \mathbf{y}\rangle\big). \tag{2.28}$$

With this definition of $K^{(s)}$ the reproducing kernel properties

$$\forall \mathbf{y} \in \mathbb{S}^d : K^{(s)}(\langle \cdot, \mathbf{y}\rangle) \in H^s(\mathbb{S}^d) \text{ and } \forall f \in H^s(\mathbb{S}^d)\ \forall \mathbf{x} \in \mathbb{S}^d : f(\mathbf{x}) = \langle f, K^{(s)}(\langle \cdot, \mathbf{x}\rangle)\rangle_{H^s} \tag{2.29}$$

can be immediately verified.

For $f \in H^s(\mathbb{S}^d)$, $s > d/2$, the integration error of the QMC method with node set X_N is given by

$$Q(X_N)(f) := \frac{1}{N} \sum_{\mathbf{x} \in X_N} f(\mathbf{x}) - \int_{\mathbb{S}^d} f(\mathbf{x})\, \mathrm{d}\sigma_d(\mathbf{x}) = \langle f, R(X_N)\rangle_{H^s}\,, \tag{2.30}$$

where the function

$$R(X_N)(\mathbf{y}) := \frac{1}{N} \sum_{\mathbf{x} \in X_N} K^{(s)}(\langle \mathbf{y}, \mathbf{x}\rangle) - 1 \tag{2.31}$$

is called the *representer of the integration error*. It is now a consequence of elementary Hilbert space theory that the worst case error takes the form

$$\mathrm{wce}_{H^s}(X_N) := \sup_{\|f\|_{H^s}=1} |Q(X_N)(f)| = \|R(X_N)\|_{H^s}\,. \tag{2.32}$$

The squared norm $\|R(X_N)\|^2 = \langle R(X_N), R(X_N)\rangle$ can be expressed in terms of the kernel function $K^{(s)}$ by means of

$$\|R(X_N)\|_{H^s}^2 = \frac{1}{N^2} \sum_{\mathbf{x},\mathbf{y} \in X_N} K^{(s)}(\langle \mathbf{x}, \mathbf{y}\rangle) - 1. \tag{2.33}$$

For a more precise explanation of this formalism we refer to [40]. The expression (2.33) is a special case of an energy functional as discussed further in Section 3.

Taking a spherical t-design for the set X_N in (2.33), the first t terms in the Laplace-Fourier expansion of $K^{(s)}$ are annihilated:

$$\mathrm{wce}_{H^s}(X_N)^2 = \sum_{\ell=t+1}^{\infty} (1+\ell)^{-2s}\, Z(d,\ell)\, \frac{1}{N^2} \sum_{\mathbf{x},\mathbf{y} \in X_N} P_\ell^{(d)}(\langle \mathbf{x}, \mathbf{y}\rangle). \tag{2.34}$$

Estimating this sum trivially would give a bound $\mathcal{O}(t^{d-2s})$.

In [84] and [85] a method, which provides much better estimates for the worst case error in $H^s(\mathbb{S}^2)$ has been invented. This method was extended and generalised to higher dimensions in [39]. This has now been established as a standard technique in this context. Even if it is too technical to give a precise description here (for which we refer to [39]), we explain the two main steps. First, the truncated kernel

$$K_t^{(s)}(x) := \sum_{\ell=t+1}^{\infty} (1+\ell)^{-2s}\, Z(d,\ell)\, P_\ell^{(d)}(x)$$

is rewritten in terms of Jacobi polynomials instead of Legendre polynomials. This is done using the fact that the Legendre polynomials are special cases of Jacobi polynomials and that there exist connection formulas involving hypergeometric expressions (cf. [96]). After this transformation, the kernel $K_t^{(s)}$ is expressed as a polynomial of degree t plus a series $\widetilde{K}_t^{(s)}$ involving higher order polynomials ("kernel split method"). The polynomial part is integrated exactly by the QMC method supported in X_N; the remaining part

$$\sum_{\mathbf{x},\mathbf{y}\in X_N} \widetilde{K}_t^{(s)}(\langle \mathbf{x},\mathbf{y}\rangle)$$

is then estimated using bounds for Jacobi polynomials. This part is rather delicate, since different estimates have to be used for $\langle \mathbf{x},\mathbf{y}\rangle \in [-1+c/t, 1-c/t]$ and $|\langle \mathbf{x},\mathbf{y}\rangle| > 1-c/t$. Here, a coarse equidistribution property of spherical t-designs is used to obtain optimal order estimates: there exist constants c_1 and c_2 independent of t and N such that

$$\#\Big(X_N \cap C(\mathbf{x}, \frac{c_1}{t})\Big) \le c_2 N \sigma_d\Big(C(\mathbf{x}, \frac{c_1}{t})\Big). \tag{2.35}$$

It was proved in [110] (see also [111]) that this is a general property of positive weight quadrature formulas, which integrate polynomials of degree $\le t$ exactly; thus (2.35) holds especially for spherical t-designs.

Using the technique described above, it was proved in [39] that the worst case integration error on $H^s(\mathbb{S}^d)$ (for $s > d/2$) satisfies

$$\mathrm{wce}_{H^s}(X_N) = \mathcal{O}_{s,d}\big(t^{-s}\big). \tag{2.36}$$

Using the recent progress on the existence of spherical designs with optimal growth order (cf. [17]), this gives

$$\mathrm{wce}_{H^s}(X_N) = \mathcal{O}_{s,d}\big(N^{-s/d}\big), \tag{2.37}$$

if X_N is a spherical t-design with $N = \mathcal{O}(t^d)$. This is known to be the optimal order for the worst case error in $H^s(\mathbb{S}^d)$ (cf. [82, 83]).

The estimate (2.37) led to the definition of sequences of *QMC-designs* in [40]: let $s > d/2$. A sequence of point sets $(X_N)_N$ on $\mathbb{S}^d$ is called a *sequence of QMC-designs* for $H^s(\mathbb{S}^d)$, if (2.37) holds. The supremum of all s, for which this property holds, is called the *strength* of the sequence $(X_N)_N$. By the above description, a sequence of spherical t-designs of optimal growth order $\mathcal{O}(t^d)$ has strength ∞. For a more detailed exposition of QMC-designs and their properties, we refer to the seminal paper [40].

2.8. Applications in approximation and interpolation

Well distributed point sets can also be used as sample points for interpolation formulas. Given a continuous function $f : \mathbb{S}^d \to \mathbb{R}$ and a set of points X_N with $N \geq Z(d+1,t)$ points; observe that

$$Z(d+1,t) = \sum_{k=0}^{t} Z(d,k)$$

is the dimension of the space of all polynomials of total degree $\leq t$ on $\mathbb{S}^d$. Then we look for a polynomial p of degree $\leq t$, such that

$$p(\mathbf{x}_i) = f(\mathbf{x}_i) \qquad \text{for } i = 1, \ldots, N \tag{2.38}$$

holds. Choosing $Y_{\ell,k}$ ($\ell = 0, \ldots, t$, $k = 1, \ldots, Z(d,\ell)$) as a basis for the polynomials and $N = Z(d+1,t)$, we have to solve a system of N linear equations; the points have to be chosen so that this system has full rank. One possibility for choosing the points X_N is to maximise the modulus of the determinant of the system, which optimises the numerical stability of solving the system. This is an approach, which is in the spirit of finding the extremal value of a functional depending on the points, such as the energy functionals discussed in Section 3. This has been worked out in [118] for $d = 2$.

