POINT SETS OF MINIMAL ENERGY

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Dedicated to Harald Niederreiter on the occasion of his 70th birthday

1. Introduction

Different types of constructions have been used to find "good" configurations of N points $X_N = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ on a manifold M, especially the unit sphere $\mathbb{S}^d$ in $\mathbb{R}^{d+1}$. Of course the construction depends on what quantitative measure is used for the configuration. In this survey we will discuss two such measures and their interrelation. We will mostly emphasise on the discussion of the latest results and developments in the context of minimal energy point configurations.

Discrepancy of a point set X_N is given by

$$D(X_N) = \sup_C \left| \frac{1}{N} \sum_{n=1}^{N} \chi_C(\mathbf{x}_n) - \sigma(C) \right|, \tag{1.1}$$

where the supremum is extended over a system of Riemann-measurable subsets of M (for instance all spherical caps in the case of the sphere), χ_C denotes the indicator function of the set C, and σ is a normalised measure on M (the normalised surface area measure in the case of the sphere). This is a classical measure for the quality of a finite point distribution approximating a measure, which has been studied intensively in the theory of uniform distribution (cf. [20, 30]) as well as in the theory of irregularities of distribution (cf. [2]).

Energy of a point set X_N is defined as

$$E_s(X_N) = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \|\mathbf{x}_i - \mathbf{x}_j\|^{-s} \tag{1.2}$$

for a positive real parameter s. This is a discrete version of the energy integral

$$I_s(\mu) = \iint\limits_{M \times M} \|\mathbf{x} - \mathbf{y}\|^{-s} \, d\mu(\mathbf{x}) \, d\mu(\mathbf{y}). \tag{1.3}$$

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The discrete distributions of point sets X_N^* minimising E_s,

$$\nu_N = \frac{1}{N}\sum_{n=1}^{N} \delta_{\mathbf{x}_n^*},$$

are studied then for $N \to \infty$. The minimisation of such discrete energy expressions is a problem attributed to Fekete. Minimal energy point sets are thus called Fekete-points. The case $s < \dim(M)$ can be investigated by methods from classical potential theory (cf. [31]). In this case the unique minimiser $\mu_M^{(s)}$ of $I_s(\mu)$ is the weak limit of the measures ν_N (cf. [31]). For $s \geq \dim(M)$, the situation changes completely. The corresponding energy integral diverges for all probability measures. Techniques from geometric measure theory could be applied in [6, 7, 26, 27] to show that the limiting distribution $\mu_M^{(s)}$ of the minimal energy distributions is the normalised $\dim(M)$-dimensional Hausdorff measure on M, if M is rectifiable.

2. Generalised energy and uniform distribution on the sphere

Using mutually repelling forces on N particles to distribute them on a surface M is a rather compelling idea. The motivation for this could be taken from physical experiments, where electric charges distribute themselves in a way that minimises the sum of the mutual energies (1.2) for $s = \dim(M) - 1$ (cf. [21, 38]). The study of the precise distribution of the charges is the subject of classical potential theory (cf. [31]), which shows that the energy integral (1.3) has a unique minimiser amongst all Borel probability measures supported on M; in the case $s = \dim(M) - 1$ this is the harmonic measure on M. The minimising measure depends highly on the curvature of the surface and the value of the parameter s, and thus differs from the surface measure, except for surfaces with high symmetry, like the sphere. For values of $s \neq \dim(M) - 1$ (and $\dim(M) \neq 2, 3$), there is no physical experiment, which can be used to describe the charge distribution, nevertheless, the intuition and the result remain the same – there exists a unique equilibrium measure depending on s on M – if $s < \dim(M)$.

In the following we will study the general potential theoretic situation of a strictly positive definite continuous kernel $g : [-1, 1) \to \mathbb{R}$ (cf. [31]). Here a function g is called positive definite, if the *energy integral*

$$I_g(\mu) = \iint\limits_{\mathbb{S}^d \times \mathbb{S}^d} g(\langle \mathbf{x}, \mathbf{y}\rangle)\, d\mu(\mathbf{x})\, d\mu(\mathbf{y}) \geq 0, \tag{2.1}$$

for all signed Borel measures μ on $\mathbb{S}^d$, and $I_g(\mu)$ is finite for at least one Borel measure μ. It is called *strictly* positive definite, if equality in (2.1) only occurs for the zero measure.

