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Discrepancy, separation and Riesz energy of finite point sets on the unit sphere

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Abstract For $d \geqslant 2$, we consider asymptotically equidistributed sequences of $\mathbb{S}^d$ codes, with an upper bound δ on spherical cap discrepancy, and a lower bound Δ on separation. For such sequences, if $0 < s < d$, then the difference between the normalized Riesz s energy of each code, and the normalized s-energy double integral on the sphere is bounded above by $\mathrm{O}\left(\delta^{1-s/d}\,\Delta^{-s}\,N^{-s/d}\right)$, where N is the number of code points. For well separated sequences of spherical codes, this bound becomes $\mathrm{O}\left(\delta^{1-s/d}\right)$. We apply these bounds to minimum energy sequences, sequences of well separated spherical designs, sequences of extremal fundamental systems, and sequences of equal area points.

Keywords sphere · spherical cap discrepancy · separation · Riesz energy

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1 Introduction and Main Results

Consider the unit sphere $\mathbb{S}^d := \left\{x \in \mathbb{R}^{d+1} \mid \|x\| = 1\right\}$, for $d \geqslant 2$. Call a finite set of points of $\mathbb{S}^d$ a *spherical code*. There is a continuing interest in the generation and use of spherical codes which are in some sense well distributed, and the properties which can be used to distinguish better distributed codes from more poorly distributed ones. This paper examines the relationship between three such properties of sequences of spherical codes. These properties are the Riesz s energy, the spherical cap discrepancy, and the separation of code points.

It is known that a sequence of spherical codes with minimal Riesz s energy and increasing numbers of points has "good" spherical cap discrepancy, and "good" separation, in a sense which is made more precise below. The question addressed in this paper concerns a partial converse to this result:

> When does a sequence of spherical codes with "good" spherical cap discrepancy and "good" separation also have "good" Riesz s energy?

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The following definitions make these concepts more precise. The normalized *Riesz s energy* of a spherical code X is $\mathrm{E}(X)\,U_s$, where $U_s(r) := r^{-s}$, the Riesz potential function, and $\mathrm{E}(X)$ is the normalized discrete energy functional

$$\mathrm{E}(X)\,u := \frac{1}{|X|^2} \sum_{x \in X} \sum_{\substack{y \in X \\ y \neq x}} u\,(\|x-y\|)\,.$$

The corresponding normalized continuous energy functional is given by the double integral

$$\mathscr{I}\,u := \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} u\,(\|x-y\|)\,d\sigma(x)\,d\sigma(y),$$

where σ is the spherical probability measure, the uniform measure on $\mathbb{S}^d$ normalized so that $\sigma(\mathbb{S}^d) = 1$. It is well known that for $0 < s < d$, the normalized energy double integral of U_s has the value

$$\mathscr{I}\,U_s = 2^{d-s-1} \frac{\Gamma\big((d+1)/2\big)\,\Gamma\big((d-s)/2\big)}{\sqrt{\pi}\,\Gamma(d-s/2)}. \tag{1}$$

The normalized *spherical cap discrepancy* of a spherical code is the supremum over all spherical caps of the difference between the normalized area of the cap and the proportion of code points which lie in the cap. In other words, for $y \in \mathbb{S}^d$, $r \in (0,2]$, let $S(y,r)$ be the closed spherical cap $\{x \mid \|x-y\| \leqslant r\}$, and let σ_X be the normalized counting measure defined for $Y \in \mathbb{S}^d$ by

$$\sigma_X(Y) := \frac{|X \cap Y|}{|X|}.$$

Then the normalized spherical cap discrepancy of X is

$$\mathscr{D}(X) := \sup_{y \in \mathbb{S}^d, r \in (0,2]} \left|\sigma\left(S(y,r)\right) - \sigma_X\left(S(y,r)\right)\right|.$$