In [4] it is proposed to use spherical t-designs as interpolation points; for $N \geq Z(d+1,t)$ the determinant of the matrix

$$H_t := \left(\sum_{j=1}^{N} Y_{\ell,k}(\mathbf{x}_j) Y_{\ell',k'}(\mathbf{x}_j) \right)_{(\ell,k),(\ell',k')} \qquad 1 \leq \ell, \ell' \leq t, \quad 1 \leq k \leq Z(d,\ell), \quad 1 \leq k' \leq Z(d,\ell'),$$

under the constraint that the point set X_N is a spherical t-design, is maximised. This leads to the definition of *well conditioned* designs.

In [4] this is worked out for $d = 2$. It should be mentioned that based on the numerical experiments [70, 80] there exist t-designs with $\lfloor (t+1)^2/2 \rfloor$ points (at least for $t \leq 100$). In the context of interpolation, the number of points has to be chosen $\geq (t+1)^2$, which gives further freedom for choosing the points, which can be used to maximise the determinant of H_t.

In [5] the application of spherical designs in the context of approximation of functions $f : \mathbb{S}^d \to \mathbb{R}$ is proposed. Usually, the approximation is computed by integrating f against an approximation kernel G_L, which is a polynomial of degree L in $\langle \mathbf{x}, \mathbf{y} \rangle$ (cf. [14, 112]). In [5] the integral is replaced by the equal weight quadrature rule given by a $2L$-design X_N. This approach is worked out for $d = 2$ and various classical approximation kernels. In order to make this procedure numerically more stable, a regularisation procedure is proposed: p is chosen to minimise

$$\sum_{j=1}^{N} \left(p(\mathbf{x}_j) - f(\mathbf{x}_j) \right)^2 + \lambda \sum_{j=1}^{N} \left(\mathcal{R} p(\mathbf{x}_j) \right)^2 \tag{2.39}$$

amongst all polynomials of degree L; here $\mathcal{R}$ is an operator on the space of polynomials, and $\lambda > 0$ is the regularisation parameter. The fact that X_N is chosen as a $2L$-design makes the linear algebra behind the least square approximation especially simple.

3. Energy

3.1. Minimal energy in applications

A surprising number of rather diverse applications can be formulated as a discrete or continuous minimal energy problem (or a mixture of both). In the discrete case this means to find a collection of N points in a subset A of $\mathbb{R}^p$, $p \geq 1$, that minimise a *discrete* K*-energy functional*

$$E_{\mathrm{K},Q}(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \sum_{\substack{i=1 \\ i \neq j}}^{N} \sum_{j=1}^{N} \Big[\mathrm{K}(\mathbf{x}_i, \mathbf{x}_j) + \mathrm{Q}(\mathbf{x}_i) + \mathrm{Q}(\mathbf{x}_j) \Big]$$

incorporating an *external field* Q (which is often taken to be zero), among all N-point tuples from A^N. The diagonal (self-interaction) terms are removed to allow singular kernels K. Evidently, further requirements on the set A, the kernel K and the external field Q are needed to ensure existence of a solution. A suitable Q compatible with K prevents points from escaping to infinity and thus introduces soft boundaries (allowing even $A = \mathbb{R}^p$) whereas by restricting the points to a finite set, a fractal, a torus or a sphere of Hausdorff dimension $d \leq p$, fractal or topological aspects enter the picture. A standard assumption is that K is symmetric and lower semi-continuous on $A \times A$ and that Q is also lower semi-continuous on A. This will (roughly speaking) guarantee that the *minimal* K*-energy problem with external field* Q has a solution when solved for an infinite compact set A; i.e.,

$$\mathcal{E}_{\mathrm{K},Q}(A; N) := \inf \Big\{ E_{\mathrm{K},Q}(\mathbf{x}_1, \ldots, \mathbf{x}_N) : \mathbf{x}_1, \ldots, \mathbf{x}_N \in A \Big\} = E_{\mathrm{K},Q}(\mathbf{x}_1^*, \ldots, \mathbf{x}_N^*)$$

for an N*-point minimal* K*-energy configuration* $X_N^* = \{\mathbf{x}_1^*, \ldots, \mathbf{x}_N^*\}$ *associated with* Q. Furthermore, the quantities $N(N-1)/\mathcal{E}_{\mathrm{K},Q}(A; N)$ form a non-increasing sequence that is bounded from below by semi-continuity. Thus the limit exists and it discriminates between two types of sets A depending on whether or not this limit vanishes. This gives rise to two different regimes characterised by a complete change in the nature of the minimisation problem with regard to properties of the solution and methods that are used to study it. In the field-free setting ($\mathrm{Q} \equiv 0$), the normalised *discrete minimal* N*-point energy of* A, given by $\mathcal{E}_{\mathrm{K},0}(A; N)/[N(N-1)]$, is also known as the N-th diameter of A. The limit in the extended sense (as $N \to \infty$) is called the *transfinite diameter of* A.

A fundamental question concerns the "limit distribution" (if such exists) of a sequence (X_N^*) of minimal energy configurations X_N^* on A as $N \to \infty$; i.e., is there a (unique) Borel probability measure μ_A^* supported on A that is the weak limit of the sequence formed by the discrete equal weight distribution supported on X_N^*,

$$\mu_{X_N^*} := \frac{1}{N} \sum_{j=1}^{N} \delta_{\mathbf{x}}.$$

Let $\mathcal{M}(A)$ denote the collection of Borel probability measures supported on A. The analogue continuous energy problem concerns the finding of a measure supported on A

that minimises the *weighted* K-*energy associated with* Q,

$$\mathcal{I}_{\mathrm{K,Q}}(\mu) := \mathcal{I}_{\mathrm{K}}(\mu) + 2\int_A \mathrm{Q}(\mathbf{x})\,\mathrm{d}\sigma_d(\mathbf{x}),$$

which is defined by means of the K-*energy of the measure* μ *on* A,

$$\mathcal{I}_{\mathrm{K}}(\mu) := \int_A\int_A \mathrm{K}(\mathbf{x},\mathbf{y})\,\mathrm{d}\mu(\mathbf{x})\mathrm{d}\mu(\mathbf{y}),$$

among all Borel probability measures supported on A. A minimising measure $\mu_{\mathrm{K,Q};A} \in \mathcal{M}(A)$ with

$$\mathcal{I}_{\mathrm{K,Q}}(\mu_{\mathrm{K,Q};A}) = W_{\mathrm{K,Q}}(A) := \inf\Big\{\mathcal{I}_{\mathrm{K,Q}}(\mu) \;\Big|\; \mu \in \mathcal{M}(A)\Big\},$$

is called a K-*extremal (or positive equilibrium) measure on* A *associated with* Q. In the field free setting $\mathrm{Q} \equiv 0$, a minimising measure $\mu_{K;A}$ is called K-*equilibrium measure on* A. In this case, the K-energy $\mathcal{I}_{\mathrm{K}}(\mu_{K;A})$ is equal to the *Wiener energy of* A,

$$W_{\mathrm{K}}(A) := \inf\Big\{\mathcal{I}_{\mathrm{K}}(\mu) \;\Big|\; \mu \in \mathcal{M}(A)\Big\}.$$

A fundamental question concerns the relation between the Wiener energy of A, the transfinite diameter of A and the Chebyshev constant of A which is the limit as $N \to \infty$ of the N-th Chebyshev constant of A defined as

$$M_N(A) := \sup_{\mathbf{x}_1,\ldots,\mathbf{x}_N \in A} \inf_{\mathbf{x}\in A} \frac{1}{N}\sum_{j=1}^{N} \mathrm{K}(\mathbf{x},\mathbf{x}_j);$$

see [59] and references cited therein for further details.

