MESH RATIOS FOR BEST-PACKING AND LIMITS OF MINIMAL ENERGY CONFIGURATIONS

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ABSTRACT. For N-point best-packing configurations ω_N on a compact metric space (A, ρ), we obtain estimates for the mesh-separation ratio $\gamma(\omega_N, A)$, which is the quotient of the covering radius of ω_N relative to A and the minimum pairwise distance between points in ω_N. For best-packing configurations ω_N that arise as limits of minimal Riesz s-energy configurations as $s \to \infty$, we prove that $\gamma(\omega_N, A) \leq 1$ and this bound can be attained even for the sphere. In the particular case when $N = 5$ on S^2 with ρ the Euclidean metric, we prove our main result that among the infinitely many 5-point best-packing configurations there is a unique configuration, namely a square-base pyramid ω_5^*, that is the limit (as $s \to \infty$) of 5-point s-energy minimizing configurations. Moreover, $\gamma(\omega_5^*, S^2) = 1$.

1. Introduction

Let A be a compact infinite metric space with metric $\rho : A \times A \to [0, \infty)$ and let $\omega_N = \{x_i\}_{i=1}^N \subset A$ denote a configuration of $N \geq 2$ points in A. We are chiefly

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concerned with two 'quality' measures of ω_N; namely, the *separation distance of* ω_N defined by

$$\delta(\omega_N) = \delta^\rho(\omega_N) := \min_{1\le i\neq j\le N} \rho(x_i, x_j), \tag{1}$$

and the *mesh norm of* ω_N *with respect to* A defined by

$$\eta(\omega_N, A) = \eta^\rho(\omega_N, A) := \max_{y\in A} \min_{1\le i\le N} \rho(y, x_i). \tag{2}$$

This quantity is also known as the *fill radius* or *covering radius* of ω_N relative to A. The optimal values of these quantities are also of interest and we consider, for $N \geq 2$, the N*-point best-packing distance on* A given by

$$\delta_N(A) = \delta_N^\rho(A) := \max\{\delta(\omega_N) \colon \omega_N \subset A,\ \#\omega_N = N\}, \tag{3}$$

and the N*-point mesh norm* of A given by

$$\eta_N(A) = \eta_N^\rho(A) := \min\{\eta(\omega_N, A) \colon \omega_N \subset A,\ \#\omega_N = N\}, \tag{4}$$

where $\#S$ denotes the cardinality of set S. A configuration ω_N of N points in A is called a *best-packing configuration for* A if $\delta(\omega_N) = \delta_N(A)$.

In the theory of approximation and interpolation (for example, by splines or radial basis functions (RBFs)), the separation distance is often associated with some measure of 'stability' of the approximation, while the mesh norm arises in the error of the approximation. In this context, the *mesh-separation ratio* (or *mesh ratio*)

$$\gamma(\omega_N, A) := \eta(\omega_N, A)/\delta(\omega_N),$$

can be regarded as a 'condition number' for ω_N relative to A. If $\{\omega_N\}_{N=2}^\infty$ is a sequence of N-point configurations such that $\gamma(\omega_N, A)$ is uniformly bounded in N, then the sequence is said to be *quasi-uniform on* A. Quasi-uniform sequences of configurations are important for a number of methods involving RBF approximation and interpolation (see [9, 13, 16, 17]).

We remark that in some cases it is easy to obtain positive lower bounds for the mesh-separation ratio. For example, if A is connected, then $\gamma(\omega_N, A) \geq 1/2$. Furthermore, letting

$$B(x,r) := \{y \in A : \rho(y,x) \leq r\}$$

denote the closed ball in A with center x and radius r, then $\gamma(\omega_N, A) \geq \beta/2$ for any N-point configuration $\omega_N \subset A$ whenever A and $\beta \in (0,1)$ have the property that for any $r \in (0, \operatorname{diam}(A)]$ and any $x \in A$, the annulus $B(x,r) \setminus B(x, \beta r)$ is nonempty. The *diameter* of A is defined by

$$\operatorname{diam}(A) := \max\{\rho(x,y) \colon x \in A,\ y \in A\}.$$

The outline of the paper is as follows. In Section 2 we present two simple but basic results concerning the mesh-separation ratio for best-packing configurations on general sets. In Section 3, we obtain lower bounds for this ratio for any best-packing configuration on the sphere in $\mathbb{R}^n$ and, in Section 4, we study the special case of minimal Riesz s-energy 5-point configurations on S^2 and determine their limiting best-packing configuration as $s \to \infty$. Section 5 is devoted to a brief discussion of some special best-packing configurations on S^n.