A sequence $\mathscr{X} := (X_1, X_2, \ldots)$, of spherical codes with corresponding cardinalities $N_\ell := |X_\ell|$ is *asymptotically equidistributed* [10, Remark 4, p. 236], if the normalized spherical cap discrepancy is bounded above by a positive decreasing function $\delta : \mathbb{N} \to (0,2]$, with $\delta(N) \to 0$ as $N \to \infty$. Specifically,

$$\mathscr{D}(X_\ell) < \delta(N_\ell). \tag{2}$$

The sequences of spherical codes of most interest for this paper are those such that the minimum distance between code points is bounded below by a positive decreasing function $\Delta : \mathbb{N} \to (0,2]$,

$$\|x-y\| > \Delta(N_\ell) \quad \text{for all } x, y \in X_\ell. \tag{3}$$

An easy area argument shows that the order of the lower bound $\Delta(N)$ for the separation of the solution of the *Tammes problem* [38] (the sequence which has the largest separation for each N) is $\Omega(N^{-1/d})$ [33, Theorem 2]. Therefore, for all sequences of $\mathbb{S}^d$ codes, $\Delta(N_\ell)N_\ell^{1/d}$ is bounded above by a constant. In other words, we must have

$$\Delta(N_\ell) = \mathrm{O}(N_\ell^{-1/d}). \tag{4}$$

A sequence of $\mathbb{S}^d$ codes is called *well separated* if there exists a *separation constant* $\gamma > 0$ such that we can set $\Delta(N) = \gamma N^{-1/d}$.

For the purposes of this paper, we define an *admissible sequence* of spherical codes to be a sequence $\mathscr{X}$, such that a discrepancy function δ, and a separation function Δ exist, satisfying the bounds (2) and (3) respectively.

Before stating our main result, we note here that this paper uses "big-Oh" and "big-Omega" notation with *inequalities* in a somewhat unusual way, to avoid a proliferation of unknown constants. For upper bounds, when we say that

$$f(n) \leqslant g(n) + \mathrm{O}\left(h(n)\right) \quad \text{as } n \to \infty,$$

we mean that there exist positive constants C and M such that

$$f(n) \leqslant g(n) + C\big(h(n)\big) \quad \text{for all } n \geqslant M.$$

For lower bounds, when we say that

$$f(n) \geqslant g(n) + \Omega\left(h(n)\right) \quad \text{as } n \to \infty,$$

we mean that there exist positive constants C and M such that

$$f(n) \geqslant g(n) + C\big(h(n)\big) \quad \text{for all } n \geqslant M.$$

If more than one O or Ω expression is used in an inequality, the implied constants may be different from each other.

We now state our main result.

Theorem 1.1 *For an admissible sequence $\mathscr{X}$ of $\mathbb{S}^d$ spherical codes, with discrepancy function δ, and separation function Δ, the normalized Riesz s energy for $0 < s < d$ is bounded by*

$$\left(\mathrm{E}(X_\ell) - \mathscr{I}\right) U_s \leqslant \mathrm{O}\left(\delta(N_\ell)^{1-s/d}\, \Delta(N_\ell)^{-s}\, N_\ell^{-s/d}\right), \quad \textit{and} \tag{5}$$

$$\left(\mathscr{I} - \mathrm{E}(X_\ell)\right) U_s \leqslant \mathrm{O}\left(\delta(N_\ell)^{1-s/d}\right). \tag{6}$$

This result immediately implies the following.

Corollary 1.2 *For a well separated admissible sequence $\mathscr{X}$ of $\mathbb{S}^d$ spherical codes, with discrepancy function δ, the normalized Riesz s energy for $0 < s < d$ satisfies*

$$\mathrm{E}(X_\ell)\, U_s = \mathscr{I}\, U_s + \mathrm{O}\left(\delta(N_\ell)^{1-s/d}\right). \tag{7}$$

Remarks

Bounds in the best case

As stated by Beck [1, p. 10], for any sequence of spherical codes, the normalized spherical cap discrepancy is bounded below such that

$$\delta(N_\ell) = \Omega\left(N_\ell^{-1/2-1/(2d)}\right). \tag{8}$$

Thus, for a well separated sequence with the best possible normalized spherical cap discrepancy, if the sequence is well separated, then the estimate (7) gives an upper bound for the normalized Riesz s energy of no better than

$$\mathrm{E}(X_\ell)\,U_s - \mathscr{I}\,U_s \leqslant \mathrm{O}\left(N_\ell^{(s-d)(d+1)/(2d^2)}\right).$$

In contrast, the best known upper bound for $\mathrm{E}(X_N)\,U_s - \mathscr{I}\,U_s$ for a minimum s-energy sequence Ω_s, for $d \geqslant 2$ and $s \in (0,d)$, is

$$\mathrm{E}(\Omega_{s,N})\,U_s - \mathscr{I}\,U_s \leqslant -cN^{s/d-1}, \quad \text{with } c > 0, \tag{9}$$

as given by Kuijlaars and Saff [24, (1.6)].