Next, we discuss applications which make use of the minimal energy problem.

The Thomson problem and its generalisation. A classical problem in electrostatics is to find the distribution of N unit point charges on a conductor in the most-stable equilibrium (the charges interact according to the Coulomb potential $1/r$, where r is the Euclidean distance between two interacting charges). This leads to a minimisation problem for the potential energy of the discrete charge system named after J. J. Thomson who posed it for the sphere [124]. A generalisation of Thomson problem using general laws of interactions (Riesz s-potential $1/r^s$) include multi-electron bubbles and arrangements of protein subunits which form the shells (or capsid) of spherical viruses; see [24] (cf. [25]) for a discussion.

For small number of points numerical optimisation can be used to find minimal Riesz s-energy configurations. As observed in [99], for each N there may be one or more "basic configuration" which compete for smallest energy as s grows from 1 to large values. For example, no configuration of five points can be optimal for

all values of s (cf. [49]). In fact, there are two basic configuration (double pyramid and quadratic pyramid) which compete. According to the numerical results for $2 \leq s \leq 15.048077392\ldots$ the regular triangular bi-pyramid is the putative energy-minimising configuration whereas for higher values of s it seems to be the square pyramid (with adjusted height); see also [105] for a finer analysis. In the last paper monotonicity properties of the second discrete derivative were considered which lead to new putative low-energy configurations in two cases.

Half-toning. Loosely speaking, half-toning is some way of creating an illusion of a grey-value image by appropriately distributing black dots. (One can variate from this by having only a limited number of colours available.) In [71] the authors show how the process of half-toning can be seen as a numerical integration process with the aim to minimise a worst-case error or how it can be interpreted as an external field problem where the picture drives the external field which guides the interacting points; see also [123].

Maximising Determinants. I. Sloan and R. S. Womersley [118] considered points that maximise a Vandermonde-type determinant that appears in the polynomial Lagrange interpolation formula. See also [98].

Diffusion on a sphere with localised traps. As an application in cellular signal transport the authors of [53] calculate the principal eigenvalue for the Laplacian on the unit sphere in the presence of N traps on the surface of the sphere of asymptotically small radii. The positions of the traps are chosen to minimise the discrete logarithmic energy (cf. Section 3.2).

3.2. The discrete and continuous minimal logarithmic and Riesz energy problem

The discrete logarithmic energy problem on $\mathbb{S}^d$ is concerned with the properties of N-point configurations $\{\mathbf{x}_1^*, \ldots, \mathbf{x}_N^*\} \subset \mathbb{S}^d$ that maximise the product of all mutual pairwise Euclidean distances

$$\prod_{\substack{i=1 \\ i\neq j}}^{N} \prod_{j=1}^{N} \|\mathbf{x}_i - \mathbf{x}_j\|\,, \tag{3.1}$$

or equivalently, minimise the discrete logarithmic energy

$$E_{\log}(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \sum_{\substack{i=1 \\ i\neq j}}^{N} \sum_{j=1}^{N} \log \frac{1}{\|\mathbf{x}_i - \mathbf{x}_j\|}$$

over all N-point configurations $(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ on $\mathbb{S}^d$. The discrete logarithmic energy is the limiting case (as $s \to 0$) of the Riesz s-energy

$$E_s(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \sum_{\substack{i=1 \\ i\neq j}}^{N} \sum_{j=1}^{N} \frac{1}{\|\mathbf{x}_i - \mathbf{x}_j\|^s}.$$

The discrete Riesz s-energy problem for $s > 0$ is concerned with the properties of N-point configurations $\{\mathbf{x}_1^*, \ldots, \mathbf{x}_N^*\} \subset \mathbb{S}^d$ that minimise the Riesz s-energy over all N-point configurations $(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ on $\mathbb{S}^d$. For convenience we set $\mathrm{k}_s(\mathbf{x}, \mathbf{y}) := -\log \|\mathbf{x} - \mathbf{y}\|$ for $s = \log$ and $\mathrm{k}_s(\mathbf{x}, \mathbf{y}) := 1/\|\mathbf{x} - \mathbf{y}\|^s$ for $s \in \mathbb{R}$. Then for $N \geq 2$ we are interested in the *optimal N-point s-energy* of a compact set $A \subset \mathbb{R}^{d+1}$ defined by

$$\mathcal{E}_s(A; N) := \begin{cases} \min\left\{E_s(\mathbf{x}_1, \ldots, \mathbf{x}_N) \mid \mathbf{x}_1, \ldots, \mathbf{x}_N \in A\right\} & \text{for } s = \log \text{ or } s > 0, \\ \max\left\{E_s(\mathbf{x}_1, \ldots, \mathbf{x}_N) \mid \mathbf{x}_1, \ldots, \mathbf{x}_N \in A\right\} & \text{for } s < 0. \end{cases}$$

The Riesz s-kernel is conditionally positive definite of order 1 for $-2 < s < 0$. Alternatively, as in the setting of numerical integration on $\mathbb{S}^d$, one can minimise

$$2\int_A \int_A \|\mathbf{x} - \mathbf{y}\|^{-s} \, \mathrm{d}\sigma_d(\mathbf{x}\mathrm{d}\sigma_d(\mathbf{y}) - \sum_{i=1}^N \sum_{j=1}^N \|\mathbf{x}_i - \mathbf{x}_j\|^{-s}$$

in this case.

The *s-potential* and the *s-energy* of a measure μ in the class $\mathcal{M}(A)$ of Borel probability measures supported on A are given, respectively, by

$$U_s^\mu(\mathbf{x}) := \int_A \mathrm{k}(\mathbf{x}, \mathbf{y}) \, \mathrm{d}\mu(\mathbf{y}), \quad \mathbf{x} \in \mathbb{R}^{d+1}, \qquad \mathcal{I}_s(\mu) := \int_A \int_A \mathrm{k}(\mathbf{x}, \mathbf{y}) \, \mathrm{d}\mu(\mathbf{x})\mathrm{d}\mu(\mathbf{y}). \tag{3.2}$$

The *s-capacity* of A is for $s > 0$ the reciprocal of the Wiener energy $\inf\{\mathcal{I}_s(\mu) \mid \mu \in \mathcal{M}(A)\}$. (If the Wiener energy is finite, it will be denoted by $W_s(A)$.) The logarithmic capacity is defined by $\mathrm{cap}_{\log}(A) := \exp(-\inf\{\mathcal{I}_{\log}(\mu) \mid \mu \in \mathcal{M}(A)\})$. The infimum is denoted by $W_{\log}(A)$, if it is finite. The lower semi-continuous logarithmic kernel is bounded from below and thus the kernel k_s (plus a constant if needed) is strictly positive definite for $s = \log$ and $0 < s < p$. Consequently, the s-equilibrium measure $\mu_{A,s}$ on A is unique for every compact set $A \subset \mathbb{R}^p$ with finite s-energy; cf. [23, 91]. For the range $-2 < s < 0$, one also has a unique s-equilibrium measure on A; cf. [16] for the potential theoretic quantities and variational inequalities.