Let g be given by its Laplace expansion (cf. [34])

$$g(t) = \sum_{n=0}^{\infty} a_n Z(d, n) P_n^{(d)}(t) \tag{2.2}$$

in terms of the Legendre-Gegenbauer polynomials $P_n^{(d)}$. These are the orthogonal polynomials with respect to the weight function $(1-t^2)^{\frac{d-2}{2}}$ normalised so that $P_n^{(d)}(1) = 1$. Then the requirement of strict positive definiteness is expressed by the strict positivity of all coefficients a_n (cf. [41]). Furthermore, $Z(d,n)$ denotes the dimension of the space of spherical harmonics of degree n on $\mathbb{S}^d$;

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

Assume further that g is integrable,

$$\forall \mathbf{y} \in \mathbb{S}^d : \int_{\mathbb{S}^d} g(\langle \mathbf{x}, \mathbf{y}\rangle)\, d\sigma_d(\mathbf{x}) = a_0 \omega_d,$$

where σ_d denotes the surface measure on $\mathbb{S}^d$ and $\omega_d = \sigma_d(\mathbb{S}^d)$.

Under the assumptions of continuity on $[-1,1)$ and integrability, the function g is represented by (2.2) in the sense of Abel-summability, namely

$$\lim_{r\to 1-} \sum_{n=0}^{\infty} r^n a_n Z(d,n) P_n^{(d)}(t) = g(t); \tag{2.3}$$

this relation holds uniformly on any interval $[-1, 1-\varepsilon]$ for $\varepsilon > 0$ by positivity of the Poisson-kernel

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

Remark 2.1. Notice that the series (2.2) can diverge for certain kernel functions; for instance, the series diverges for $g(t) = (1-t)^{-s/2}$ for $\frac{d+1}{2} < s < d$, which corresponds to the classical Riesz kernels. Thus we had to use a summation method, in order to ensure convergence. We chose Abel-summation for simplicity. For a comprehensive discussion of applications of summation methods to Laplace series, we refer to [3].

In general g will have a singularity at $t = 1$, namely

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

which also means that the series

$$\sum_{n=0}^{\infty} Z(d,n) a_n$$

diverges. If g is continuous on $[-1,1]$, we call g a *regular* kernel, whereas if it has a singularity at $t = 1$ but is still integrable, we call g *singular*.

For a regular or singular kernel g, the energy integral (2.1) is uniquely minimised by $\frac{1}{\omega_d}\sigma_d$ amongst all Borel probability measures on $\mathbb{S}^d$. By our assumptions on g we have for every probability measure ν

$$a_0 \le \lim_{r\to 1-} \iint_{\mathbb{S}^d\times\mathbb{S}^d} \sum_{n=0}^{\infty} r^n a_n Z(d,n) P_n^{(d)}(\langle \mathbf{x}, \mathbf{y}\rangle)\, d\nu(\mathbf{x})\, d\nu(\mathbf{y}) = \iint_{\mathbb{S}^d\times\mathbb{S}^d} g(\langle \mathbf{x}, \mathbf{y}\rangle)\, d\nu(\mathbf{x})\, d\nu(\mathbf{y}),$$

where the second equality follows from the uniform convergence in (2.3). Equality holds, if and only if

$$\iint_{\mathbb{S}^d\times\mathbb{S}^d} P_n^{(d)}(\langle\mathbf{x},\mathbf{y}\rangle)\,d\nu(\mathbf{x})\,d\nu(\mathbf{y})=0$$

for $n\geq 1$, which is equivalent to $\nu=\frac{1}{\omega_d}\sigma_d$.

For a finite set $X_N=\{\mathbf{x}_1,\dots,\mathbf{x}_N\}\subset\mathbb{S}^d$ of N (pairwise distinct!) points we define the g-energy as

$$E_g(X_N)=\sum_{i\neq j} g(\langle\mathbf{x}_i,\mathbf{x}_j\rangle). \tag{2.4}$$