Asymptotic equidistribution and weak-star convergence

It has long been known that such a sequence $\mathscr{X}$ of spherical codes is asymptotically equidistributed if and only if it is weak-star convergent, i.e. the corresponding sequence (σ_{X_ℓ}) of normalized counting measures converges weakly to σ,

$$\int_{\mathbb{S}^d} f(x)\,d\sigma_{X_\ell}(x) := \frac{1}{N_\ell}\sum_{x\in X_\ell} f(x) \to \int_{\mathbb{S}^d} f(x)\,d\sigma(x)$$

as $\ell \to \infty$ for all continuous $f : \mathbb{S}^d \to \mathbb{R}$.

Theorem 4.1 of R. Ranga Rao [34, p. 665] states that given a measure μ on $\mathbb{R}^{d+1}$ such that $\mu\mathscr{L}^{-1}$ is continuous for every linear function $\mathscr{L}$ on $\mathbb{R}^{d+1}$, a sequence of measures converges weakly to μ if and only if it converges to μ for certain discrepancies defined on half spaces. This theorem can be used to show that a sequence of $\mathbb{S}^d$ codes is weak-star convergent if and only if it converges to zero in normalized spherical cap discrepancy. Brauchart [7, Lemma 1.4] proves this equivalence relationship in another way, by appealing to Grabner's [18] Erdős-Turán inequality on the sphere. Blümlinger extends this result to compact Riemannian manifolds [3].

Measures with bounded density

Götz obtains a result [17, Proposition 13] similar to Corollary 1.2, that is, an estimate of Riesz energy in terms of ball discrepancy, but his result is for the difference in energy double integral between two probability measures satisfying a density bound [17, (12)], and so the result does not apply in our case. It is interesting to note, though, that if we set $\beta = d$ in [17, (12)], then the energy difference given by [17, Proposition 13] is also bounded by $C\,\delta^{1-s/d}$, where in this case δ is the discrepancy between the two probability measures.

Applications of Theorem 1.1

It is known that the following sequences of spherical codes are admissible.

1. Minimum energy sequences.
   See Section 2.
2. Well separated sequences of spherical designs.
   See Section 3.

3. Sequences of extremal fundamental systems.
   Let $\{p_1, \ldots, p_{D_t}\}$ be a basis for the spherical polynomials of degree at most t. An *extremal fundamental system* is a spherical code X which maximizes the determinant $\det A(X)$, where A is the interpolation matrix of size $D_t \times D_t$ with entries $A_{i,j} := p_i(x_j)$. See [35,36] for details. A sequence Ξ of extremal fundamental systems with increasing degree t is known to be well separated [35]. Marzo and Ortega-Cerdà [30] have recently shown that Ξ is asymptotically equidistributed. Corollary 1.2 therefore implies that the normalized Riesz s energy of Ξ converges to the normalized energy double integral for all $s \in (0,d)$.
4. Well separated, diameter-bounded equal area sequences.
   The sequence $\mathrm{EQP}(d)$ of recursive zonal equal area spherical codes, as described in the author's PhD thesis [27, 4.1], is well separated [27, Theorem 4.3.2] and has normalized spherical cap discrepancy $\mathscr{D}\left(\mathrm{EQP}(d,N)\right) = \mathrm{O}\left(N^{-1/d}\right)$ [27, Theorem 5.4.1]. Our estimate (7) therefore yields the normalized energy estimate

$$\mathrm{E}(\mathrm{EQP}(d,N))\, U_s = \mathscr{I}\, U_s + \mathrm{O}\left(N^{(s-d)/d^2}\right).$$