2. Mesh-separation ratio for general sets

The following simple result is of the same spirit as that of Proposition 2.1 of [12].

Theorem 1. *Let (A, ρ) be a compact infinite metric space. Then, for each $N \geq 2$, there exists an N-point best-packing configuration ω_N on A such that $\gamma(\omega_N, A) \leq 1$. In particular, this holds for any best-packing configuration $\omega_N = \{x_1, \ldots, x_N\}$ having the minimal number of pairs of points $\{x_i, x_j\}$ such that $\rho(x_i, x_j) = \delta_N(A)$.*

Proof. Let ω_N be a best-packing configuration on A having the minimal number of unordered pairs of points $\{x_i, x_j\}$ such that $\rho(x_i, x_j) = \delta_N(A)$. If $\eta(\omega_N, A) > \delta_N(A)$, then select a point $a \in A$ such that $\rho(a, x_i) > \delta_N(A)$ for $i = 1, \ldots, N$, and choose a point x_ℓ from some pair $\{x_k, x_\ell\}$ such that $\rho(x_k, x_\ell) = \delta_N(A)$. Let ω'_N be the best-packing configuration obtained by replacing a in ω_N by x_ℓ. Clearly, ω'_N has fewer unordered pairs of points $\{x_i, x_j\}$ such that $\rho(x_i, x_j) = \delta_N(A)$ than ω_N. This contradiction proves Theorem 1. □

On the other hand, there exist examples of compact metric spaces (A, ρ) for which

$$\limsup_{N\to\infty} \sup\{\gamma(\omega_N, A) \mid \delta(\omega_N) = \delta_N(A)\} = \infty, \tag{5}$$

as we now show.

Example 1. Let A be the standard 1/3 Cantor set in [0,1] and let ρ be the Euclidean metric. For each $N \in \mathbb{N}$, the set A is contained in the union of 2^N disjoint intervals of length 3^{-N} with endpoints $0 = x_1^N < x_2^N < \ldots < x_{2^{N+1}}^N = 1$ which belong to A. For any configuration of 2^N+1 points in A, at least one of the intervals of length 3^{-N} must contain at least two points from the configuration showing that $\delta_{2^N+1}(A) \le 3^{-N}$. On the other hand, the configuration $\omega_{2^N+1} := \{x_1^N, \ldots, x_{2^N+1}^N = 2/3\}$ is a best-packing configuration since $\delta(\omega_{2^N+1}) = \delta_{2^N+1}(A) = 3^{-N}$ and has mesh norm $\eta(\omega_{2^N+1}, A) = 1/3$. Thus (5) holds.

Best-packing configurations arise as limits of minimum energy configurations as we now describe. For a configuration $\omega_N := \{x_1, \ldots, x_N\} \subset A$ of $N \ge 2$ distinct points and $s > 0$, the *Riesz s-energy of* ω_N is defined by

$$E_s(\omega_N) = E_s^\rho(\omega_N) := \sum_{1\le i\ne j\le N} \frac{1}{\rho(x_i, x_j)^s} = \sum_{i=1}^{N} \sum_{\substack{j=1\\ j\ne i}}^{N} \frac{1}{\rho(x_i, x_j)^s},$$

while the *N-point Riesz s-energy of A* is defined by

$$\mathcal{E}_s(A, N) = \mathcal{E}_s^\rho(A, N) := \inf\{E_s(\omega_N) : \omega_N \subset A, \#\omega_N = N\}. \tag{6}$$

An N-point configuration $\omega_N \subset A$ is said to *s-energy minimizing* if $E_s(\omega_N) = \mathcal{E}_s(A, N)$.

Proposition 2 ([4]). *Let (A, ρ) be an infinite compact metric space. For each fixed $N \geq 2$,*

$$\lim_{s\to\infty} \mathcal{E}_s(A, N)^{1/s} = \frac{1}{\delta_N(A)}.$$

Moreover, every cluster point as $s \to \infty$ of s-energy minimizing N-point configurations on A is an N-point best-packing configuration on A.

The following theorem concerning the mesh-separation ratio of best-packing configurations that arise as cluster points of s-energy minimizing configurations generalizes, simplifies, and improves Theorem 7 of [11].

Theorem 3. *For a fixed $N \geq 2$, let ω_N be a cluster point as $s \to \infty$ of a family of N-point s-energy minimizing configurations on a compact metric space (A, ρ). Then $\gamma(\omega_N, A) \leq 1$.*

The upper bound for $\gamma(\omega_N, A)$ in this theorem can be attained even for the case when A is a sphere and ρ is the Euclidean metric. For $N = 11$ on S^2, equality follows from the uniqueness result for best-packing of Böröczky [3]. For $N = 5$ on S^2, it follows from Theorem 7 in Section 4.

