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ASYMPTOTICS FOR MINIMAL DISCRETE ENERGY ON THE SPHERE

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Abstract. We investigate the energy of arrangements of N points on the surface of the unit sphere S^d in $\mathbf{R}^{d+1}$ that interact through a power law potential $V = 1/r^s$, where $s > 0$ and r is Euclidean distance. With $\mathcal{E}_d(s, N)$ denoting the *minimal* energy for such N-point arrangements we obtain bounds (valid for all N) for $\mathcal{E}_d(s, N)$ in the cases when $0 < s < d$ and $2 \le d < s$. For $s = d$, we determine the precise asymptotic behavior of $\mathcal{E}_d(d, N)$ as $N \to \infty$. As a corollary, lower bounds are given for the separation of any pair of points in an N-point minimal energy configuration, when $s \ge d \ge 2$.

For the unit sphere in $\mathbf{R}^3$ ($d = 2$), we present two conjectures concerning the asymptotic expansion of $\mathcal{E}_2(s, N)$ that relate to the zeta function $\zeta_L(s)$ for a hexagonal lattice in the plane. We prove an asymptotic upper bound that supports the first of these conjectures. Of related interest, we derive an asymptotic formula for the partial sums of $\zeta_L(s)$ when $0 < s < 2$ (the divergent case).

1. Introduction and statement of results

Let $S^d = \{x \in \mathbf{R}^{d+1} \mid |x| = 1\}$ be the unit sphere in $\mathbf{R}^{d+1}$. We denote by σ the normalized Lebesgue measure on S^d (total mass one). The Euclidean distance between two points x, y is denoted by $|x - y|$ and their inner product by $\langle x, y\rangle$.

For a given $s > 0$, the discrete *s-energy* associated with a finite subset $\omega_N = \{x_1, \dots, x_N\}$ of points on S^d is

$$E_d(s, \omega_N) := \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|^s}. \tag{1.1}$$

We are interested in the minimal s-energy for N points on the sphere

$$\mathcal{E}_d(s, N) := \inf_{\omega_N} E_d(s, \omega_N),$$

where the infimum is taken over all N-point subsets of S^d. Any configuration ω_N for which the infimum is attained is called an *s-extremal configuration.*

The determination of s-extremal configurations and the associated minimal s-energy is a problem which is of interest in physics, chemistry and computer science. The important special case $d = 2$, $s = 1$ corresponds to points on the sphere in

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three dimensional space interacting according to the Coulomb potential [2], [10], [11]. General values of s are considered in [2], [15]; for the case of logarithmic interactions, see [3], [20].

In this paper we consider the asymptotic behavior of the minimal s-energy $\mathcal{E}_d(s,N)$ as N tends to infinity. The asymptotics were studied by G. Wagner [23], [24] for the case $0 < s < d$ (and also for $s < 0$, but we will not consider such values here). For $0 < s < d$, the energy integral

$$I_{d,s}(\mu) := \int_{S^d}\int_{S^d} \frac{1}{|x-y|^s} d\mu(x) d\mu(y),$$

taken for probability measures μ on S^d, is minimal for the normalized Lebesgue measure σ. This follows from well-known results on the existence and uniqueness of a minimizing measure, see e.g. [14, Chapter II], and the rotational invariance. This leads easily to the main term of the asymptotics for $\mathcal{E}_d(s,N)$:

$$\mathcal{E}_d(s,N) = \frac{1}{2}V_d(s)N^2 + o(N^2) \quad (N \to \infty), \qquad 0 < s < d,$$

where

$$V_d(s) := I_{d,s}(\sigma) = \frac{\Gamma((d+1)/2)\Gamma(d-s)}{\Gamma((d-s+1)/2)\Gamma(d-s/2)} \tag{1.2}$$

Concerning the second term, Wagner [23] obtained the lower bounds

$$\mathcal{E}_d(s,N) \geq \frac{1}{2}V_d(s)N^2 - CN^{1+s/d}, \qquad d-2 < s < d, \tag{1.3}$$

$$\mathcal{E}_d(s,N) \geq \frac{1}{2}V_d(s)N^2 - CN^{1+s/(2+s)}, \qquad d \geq 3, \quad 0 < s \leq d-2. \tag{1.4}$$

The bound for the range $0 < s < d-2$ is probably not best possible. (Here and in the following, C denotes a positive constant that may depend on s and d, but not on N.)

Wagner [24] also derived an upper bound for the case $d = 2$:

$$\mathcal{E}_2(s,N) \leq \frac{1}{2}V_2(s)N^2 - CN^{1+s/2}, \qquad 0 < s < 2. \tag{1.5}$$

Recently, E. A. Rakhmanov, E. B. Saff and Y. M. Zhou [17] gave an alternative proof of this upper bound. Their method is much simpler than Wagner's and lends itself easily to generalization to higher dimensions. This is our first result.

Theorem 1. *Let $d \geq 2$ and $0 < s < d$. There is a constant $C > 0$ such that*

$$\mathcal{E}_d(s,N) \leq \frac{1}{2}V_d(s)N^2 - CN^{1+s/d}. \tag{1.6}$$

The combination of (1.3) and (1.6) leads to the correct order of $\mathcal{E}_d(s,N) - \frac{1}{2}V_d(s)N^2$ for the case $d-2 < s < d$.