Furthermore, we denote by

$$\mathcal{E}_g(\mathbb{S}^d,N)=\min_{X_N} E_g(X_N)$$

the minimal g-energy of an N-point set on the sphere $\mathbb{S}^d$. We denote point sets minimising the energy by X_N^* (suppressing the dependence on g in this notation). To any point set X_N we associate the measure

$$\nu_N=\frac{1}{N}\sum_{i=1}^N\delta_{\mathbf{x}_i}.$$

Theorem 2.1. *Let g be a strictly positive definite regular or singular integrable kernel function, which is continuous on $[-1,1)$. Let $(X_N)_N$ be a sequence of point sets on the unit sphere $\mathbb{S}^d$ such that*

$$\lim_{N\to\infty}\frac{1}{N^2}E_g(X_N)=\frac{1}{\omega_d}\int_{\mathbb{S}^d} g(\langle\mathbf{x},\mathbf{y})\,d\sigma_d(\mathbf{x})=a_0. \tag{2.5}$$

Then the associated measures ν_N tend weakly to the normalised surface measure $\frac{1}{\omega_d}\sigma_d$. Especially, the measures associated to a sequence of energy minimising configurations $(X_N^*)_N$ tend to $\frac{1}{\omega_d}\sigma_d$.

Proof. We first notice that $I_g(\mu)$ is uniquely minimised amongst all Borel probability measures by the normalised surface measure $\frac{1}{\omega_d}\sigma_d$. This is an immediate consequence of the addition theorem for spherical harmonics (cf. [34]) and the fact that every measure on $\mathbb{S}^d$ is characterised by its Fourier coefficients.

We will only give a proof of the theorem for singular g; the case of regular kernels can be treated in a much simpler way by harmonic analysis. Assume that we have a sequence of point sets $(X_N)_N$ such that the associated measures ν_N weakly tend to a limiting measure ν. Then we also have

$$\frac{1}{N^2}\sum_{i\neq j}\delta_{(\mathbf{x}_i,\mathbf{x}_j)}\rightharpoonup\nu\otimes\nu.$$

For $M > 0$, let $g_M(t) = \min(g(t), M)$. Then $(g_M)_M$ is a pointwise monotonically increasing family of continuous functions; we have

$$\lim_{M\to\infty}\lim_{N\to\infty}\frac{1}{N^2}\sum_{i\neq j} g_M(\langle \mathbf{x}_i,\mathbf{x}_j\rangle) = \lim_{M\to\infty}\iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} g_M(\langle \mathbf{x},\mathbf{y}\rangle)\,d\nu(\mathbf{x})\,d\nu(\mathbf{y})$$
$$= \iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} g(\langle \mathbf{x},\mathbf{y}\rangle)\,d\nu(\mathbf{x})\,d\nu(\mathbf{y}).$$

On the other hand, by the monotonicity of $(g_M)_M$, we have

$$\lim_{N\to\infty}\frac{1}{N^2}\sum_{i\neq j} g_M(\langle \mathbf{x}_i,\mathbf{x}_j\rangle) \le \liminf_{N\to\infty}\frac{1}{N^2}\sum_{i\neq j} g(\langle \mathbf{x}_i,\mathbf{x}_j\rangle),$$

from which we derive

$$\iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} g(\langle \mathbf{x},\mathbf{y}\rangle)\,d\nu(\mathbf{x})\,d\nu(\mathbf{y}) \le \liminf_{N\to\infty}\frac{1}{N^2}\sum_{i\neq j} g(\langle \mathbf{x}_i,\mathbf{x}_j\rangle).$$

Now take a sequence $(X_N)_N$ satisfying the assumptions of the theorem and assume that ν is cluster point of the sequence of measures $(\nu_N)_N$; such a cluster point exists by the Banach-Alaoglu theorem. Since $I_g(\nu) = a_0 = I_g(\frac{1}{\omega_d}\sigma_d)$ and the fact that the energy integral (2.1) is uniquely minimised by $\frac{1}{\omega_d}\sigma_d$, we obtain $\nu = \frac{1}{\omega_d}\sigma_d$. Since this is the only possible cluster point and under our assumptions, we have $\nu_N \rightharpoonup \frac{1}{\omega_d}\sigma_d$. Applying this argument to a sequence $(X_N^*)_N$ of energy minimising point sets gives the second assertion. $\square$

We recall an averaging argument from [37], which shows the existence of point sets X_N with $E_g(X_N) \le a_0 N^2$. Let $(D_i)_{i=1}^N$ be an area regular partition of $\mathbb{S}^d$, namely a collection of closed subsets of $\mathbb{S}^d$ satisfying

$$\begin{aligned}
&(i) && \bigcup_{i=1}^N D_i = \mathbb{S}^d,\\
&(ii) && D_i^\circ \cap D_j^\circ = \emptyset \text{ for } 1\le i<j\le N,\\
&(iii) && \sigma_d(D_i) = \frac{\omega_d}{N} \text{ for } 1\le i\le N,\\
&(iv) && \sigma_d(\partial D_i) = 0 \text{ for } 1\le i\le N.
\end{aligned}$$