2 Minimum energy sequences

Minimum Riesz s energy

For $q > 0$, let $\Omega_q = (\Omega_{q,1}, \Omega_{q,2}, \ldots)$ be a sequence of $\mathbb{S}^d$ codes such that $|\Omega_{q,N}| = N$ and such that $\Omega_{q,N}$ has the minimum Riesz q energy of any $\mathbb{S}^d$ code with N code points. It is known that for $q \in (0,d)$, Ω_q is asymptotically equidistributed [26, Ch. 2, pp. 160–162] [10, Theorem 3] [20, Theorem 1.1]. Brauchart [6, Theorem 2.2] gives a bound for the normalized spherical cap discrepancy of Ω_q of

$$\mathscr{D}(\Omega_{q,N}) = \mathrm{O}\left(N^{-\alpha/d}\right). \tag{10}$$

where $\alpha := (d-q)/(d-q+2)$.

For $q \in (d-2, d)$, Ω_q is also known to be well separated [15, Theorem 1.5]. Therefore, for $q \in (d-2,d)$ and $s \in (0,d)$, Corollary 1.2 implies that $\mathrm{E}(\Omega_{q,N})\, U_s \to \mathscr{I}\, U_s$ as $N \to \infty$. Using Brauchart's bound (10) we obtain, for this case, the estimate

$$\mathrm{E}(\Omega_{q,N})\, U_s = \mathscr{I}\, U_s + \mathrm{O}\left(N^{-(1-s/d)\,\alpha/d}\right) = \mathscr{I}\, U_s + \mathrm{O}\left(N^{-(1-s/d)(1-q/d)/(d-q+2)}\right).$$

For general $q > 0$, the situation is more complicated, and the known results on discrepancy and separation split into a number of cases. Let $\phi_{q,s}(N)$ be the order in N of the upper bound on $\mathrm{E}(\Omega_{q,N})\, U_s - \mathscr{I}\, U_s$ given by (5) above, given the current best known values of the upper bound $\delta(N)$ and lower bound $\Delta(N)$ for Ω_q. Table 1 lists these results, giving references.

The result for $q = d$ in Table 1 is peculiar. When $s < d/3$, the upper bound

$$\phi_{d,s}(N) = (\log N)^{(3s/d-1)/2}\, (\log\log N)^{(1-s/d)/2}$$

decreases to 0 as $N \to \infty$, but when $s \geqslant d/3$, this upper bound increases with increasing N. Kuijlaars and Saff comment that the order of the separation bound $\Delta(N)$ for Ω_d "most likely is not best possible" [24, p. 525]. This seems reasonable, since both $\Omega_{d+\varepsilon}$ and $\Omega_{d-\varepsilon}$ are known to be well separated.

q	$\delta(N)$	$\Delta(N)$	$\phi_{q,s}(N)$
$(0,d-2]$ $(d \geqslant 3)$	$\mathrm{O}\left(N^{-\alpha/d}\right)$ [6, Ch. 2]	$\Omega\left(N^{-1/(q+2)}\right)$ [13, Th. 3.5]	$\mathrm{O}\left(N^{-(1-s/d)\,\alpha/d-s/d+s/(q+2)}\right)$
$(d-2,d-1)$	$\mathrm{O}\left(N^{-\alpha/d}\right)$ [6, Ch. 2]	$\Omega\left(N^{-1/d}\right)$ [15, Th. 1.5]	$\mathrm{O}\left(N^{-(1-s/d)\,\alpha/d}\right)$
$d-1$	$\mathrm{O}\left(N^{-1/d}\log N\right)$ [16, Th. 4]	$\Omega\left(N^{-1/d}\right)$ [16, Th. 3]	$\mathrm{O}\left(N^{-(1-s/d)/d}(\log N)^{-(1-s/d)}\right)$
$(d-1,d)$	$\mathrm{O}\left(N^{-\alpha/d}\right)$ [6, Ch. 2]	$\Omega\left(N^{-1/d}\right)$ [25, Th. 8]	$\mathrm{O}\left(N^{-(1-s/d)\,\alpha/d}\right)$
d	$\mathrm{O}\left(\sqrt{\frac{\log\log N}{\log N}}\right)$ [11, Th. 1]	$\Omega\left((N\log N)^{-1/d}\right)$ [24, (1.13)]	$\mathrm{O}\left((\log N)^{(3s/d-1)/2}\,(\log\log N)^{(1-s/d)/2}\right)$
(d,∞)	$\to 0$ [20, Th. 2.2]	$\Omega\left(N^{-1/d}\right)$ [24, (1.12)]	$\to 0$