The main results of this paper deal with the case $s \geq d$. This case seems not to have been investigated before. In the limit, for N fixed and $s \to \infty$, we arrive at the best packing problem on S^d—that is, the problem of maximizing the minimal distance among N points on the sphere. For $d = 2$, W. Habicht and B. L. van der Waerden [12], [22] proved that the maximal minimal distance among N points satisfies

$$\left(\frac{8\pi}{\sqrt{3}}\right)^{1/2} N^{-1/2} + O(N^{-2/3}) \qquad (N \to \infty). \tag{1.7}$$

For results in higher dimensions, see [8].

For $s \geq d$, the energy integral $I_{d,s}(\mu)$ diverges for every measure μ. This means that the nearest neighbor interactions are dominating, and they determine the order of the first term of the asymptotics for $\mathcal{E}_d(s, N)$.

Theorem 2. *Let $d \geq 2$ and $s > d$. There are constants $C_1, C_2 > 0$ such that*

$$C_1 N^{1+s/d} \leq \mathcal{E}_d(s, N) \leq C_2 N^{1+s/d}, \qquad s > d. \tag{1.8}$$

The estimates (1.8) suggest that the limit

$$\lim_{N\to\infty} N^{-1-s/d}\mathcal{E}_d(s, N), \quad s > d, \tag{1.9}$$

exists. As yet, we have not been able to prove this.

For the case $s = d$, the order of the first term of the asymptotics for $\mathcal{E}_d(s, N)$ is $N^2 \log N$, and in this case we are able to determine the precise constant.

Theorem 3. *Let $d \geq 2$. Then*

$$\lim_{N\to\infty} (N^2 \log N)^{-1}\mathcal{E}_d(d, N) = \frac{1}{2d}\gamma_d, \tag{1.10}$$

where

$$\gamma_d := \frac{\Gamma((d+1)/2)}{\Gamma(d/2)\Gamma(1/2)}. \tag{1.11}$$

As a by-product, the proofs of Theorems 2 and 3 yield lower bounds for the separation of points in an s-extremal configuration.

Corollary 4. *Let $s \geq d \geq 2$ and let $\omega_N = \{x_1, \dots, x_N\}$ be a configuration of points on S^d that minimizes the s-energy. Then there is a constant C, depending only on s and d, such that for $i \neq j$,*

$$|x_i - x_j| \geq CN^{-1/d}, \qquad s > d, \tag{1.12}$$

and

$$|x_i - x_j| \geq CN^{-1/d}(\log N)^{-1/d}, \qquad s = d. \tag{1.13}$$

The order of the estimate (1.12) is best possible, but the order of the estimate (1.13) most likely is not. A separation result like (1.12) was proved by B.E.J. Dahlberg [9] for the case $s = d - 1$. For the case of logarithmic interactions and $d = 2$, see [18].

In Section 2 we consider the case $d = 2$ in more detail. We present heuristic evidence that the limit (1.9) exists, and we give a conjecture about the value (see Conjecture 1). Our Theorem 5 (see below) supports this conjecture. Furthermore, this conjecture is extended to the range $0 < s < 2$ to give a conjectured value of the constant with the second term in the asymptotics (see Conjecture 2).

The proofs of the theorems are in Sections 3–7.

2. Some conjectures for $d = 2$

Although we are unable to prove that the limit (1.9) exists, for the case $d = 2$ we shall present a partial result as well as a conjecture about the limit. We begin with some motivational discussion.

For $d = 2$, extensive numerical calculations have been performed by several investigators, especially for the important special case $s = 1$. It can be observed that configurations that minimize some s-energy have in some sense the same structure.

The Voronoi cell associated with a point x_i of a configuration $\omega_N = \{x_1, \dots, x_N\}$ is the set

$$\{x \in S^2 \mid |x - x_i| \leq |x - x_j| \text{ for all } j\}.$$

In an s-extremal configuration with $N \geq 12$ the Voronoi cells appear to partition the sphere into 12 pentagons and $N-12$ hexagons. These hexagons have approximately the same size and are nearly regular. This leads to the impression that the extremal configurations tend to imitate a regular planar hexagonal lattice. This imitation becomes better as the number of points increases. We are therefore led to a study of the planar hexagonal lattice.

Let L denote the hexagonal lattice in $\mathbf{R}^2$ normalized so that the minimal distance is 1. The Voronoi cell of a point in L is a hexagon with area $\frac{1}{2}\sqrt{3}$. If we take $(0,0) \in L$ and $(1,0) \in L$, then a general point in L has the form $m(1,0) + n(1/2, \sqrt{3}/2)$, $m, n \in \mathbf{Z}$. We need the zeta function for L:

$$\zeta_L(s) := \sum_{0 \neq X \in L} |X|^{-s} = \sum_{(m,n) \in \mathbf{Z}^2 \setminus (0,0)} (m^2 + mn + n^2)^{-s/2}. \tag{2.1}$$

This series converges for $s > 2$.

Let $\omega_N^* = \{x_1, \dots, x_N\}$ be a configuration that minimizes the s-energy. Assuming that our observation is correct, the Voronoi cell of a typical point x_i would be a hexagon which is part of a hexagonal lattice scaled so that the minimal distance is δ_N, where δ_N is such that $\frac{1}{2}\sqrt{3}\delta_N^2 = 4\pi/N$; that is,

$$\delta_N = \left(\frac{8\pi}{\sqrt{3}}\right)^{1/2} N^{-1/2}.$$

Note that δ_N is equal to the first term in (1.7). (Here we ignore the 12 pentagonal cells.)