An *external field* will be a lower semi-continuous function $Q : \mathbb{S}^d \to (-\infty, \infty]$ such that $Q(\mathbf{x}) < \infty$ on a set of positive Lebesgue surface measure. We note that the lower semi-continuity implies the existence of a finite c_Q such that $Q(\mathbf{x}) \geq c_Q$ for all $\mathbf{x} \in \mathbb{S}^d$. The *weighted energy associated with $Q(\mathbf{x})$* is then given by

$$I_{Q,s}(\mu) := \mathcal{I}_s(\mu) + 2\int Q(\mathbf{x})\mathrm{d}\mu(\mathbf{x}), \qquad \mu \in \mathcal{M}(\mathbb{S}^d). \tag{3.3}$$

We recall from [58] the following Frostman-type result which deals with existence and uniqueness of the s-extremal measure on A associated with Q and its characterisation in terms of weighted potentials. The potential theory used in the context of this survey can be found in G. Björck [16] (dealing with Riesz potential with negative exponent), E. B. Saff and V. Totik [113] (logarithmic external field problem in the plane), N. S. Landkof [91] (Riesz and logarithmic potential and general reference) and, in particular, for Riesz external field problems N. V. Zorič [130, 131].

Proposition 3.1. *Let $0 < s < d$.*[3] *For the minimal energy problem on $\mathbb{S}^d$ with external field Q the following properties hold:*

(a) *$W_{Q,s}$ is finite.*

(b) *There exists a unique s-extremal measure $\mu_{Q,s} \in \mathcal{M}(\mathbb{S}^d)$ associated with Q. Moreover, the support $S_{Q,s} := \operatorname{supp}(\mu_{Q,s})$ of this measure is contained in the compact set $E_M := \{\mathbf{x} \in \mathbb{S}^d : Q(\mathbf{x}) \leq M\}$ for some $M > 0$.*

(c) *The measure $\mu_{Q,s}$ satisfies the variational inequalities*

$$U_s^{\mu_{Q,s}}(\mathbf{x}) + Q(\mathbf{x}) \geq F_{Q,s} \quad q.e.\ on\ \mathbb{S}^d, \tag{3.4}$$

$$U_s^{\mu_{Q,s}}(\mathbf{x}) + Q(\mathbf{x}) \leq F_{Q,s} \quad everywhere\ on\ S_{Q,s}, \tag{3.5}$$

where

$$F_{Q,s} := W_{Q,s} - \int Q(\mathbf{x}) \mathrm{d}\mu_{Q,s}(\mathbf{x}). \tag{3.6}$$

(d) *Inequalities* (3.4) *and* (3.5) *completely characterise the s-extremal measure μ_Q in the sense that if $\nu \in \mathcal{M}(\mathbb{S}^d)$ is a measure with finite s-energy such that for some constant C we have*

$$U_s^{\nu}(\mathbf{x}) + Q(\mathbf{x}) \geq C \quad q.\ e.\ on\ \mathbb{S}^d, \tag{3.7}$$

$$U_s^{\nu}(\mathbf{x}) + Q(\mathbf{x}) \leq C \quad everywhere\ on\ \operatorname{supp}(\nu), \tag{3.8}$$

then $\nu = \mu_{Q,s}$ and $C = F_{Q,s}$.

We recall that a property is said to hold *quasi everywhere* ("q. e." for short), if it holds outside of a set of zero capacity.

Observe that, if the external field Q is continuous on $\mathbb{S}^d$, then the inequality in (3.7) holds everywhere on $\mathbb{S}^d$.

3.3. The distribution of minimal logarithmic and Riesz energy points

Let A be an infinite compact set $A \subset \mathbb{R}^p$ with Hausdorff dimension d having finite logarithmic or Riesz s-energy and $Q \equiv 0$. Classical potential theory implies that the minimal energy N-point configurations X_N^* on A are distributed according to the unique equilibrium measure μ_A on A and the discrete measures $\mu_{X_N^*}$ will have μ_A as a weak limit. Except for the unit sphere $\mathbb{S}^d$, this will be **not** the normalised uniform measure on A. This phenomenon can be observed particularly well in the case of the circular torus $A = \mathbb{T}^2$. D. P. Hardin, E. B. Saff and H. Stahl [75] showed that the logarithmic equilibrium measure $\mu_{\mathbb{T}}$ on the torus $\mathbb{T}^2$ is supported on a proper subset of the surface part with positive curvature. (The precise form of the logarithmic measure on the torus is still unknown.) Moreover, it could be shown in [34, 35] that the support of the Riesz s-equilibrium measure

[3] A similar result holds for the logarithmic case.

on $\mathbb{T}$ for small $s > 0$ is a proper subset of the torus. On the other hand, it is well-known (cf. Landkof [91]) that in the harmonic case ($s = d - 1$) the support of the equilibrium measure is always all of A. In general, the equilibrium measure μ_A will be supported on part of the *outer boundary* (i.e., the boundary of A shared with the unbounded component of the ambient space $\mathbb{R}^p$) if the energy kernel is strictly superharmonic, all of the outer boundary if the kernel is harmonic and supported on (part of) the volume as well if the kernel is strictly subharmonic. Consequently, the minimal energy points are forced out of the volume (if there is one) onto the outer boundary in the first case, spread out over all of the outer boundary as their number increases (the "interior" becomes effectively field-free, "Faraday-cage effect") and in part injected into the volume (if there is one) to decrease the discrete energy in the last case. This is the potential theoretic regime of D. P. Hardin and E. B. Saff's *Poppy-seed Bagel Theorem* where the poppy seeds represent the minimal energy points and the Bagel is an interesting manifold. The intuition is that in this regime $s = \log$ or $0 < s < d$ (d the Hausdorff dimension of A) global effects dominate (points interact as if they are subject to long-range forces and the range increases as s becomes smaller). In the hypersingular case $s > d$, local effects dominate (points interact as if they are responding to a short range force). Both kind of interaction intermingle when $s = d$.

The energy integral diverges for every probability measure supported on $\mathbb{S}^d$ in the hypersingular case $s \geq d$. Techniques from geometric measure theory were applied to obtain that the limiting distribution of the minimal Riesz s-energy N-point sets on A (even asymptotically s-energy minimising would suffice) is uniformly distributed with respect to the d-dimensional Hausdorff measure $\mathcal{H}_d$; i.e.,

$$\mu_{X_N^*} \rightharpoonup \frac{\mathrm{d}\mathcal{H}_d\big|_A}{\mathcal{H}_d(A)} \qquad N \to \infty,$$

where X_N^* are minimal N-point Riesz s-energy configurations on A ($s > \dim(A)$ and $\mathcal{H}_d(A) > 0$) and, say, A is a rectifiable set (see [21] and earlier work [20, 73, 74]). It should be noted that in the case $s = \dim(A)$ an additional regularity assumption on A is required. The paper [21] also shows analogue results for weighted Riesz s-energy

$$\sum_{\substack{i=1 \\ i \neq j}}^{N} \sum_{j=1}^{N} \frac{w(\mathbf{x}_i, \mathbf{x}_j)}{\|\mathbf{x}_i - \mathbf{x}_j\|^s},$$

where w is a CPD weight function (CPD stands for (almost everywhere) continuous and positive on the diagonal). We remark that the case $s = d$ for $\mathbb{S}^d$ has already been dealt with in [64] using results in [89]. Furthermore, [42] showed that the s-equilibrium measures on A for $0 < s < d$ converge to the normalised d-dimensional Hausdorff measure restricted to A under rather general assumptions on A. We remark that I. Pritzker [108] studied the discrete approximation of the equilibrium measure on a compact set $A \subset \mathbb{R}^p$, $p \geq 2$, with positive s-capacity by means of points which do not need to lie inside A. He also obtained discrepancy estimates in the harmonic case.