Table 1 Discrepancy, separation and s-energy bounds for minimum q-energy sequences

The result for $q \in (0,d-2)$ in Table 1 is also remarkable. The exponent

$$f(d,q,s) := -(1-s/d)(d-q)/(d-q+2)/d - s/d + s/(q+2)$$

is not always negative. In particular for $\phi_{s,s}(N)$, the upper bound from (5) for the normalized Riesz s energy of the optimal Riesz s energy points, the exponent $f(d,s,s)$ is not always negative:

$$\begin{aligned} f(d,s,s) &= -(1-s/d)(d-s)/(d-s+2)/d - s/d + s/(s+2) \\ &= \frac{(d-1)s^3 + (-2d^2+2d-2)s^2 + (d^3-d^2)s - 2d^2}{d^2\,(s+2)\,(d-s+2)}. \end{aligned}$$

For $d \geqslant 5$, $f(d,s,s)$ takes on positive values for s in some interval within $(0,d-2)$. For example, $f(5,s,s) > 0$ for $s \in (4-\sqrt{11}, 5/2)$, and our upper bound therefore diverges for this range of s.

In fact, our upper bound $\phi_{s,s}(N)$ is never tight for any $s \in (0,d)$, since it is always positive, and the best known upper bound for $\mathrm{E}(\Omega_{s,N})\,U_s - \mathscr{I}\,U_s$ is given by (9), which is negative.

Minimum logarithmic energy

For $d \geqslant 2$, the normalized *logarithmic energy* of a spherical code X is given by $\mathrm{E}(X)\,U_{\log}$, where $U_{\log}(r) := -\log(r)$ is the logarithmic potential function. Let $\Omega_{\log}$ be a sequence of $\mathbb{S}^d$ codes with such that $|\Omega_{\log,N}| = N$ and such that $\Omega_{\log,N}$ has the minimum normalized logarithmic energy for any $\mathbb{S}^d$ code with N code points. The best known bound on the normalized spherical cap discrepancy of $\Omega_{\log}$ is Brauchart's bound [7, Theorem 1.6], $\mathscr{D}(\Omega_{\log,N}) = \mathrm{O}\left(N^{-1/(d+2)}\right)$.

For $d = 2$, the logarithmic energy points are also known to be well separated [32, Theorem 1]. In this case, our estimate (7) implies the normalized energy estimate

$$\mathrm{E}(\Omega_{\log,N})\, U_s = \mathscr{I}\, U_s + \mathrm{O}\left(N^{-(1-s/2)/4}\right) \quad \text{for } s \in (0,2).$$

3 Well separated sequences of spherical designs

A spherical t-design is a spherical code such that the corresponding normalized counting measure gives an equal weight quadrature functional which exactly integrates all spherical polynomials of degree at most t [14]. In [22] it is proved that for a well separated sequence of spherical designs on $\mathbb{S}^2$ such that each t-design has $(t+1)^2$ points, the normalized Coulomb energy (i.e. Riesz 1 energy) has the same first term and a second term of the same order as the minimum normalized Coulomb energy for $\mathbb{S}^2$ codes. Hesse [21] generalizes these to cover the Riesz s energy for $0 < s < 2$.