Then integrating

$$\sum_{i\neq j} g(\langle \mathbf{x}_i,\mathbf{x}_j\rangle)$$

with respect to the product of the measures $\sigma_i^* = \frac{N}{\omega_d}\sigma_d|_{D_i}$ (restriction of σ_d to D_i) gives

$$\int_{D_1}\cdots\int_{D_N}\sum_{i\neq j} g(\langle \mathbf{x}_i,\mathbf{x}_j\rangle)\,d\sigma_1^*(\mathbf{x}_1)\cdots d\sigma_N^*(\mathbf{x}_N)$$
$$= N^2 I_g\left(\frac{1}{\omega_d}\sigma_d\right) - \frac{N^2}{\omega_d^2}\sum_{i=1}^{N}\iint_{D_i\times D_i} g(\langle\mathbf{x},\mathbf{y}\rangle)\,d\sigma_d(\mathbf{x})\,d\sigma_d(\mathbf{y}).$$

Since the value on the right hand side is smaller than a_0N^2, this shows the existence of point sets with small energy.

Remark 2.2. Notice that Bondarenko, Radchenko, and Viazovska [4] in the course of proving the existence of well-separated spherical designs of optimal asymptotic growth order [5] showed the existence of area regular partitions with geodesically convex sets D_i and diameter $\operatorname{diam}(D_i) = \mathcal{O}(N^{-1/d})$ (the optimal order).

Remark 2.3. Notice that the classical Riesz kernels $g_s(\langle\mathbf{x},\mathbf{y}\rangle) = \|\mathbf{x}-\mathbf{y}\|^{-s}$ for $0 < s < d$ satisfy the hypotheses of Theorem 2.1. Thus in the classical potential theoretic situation the discrete minimising configurations are asymptotically uniformly distributed (see also [31]). Furthermore, the cases $s = 0$ with the modified kernel function $g_0(\langle\mathbf{x},\mathbf{y}\rangle) = \log\frac{1}{\|\mathbf{x}-\mathbf{y}\|}$ and $-2 < s < 0$ with $g_s(\langle\mathbf{x},\mathbf{y}\rangle) = 2^{-s} - \|\mathbf{x}-\mathbf{y}\|^{-s}$ are covered by this theorem.

Remark 2.4. Discrete energies on the sphere $\mathbb{S}^d$ have also been studied for negative values of $s > -2$, i.e. positive exponents of the distance (cf. [35, 43, 44, 46]). For the case $s \leq -2$, the kernel has to be modified further, to ensure the positivity of all coefficients in its Laplace expansion; furthermore, in the case of $s = -2k$ being a negative even integer, the kernel $g_{-2k}(\langle\mathbf{x},\mathbf{y}\rangle) = \|\mathbf{x}-\mathbf{y}\|^{2k}\log\frac{1}{\|\mathbf{x}-\mathbf{y}\|} + p_k(\langle\mathbf{x},\mathbf{y}\rangle)$ is used instead, where the function p_k has to be added to ensure positive definiteness; its Laplace series is given in [11]. Without the logarithmic factor the kernel would be a polynomial in this case.

Remark 2.5. Discrete energies for negative values of s play an important rôle in the study of numerical integration errors for certain Sobolev spaces H. In this context the energy can be interpreted as the square of the worst case error of integration on the underlying function space H

$$\operatorname{wce}_H(X_N) = \sup_{\substack{f\in H\\ \|f\|\leq 1}}\left|\frac{1}{N}\sum_{n=1}^{N} f(\mathbf{x}_n) - \frac{1}{\omega_d}\int_{\mathbb{S}^d} f(\mathbf{x})\,d\sigma_d(\mathbf{x})\right|.$$

It is a general feature of reproducing kernel Hilbert spaces that the square of the worst case error can be expressed in terms of a generalised discrete energy. This can be seen as a generalisation of Stolarsky's invariance principle (cf. [**?**, 12, 43, 44]), which relates the sum of distances of the point set X_N (this is the case $s = -1$) to the L^2-discrepancy defined in (4.4) below. In turn the L^2-discrepancy and similar energy functionals with regular kernels can be interpreted as the mean square integration error, if the function space is equipped with an appropriate Wiener measure (cf. [24]). Furthermore, the relation between the worst case integration error in Sobolev spaces and general energy functionals is used in [15] to define sequences of QMC-designs $(X_N)_N$ as sequences of point sets achieving optimal order of magnitude for the integration error.