Summarising, for $-2 < s < 0$, $s = \log$ and $s > 0$, the (asymptotically) s-energy minimising N-point configuration on $\mathbb{S}^d$ are uniformly distributed with respect to the surface area measure σ_d.

In certain applications one would prefer to generate well-distributed N-point sets on a compact d-rectifiable set in $\mathbb{R}^p$ which have a prescribed non-uniform asymptotic distribution ρ with respect to $\mathcal{H}_d$ as $N \to \infty$. It is shown in [76] that such points can be obtained by minimising the energy of N points on A interacting via a weighted power law potential $w(\mathbf{x}, \mathbf{y})/\|\mathbf{x} - \mathbf{y}\|^s$, where $s > d$ and $w(\mathbf{x}, \mathbf{y}) := [\rho(\mathbf{x})\rho(\mathbf{y})]^{-s/(2d)}$; furthermore, such point sets are "quasi-uniform" in the sense that the ratio of the covering radius (fill radius) to the separation distance is uniformly bounded in N. As mentioned in the introduction, quasi-uniformity is crucial for a number of numerical methods (cf. [62, 92, 115]). S. V. Borodachov, D. P. Hardin and E. B. Saff show in [22] that it suffices to use a varying truncated weight $w(\mathbf{x}, \mathbf{y})\, \Phi(\|\mathbf{x} - \mathbf{y}\|/r_N)$, thus keeping only those pairs of points in the energy sums that are located at a distance of at most $r_N = C_N\, N^{-1/d}$ from each other. (The positive sequence (C_N) tends to ∞ as slowly as desired.) In this way, under suitable assumptions, the complexity of the energy computation can be greatly reduced leading to order $N\, C_N^d$ computations for generating "low energy" N-point approximations.

A point charge approaching the sphere subject to the same law of interaction as the points on the sphere affects the charge distribution on the sphere. If the point charge is sufficiently close to the sphere, it will free up a part of charges. The papers [26, 32, 33], in particular, provide explicit representations of the charge distributions due to a canonical single external charge. They also address a question attributed to A. A. Gonchar, namely to find a critical distance of the external field generating charge from the sphere surface so that the support of the s-extremal measure on $\mathbb{S}^d$ for this external field is just all of the sphere. In the harmonic case this distance is characterised by a zero of a class of polynomials dubbed Gonchar polynomials. (The golden ratio and the plastic number play a prominent role for $d = 2$ and $d = 4$.)

3.4. Asymptotic expansion of minimal Riesz energy

Let $s > 0$. The leading term of the asymptotic expansion for a compact set A in $\mathbb{R}^p$ is well-understood if A has positive s-capacity (i.e., finite Riesz s-energy). This is the *potential-theoretic regime*. A standard argument from classical potential theory yields that the positive quantities $N(N-1)/\mathcal{E}_s(A; N)$ form a monotonically decreasing sequence. The limit $\operatorname{diam}_s(A)$, called the *generalised transfinite diameter of* A, is equal to the s-capacity of A (cf. [107]). Thus, the leading term of $\mathcal{E}_s(A; N)$ grows like N^2 as $N \to \infty$ and the leading coefficient is given by the Riesz s-energy of A, or equivalently, by the reciprocals of the s-capacity and transfinite diameter of A:

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A; N)}{N^2} = W_s(A) = \frac{1}{\operatorname{cap}_s(A)} = \frac{1}{\operatorname{diam}_s(A)}. \tag{3.9}$$

For $0 < s < d$, the Riesz s-energy of the sphere $\mathbb{S}^d$ has the explicit form

$$W_s(\mathbb{S}^d) = \mathcal{I}_s[\sigma_d] = 2^{d-1-s} \frac{\Gamma((d+1)/2)\, \Gamma((d-s)/2)}{\sqrt{\pi}\, \Gamma(d - s/2)}, \tag{3.10}$$

expressed in terms of the Gamma function Γ. By identifying $W_s(\mathbb{S}^d)$ with the analytic continuation of the right-hand side above to the complex s-plane[4], we can define the Riesz s-energy of $\mathbb{S}^d$ for Riesz parameter s for which the s-energy integral (3.2) is $+\infty$ for every Borel probability measure on $\mathbb{S}^d$. The combined effort of [27, 89, 109, 127, 128] resulted in the following bounds for the second term of the minimal energy asymptotics[5]: There exist constants $c, C > 0$ depending only on $d \geq 2$ and $0 < s < d$ such that

$$c\, N^{1+s/d} \leq \mathcal{E}_s(\mathbb{S}^d; N) - W_s(\mathbb{S}^d)\, N^2 \leq C\, N^{1+s/d}, \qquad N \geq 2.$$

This estimates give the correct order of growth and sign for the second-order term. It is an open problem if the sequence $\big(\mathcal{E}_s(\mathbb{S}^d; N) - W_s(\mathbb{S}^d)\, N^2\big)/N^{1+s/d}$ has a limit as $N \to \infty$. A. A. Berezin [15] used a semicontinuum approach (a classical method from solid state physics, cf. [65]) to derive the plausible asymptotics

$$\mathcal{E}_s(\mathbb{S}^2; N) \approx N^2 \frac{2^{1-s}}{2-s}\left[1 - (n/N)^{1-s/2}\right] + N^{1+s/2}\left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} \times \left\{\frac{6}{1^s} + \frac{6}{(\sqrt{3})^s} + \frac{6}{2^s} + \frac{12}{(\sqrt{7})^s} + \frac{6}{3^s} + \frac{6}{(2\sqrt{3})^s} + \frac{12}{(\sqrt{13})^s} + \cdots\right\}$$

based on the assumptions that a typical point (and most of its immediate neighbours) in a minimal Riesz s-energy N-point configuration on $\mathbb{S}^2$ gives rise to a hexagonal Voronoi cell (sixfold symmetry) whereas the defects according to the curved surface of the sphere will have no significant role for the second term in the asymptotics. Thus the contribution to the Riesz s-energy due to a typical point can be split into a local part which uses n nearest neighbour points from a suitably adjusted (thus the geometric scaling factor) flat hexagonal lattice and a distant part where the $N-n$ points are replaced by the continuous uniform distribution. The expression in curly braces gives the formal series expansion of the Epstein zeta function of the hexagonal lattices truncated to include only the $n-1$ shortest distances in the lattice[6]. (In order to get a non-trivial expansion, n has to grow weakly to infinity. The paper [15] mentions some numerical experiments for slowly growing n but a rigorous investigation has not been undertaken.) The discussion leading to Conjecture 1 below suggests that the semicontinuum approach would also work for $d = 4$, 8 and 24. In general, it is not clear what local approximation should be used.