Proof. Let $N \geq 2$ be fixed and, for $s > 0$, let $\omega_{N,s}$ be an N-point s-energy minimizing configuration on A. Clearly, $E_s(\omega_{N,s}) \geq \delta(\omega_{N,s})^{-s}$. This implies that there exists a point $x_s \in \omega_{N,s}$ such that

$$\sum_{y\in\omega_{N,s}\setminus\{x_s\}} \rho(x_s, y)^{-s} \geq N^{-1}E_s(\omega_{N,s}) \geq N^{-1}\delta(\omega_{N,s})^{-s}.$$

If $\eta(\omega_{N,s}, A) > N^{2/s}\delta(\omega_{N,s})$, then $E_s(\omega'_{N,s}) < E_s(\omega_{N,s})$, where $\omega'_{N,s} := \omega_{N,s}\cup\{a\}\setminus\{x_s\}$, and a is a point of A such that $\rho(t, a) \geq \eta(\omega_{N,s}, A)$, for all $t \in \omega_{N,s}$, which yields a contradiction. Hence,

$$\eta(\omega_{N,s}, A) \leq N^{2/s}\delta(\omega_{N,s}), \tag{7}$$

and letting $s \to \infty$ in (7) and using Proposition 2, we obtain the statement of Theorem 3. □

3. Lower bounds for the mesh-separation ratio on the sphere

In this section we derive some lower bounds for the mesh-separation ratio of a best-packing N-point configuration on the unit sphere $S^n \subset \mathbb{R}^{n+1}$ with ρ the Euclidean metric. Let Δ_n and Θ_n be the sphere packing and covering constants in $\mathbb{R}^n$, respectively:

$$\Delta_n := \lim_{N\to\infty} N(\delta_N(U_n)/2)^n\beta_n \quad \text{and} \quad \Theta_n := \lim_{N\to\infty} N\eta_N(U_n)^n\beta_n, \tag{8}$$

where $U_n := [0,1]^n$ denotes the unit cube in $\mathbb{R}^n$ and β_n denotes the volume of the unit ball in $\mathbb{R}^n$ (see, e.g. [7, 14]). First we prove the following asymptotic result for best-packing configurations on S^n.

Theorem 4. *Let $\{\omega_N\}$ denote a sequence of N-point best-packing configurations on S^n. Then*

$$\gamma(\omega_N, S^n) \geq \frac{1}{2}\left(\frac{\Theta_n}{\Delta_n}\right)^{1/n} + o(1), \quad N \to \infty. \tag{9}$$

Proof. Since the collection of spherical caps with centers in the points of ω_N of the radius $\eta(\omega_N, S^n)$ covers S^n, a standard projection argument implies

$$N\beta_n \left(\eta(\omega_N, S^n)\right)^n \geq \Theta_n \text{Area}(S^n) + o(1), \quad N \to \infty. \tag{10}$$

Similarly we have

$$N\beta_n \left(\frac{\delta(\omega_N)}{2}\right)^n \leq \Delta_n \text{Area}(S^n) + o(1), \quad N \to \infty. \tag{11}$$

Thus, we obtain (9) directly from (10) and (11). □

It is interesting to investigate the asymptotic behavior of the constant on the right-hand side of (9) as $n \to \infty$. The best known asymptotic upper bound for Δ_n is the Kabatyanski-Levenshtein bound $\Delta_n \le 2^{-0.599n+o(n)}$ as $n \to \infty$ and the best known lower bound for the covering constant is $\Theta_n \ge cn$, where c is a positive absolute constant (cf. [7, pages 40 and 247]). Thus the inequality (9) implies the following: if n is large enough and $N > C(n)$, then the inequality

$$\gamma(\omega_N, S^n) \ge (1/2)2^{0.599} + o(1) \ge 0.757, \qquad n \to \infty,$$

holds for an arbitrary best-packing configuration ω_N on S^n. Further upper bounds for Δ_n and lower bounds for Θ_n can be found in [5] and [7]. In particular, it is known that for $n = 2$ the hexagonal lattice provides both $\Delta_2 = \pi/\sqrt{12}$, and $\Theta_2 = 2\pi/\sqrt{27}$. Hence

$$\gamma(\omega_N, S^2) \ge \frac{1}{\sqrt{3}} + o(1), \quad N \to \infty,$$

for an arbitrary best packing configuration ω_N on S^2. However, by special arguments working only for $n = 2$ we are able to improve this result to the following:

Theorem 5. *Let $\{\omega_N\}$ denote a sequence of N-point best-packing configurations on S^2. Then*

$$\gamma(\omega_N, S^2) \ge \frac{1}{2\cos\pi/5} + o(1) = \frac{2}{1+\sqrt{5}} + o(1), \quad N \to \infty. \tag{12}$$

Proof. It suffices to only consider sequences such that $\gamma(\omega_N, S^2) = O(1)$ as $N \to \infty$. For a fixed $N \ge 4$, consider the Voronoi decomposition of S^2 generated by ω_N, with X_i denoting the cell associated with x_i; that is,

$$X_i := \{v \in S^2 \mid |v - x_i| = \min_{x \in \omega_N} |v - x|\}.$$

Euler's formula for convex polyhedra implies that there is a cell X_j having at most 5 edges (each cell is a spherical polygon with edges consisting of arcs of great circles), see [10]. Since

$$B(x_i, \delta(\omega_N)/2) \cap S^2 \subset X_i \subset B(x_i, \eta(\omega_N, S^2)),$$

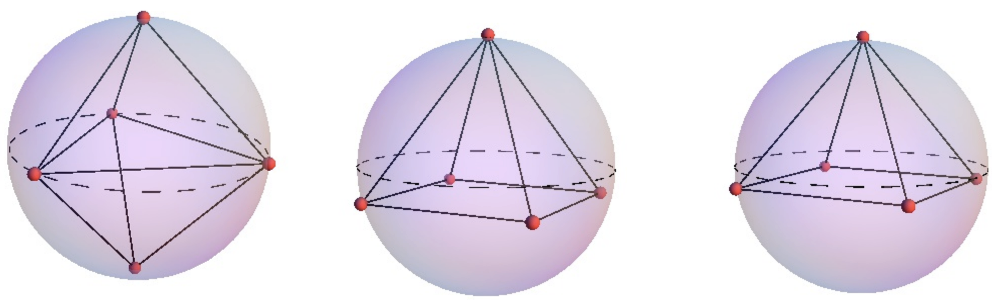
and $\eta(\omega_N, S^2) = O(\delta(\omega_N))$, it follows by a projection argument that there is at least one interior angle from x_j to consecutive vertices of X_j with angle $2\pi/5 + o(1)$, and hence the distance from x_j to some vertex of X_j is at least

$$\frac{\delta(\omega_N)}{2\cos\pi/5} + o(\delta(\omega_N)), \quad N \to \infty.$$

This yields (12).

□

4. Limit of minimal energy for 5 points on S^2



(a) (b) (c)

FIGURE 1. 'Optimal' 5-point configurations on $\mathbb{S}^2$: (a) bipyramid BP, (b) optimal square-base pyramid SBP(1) , (c) optimal square-base pyramid SBP(16).

It was observed in [15] from numerical experiments that 5-point minimum Riesz s-energy configurations on S^2 with the Euclidean metric appear to depend on s and to be of two general types: (i) the bipyramid (BP) consisting of 2 antipodal points and 3 equally spaced points on the associated equator, and (ii) the square-base pyramid (SBP(s)) with one vertex at the north pole and 4 vertices of the same latitude depending on s and forming a square (see Figure 1). A comparison of the s-energy for the BP and the SBP(s) configurations is given in Figure 2 and suggests (as in [15]) that BP is optimal for $s < s^* \approx 15.04808$, while SBP(s) is optimal for $s > s^*$.

R. Schwartz [18] using a mathematically rigorous computer-aided solution proved (in a manuscript of 67 pages) that, for $N = 5$, BP is the unique minimizer of the Riesz s-energy for $s = 1$ and $s = 2$. (For the logarithmic energy, the optimality of BP is established in [8].) Currently there are no other values of $s > 0$ for which a rigorous optimality proof is known. Regarding the stability of BP and SBP(s), in Figure 3 we plot the minimum eigenvalue of the Hessian of their s-energies. These graphs suggest that BP is not a local minimizing configuration for $s > 21.148$ (also observed by H. Cohn), while SBP(s) is not a local minimizing configuration for $s < 13.5204$.

According to Proposition 2, every cluster point of s-energy minimizing configurations as $s \to \infty$ is a best-packing configuration. However, as is known, there are infinitely many non-isometric 5-point best-packing configurations on S^2 (see e.g. [2]).