3. Hyper-singular energies and uniform distribution

For $s \geq \dim(M)$, the situation changes completely. The energy integral (1.3) diverges for all measures μ. But minimising point configurations of the energy sum (1.2) can still be studied. By a result of Hardin and Saff [26, 27] from 2004, the energy mimimising points distribute asymptotically according to the normalised surface measure for a rectifiable manifold. In the following, $\mathcal{H}_d$ will denote the d-dimensional Hausdorff measure, normalised so that $\mathcal{H}_d([0,1]^d) = 1$.

Theorem 3.1 (Theorems 2.1 and 2.2 in [27])**.** *Let $A \subset \mathbb{R}^d$ be a compact set and $s > d$. Let*

$$\mathcal{E}_s(A, N) = \min_{X_N \subset A} E_s(X_N)$$

be the minimal s-energy of a point set $X_N \subset A$. Then the limit $\lim_{N\to\infty} \mathcal{E}_s(A, N) N^{-1-\frac{s}{d}}$ exists and is given by

$$\lim_{N\to\infty} \frac{1}{N^{1+\frac{s}{d}}} \mathcal{E}_s(A, N) = \frac{C_d(s)}{\mathcal{H}_d(A)^{\frac{s}{d}}}, \tag{3.1}$$

where $C_d(s)$ is a positive constant depending only on s and d; the constant occurs as the limit for the case $A = U_d = [0,1]^d$,

$$C_d(s) = \lim_{N\to\infty} \frac{\mathcal{E}(U_d, N)}{N^{1+\frac{s}{d}}}.$$

Furthermore, if A has positive d-dimensional Hausdorff-measure $\mathcal{H}_d(A) > 0$ and $(X_N)_N$ ($X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset A$) is a sequence of point sets with

$$\lim_{N\to\infty} \frac{1}{N^{1+\frac{s}{d}}} E_s(X_N) = \frac{C_d(s)}{\mathcal{H}_d(A)^{\frac{s}{d}}},$$

then the corresponding measures ν_N tend weakly to the normalised Hausdorff measure on A,

$$\frac{1}{N} \sum_{i=1^N} \delta_{\mathbf{x}_i} \rightharpoonup \frac{\mathcal{H}_d|_A}{\mathcal{H}_d(A)}. \tag{3.2}$$

Remark 3.1. In the case $s = d$ a similar result holds with $N^{1+s/d}$ replaced by $N^2 \log N$. In this case also the constant $C'_d(d)$ is explicitly known, namely

$$C'_d(d) = \mathcal{H}_d(B_d) = \frac{\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2} + 1\right)},$$

where B_d is the d-dimensional unit ball in $\mathbb{R}^d$.

This result has several interesting features that we shall discuss briefly:

- the limiting measure is independent of s, which is in obvious contrast to the case $s < d$, where the measure depends highly on s (except for manifolds of high symmetry such as the sphere; this is the reason that we restricted to the sphere in Section 2);
- the limiting measure has a geometrical interpretation ("surface");
- the proof shows that in contrast to the situation for $s < d$ only local (short range) interactions contribute to the asymptotic behaviour of $E_s(X_N)$.

The proof of the existence of the limit

$$\lim_{N\to\infty} \frac{1}{N^{1+\frac{s}{d}}} \mathcal{E}_s(N)$$

for $s > d$ and the fact that the corresponding distribution measures tend to the normalised surface area measure, the normalised Hausdorff measure $\mathcal{H}_d$ on A, is rather intricate and technical; we refer the reader to [27]. Furthermore, there is an excellent survey in [26] on the result, which recollects the proof of the result for the unit cube.