For a compact set A in $\mathbb{R}^p$ of vanishing s-capacity, the leading term is rather well-understood. In the *(strictly) hypersingular regime* $s > d$, where d is the Hausdorff dimension of A, Hardin and Saff [74] (for rectifiable d-dimensional manifolds including the

[4]The meromorphic function $W_s(\mathbb{S}^d)$, which appears in the conjecture for the asymptotics in the hypersingular case, has simple poles (finitely many if d is even and infinitely many if d is odd). The effect of this dichotomy on the asymptotic expansion of the minimal Riesz s-energy is completely open for $d \geq 2$ and leads to $\log N$ terms for the unit circle, cf. [36].

[5]Similar estimates but with negative constants c, C holds for the sum of generalised distances (i.e., $-2 < s < 0$); cf. [1, 2, 3, 13, 81, 120, 121] and culminating in [127, 128].

[6]Indeed, the first few most frequent distances in a putative minimal energy configuration emulate remarkably well the first few distances in a hexagonal lattice (cf., in particular, [38, Figure 1]).

sphere $\mathbb{S}^d$) and Borodachov, Hardin and Saff [21] (for infinite compact d-rectifiable sets[7]) established for a large class of compact sets A the existence of a constant $C_{s,d}$ such that[8]

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A;N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d(A)]^{s/d}}. \tag{3.11}$$

This result is also referred to as the *Poppy-seed Bagel Theorem* because of its interpretation for distributing points on a torus.[9] Here and hereafter, $\mathcal{H}_d$ denotes the d-dimensional Hausdorff measure in $\mathbb{R}^p$ normalised such that the d-dimensional unit cube has $\mathcal{H}_d$-measure 1. Except for one-dimensional sets (when $C_{s,1}$ is twice the Riemann zeta function at s, see [97, Thm. 3.1]), the precise value of $C_{s,d}$ is not known. Its determination is a challenging open problem. The significance and difficulty of obtaining $C_{s,d}$ is due to the deep connection to densest packings. In [20] it is shown that $C_{s,d}$ is tied to the largest sphere packing density Δ_d in $\mathbb{R}^d$ and the best-packing distance δ_N^* of N-points on $\mathbb{S}^d$ by means of the limit relations[10]

$$\lim_{s\to\infty} [C_{s,d}]^{-1/s} = 2\left[\frac{\Delta_d}{\mathcal{H}_d(\mathbb{B}^d)}\right]^{1/d} = \lim_{N\to\infty} N^{1/d}\delta_N^*. \tag{3.12}$$

(Here, $\mathcal{H}_d(\mathbb{B}^d)$ is the volume of the unit ball in $\mathbb{R}^d$.) We recall that Δ_d is only known for three cases: $\Delta_1 = 1$, $\Delta_2 = \pi/\sqrt{12}$ (A. Thue in 1892 and L. Fejes Tóth [61]) and $\Delta_3 = \pi/\sqrt{18}$ (Kepler conjecture proved by Hales [72]). The connection to (regular) lattices is evident in the upper estimate of the constant $C_{s,d}$ in terms of the Epstein zeta function $\zeta_\Lambda(s)$ of a lattice Λ in $\mathbb{R}^d$ which can be obtained by considering the Riesz s-energy of the $N = n^d$ points of the rescaled lattice $\frac{1}{n}\Lambda$ lying in the fundamental parallelotope Ω of Λ and which implies that $\mathcal{E}_s(\Omega;N) \le n^{d+s}\,\zeta_\Lambda(s) = N^{1+s/d}\,\zeta_\Lambda(s)$ and thus for $s > d$ (cf. [36, Prop. 1]),

$$C_{s,d} \le \min_{\Lambda} |\Lambda|^{s/d}\,\zeta_\Lambda(s), \tag{3.13}$$

where the minimum is extended over all lattices Λ in $\mathbb{R}^d$ with positive covolume $|\Lambda|$. Because of (3.12), the sharpness of this inequality touches on questions regarding densest lattice sphere packings and which (if so) solve the sphere packing problem. For $1 \le d \le 8$ and $d = 24$, the unique densest lattice in $\mathbb{R}^d$ up to scaling and isometries is the root lattice A_1, A_2, A_3, D_4, D_5, E_6, E_7, E_8 and the Leech lattice, respectively (cf. [50]). Among those the hexagonal lattice A_2 in $\mathbb{R}^2$, the E_8 root lattice in $\mathbb{R}^8$ and the Leech lattice in $\mathbb{R}^{24}$ are conjectured to be optimal for all values of $s > d$ (*universally optimal*) whereas the remaining lattices are provably not universally optimal (cf. [49, 51]). See [114] for local optimality results and [55] for improvements. Montgomery [100] proved that the hexagonal lattice is universally optimal among all lattices in $\mathbb{R}^2$ (which is weaker than universal optimality among all periodic point configurations). Cohn and Elkis [48] conjectured that

[7] A d-rectifiable set is the Lipschitz image of a bounded set in $\mathbb{R}^d$.

[8] The boundedness of $\mathcal{E}_s(\mathbb{S}^d;N)/N^{1+s/d}$ has already been shown in [89].

[9] Cf. `http://news.vanderbilt.edu/2004/11/the-poppy-seed-bagel-theorem-59497/`

[10] Indeed, one can recasts this relation as $\Delta_d = \lim_{s\to\infty}\lim_{N\to\infty}\left[\mathcal{E}_s(\frac{1}{2}\mathbb{B}^d;N)/N^{1+s/d}\right]^{-d/s}$.

E_8 and the Leech lattice solve the sphere packing problem in their dimension. It is generally expected that for sufficiently large d, lattice packings are not densest packings and [125] suggests that best-packings are highly "disordered" as $d \to \infty$. This motivates the following conjecture[11].

Conjecture 1 ([36]). *For $d = 2$, 4, 8 and 24, one has $C_{s,d} = |\Lambda_d|^{s/d} \zeta_{\Lambda_d}(s)$, where Λ_d denotes, respectively, the hexagonal lattice A_2, the root lattices D_4 and E_8, and the Leech lattice.*

We remark that in [38] very coarse lower and upper bounds are obtained for $\mathcal{E}_s(\mathbb{S}^d; N)$. Although, the leading term has the wrong coefficient, curiously, the second order term in the lower bound has the conjectured form. As a consequence of these bounds, [38] could give the estimates

$$\frac{d}{s-d}\left[\frac{1}{2}\frac{\Gamma((d+1)/2)\,\Gamma(1+(s-d)/2)}{\sqrt{\pi}\,\Gamma(1+s/2)}\right]^{s/d} \le \frac{C_{s,d}}{[\mathcal{H}_d(\mathbb{S}^d)]^{s/d}} \le \left[\frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)(1-d/s)}\right]^{s/d},$$

valid for $s > d \ge 2$ and $(s-d)/2$ not an integer.