Proposition 6. $\delta_5(S^2) = \sqrt{2}$ *and all 5-point best-packing configurations on* S^2 *consist of two antipodal points (poles) and a triangle on the equator having all angles greater than or equal to* $\pi/4$.

It appears from Figure 2 that the unique (up to isometry) cluster point of 5-point s-energy minimizing configurations is SBP(∞); that is, the square base pyramid with base on the equator. We shall next provide a rigorous proof that this is indeed the case.

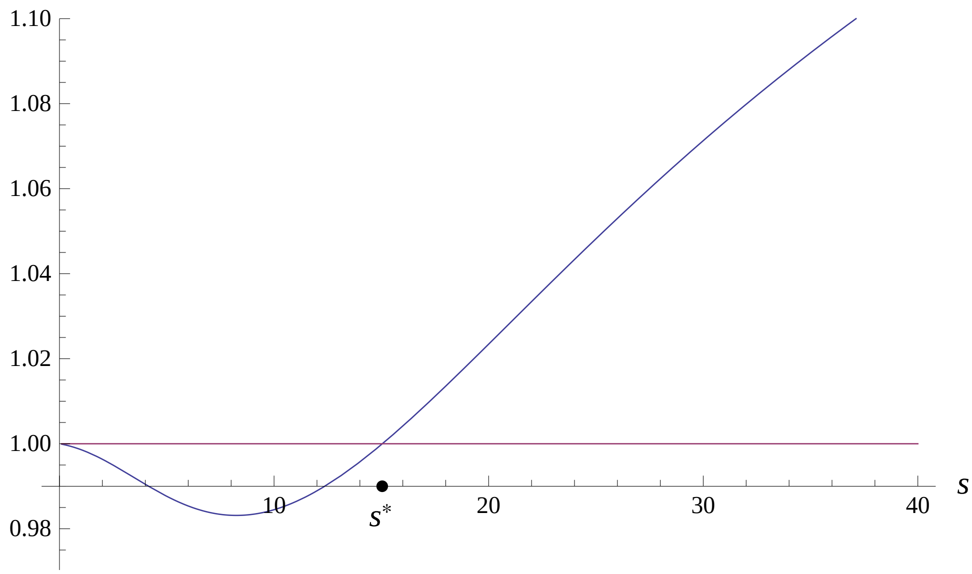
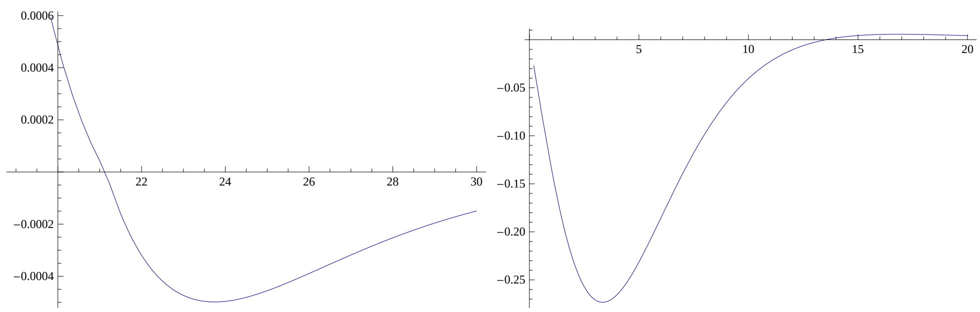


FIGURE 2. The ratio of the s-energy of BP to the s-energy of SBP(s).



(a) (b)

FIGURE 3. The minimum eigenvalue of the Hessian for the s-energy of (a) the BP configuration and (b) the SBP(s) configuration.

Theorem 7. *Let Q' be a cluster point of a family of 5-point s-energy minimizing configurations on S^2 as $s \to \infty$. Then Q' is isometric to*

$$Q = \mathrm{SBP}(\infty) := \{\mathrm{e}_1, -\mathrm{e}_1, \mathrm{e}_2, \mathrm{e}_3, -\mathrm{e}_3\}, \tag{13}$$

where $\mathrm{e}_1 = (1, 0, 0)$, $\mathrm{e}_2 = (0, 1, 0)$, *and* $\mathrm{e}_3 = (0, 0, 1)$.

It is perhaps surprising that this configuration has the maximum number of common pairwise distances (eight) of length $\sqrt{2}$ among all 5-point best-packings.

We start the proof with an upper estimate for the minimum 5-point s-energy on S^2.