Facts and conjectures about energy. In [9, 29, 37, 39, 47, 49] the asymptotic behaviour of the minimal energy of N point configurations on the sphere $\mathbb{S}^d$ for all positive values of the parameter s has been studied. For the case $0 < s < d$, it was shown that there exist positive constants C_1, C_2 such that

$$I_s\left(\frac{1}{\omega_d}\sigma_d\right) N^2 - C_1 N^{1+s/d} \le \mathcal{E}_s(\mathbb{S}^d, N) \le I_s\left(\frac{1}{\omega_d}\sigma_d\right) N^2 - C_2 N^{1+s/d}. \tag{3.3}$$

For $s = d$, a phase change occurs, namely

$$\mathcal{E}_d(\mathbb{S}^d, N) \sim C N^2 \log N,$$

this could be explained by the "collapse" of the two terms in the lower and upper bounds in (3.3) ($1 + s/d = 2$ in this case). The coincidence of two asymptotic terms often produces phase change phenomena. The behaviour of the minimal energy for $s \ge d$ – the hypersingular case – was only understood after the work of Hardin and Saff [27] which we stated as Theorem 3.1. The proof shows the existence of the constant $C_d(s)$, the exact value of this constant is still conjectural.

For $d = 2$, the value $C_2(s)$ ($s > 2$) is conjectured to be

$$C_2(s) = \left(\frac{\sqrt{3}}{2}\right)^{s/2} \zeta_{\mathsf{A}_2}(s),$$

where ζ_{A_2} denotes the Epstein zeta function,

$$\zeta_{\mathsf{A}_2}(s) = \sum_{\substack{\mathbf{z}\in\mathsf{A}_2\\ \mathbf{z}\neq\mathbf{0}}} \|\mathbf{z}\|^{-s},$$

of the hexagonal lattice A_2 spanned by the vectors $(1, 0)$ and $(\frac{1}{2}, \frac{1}{2}\sqrt{3})$. The conjecture is supported by the fact that the hexagonal lattice is the solution of the two-dimensional best packing problem, as well as the fact that this lattice is universally optimal (cf. Section 5) among two-dimensional lattices by [33]. Furthermore, it has been conjectured in [14] that the inequality (3.3) can be sharpened to an asymptotic relation

$$\mathcal{E}_s(\mathbb{S}^d, N) = I_s\left(\frac{1}{\omega_d}\sigma_d\right) N^2 - \frac{C_d(s)}{\mathcal{H}_d(\mathbb{S}^d)^{\frac{s}{d}}} N^{1+\frac{s}{d}} + o\left(N^{\min(2,1+\frac{s}{d})}\right),$$

valid for $s \in (-2,0) \cup (0,d) \cup (d, d+1)$; the constant $C_d(s)$ for s in this range is conjectured to be the analytic continuation of $C_d(s)$ for $s > d$ to the complex plane; the value $I_s(\frac{1}{\omega_d}\sigma_d)$ has to be interpreted as the analytic continuation of the expression $I_s(\frac{1}{\omega_d}\sigma_d)$ for $s < d$ to complex values of s. This was coined "the principle of analytic continuation" in [14]. Notice that the two first asymptotic terms change their rôle at $s = d$; for this value of s, $I_s(\frac{1}{\omega_d}\sigma_d)$ and $C_d(s)$ have a singularity, which is mirrored by a $N^2 \log N$ term in the asymptotic expression. The conjecture includes the value of the constant $C_d(s)$ in terms of the Epstein zeta function of a lattice minimising the energy (for $s \geq 0$, $s \neq d$). It is supported by the fact that a corresponding principle holds for $d = 1$ (cf. [13]). Moreover, for $d = 2, 4, 8, 24$, it is conjectured that $C_d(s) = |\Lambda_d|^{s/d}\zeta_{\Lambda_d}(s)$, where Λ_d denotes, respectively, the hexagonal lattice A_2, D_4, E_8, and the Leech lattice Λ_{24}.

For dimensions $d \geq 3$, the situation seems to be much more complicated. In general it is known that the limit

$$\lim_{s\to\infty} C_d(s)^{1/s}$$

exists and is related to the best-packing constant in dimension d.

Of course, not all Voronoï cells of a minimal energy configuration on the sphere $\mathbb{S}^2$ can be hexagonal; there have to be at least 12 pentagons by Euler's polyhedral formula. Numerical experiments with large numbers of points show that not only pentagonal cells, but also structures of pentagons and heptagons occur, which seem to organise themselves along curves, called "scars" (cf. [1, 8, 26]).