For every $R > 0$, let $n(R)$ be the number of points X in the lattice L with $|X| \leq R$. For N large, the $n(R) - 1$ points closest to a typical point $x_i \in \omega_N^*$ will, heuristically speaking, constitute a part of a hexagonal lattice scaled by the factor δ_N. The contribution of these points to the sum $\sum_{j \neq i} |x_i - x_j|^{-s}$ is

$$(\delta_N)^{-s} \sum_{0 < |X| \leq R} |X|^{-s} = \left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} N^{s/2} \sum_{0 < |X| \leq R} |X|^{-s}. \tag{2.2}$$

Assuming that the extremal configuration is uniformly distributed with respect to $d\sigma$, the $n(R)-1$ points can be visualized as occupying a spherical cap $C(x_i)$ around x_i with normalized area $n(R)/N$. The remaining $N - n(R)$ points are uniformly distributed over the rest of the sphere. We approximate their contribution to the sum by the integral

$$(N - n(R)) \int_{S^2 \setminus C(x_i)} |x_i - y|^{-s} d\sigma(y) = \frac{2n(R)^{1-s/2}}{2^s(s-2)} N^{s/2} + o(N^{s/2}). \tag{2.3}$$

Thus, combining (2.2) and (2.3), we are led to the approximation

(2.4)
$$\sum_{j=1, j \neq i}^{N} |x_i - x_j|^{-s} \approx \left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} \left[\sum_{0 < |X| \leq R} |X|^{-s} + \left(\frac{2\pi}{\sqrt{3}}\right)^{s/2} \frac{2n(R)^{1-s/2}}{(s-2)}\right] N^{s/2}.$$

Now letting $R \to \infty$, we obtain, for $s > 2$,

$$\sum_{j=1, j\neq i}^{N} |x_i - x_j|^{-s} \approx \left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} \zeta_L(s) N^{s/2}.$$

This suggests that the minimal discrete s-energy satisfies

$$\mathcal{E}_2(s, N) \approx \frac{1}{2}\left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} \zeta_L(s) N^{1+s/2},$$

and this leads to the following conjecture when $d = 2$.

Conjecture 1. *For $s > 2$ the limit*

$$\lim_{N\to\infty} N^{-1-s/2}\mathcal{E}_2(s, N) = C_s$$

exists, and

$$C_s := \frac{1}{2}\left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} \zeta_L(s). \tag{2.5}$$

Our final result supports this conjecture.

Theorem 5. *If $s > 2$, then*

$$\limsup_{N\to\infty} N^{-1-s/2}\mathcal{E}_2(s, N) \leq C_s, \tag{2.6}$$

where C_s is given by (2.5).

The function $\zeta_L(s)$ appears in number theory as the zeta function of the quadratic number field $\mathbf{Q}(\sqrt{-3})$. The integers in $\mathbf{Q}(\sqrt{-3})$ can be identified with the lattice points of the hexagonal lattice L. It is known [7, Ch. X, Sec. 7] that $\zeta_L(s)$ admits a factorization

$$\zeta_L(s) = 6\zeta(s/2)L_{-3}(s/2), \qquad s > 2, \tag{2.7}$$

where ζ is the Riemann zeta function

$$\zeta(s) = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{4^s} \cdots$$

and L_{-3} is a Dirichlet L-function

$$L_{-3}(s) = 1 - \frac{1}{2^s} + \frac{1}{4^s} - \frac{1}{5^s} + \frac{1}{7^s} - \cdots .$$

This factorization provides a convenient way to evaluate $\zeta_L(s)$.

The considerations that led to Conjecture 1 can be extended to the range $0 < s < 2$. Recall from (1.3) and (1.5) that $\mathcal{E}_2(s, N) - \frac{1}{2}V_2(s)N^2$ is of order $N^{1+s/2}$. For $s = 1$, conjectures on the value of the coefficient for the $N^{1+s/2}$-term were stated by Berezin [2], Glasser-Every [11] and Rakhmanov-Saff-Zhou [17]. We present an extended and more explicit version of these conjectures. For $0 < s < 2$, we get for the right-hand side of (2.3)

$$V_2(s)N - \frac{2n(R)^{1-s/2}}{2^s(2-s)} N^{s/2} + o(N^{s/2}).$$

Then

(2.8)
$$\sum_{j=1, j\neq i}^{N} |x_i - x_j|^{-s}$$
$$\approx V_2(s)N - \left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} \left[\sum_{0<|X|\leq R} |X|^{-s} - \left(\frac{2\pi}{\sqrt{3}}\right)^{s/2} \frac{2}{2-s} n(R)^{1-s/2}\right] N^{s/2}.$$

Letting $R \to \infty$, we are led to believe that the limit

$$\lim_{R\to\infty} \left[\sum_{0<|X|\leq R} |X|^{-s} - \left(\frac{2\pi}{\sqrt{3}}\right)^{s/2} \frac{2}{2-s} n(R)^{1-s/2}\right], \qquad 0 < s < 2, \tag{2.9}$$

exists. This is indeed the case, and, in fact, it can be proved that the limit is equal to $6\zeta(s/2)L_{-3}(s/2)$. Since we have not been able to find a reference for this result in the literature, we have included a proof in the appendix. Note that according to (2.7) the limit $6\zeta(s/2)L_{-3}(s/2)$ is equal to the analytic continuation of $\zeta_L(s)$ to $0 < s < 2$. See Borwein-Borwein-Shail-Zucker [5] for a similar phenomenon related to the square lattice.

Thus (2.8) leads to the following conjecture.