Lemma 8.

$$\limsup_{s\to\infty} 2^{s/2}\mathcal{E}_s(S^2,5) \leq 8.$$

Proof. For arbitrary $0 < t < 1$, we define the following 5-point configuration on S^2:

$$Q_t := \{(\pm\sqrt{1-t^2}, -t, 0), (0, -t, \pm\sqrt{1-t^2}), \mathrm{e}_2\}, \tag{14}$$

which, for a suitable choice of t (depending on s), is a conjectured minimum energy configuration on S^2 for every s large enough. The s-energy of this configuration is given by

$$E_s(Q_t) := 4\cdot 2^{-s}(1-t^2)^{-s/2} + 8\cdot 2^{-s/2}(1-t^2)^{-s/2} + 8\cdot 2^{-s/2}(1+t)^{-s/2}.$$

Letting now $t = s^{-2/3}$, we obtain that

$$\lim_{s\to\infty}(1-t^2)^{-s/2} = 1 \quad \text{and} \quad \lim_{s\to\infty}(1+t)^{-s/2} = 0,$$

and so

$$\limsup_{s\to\infty} 2^{s/2}\mathcal{E}_s(S^2,5) \leq \lim_{s\to\infty} 2^{s/2}E_s(Q_t)$$
$$= \lim_{s\to\infty}(4\cdot 2^{-s/2}(1-t^2)^{-s/2} + 8(1-t^2)^{-s/2} + 8(1+t)^{-s/2}) = 8.$$

□

We further need the following statement.

Lemma 9. *Let A, B, and M be fixed positive constants. Then*

$$f(x) := M(1-Ax)^{-s} + (1+Bx)^{-s} \geq M + \min\{1, AM/B\}$$

for every $x \in [0, 1/A)$ and $s > 0$.

Proof. It is not difficult to see that f attains its minimum on $[0, 1/A)$ at the point $x_0 = 0$ if $B \leq AM$ and at the point

$$x_1 = \frac{(B/(AM))^{1/(s+1)} - 1}{B + A(B/(AM))^{1/(s+1)}}$$

if $B > AM$. In the first case we have

$$f(x) \geq f(0) = M + 1, \quad x \in [0, 1/A), \quad s > 0.$$

In the second case, since

$$x_1 \leq \frac{1}{B}\left[(B/(AM))^{1/(s+1)} - 1\right],$$

we have

$$f(x) \geq f(x_1) \geq M + (1 + Bx_1)^{-s} \geq M + (B/(AM))^{-s/(s+1)} > M + AM/B$$

for all $x \in [0, 1/A)$ and $s > 0$. Combining the results in both cases, we obtain the assertion of the lemma. □

Proof of Theorem 7. As we mentioned in Proposition 2 above, any cluster point of a family of s-energy minimizing configurations as $s \to \infty$ is a best-packing configuration. Thus, by Proposition 6, it is sufficient to show that no 5-point configuration consisting of two opposite poles and an acute triangle on the equator (which we call an *acute configuration*) could be such a cluster point. We will prove this by contradiction. For s large, consider a minimal s-energy configuration that is 'close' to a fixed acute configuration. We may assume that this minimal s-energy configuration $\omega_5(s)$ consists of three points

$$A_1 = A_{1s} = (a_{11s}, a_{12s}, h),\ A_2 = A_{2s} = (a_{21s}, a_{22s}, h),\ A_3 = A_{3s} = (a_{31s}, a_{32s}, h),$$

where $h = h_s = o(1)$ as $s \to \infty$, that are close to the vertices of a fixed acute triangle on the equator, and two points $A_4 = A_{4s}$ and $A_5 = A_{5s}$ that are close to $(0, 0, 1)$ and $(0, 0, -1)$, respectively. Denote by

$$E_1 := E_{1s} = \sum_{i=1}^{3} |A_4 - A_i|^{-s}, \quad \text{and} \quad E_2 := E_{2s} = \sum_{i=1}^{3} |A_5 - A_i|^{-s}.$$

Clearly, the total s-energy $E_s(\omega_5(s)) > 2E_1 + 2E_2$.

Let us first estimate E_1 from below. Denote by O the point $(0, 0, h)$, by B the projection of A_4 to the plane $A_1A_2A_3$, and by x the length $|O - B|$. Without lost of generality we may assume that B lies in the triangle OA_2A_3. Here we use the facts that $x = x_s = o(1)$ as $s \to \infty$, and that $A_1A_2A_3$ is 'close' to a fixed acute triangle implying that O lies inside the triangle $A_1A_2A_3$. Denote by $\alpha = \alpha_s$, $\beta = \beta_s$, and $\gamma = \gamma_s$ the angles A_2OB, A_3OB, A_2OA_1, respectively (see Figure 4).