4. Discrepancy estimates

Discrepancy given by (1.1) is an easy to understand concept; $D(X_N)$ just measures the maximal deviation of the discrete distribution from the limiting distribution σ (in statistics this is called the Kolmogorov-Smirnov statistics). On the other hand, the precise value of the discrepancy of a point set is rather difficult to compute. Thus discrepancy is usually estimated rather than computed directly. In the simplest one-dimensional case there are two classical estimates for discrepancy, namely the Erdős-Turán inequality and LeVeque's inequality (cf. [30]). Both inequalities have been generalised to the spherical case and used for estimating the discrepancy of point sets constructed by the various methods.

The $\mathbb{S}^d$ version of the Erdős-Turán inequality has been given independently by the author [23] and Li and Vaaler [32] and reads as

$$D(X_N) \leq \frac{C_1(d)}{M} + \sum_{\ell=1}^{M} \frac{C_2(d)}{\ell} \sum_{m=1}^{Z(d,\ell)} \frac{1}{N} \left| \sum_{n=1}^{N} Y_{\ell,m}(\mathbf{x}_n) \right|, \tag{4.1}$$

valid for all positive integer values of M. Here $C_1(d)$ and $C_2(d)$ denote (explicitly known) constants, $Y_{\ell,m}$ ($m = 1, \ldots, Z(d,\ell)$) denote an orthonormal system of real spherical harmonics of order ℓ, and $Z(d,\ell)$ denotes the dimension of the space of these spherical harmonics.

Only recently, a spherical version of the LeVeque inequality was found (cf. [35]):

$$D(X_N) \leq A(d) \left(\sum_{\ell=0}^{\infty} \ell^{-(d+1)} \sum_{m=1}^{Z(d,\ell)} \left(\frac{1}{N} \sum_{n=1}^{N} Y_{\ell,m}(\mathbf{x}_n) \right)^2 \right)^{\frac{1}{d+2}} \tag{4.2}$$

with an explicit constant $A(d)$. Both inequalities (4.1) and (4.2) specialise to their classical versions for $d = 1$. It is interesting to mention that the LeVeque inequality also has an opposite version providing a lower bound (cf. [35])

$$D(X_N) \geq B(d) \left(\sum_{\ell=0}^{\infty} \ell^{-(d+1)} \sum_{m=1}^{Z(d,\ell)} \left(\frac{1}{N} \sum_{n=1}^{N} Y_{\ell,m}(\mathbf{x}_n) \right)^2 \right)^{\frac{1}{2}} \tag{4.3}$$

with some explicit positive constant $B(d)$. It should also be mentioned that the expression raised to the $d+2$ power in (4.2) is equivalent to the L^2-discrepancy

$$\int_0^{\pi} \int_{\mathbb{S}^d} \left(\frac{1}{N} \sum_{n=1}^{N} \mathbb{1}_{C(\mathbf{x}_n,\varphi)}(\mathbf{x}) - \frac{1}{\omega_d} \sigma_d(C(\cdot,\varphi)) \right)^2 \sin(\varphi)^{d-1} \, d\sigma_d(\mathbf{x}) \, d\varphi, \tag{4.4}$$

where $C(\mathbf{x},\varphi) = \{\mathbf{y} \in \mathbb{S}^d \mid \langle \mathbf{x}, \mathbf{y} \rangle \geq \cos(\varphi)\}$ denotes the spherical cap centered at $\mathbf{x}$ with angle φ. A similar inequality relating the discrepancy $D(X_N)$ to the L^2-discrepancy has been given in [36] in the Euclidean case and in [45] in the general case of a metric space, which specialises to a similar inequality as (4.2) in the case of the sphere.

Although the limiting distribution of minimal energy point sets X_N^* for $s \geq d$ on the sphere has been determined in [27], almost nothing is known about quantitative results. The only – and very weak – estimate for the discrepancy of minimal energy point sets in the singular case is due to Damelin and the author [19] and gives

$$D(X_N^*) = \mathcal{O}\left(\sqrt{\frac{\log \log N}{\log N}} \right) \tag{4.5}$$

for $s = d$. This estimate is proved by approximating the d-energy by a limiting process $s \to d-$.

In the harmonic case $s = d-1$, Götz [22] could prove that minimal energy configurations X_N^* satisfy

$$D(X_N^*) \ll N^{-\frac{1}{d}} \log N,$$

solving a conjecture of Korevaar (cf. [28]) – up to the logarithmic factor. This improves the exponent $-\frac{1}{2d}$ given by Sjögren [42].