Conjecture 2. *Let* $0 < s < 2$. *Then*

$$\mathcal{E}_2(s, N) = \frac{1}{2}V_2(s)N^2 + C_s N^{1+s/2} + o(N^{1+s/2}),$$

where

$$C_s := 3\left(\frac{\sqrt{3}}{8\pi}\right)^{s/2} \zeta(s/2)L_{-3}(s/2). \tag{2.10}$$

Note that the number C_s in (2.10) is negative, since the Riemann zeta function has negative values between 0 and 1.

For $s = 1$, we find $C_s = -0.5530\cdots$, which is fairly close to the constant -0.5523 which was found in [17] on the basis of extensive numerical computations. We intend to return to these issues in a later paper.

To illustrate our results and conjectures, we have made additional numerical computations. In all cases it can be observed that the convergence is very slow. Probably one needs accurate calculations with several thousand points to obtain precise values. This is way beyond present computer capacities.

The following table contains results of computing extremal energies with $d = 2$ and $s = 2$ and $s = 4$, respectively, for configurations up to $N = 80$ points. By Theorem 3 the limit $\lim_N (N^2 \log N)^{-1}\mathcal{E}_2(2, N)$ exists and is equal to $1/8$. The slow convergence is obvious from the table. For $s = 4$, Conjecture 1 says that the limit $\lim_N N^{-3}\mathcal{E}_2(4, N)$ exists and that its value is $\pi^2/512 = 0.01927\cdots$. The last column indeed shows a tendency to converge, but again the convergence is slow.

We wish to thank Jeroen Voogd (University of Amsterdam) for performing the computer calculations.

N	$\mathcal{E}_2(2,N)$	$(N^2 \log N)^{-1}\mathcal{E}_2(2,N)$	$\mathcal{E}_2(4,N)$	$N^{-3}\mathcal{E}_2(4,N)$
5	4.2500000	.10562693	1.8958333	.015166666
10	25.041359	.10875324	16.626089	.016626089
15	67.486184	.11075813	58.557123	.017350258
20	133.93697	.11177315	140.69671	.017587089
25	226.54507	.11260829	278.84214	.017845897
30	346.26363	.11311821	483.74928	.017916640
35	494.81643	.11361244	773.84929	.018048963
40	672.30935	.11390812	1155.1985	.018049977
45	880.35796	.11420625	1648.5414	.018090989
50	1119.5995	.11447780	2267.7140	.018141712
55	1390.9691	.11474576	3031.5112	.018220954
60	1693.7946	.11491424	3934.0984	.018213418
65	2030.2336	.11511358	5014.5816	.018259741
70	2399.2395	.11525038	6261.6290	.018255478
75	2802.5708	.11539923	7711.1666	.018278321
80	3239.5225	.11551171	9355.4887	.018272438
∞		.12500000		$.01927\cdots$ (?)

3. Preliminaries

Here we collect some well-known facts about the integration of functions on S^d. As before, σ denotes the normalized Lebesgue measure on S^d. We denote by $\langle x, y\rangle$ the inner product of $x, y \in \mathbf{R}^{d+1}$.

We note the following basic rule (see [16, p.20]):

$$\int_{S^d} f(\langle x, x_0\rangle)d\sigma(x) = \gamma_d \int_{-1}^{1} f(t)(1-t^2)^{d/2-1}dt, \tag{3.1}$$

where γ_d is defined in (1.11). Here $x_0 \in S^d$ is some fixed point and $f : [-1,1] \to \mathbf{R}$ is integrable with respect to the weight $(1-t^2)^{d/2-1}$.

A spherical cap with center $x_0 \in S^d$ and radius r is

$$C(x_0, r) := \{x \in S^d \mid |x - x_0| \le r\} = \{x \in S^d \mid \langle x, x_0\rangle \ge 1 - r^2/2\}. \tag{3.2}$$

The normalized area of $C(x_0, r)$ can be computed from (3.1). We find that

$$\sigma(C(x_0, r)) = \gamma_d \int_{1-r^2/2}^{1} (1-t^2)^{d/2-1}dt.$$

From this it is easy to obtain the asymptotic formula

$$\sigma(C(x_0, r)) = \frac{1}{d}\gamma_d r^d + \mathcal{O}(r^{d+2}), \qquad (r \to 0), \tag{3.3}$$

and also the estimate

$$\sigma(C(x_0, r)) \le \frac{1}{d}\gamma_d r^d, \qquad d \ge 2. \tag{3.4}$$

For $s \geq d$ the integral $\int_{S^d} |x-y|^{-s} d\sigma(y)$ diverges, but it converges if we delete a spherical cap around x. We have, from (3.1),

(3.5)
$$\int_{S^d \setminus C(x,r)} |x-y|^{-s} d\sigma(y) = \gamma_d 2^{-s/2} \int_{-1}^{1-r^2/2} (1-t)^{-s/2+d/2-1}(1+t)^{d/2-1} dt.$$

To obtain the asymptotic behavior for $r \to 0$, we may replace the factor $1+t$ in the integrand of the right-hand side of (3.5) by 2. This leads to

$$\int_{S^d \setminus C(x,r)} |x-y|^{-s} d\sigma(y) = \frac{1}{s-d}\gamma_d r^{d-s} + o(r^{d-s}) \quad (r \to 0), \qquad s > d, \tag{3.6}$$

and

$$\int_{S^d \setminus C(x,r)} |x-y|^{-d} d\sigma(y) = \gamma_d \left[-\log r\right] + \mathcal{O}(1) \quad (r \to 0), \qquad s = d. \tag{3.7}$$