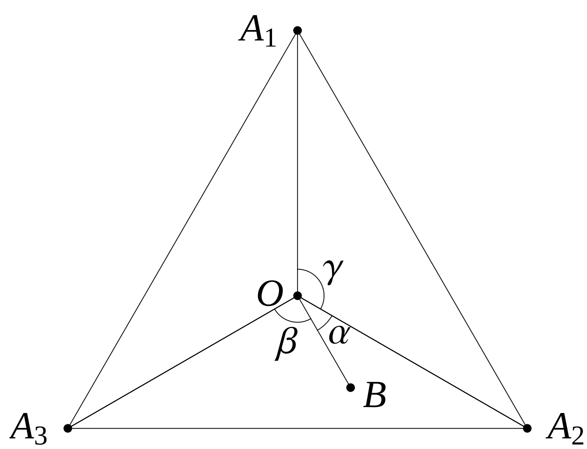


FIGURE 4. Projection B of A_4 on horizontal $A_1A_2A_3$ plane.

Since

$$E_1 = \sum_{i=1}^{3} |A_4 - A_i|^{-s} = \sum_{i=1}^{3} \left(|B - A_4|^2 + |B - A_i|^2\right)^{-s/2},$$

we have, by the law of cosines and the fact that $|B - A_4| = \sqrt{1 - x^2} - h$,

$$\begin{aligned}E_1 &= (2 - 2h\sqrt{1-x^2} - 2x\sqrt{1-h^2}\cos\alpha)^{-s/2}\\ &\quad + (2 - 2h\sqrt{1-x^2} - 2x\sqrt{1-h^2}\cos\beta)^{-s/2}\\ &\quad + (2 - 2h\sqrt{1-x^2} - 2x\sqrt{1-h^2}\cos(\alpha+\gamma))^{-s/2}.\end{aligned}$$

The crucial observation is the fact that $\alpha + \beta < \tau < \pi$, for some τ that does not depend on s. Now monotonicity and convexity of the function $t^{-s/2}$, $t > 0$, immediately imply

$$\begin{aligned}E_1 &\geq 2\left(2 - 2h\sqrt{1-x^2} - x\sqrt{1-h^2}(\cos\alpha + \cos\beta)\right)^{-s/2}\\ &\qquad\qquad + (2 - 2h\sqrt{1-x^2} + 2x)^{-s/2}\\ &\geq 2\left(2 - 2h\sqrt{1-x^2} - x\sqrt{1-h^2}(1 + \cos\tau)\right)^{-s/2}\\ &\qquad\qquad + (2 - 2h\sqrt{1-x^2} + 2x)^{-s/2}.\end{aligned} \tag{15}$$

From the facts that $x = o(1)$, and $h = o(1)$ as $s \to \infty$ and the inequality $1 - x \leq \sqrt{1-x^2} \leq 1$, we get that

$$E_1 \geq 2\,(2 - 2h - \theta_1 x)^{-s/2} + (2 - 2h + 3x)^{-s/2},$$

for some absolute constant $\theta_1 > 0$. Then, by Lemma 9,

$$E_1 \geq (2 + \theta_2)(2 - 2h)^{-s/2},$$

for some absolute constant $\theta_2 > 0$. Similarly we obtain

$$E_2 \geq (2 + \theta_2)(2 + 2h)^{-s/2},$$

and so again applying the convexity of $t^{-s/2}$ we finally deduce that, for s sufficiently large,

$$E_s(\omega_5(s)) > 2(E_1 + E_2) \geq (8 + 4\theta_2)\,2^{-s/2}. \tag{16}$$

On the other hand, from Lemma 8, we know that $\mathcal{E}_s(S^2,5) \le (8+o(1))2^{-s/2}$. Therefore, by (16), an acute configuration cannot be a cluster point of minimal s-energy configurations as $s \to \infty$. □

We can now obtain the dominant term in the asymptotic expansion for the minimal 5-point s-energy.

Theorem 10. *We have*

$$\lim_{s\to\infty} 2^{s/2}\mathcal{E}_s(S^2,5) = 8.$$

Proof. By Lemma 8 it is enough to prove that

$$\liminf_{s\to\infty} 2^{s/2}\mathcal{E}_s(S^2,5) \ge 8. \tag{17}$$

For a fixed $s>0$ consider a minimal s-energy configuration $\omega_5(s) = \{A_1,\dots,A_5\} := \{A_{1s},\dots,A_{5s}\}$. By Theorem 7 we may assume that both distances $|A_2 - A_3|$ and $|A_4 - A_5|$ have limit 2 as $s \to \infty$. Observe that if the triangle $A_1A_2A_3$ is not acute, then