In [35] the LeVeque type inequality (4.2) for the spherical cap discrepancy was proved and applied to minimal energy point sets X_N^* for g_s with $-1 < s < 0$. This gives bounds for the discrepancy

$$D(X_N^*) \ll N^{-\frac{d-s}{d(d+2)}}. \tag{4.6}$$

For $s = 0$, in [10] the bound

$$D(X_N^*) \ll N^{-\frac{1}{d+2}} \tag{4.7}$$

had been obtained before.

It should be mentioned that from the theory of irregularities of distribution [2] it is known that for all sets $X_N \subset \mathbb{S}^d$ the inequality

$$D(X_N) \gg N^{-\frac{1}{2}-\frac{1}{2d}} \tag{4.8}$$

holds for the spherical cap discrepancy. Inequality (4.3) together with lower bounds for the energy from [47] was used to reprove this result in [35]. This indicates the sharpness of the inequality (4.3) as a lower bound for the discrepancy in terms of sums over spherical harmonics.

It is also known that inequality (4.8) is best possible up to a factor $\sqrt{\log N}$. The existence of point sets X_N with

$$D(X_N) \ll N^{-\frac{1}{2}-\frac{1}{2d}}\sqrt{\log N}$$

uses a probabilistic argument resembling the averaging argument that we used to prove the existence of point sets of small energy; up to now no explicit construction of such a point set is known. All the known estimates for the discrepancy of point sets differ from the lower bound (4.8) by a power of N. The bounds (4.5), (4.6), and (4.7) should be compared to (4.8).

Remark 4.1. Discrepancy estimates for point sets of minimal energy are known in the case of $-2 < s \le 0$ (giving sums of positive powers of the distance) from the work of Wagner [48]. These results have been partly rediscovered and refined in [35]. Estimates for the discrepancy in terms of g-energy of the point set for singular g satisfying an additional technical hypothesis have been given in [19]. This gives estimates for the discrepancy of point sets minimising the Riesz s-energy for $-2 < s \le d$. All these estimates have the disadvantage that they have been derived via harmonic analysis and that this method has to use estimates for the Fourier coefficients of certain functions in an unfavourable way; thus it can be expected that these estimates for the discrepancy of minimal energy point sets are far away from the correct order of magnitude. Furthermore, nothing is known about the discrepancy of energy minimising point sets for $s > d$. This is due to the fact that harmonic analysis is not applicable in that case.

5. Some remarks on lattices

As was pointed out in the discussion of the local structure of minimal energy point configurations at the end of Section 3, there seems to be an intricate connection to lattices which minimise a corresponding energy functional. Therefore, we add a short description of the appropriate notions for lattices and the state of knowledge about them.

The optimal density of sphere packings in $\mathbb{R}^d$ is a classical question that found new interest by Hales's proof of the Kepler conjecture [25]. In [16] new upper bounds for the density of sphere packings in dimensions $3 < d \leq 36$ could be derived from linear programming bounds based on Fourier transform. This led to the definition of *universally optimal lattices* as those lattices Λ, which minimise

$$\sum_{\lambda\in\Lambda} e^{-t\|\lambda\|^2}$$

for all real parameters $t > 0$ amongst all lattices of covolume 1.

As was pointed out in Section 3 the conjectured local structure of minimal energy point sets in the case $s > \dim(M)$ is related to lattices Λ of covolume 1 which minimise the Riesz energy

$$\sum_{\lambda\in\Lambda\setminus\{0\}} \|\lambda\|^{-s} \tag{5.1}$$

for $s > d$; this equals the classical Epstein zeta function of the lattice Λ. For recent progress on minimisation of values of the Epstein zeta function we refer to [40]. By Mellin transform universally optimal lattices also minimise the Riesz energy (5.1).

The sphere packing problem is naturally related to the study of periodic point sets with minimal energy. As in the case of spherical codes, one may ask if there exist *universally optimal periodic sets*, that is, periodic sets that minimise the energy

$$\sum_{\lambda\in\Lambda} f(\|\lambda\|) \tag{5.2}$$

for all completely monotonic functions f. Up to now, no such universally optimal periodic set is known. However, exceptional lattices as the hexagonal lattice A_2, the root lattice E_8, and the 24-dimensional Leech lattice Λ_{24} are conjectured to be examples (see [17]). Some candidates for universally optimal lattices have been found numerically (cf. [18]), proofs are still missing.

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