To compare the results of [22] and [21] to energy bounds of the type treated here, we need a variant of Corollary 1.2. From [18, Theorem 1] [19, (2.1)] we know that there is a constant C_G such that for any spherical t-design X_t on $\mathbb{S}^2$, we have

$$\mathscr{D}(X_t) \leqslant \frac{C_G}{t+1}. \tag{11}$$

We therefore need to modify Corollary 1.2 to treat sequences $\mathscr{X}$ of spherical codes with normalized spherical cap discrepancy bounded by

$$\mathscr{D}(X_\ell) < \delta(\ell). \tag{12}$$

Corollary 3.1 *For a well separated sequence $\mathscr{X}$ of $\mathbb{S}^d$ spherical codes, with normalized spherical cap discrepancy bounded by* (12)*, the normalized Riesz s energy for $0 < s < d$ satisfies*

$$\mathrm{E}(X_\ell)\, U_s = \mathscr{I}\, U_s + \mathrm{O}\left(\delta(\ell)^{1-s/d}\right). \tag{13}$$

We define a well separated admissible sequence of $\mathbb{S}^d$ designs with separation constant γ to be a sequence of spherical designs $\mathscr{X} = (X_1, X_2, \ldots)$, with each spherical design X_t having strength t, where $\mathscr{X}$ is well separated, with separation constant γ. We can now compare the results of [22] and [21] with the result obtained by combining the estimate (13) with the bound (11) on the normalized spherical cap discrepancy of spherical designs. First we restate the main results from [22] with notation adjusted to match this paper, and recall from (1) the well known result that $\mathscr{I}\, U_1 = 1$.

Theorem 3.2 *Let $\mathscr{X}$ be a well separated admissible sequence of $\mathbb{S}^2$ designs with separation constant γ. Then the normalized Coulomb energy $\mathrm{E}(X_t)\, U_1$ of each spherical design $X_t \in \mathscr{X}$ of cardinality N_t is bounded above by*

$$\mathrm{E}(X_t)\, U_1 \leqslant 1 + C_\gamma (t+1)^{-3/2} N_t^{1/4} - \frac{1}{2}\frac{1}{t+3/2} - \frac{1}{2}\frac{(t+1)(t+2)}{t+3/2} N_t^{-1}.$$

The constant $C_\gamma \geqslant 0$ depends on the separation constant γ, but is independent of t.

Theorem 3.3 *Let $\mathscr{X}$ be a well separated admissible sequence of $\mathbb{S}^2$ designs with separation constant γ, such that for some positive constant μ, $|X_t| = N_t \leqslant \mu(t+1)^2$. Then the normalized Coulomb energy of each $X_t \in \mathscr{X}$ is bounded above by*

$$\mathrm{E}(X_t)\,U_1 \leqslant 1 + C_{(\gamma,\mu)}\,N_t^{-1/2},$$

where $C_{(\gamma,\mu)} \geqslant 0$ is independent of t.

It is not yet known whether an infinite sequence of spherical designs exists which satisfies the premise of Theorem 3.3. In [4], Bondarenko et al. show that a sequence exists satisfying the required bound on cardinality, but their paper does not address the question of separation of the points. If a sequence $\mathscr{X}$ satisfying the premise of Theorem 3.3 exists, the theorem implies that its normalized Coulomb energy converges to the corresponding normalized energy double integral at the rate of $\mathrm{O}\left(t^{-1}\right)$, that is

$$\mathrm{E}(X_t)\,U_1 \leqslant 1 + \mathrm{O}\left(t^{-1}\right).$$

Applying our estimate (13) and the bound (11) to a well separated admissible sequence $\mathscr{X}$ of spherical designs on $\mathbb{S}^2$, we obtain

$$\mathrm{E}(X_t)\,U_1 \leqslant 1 + \mathrm{O}\left(t^{-1/2}\right).$$

This is a slower rate of convergence than predicted by Theorem 3.3, but the result does not depend on the relationship between cardinality and strength required by Theorem 3.3.

If we use Theorem 3.2 with the infinite sequence of spherical designs of Korevaar and Meyers [23, Theorem 2.3], which has cardinality $\mathrm{O}\left(t^3\right)$, we obtain

$$\mathrm{E}(X_t)\,U_1 \leqslant 1 + \mathrm{O}\left(t^{-3/4}\right).$$

This assumes that this sequence is well separated. Judging from the construction given in [23, Section 5], this assumption seems reasonable. Thus Theorem 3.2 gives a faster rate of convergence for this sequence than is predicted by Corollary 3.1.