$$|A_1 - A_2|^{-s} + |A_1 - A_3|^{-s} \ge |A_1' - A_2|^{-s} + |A_1' - A_3|^{-s} \ge 2^{1-s/2},$$

where A_1' is the midpoint of the circular arc (of length less than π) joining A_2 and A_3 and containing A_1. A similar statement holds for triangle $A_1A_4A_5$. Therefore we may assume that at least one of the triangles $A_1A_2A_3$ or $A_1A_4A_5$ is acute since otherwise the desired lower bound for the s-energy follows. Without lost of generality, we assume that $A_1A_2A_3$ is acute. We adopt the same notation as in the proof of Theorem 7 and obtain a finer lower bound for E_1 and E_2.

There are three possible cases to consider, depending on the location of the projection B of A_4 onto the plane containing A_1, A_2, and A_3: (i) B is inside the sector A_2OA_3; (ii) B is inside the sector A_1OA_2; and (iii) B is inside the sector A_1OA_3.

Let us assume first that B is inside the sector A_2OA_3 as in Figure 4. From (15), we get

$$E_1 \geq 2(2 - 2h\sqrt{1-x^2} - x\sqrt{1-h^2}(\cos\alpha + \cos\beta))^{-s/2} \geq 2(2 - 2h\sqrt{1-x^2})^{-s/2}.$$

In both other cases (ii) and (iii) we get the same inequality. Letting D denote the projection of A_5 onto the plane $A_1A_2A_3$ and setting $y = |O - D|$, we similarly get

$$E_2 \geq 2(2 + 2h\sqrt{1-y^2})^{-s/2}.$$

Thus,

$$E_s(\omega_5(s)) > 4\left[(2 - 2h\sqrt{1-x^2})^{-s/2} + (2 + 2h\sqrt{1-y^2})^{-s/2}\right].$$

Finally applying Lemma 9 to the last inequality and using the fact that $x = o(1)$ and $y = o(1)$ as $s \to \infty$ we immediately obtain (17). □

5. Special best-packing configurations on S^n

In the case $A = S^n$ with $n \geq 2$ and Euclidean distance, there are best-packing configurations ω_N such that $\eta(\omega_N, S^n) = \delta(\omega_N) = \sqrt{2}$ for $N = n+3, \ldots, 2n+1$, yielding $\gamma(\omega_N, S^n) = 1$ (see Theorem 6.2.1 [2]). For $N = 5$ on S^2, such a configuration is given by SBP(∞) defined in (13).

By the proof of Theorem 1, we have $\eta(\omega_N, A) \geq \delta(\omega_N)$ for some best-packing configuration ω_N if and only if $\delta_N(A) = \delta_{N+1}(A)$, which should be a very rare event, at least for $A = S^n$. For S^2 and $N = 11$ there exists a unique (up to isometry) best-packing configuration ω_{11} consisting of the regular icosahedron minus one of its vertices (see [3]). Hence,

$$\eta_{11}(S^2) = \delta_{11}(S^2) \text{ and } \gamma(\omega_{11}, S^2) = 1. \tag{18}$$

The unique best-packing configuration of 120 points on S^3 is the 600-cell configuration which has many other fascinating extremal properties, see [1, 6]. Moreover, in [19], the numerical evidence is given that

$$\delta_{113}(S^3) = \ldots = \delta_{120}(S^3) = (\sqrt{5}-1)/2. \tag{19}$$

Assuming (19), we are able to construct a best-packing configuration of 113 points on the sphere with $\eta(\omega_{113}, S^3) > \delta_N(\omega_{113})$. It consists of 600-cell without certain 7 points which we describe below.

In the 600-cell each point has 12 other points at the closest distance $(\sqrt{5}-1)/2$, and each pair of points at this distance has exactly 5 other points having the same distance to both points of the pair. So we will remove two points x_1, x_2, such that $|x_1 - x_2| = (\sqrt{5}-1)/2$, and also 5 points $y_1, \ldots y_5$, such that $|x_i - y_j| = (\sqrt{5}-1)/2$, $i = 1, 2$, $j = 1, \ldots, 5$. Recall that the second largest distance between points of the 600-cell is 1. Thus,

$$\eta(\omega_{113}, S^3) \geq \min_{x \in \omega_{113}} \left| \frac{x_1 + x_2}{|x_1 + x_2|} - x \right| = \sqrt{2 - \frac{3+\sqrt{5}}{\sqrt{10+2\sqrt{5}}}} \approx 1.2778\, \delta(\omega_{113}).$$

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