We also need some basic facts from spherical harmonics; see [16]. Following [21] we denote the ultrapherical polynomials by P_n^λ, and we recall the Rodrigues formula

$$P_n^\lambda(t) = \frac{(-2)^n}{n!} \frac{\Gamma(n+\lambda)\Gamma(n+2\lambda)}{\Gamma(\lambda)\Gamma(2n+2\lambda)} (1-t^2)^{1/2-\lambda} \left(\frac{d}{dt}\right)^n (1-t^2)^{n+\lambda-1/2}. \tag{3.8}$$

From the addition formula for spherical harmonics [16, p. 20], we get

(3.9)
$$P_n^{(d-1)/2}(\langle x_1, x_2\rangle) = \frac{2n+d-1}{d-1} \int_{S^d} P_n^{(d-1)/2}(\langle x_1, y\rangle) P_n^{(d-1)/2}(\langle x_2, y\rangle) d\sigma(y).$$

If K is a continuous function on $[-1,1]$ with ultrapherical expansion

$$K(t) = \sum_{n=0}^{\infty} a_n P_n^{(d-1)/2}(t),$$

then (3.9) gives us, for any configuration $\{x_1, \dots, x_N\}$ of points on S^d,

$$\sum_{i=1}^N \sum_{j=1}^N K(\langle x_i, x_j\rangle) = \sum_{n=0}^\infty a_n \frac{2n+d-1}{d-1} \int_{S^d} \left(\sum_{i=1}^N P_n^{(d-1)/2}(\langle x_i, y\rangle)\right)^2 d\sigma(y).$$

In case the coefficients $a_1, a_2, \dots$ are all *non-negative*, we deduce from this the inequality

$$\sum_{i=1}^N \sum_{j=1}^N K(\langle x_i, x_j\rangle) \geq a_0 N^2$$

and also

$$\sum_{i \neq j} K(\langle x_i, x_j\rangle) \geq a_0 N^2 - K(1) N. \tag{3.10}$$

Note that functions K whose coefficients a_n in the ultraspherical expansion are non-negative are sometimes called *positive definite functions*; see [19]. The estimate (3.10) for positive definite functions follows immediately from the results of I. J. Schoenberg [19].

4. Proof of Theorem 1

The proof is as in [17].

Proof. Let $\mathcal{P}_N = \{D_1, \dots, D_N\}$ be a partition of the sphere S^d into N parts such that $\sigma(D_j) = 1/N$ and the diameter of D_j is $\leq CN^{-1/d}$ for $j = 1, 2, \dots, N$. Here C is a constant that does not depend on N. In [17] such a partition is called an area-regular partition of the sphere.

Area-regular partitions are not so easy to construct explicitly, and a rigorous proof would be quite tedious. In [17] this was done for the case $d = 2$. Area-regular partitions were also used by J. Beck and W. Chen [1, pp. 237-238] and J. Bourgain and J. Lindenstrauss [6].

Let σ_j^* be the restriction of the measure $N\sigma$ to D_j. Then each σ_j^* is a probability measure, and, integrating $E_d(s, \{x_1, \dots, x_N\})$ with respect to the probability measure $d\sigma_1^*(x_1)d\sigma_2^*(x_2)\cdots d\sigma_N^*(x_N)$, we get

$$\begin{aligned} 2\mathcal{E}_d(s,N) &\leq \int \cdots \int \sum_{i\neq j} |x_i - x_j|^{-s} d\sigma_1^*(x_1)\cdots d\sigma_N^*(x_N) \\ &= N^2 \int\int |x-y|^{-s} d\sigma(x)d\sigma(y) - \sum_{j=1}^N \int_{D_j}\int_{D_j} |x-y|^{-s} d\sigma_j^*(x)d\sigma_j^*(y) \\ &\leq V_d(s)N^2 - \sum_{j=1}^N (\operatorname{diam} D_j)^{-s}. \end{aligned}$$

Because the diameter of each D_j is at most $CN^{-1/d}$, the estimate (1.6) follows. $\square$

5. Proof of Theorem 2

Proof of the lower bound. Let $\omega_N = \{x_1, \dots, x_N\}$ be any configuration of N points on S^d. For each i, we define

$$r_i := \min_{j\neq i} |x_i - x_j|.$$

Then it is easy to see that the caps $C(x_i, r_i/2)$ are disjoint. Using the fact that $\sigma(C(x_i, r_i/2)) \geq Ar_i^d$ for some absolute constant A (cf. (3.3)), we get

$$A\sum_{i=1}^N r_i^d \leq \sum_{i=1}^N \sigma(C(x_i, r_i/2)) \leq 1. \tag{5.1}$$

An easy argument based on Lagrange multipliers shows that (5.1) implies

$$\sum_{i=1}^N r_i^{-s} \geq A^{s/d} N^{1+s/d}. \tag{5.2}$$

This gives $E_d(s, \omega_N) \geq \frac{1}{2}A^{s/d}N^{1+s/d}$, and so $\mathcal{E}_d(s,N) \geq C_1 N^{1+s/d}$, which is the desired lower bound. $\square$

Proof of the upper bound. Let $\omega_N = \{x_1, \dots, x_N\}$ be a configuration of N points on the unit sphere that minimizes the s-energy. For each i let $D_i := S^d \setminus C(x_i, N^{-1/d})$, and put $D := \bigcap_{i=1}^N D_i$. From (3.4) it follows that

$$\sigma(D) \geq 1 - \frac{1}{d}\gamma_d > 0. \tag{5.3}$$

Consider, for a given index i, the function

$$U_i(x) := \sum_{j \neq i} |x - x_j|^{-s}, \qquad x \in S^d. \tag{5.4}$$

Then we have

$$\begin{aligned} \int_D U_i(x) d\sigma(x) &= \sum_{j \neq i} \int_D |x - x_j|^{-s} d\sigma(x) \leq \sum_{j \neq i} \int_{D_j} |x - x_j|^{-s} d\sigma(x) \\ &\leq CN^{s/d}, \end{aligned} \tag{5.5}$$

where for the last inequality we used (3.6).