In the *hypersingular case* $s = d$, where d is the Hausdorff dimension of the compact set A in $\mathbb{R}^p$, much more can be said. For a wide family of compact sets A, this boundary case can still be treated using a suitably renormalised energy integral and a limit process as s approach d from below (i.e., from the potential theoretic regime), cf. [42]. It has been known since [89] that the leading term of $\mathcal{E}_d(\mathbb{S}^d; N)$ grows like $N^2 \log N$ and

$$\lim_{N\to\infty} \frac{\mathcal{E}_d(\mathbb{S}^d; N)}{N^2 \log N} = \frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)} = \frac{1}{d}\frac{\omega_{d-1}}{\omega_d} = \frac{1}{d}\frac{\Gamma((d+1)/2)}{\sqrt{\pi}\,\Gamma(d/2)}. \tag{3.14}$$

The best estimates so far for the second-order term has been obtained recently in [38],

$$-c(d)\,N^2 + \mathcal{O}(N^{2-2/d}\log N) \le \mathcal{E}_d(\mathbb{S}^d; N) - \frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)}\,N^2 \log N \le \frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)}\,N^2 \log\log N + \mathcal{O}(N^2)$$

as $N \to \infty$, where the constant $c(d)$ is given by

$$c(2) = 1/2, \qquad c(d) := \frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)}\left\{1 - \log\frac{\mathcal{H}_d(\mathbb{B}^d)}{\mathcal{H}_d(\mathbb{S}^d)} + d\,[\psi(d/2) - \psi(1) - \log 2]\right\} > 0.$$

(Recall, that $\psi = \Gamma' / \Gamma$ denotes the digamma function.) The paper [38] conjectures, based on a limit process $s \to d$ in Conjecture 2, that the correct order of the second term is N^2 and provides a limit relation for the constant which is made explicit for the case $d = 2$.

[11] The conjecture for $d = 2$ appeared in [89].

Higher Order Terms – Complete Asymptotic Expansions – Fundamental Conjecture

Almost nothing is known about higher-order terms of the asymptotics of the minimal Riesz s-energy except for the unit circle. As the N-th roots of unity are universally optimal[12], the complete asymptotic expansion can be obtained by direct computation of the Riesz s-energy $\mathcal{L}_s(N)$ of the N-th roots of unity, see [34] (and cf. [37] for geodesic distance). Indeed, for $s \in \mathbb{C}$ with $s \neq 0, 1, 3, 5, \ldots$ and fixed $p = 1, 2, 3, \ldots$, one has[13]

$$\begin{aligned} \mathcal{L}_s(N) = W_s(\mathbb{S}^1)\, N^2 + \frac{2\,\zeta(s)}{(2\pi)^s}\, N^{1+s} + \sum_{n=1}^{p} \alpha_n(s) \frac{2\,\zeta(s-2n)}{(2\pi)^s}\, N^{1+s-2n} \\ + \mathcal{O}_{s,p}(N^{-1+\Re s-2p}) \qquad \text{as } N \to \infty, \end{aligned} \tag{3.15}$$

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

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

(Explicit formulas in terms of generalised Bernoulli polynomials $B_n^{(\alpha)}(x)$ are given in [37].) This expansion has two noteworthy features: (*i*) the fact that the expansion is valid for complex s and (*ii*) the essential role played by the Riemann zeta function. The former gives a unifying picture of the coefficients of the asymptotic terms. They are best understood as functions in the complex s-plane (*principle of analytic continuation*)[14]. The latter explains how a logarithmic term arises as s tends to one of the exceptional cases $1, 3, 5, \ldots$, when the argument of one of the Riemann zeta functions approaches the simple pole at 1 and the associated term needs to be matched with the N^2-term to offset the simple pole of $W_s(\mathbb{S}^1)$.

By combining the results for the potential theoretic and the hypersingular regime, the principle of analytic continuation motivates the following fundamental conjecture.

Conjecture 2 (cf. [38]). *Let $d \geq 2$. Then for $0 < s < d + 2$ with $s \neq d$,*

$$\mathcal{E}_s(\mathbb{S}^d; N) = W_s(\mathbb{S}^d)\, N^2 + \frac{C_d(s)}{[\mathcal{H}_d(A)]^{s/d}}\, N^{1+s/d} + o(N^{1+s/d}) \qquad \text{as } N \to \infty,$$

where $W_s(\mathbb{S}^d)$ is the analytic continuation of the right-hand side of (3.10) *and $C_d(s)$ is the analytic continuation of $C_{s,d}$ in* (3.11)*. Furthermore, for $d = 2, 4, 8$ and 24, $C_d(s)$ is the analytic continuation of $|\Lambda_d|^{s/d}\, \zeta_{\Lambda_d}(s)$, where Λ_d is given in Conjecture 1.*

[12]For $s \geq -1$ (and $s \neq 0$) a convexity argument can be applied to get optimality for Riesz s-energy (cf. [3, 60, 63]). The much more general result [49, Theorem 1.2] provides optimality for $s > -2$.

[13]The precise formulas for finite $N \geq 2$ are obtained in [29].

[14]This principle breaks down when the perfectly symmetric unit circle is replaced by some other smooth closed curve Γ. Then the s-equilibrium measure on Γ is not the normalised arc-length measure for each $0 < s < 1$ which plays a role in the characterisation of the coefficient of N^2 in the hypersingular regime $1 < s < 3$; cf. [19].

3.5. Asymptotic expansion of logarithmic energy

The leading term of the asymptotic expansion for a compact set A in $\mathbb{R}^p$ with positive logarithmic capacity (i.e. finite logarithmic energy) follows from classical potential theory. It should be noted that (cf. [23])

$$\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{E}_s(A;N)\Big|_{s=0^+} = \mathcal{E}_{\log}(A;N), \qquad N \geq 2. \tag{3.16}$$

For the unit sphere $\mathbb{S}^d$ one has in particular that

$$\lim_{N\to\infty} \frac{\mathcal{E}_{\log}(\mathbb{S}^d;N)}{N^2} = W_{\log}(\mathbb{S}^d) = \log \frac{1}{\mathrm{cap}_{\log}(\mathbb{S}^d)},$$

where the *logarithmic energy of* $\mathbb{S}^d$ is given by

$$W_{\log}(\mathbb{S}^d) = \frac{\mathrm{d}W_s(\mathbb{S}^d)}{\mathrm{d}s}\Big|_{s=0^+} = \log\frac{1}{2} + \frac{1}{2}\left[\psi(d) - \psi(d/2)\right].$$

Here, ψ is the digamma function. From an averaging argument using equal-area partitions of $\mathbb{S}^d$ (cf. [93]) and bounds of G. Wagner [128] and the first author [28] it follows that

$$\mathcal{E}_{\log}(\mathbb{S}^d;N) = W_{\log}(\mathbb{S}^d)\,N^2 - \frac{1}{d}\,N\log N + \mathcal{O}(N), \qquad N\to\infty.$$

Relation (3.16) and Conjecture 2 provide the basis for the following conjecture proposed in [38].

Conjecture 3. *For $d = 2$, 4, 8 and 24,*

$$\mathcal{E}_{\log}(\mathbb{S}^d;N) = W_{\log}(\mathbb{S}^d)\,N^2 - \frac{1}{d}\,N\log N + C_{\log,d}\,N + o(N) \qquad \text{as } N\to\infty,$$

where

$$C_{\log,d} = \frac{1}{d}\log\frac{\mathcal{H}_d(\mathbb{S}^d)}{|\Lambda_d|} + \zeta'_{\Lambda_d}(0).$$

For $d = 2$ one has

$$C_{\log,2} = 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.05560530494339251850\cdots < 0.$$

For more details, we refer to [38].