Since ω_N minimizes the s-energy, the function U_i attains its minimum at the point x_i. Therefore

$$U_i(x_i) \leq \frac{1}{\sigma(D)} \int_D U_i(x) d\sigma(x). \tag{5.6}$$

Then, combining (5.3), (5.5), (5.6), for every i we obtain

$$U_i(x_i) \leq CN^{s/d}, \qquad s > d. \tag{5.7}$$

Since $\sum_i U_i(x_i) = 2\mathcal{E}_d(s, N)$, the upper bound in (1.8) follows. □

From the above proof we easily get the separation result (1.12).

Proof of Corollary 4, (1.12). From (5.4) and (5.7) in the previous proof, we get

$$|x_i - x_j|^{-s} \leq CN^{s/d}, \qquad i \neq j.$$

This gives (1.12). □

6. Proof of Theorem 3

Let $d \geq 2$. We are going to prove the lower bound

$$\liminf_{N \to \infty} (N^2 \log N)^{-1} \mathcal{E}_d(d, N) \geq \frac{1}{2d} \gamma_d \tag{6.1}$$

and the upper bound

$$\limsup_{N \to \infty} (N^2 \log N)^{-1} \mathcal{E}_d(d, N) \leq \frac{1}{2d} \gamma_d. \tag{6.2}$$

To prove (6.1) we cannot use the method of Section 5. This method can be extended to give $\mathcal{E}_d(d, N) \geq CN^2 \log N$, but does not yield a precise estimate for the constant C. Instead we follow G. Wagner [23] in the use of spherical harmonics to prove lower bounds.

Proof of (6.1). Let $K(t) = (2 - 2t)^{-d/2}$, $K_\epsilon(t) = (2 - 2t + \epsilon)^{-d/2}$, and expand K_ϵ in a series with respect to the ultraspherical polynomials $P_n^{(d-1)/2}$:

$$K_\epsilon(t) = \sum_{n=0}^{\infty} a_n(\epsilon) P_n^{(d-1)/2}(t).$$

The coefficients $a_n(\epsilon)$ are given by

$$a_n(\epsilon) = A_{n,d} \int_{-1}^{1} (2 - 2t + \epsilon)^{-d/2} P_n^{(d-1)/2}(t)(1 - t^2)^{d/2-1} dt,$$

where $A_{n,d}$ is a positive constant. Using the Rodrigues formula (3.8) for $P_n^{(d-1)/2}$ and integrating by parts n times, we find that $a_n(\epsilon) > 0$ for every n. Therefore we can apply (3.10) to K_ϵ, and we get, for every configuration $\{x_1, \dots, x_N\}$ of points on S^d,

$$\sum_{i \neq j} K_\epsilon(\langle x_i, x_j \rangle) \geq a_0(\epsilon) N^2 - \epsilon^{-d/2} N.$$

Since $K(t) \geq K_\epsilon(t)$ for $t \in [-1, 1]$, we find that

$$\mathcal{E}_d(d, N) \geq \frac{1}{2}(a_0(\epsilon) N^2 - \epsilon^{-d/2} N). \tag{6.3}$$

Now the coefficient $a_0(\epsilon)$ satisfies

$$\begin{aligned} a_0(\epsilon) &= \gamma_d \int_{-1}^{1} (2 - 2t + \epsilon)^{-d/2} (1 - t^2)^{d/2 - 1} dt \\ &= \frac{1}{2} \gamma_d \left[-\log \epsilon \right] + \mathcal{O}(1) \qquad (\epsilon \to 0). \end{aligned} \tag{6.4}$$

Taking $\epsilon = N^{-2/d}$ and using (6.3), (6.4), we find that

$$\mathcal{E}_d(d, N) \geq \frac{1}{2d} \gamma_d N^2 \log N + \mathcal{O}(N^2) \qquad (N \to \infty).$$

This completes the proof of (6.1). □

Proof of (6.2). We follow the proof of the upper bound in Section 5. Let $\omega_N = \{x_1, \dots, x_N\}$ be a configuration that minimizes the d-energy. For $r > 0$ set

$$D_i(r) := S^d \setminus C(x_i, r N^{-1/d}), \quad i = 1, \dots, N, \qquad D(r) := \bigcap_{i=1}^{N} D_i(r).$$

Then we have, from (3.4),

$$\sigma(D(r)) \geq 1 - \frac{1}{d} \gamma_d r^d. \tag{6.5}$$

We fix $r > 0$ and introduce, for every i, the function

$$U_i(x) := \sum_{j \neq i} |x - x_j|^{-d}, \qquad x \in S^d.$$

Using (3.7), we obtain

$$\begin{aligned} \int_{D(r)} U_i(x) d\sigma(x) &\leq \sum_{j \neq i} \int_{D_j(r)} |x - x_j|^{-d} d\sigma(x) \\ &= \gamma_d N \left[-\log(r N^{-1/d}) \right] + \mathcal{O}(N) \qquad (N \to \infty) \\ &= \frac{1}{d} \gamma_d N \log N + \mathcal{O}(N) \qquad (N \to \infty). \end{aligned}$$

Since ω_N minimizes the d-energy, the function U_i attains its minimum at the point x_i. Therefore

$$U_i(x_i) \leq \frac{1}{\sigma(D(r))} \int_{D(r)} U_i(x) d\sigma(x) \leq \frac{1}{\sigma(D(r))} \frac{1}{d} \gamma_d N \log N + \mathcal{O}(N), \tag{6.6}$$

which leads to the estimate

$$\mathcal{E}_d(d, \omega_N) = \frac{1}{2} \sum_{i=1}^{N} U_i(x_i) \leq \frac{1}{\sigma(D(r))} \frac{1}{2d} \gamma_d N^2 \log N + \mathcal{O}(N^2).$$

Letting $r \to 0$ and using (6.5), we now obtain (6.2). □

As in Section 5, the above proof also gives a separation result.

Proof of Corollary 4, (1.13). Immediate from (6.6). □

7. Proof of Theorem 5

Proof. We start with a partition of the sphere

$$\mathcal{P}_m = \{D_1, \dots, D_m\}$$

into m parts of equal area $4\pi/m$ which have small diameters. Such a partition exists with

$$\operatorname{diam} D_k \le C m^{-1/2}, \qquad k = 1, \dots, m. \tag{7.1}$$

(It was shown in [17] that we can take $C = 7$.)

We fix m and such a partition $\mathcal{P}_m$. Let $\epsilon > 0$, and put

$$D_k(\epsilon) = \{x \in D_k \mid \text{distance from } x \text{ to } \partial D_k \ge \epsilon\}, \qquad k = 1, \dots, m.$$

We assume ϵ is so small that each $D_k(\epsilon)$ is non-empty. Let y_k be any point in $D_k(\epsilon)$, let T_k denote the tangent plane to the sphere at y_k and let π_k be the orthogonal projection from D_k onto T_k. Then π_k decreases distances and areas. From (7.1) it follows that

$$4\pi/m = \text{ area of } D_k \le (1 + B/m) \cdot (\text{area of } \pi_k(D_k)), \qquad k = 1, \dots, m. \tag{7.2}$$

The constant B is independent of k and m.

Let N be a large number. We are going to produce N points on the sphere, and there will be approximately N/m points in each part $D_k(\epsilon)$. For each k, we take δ_k so that

$$\frac{1}{2}\sqrt{3}\delta_k^2 = \{\text{area of } \pi_k(D_k(\epsilon))\} \cdot \frac{m}{N}. \tag{7.3}$$

Let L_{δ_k} be the hexagonal lattice scaled so that minimal distances are equal to δ_k. We can move the center of this lattice so that there are at least N/m lattice points in $\pi_k(D_k(\epsilon))$. This follows from the definition of δ_k in (7.3) and an argument due to Blichfeldt [4] (also used in [22]). Let ω_N^k be the collection of the pre-images (under the mapping π_k) of the lattice points in $\pi_k(D_k(\epsilon))$, and put

$$\omega_N := \bigcup_{k=1}^{m} \omega_N^k.$$

Then ω_N has at least N points. We throw away some of the points to get exactly N points. The resulting set is also denoted by ω_N.

Now let us estimate $E_2(s, \omega_N)$. Take $x_i \in \omega_N$, say $x_i \in \omega_N^k$. Then for $x_j \in \omega_N^k$, $x_j \ne x_i$, we have $|x_i - x_j| \ge |\pi_k(x_i) - \pi_k(x_j)|$, and this gives

$$\sum_{x_j \in \omega_N^k, x_j \ne x_i} |x_i - x_j|^{-s} \le \sum_{x_j \in \omega_N^k, x_j \ne x_i} |\pi_k(x_i) - \pi_k(x_j)|^{-s} \le \delta_k^{-s} \zeta_L(s).$$

The points from ω_N which are not in ω_N^k have distance at least ϵ to x_i. So their contribution to the sum $\sum |x_i - x_j|^{-s}$ is at most $\epsilon^{-s} N$. Then we have, for $x_i \in \omega_N^k$,

$$\sum_{x_j \in \omega_N, x_j \ne x_i} |x_i - x_j|^{-s} \le \delta_k^{-s} \zeta_L(s) + \epsilon^{-s} N. \tag{7.4}$$

Now if we put

$$A(\epsilon) := \min_k \{\text{area of } \pi_k(D_k(\epsilon))\},$$

then from (7.3) and (7.4) we get

$$\sum_{x_j \in \omega_N, x_j \neq x_i} |x_i - x_j|^{-s} \leq \left(\frac{\sqrt{3}}{2} \frac{1}{mA(\epsilon)} \right)^{s/2} \zeta_L(s) N^{s/2} + \epsilon^{-s} N.$$

Hence

$$\mathcal{E}_2(s,N) \leq \frac{1}{2} \left(\frac{\sqrt{3}}{2} \frac{1}{mA(\epsilon)} \right)^{s/2} \zeta_L(s) N^{1+s/2} + \frac{1}{2}\epsilon^{-s} N^2,$$

and it follows that

$$\limsup_N N^{-1-s/2} \mathcal{E}_2(s,N) \leq \frac{1}{2} \left(\frac{\sqrt{3}}{2} \frac{1}{mA(\epsilon)} \right)^{s/2} \zeta_L(s).$$

This holds for every $\epsilon > 0$. If we let ϵ tend to 0, then $\pi_k(D_k(\epsilon))$ tends to $\pi_k(D_k)$, and using the estimate (7.2) we obtain

$$\lim_{\epsilon \to 0} mA(\epsilon) \geq \frac{4\pi}{1 + B/m}.$$

Hence

$$\limsup_N N^{-1-s/2} \mathcal{E}_2(s,N) \leq \frac{1}{2} \left(\frac{\sqrt{3}}{2} \frac{(1 + B/m)}{4\pi} \right)^{s/2} \zeta_L(s).$$

Finally, letting m tend to ∞, we get (2.6). This completes the proof of Theorem 4. □

8. Appendix: asymptotics of lattice sums

In this appendix we prove that the limit (2.9) exists.