3.6. Numerical integration from the energy point of view

The reproducing kernel Hilbert space approach (cf. Section 2) allows to write the squared worst-case error as

$$\sum_{i=1}^{N}\sum_{j=1}^{N} \mathrm{K}(\mathbf{x}_i,\mathbf{x}_j) - \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} \mathrm{K}(\mathbf{x},\mathbf{y})\,\mathrm{d}\sigma_d(\mathbf{x})\mathrm{d}\sigma_d(\mathbf{y})$$

which can be interpreted as K-energy of the node set $\{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$ of the QMC method. The energy kernel here is a reproducing kernel for $H^s(\mathbb{S}^d)$. Optimal nodes then can be obtained by solving a minimal energy problem for this kernel. In [30] and [31] it is shown how the distance kernel

$$\mathrm{K}_{\mathrm{gd}}^{(s)}(\mathbf{x},\mathbf{y}) := 2W_{d-2s}(\mathbb{S}^d) - \|\mathbf{x}-\mathbf{y}\|^{2s-d}, \qquad \mathbf{x},\mathbf{y}\in\mathbb{S}^d, \tag{3.17}$$

arises in a natural way as a reproducing kernel for $H^s(\mathbb{S}^d)$ for s in $(d/2, d/2+1)$. Wagner's bounds on the sum of generalised distances ([127, 128]) yield that a sequence of N-point maximises of the generalised sum of distances with power $2s-d$ and $N\to\infty$ form a QMC design sequence for $H^s(\mathbb{S}^d)$, $d/2 < s < d/2+1$; cf. [40]. For $s \geq d/2+1$, an equivalent norm on $H^s(\mathbb{S}^d)$ can be chosen so that the corresponding reproducing kernel is essentially a distance kernel with power $2s-d$. However, the kernel function r^α (for $\alpha>0$) is only conditionally positive definite, whereas a reproducing kernel is always positive definite (in the sense of Schoenberg [116]). This fact is taken care of by introducing a logarithmic factor, if $s-d/2$ is a positive integer, and a polynomial correction in general. In [40] the correction term simply flips the negative signs whereas in [30] the correction term is induced by the considered integral representation of the reproducing kernel. Such a correction term gets annihilated when the search for optimal QMC designs for $H^s(\mathbb{S}^d)$, $s\in(d/2+L, d/2+1+L)$, L a positive integer, is restricted to spherical L-designs. In that case it suffices to minimise the energy functional (cf. [40])

$$[\mathrm{wce}_{H^s}(X_{N,L})]^2 = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}(-1)^{L+1}\,\|\mathbf{x}_{i,L}-\mathbf{x}_{j,L}\|^{2s-d} - (-1)^{L+1}W_{d-2s}(\mathbb{S}^d)$$

subject to the condition that the node set $X_{N,L}=\{\mathbf{x}_{1,L},\ldots,\mathbf{x}_{N,L}\}\subset\mathbb{S}^d$ is a spherical L-design. Note that L depends on s and is fixed, once s is fixed. The value L is "small" in the following sense: a QMC method with a more regular (in the sense of spherical designs) node set is more suitable for integrating functions from a smoother function space $H^s(\mathbb{S}^d)$. But regularity beyond a critical order will not improve the worst-case error bound; cf. optimal order (2.37). We remark that the Cui and Freeden kernel [56]

$$\mathrm{K}_{\mathrm{CF}}(\mathbf{x},\mathbf{y}) := 2 - 2\log\Big(1+\frac{1}{2}\,\|\mathbf{x}-\mathbf{y}\|\Big), \qquad \mathbf{x},\mathbf{y}\in\mathbb{S}^2,$$

can be interpreted as reproducing kernel for $H^{3/2}(\mathbb{S}^2)$ as observed in [118] and the minimising K_{CF}-energy point configurations give rise to a QMC design sequence for $H^{3/2}(\mathbb{S}^2)$.

Recently, Choirat and Seri [45, 46] derived the analogue kernel for d-spheres. The corresponding minimising configurations then form QMC design sequences for $H^{(d+1)/2}(\mathbb{S}^d)$. In the case, when $H^s(\mathbb{S}^d)$, with $d/2 < s < d/2+1$, is equipped with the reproducing kernel $\mathrm{K}_{\mathrm{gd}}^{(s)}$ from (3.17), a limiting process yields that (cf. [41])

$$\lim_{s\to(d/2)^+} \frac{\left[\mathrm{wce}_{H^s}(X_N)\right]^2 - \frac{1}{N}}{2s-d} = \frac{1}{N^2}\sum_{\substack{i=1\\ i\neq j}}^{N}\sum_{j=1}^{N} \log\frac{1}{\|\mathbf{x}_i-\mathbf{x}_j\|} - V_{\log}(\mathbb{S}^d)$$

for any N-point set $X_N = \{\mathbf{x}_1,\ldots,\mathbf{x}_N\} \subset \mathbb{S}^d$. This suggests that the function space $H^{d/2}(\mathbb{S}^d)$ (which is not a reproducing kernel Hilbert space as it cannot be continuously embedded into the space of continuous functions) is associated with the logarithmic kernel, in a natural way. In that sense the logarithmic energy of an N-point set can be understood as a limit of worst-case errors.

Stolarsky's invariance principle (cf. [121] and [31]) states that the sum of all mutual distances (a Riesz energy with Riesz parameter -1) and the spherical cap L^2-discrepancy

$$D_{L^2}(X_N) := \left(\int_0^\pi \int_{\mathbb{S}^d} \left| \frac{1}{N}\sum_{\mathbf{y}\in X_N} \mathbb{1}_{\mathbf{x}\in C(\mathbf{y},\theta)} - \sigma_d(C(\mathbf{z};\theta))\right|^2 \mathrm{d}\sigma_d(\mathbf{z})\,\sin\theta \mathrm{d}\theta\right)^{1/2}$$

is constant regardless of the choice of the node set X_N on $\mathbb{S}^d$. This principle connects in a very direct way the three areas optimal energy (maximising the sum of distances), uniform distribution (spherical cap L^2-discrepancy) and numerical integration (interpretation of the double integral minus the double sum as worst-case error for functions in $H^{(d+1)/2}(\mathbb{S}^d)$ provided with the distance kernel); i.e.,

$$\frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\|\mathbf{x}_i-\mathbf{x}_j\| + \frac{1}{C_d}\left[D_{L^2}(X_N)\right]^2 = \int_{\mathbb{S}^d}\int_{\mathbb{S}^d}\|\mathbf{x}-\mathbf{y}\|\,\mathrm{d}\sigma_d(\mathbf{x})\,\mathrm{d}\sigma_d(\mathbf{y}).$$

Furthermore, it provides a convenient way of computing the discrepancy $D_{L^2}(X_N)$ and it shows that for the particular setting of numerical integration the spherical cap L^2-discrepancy is a constant multiple of the worst-case error. The paper [30] gives an extension of this principle to general powers of the distance (risen to the power $2s-d$) involving the generalised spherical L_2-discrepancy

$$\int_0^\pi \int_{\mathbb{S}^d} \left|\Delta_{X_N,\beta}(\mathbf{z};\cos\theta)\right|^2 \mathrm{d}\sigma_d(\mathbf{z})\sin\theta\mathrm{d}\theta,$$

for the local discrepancy function (with smoothness index $s=\beta+(d-1)/2$)

$$\Delta_{X_N,\beta}(\mathbf{z};t) := \frac{1}{N}\sum_{\mathbf{x}\in X_N}(\mathbf{x}\cdot\mathbf{z}-t)_+^{\beta-1} - \int_{\mathbb{S}^d}(\mathbf{y}\cdot\mathbf{z}-t)_+^{\beta-1}\,\mathrm{d}\sigma_d(\mathbf{y}).$$

The paper [67] discusses further connections between energy and discrepancy.

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