Theorem 6. *For $0 < s < 2$, we have*

$$\lim_{R \to \infty} \left[\sum_{0 < |X| \leq R} |X|^{-s} - \left(\frac{2\pi}{\sqrt{3}} \right)^{s/2} \frac{2}{2-s} n(R)^{1-s/2} \right] = 6\zeta(s/2) L_{-3}(s/2). \tag{8.1}$$

Here the sum is over all non-zero points in the hexagonal lattice with modulus $\leq R$, and $n(R)$ denotes the number of points with modulus $\leq R$ (including 0).

Proof. For a lattice point X, let H_X denote the closed hexagonal Voronoi cell of X. The area of H_X is $\sqrt{3}/2$. Observe that for complex s with $\Re s = \sigma$, we have

$$|X|^{-s} - \frac{2}{\sqrt{3}} \int_{H_X} |Y|^{-s} dY = \mathcal{O}(|X|^{-\sigma-2}).$$

This follows from a Taylor expansion of $|Y|^{-s}$ around X and the fact that the integral of the linear term vanishes because X is the center of H_X. Therefore the series

$$\psi(s) := \sum_{X \neq 0} \left\{ |X|^{-s} - \frac{2}{\sqrt{3}} \int_{H_X} |Y|^{-s} dY \right\}$$

converges for $\Re s > 0$ and represents an analytic function.

For $s > 2$ we have

$$\begin{aligned}\psi(s) &= \sum_{X\neq 0} |X|^{-s} - \frac{2}{\sqrt{3}} \int_{\mathbf{R}^2\setminus H_0} |Y|^{-s} dY \\ &= 6\zeta(s/2)L_{-3}(s/2) - \frac{4\pi}{\sqrt{3}}\frac{1}{s-2} - \frac{2}{\sqrt{3}} \int_{D\setminus H_0} |Y|^{-s} dY,\end{aligned}$$

where D is the unit disk. By analyticity this formula holds throughout $\Re s > 0$. Since

$$\frac{2}{\sqrt{3}} \int_D |Y|^{-s} dY = \frac{4\pi}{\sqrt{3}}\frac{1}{2-s}, \qquad 0 < s < 2,$$

it follows that

$$\psi(s) = 6\zeta(s/2)L_{-3}(s/2) + \frac{2}{\sqrt{3}} \int_{H_0} |Y|^{-s} dY, \qquad 0 < s < 2.$$

Writing

$$A(R) := \bigcup \{H_X \mid |X| \leq R\}$$

and noting the definition of $\psi(s)$, we obtain from this

$$\lim_{R\to\infty} \left[\sum_{0<|X|\leq R} |X|^{-s} - \frac{2}{\sqrt{3}} \int_{A(R)} |Y|^{-s} dY \right] = 6\zeta(s/2)L_{-3}(s/2). \tag{8.2}$$

Next choose $\tilde{R}$ such that the area of the disk $D(\tilde{R})$ is equal to the area of $A(R)$. That is,

$$\pi \tilde{R}^2 = \frac{\sqrt{3}}{2} n(R). \tag{8.3}$$

Taking

$$B_1(R) := D(\tilde{R}) \setminus A(R), \qquad B_2(R) := A(R) \setminus D(\tilde{R}),$$

we have

$$\left| \int_{A(R)} |Y|^{-s} dY - \int_{D(\tilde{R})} |Y|^{-s} dY \right| = \int_{B_1(R)} |Y|^{-s} dY - \int_{B_2(R)} |Y|^{-s} dY.$$

Since $B_1(R)$ is contained in the annulus $R - 1 < |Y| \leq \tilde{R}$ and $B_2(R)$ is contained in $\tilde{R} \leq |Y| < R + 1$, we find that

$$\int_{B_1(R)} |Y|^{-s} dY \leq |B_1(R)| \, (R-1)^{-s}, \qquad \int_{B_2(R)} |Y|^{-s} dY \geq |B_2(R)| \, (R+1)^{-s},$$

where $|B_j(R)|$ is the area of $B_j(R)$, $j = 1, 2$. Since these areas are equal and of the order $\mathcal{O}(R)$, we end up with

$$\left| \int_{A(R)} |Y|^{-s} dY - \int_{D(\tilde{R})} |Y|^{-s} dY \right| = \left((R-1)^{-s} - (R+1)^{-s} \right) \mathcal{O}(R) = \mathcal{O}(R^{-s}).$$

Thus in the limit relation (8.2), $A(R)$ can be replaced with $D(\tilde{R})$. The integral over $D(\tilde{R})$ can be evaluated explicitly, and by combining this with (8.3) we arrive at (8.1). $\square$

Since $n(R) = (2\pi/\sqrt{3})R^2 + \mathcal{O}(R^{2/3})$ (see [13, II]), it also follows that

$$\lim_{R\to\infty}\left[\sum_{0<|X|\le R} |X|^{-s} - \frac{2\pi}{\sqrt{3}}\frac{2}{2-s}R^{2-s}\right] = 6\zeta(s/2)L_{-3}(s/2)$$

in case $2/3 < s < 2$.

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