If instead of the normalized Coulomb energy, we use the normalized Riesz s energy for $s \in (0,2)$, then for a well separated admissible sequence $\mathscr{X}$ of spherical designs on $\mathbb{S}^2$, the estimate (13) and the bound (11) yield

$$\mathrm{E}(X_t)\,U_s \leqslant \mathscr{I}\,U_s + \mathrm{O}\left(t^{s/2-1}\right). \tag{14}$$

Hesse's result [21, Theorem 2] implies that for a sequence $\mathscr{X}$ of spherical designs which satisfies the premise of Theorem 3.3, the Riesz s energy for $s \in (0,2)$ satisfies

$$\mathrm{E}(X_t)\,U_s \leqslant \mathscr{I}\,U_s + \mathrm{O}\left(t^{s-2}\right).$$

Again, this result is better than our corresponding result (14).

4 Results used to prove Theorem 1.1

Our proof of Theorem 1.1 needs a few well known results, which we state here. We denote the Lebesgue area measure of the sphere $\mathbb{S}^d$ by

$$\omega_d := \frac{2\pi^{(d+1)/2}}{\Gamma(\frac{d+1}{2})}.$$

This usage of ω_d agrees with Müller [31], but not with Landkof [26, Ch. 1, p. 45], who would put ω_{d+1} where we have ω_d.

Lemma 4.1 *For $R \in (0,2]$ and $x \in \mathbb{S}^d$, the normalized area integral $\mathscr{V}_d(R) := \sigma(S(x,R))$ can be evaluated by*

$$\mathscr{V}_d(R) = \frac{\omega_{d-1}}{\omega_d} \int_0^R r^{d-1} \left(1 - \frac{r^2}{4}\right)^{d/2-1} dr,$$

independent of the point x.

Corollary 4.2 *For $R \in (0,T]$, $T \in (0,2]$, the normalized area integral $\mathscr{V}_d(R)$ satisfies*

$$\mathscr{V}_d(R) \in \left[C_{L,d}(T), C_{H,d}\right) \frac{R^d}{d}, \quad \text{where}$$
$$C_{L,d}(T) := \left(1 - \frac{T^2}{4}\right)^{d/2-1} C_{H,d}, \quad \text{and} \quad C_{H,d} := \frac{\omega_{d-1}}{\omega_d}. \tag{15}$$

Lemma 4.3 *For $R \in (0,2]$ and any $x \in \mathbb{S}^d$, for any integrable function $u : (0,2] \to \mathbb{R}$, the single integral*

$$\mathscr{I}(x;R)\,u := \int_{\|x-y\| \leqslant R} u(\|x-y\|)\, d\sigma(y), \quad \text{can be evaluated by}$$
$$\mathscr{I}(x;R)\,u = \mathscr{I}_d(R)\,u := \int_0^R u(r) d\mathscr{V}_d(r) = \frac{\omega_{d-1}}{\omega_d} \int_0^R u(r)\, r^{d-1} \left(1 - \frac{r^2}{4}\right)^{d/2-1} dr, \tag{16}$$

which is independent of x.

Corollary 4.4 *For any integrable function $u : (0,2] \to \mathbb{R}$, the double integral $\mathscr{I} u$ can be evaluated by $\mathscr{I} u = \mathscr{I}_d(2)\, u$, where $\mathscr{I}_d$ is defined by* (16)*.*

Corollary 4.5 *For $s \in (0,d)$, $R \in (0,T]$, $T \in (0,2]$, the integral $\mathscr{I}_d(R)\, U_s$ satisfies*

$$\mathscr{I}_d(R)\, U_s \in \left[C_{L,d}(T), C_{H,d}\right) \frac{R^{d-s}}{d-s}, \tag{17}$$

where $C_{L,d}$ and $C_{H,d}$ are defined by (15)*.*

From the results above we derive the following estimate.

Lemma 4.6 *Let X be a spherical code with cardinality $|X| = N > 2$ and minimum Euclidean distance bounded below by $\Delta \leqslant \sqrt{2}$. For $x \in X$, for $R \in (\Delta, \sqrt{2}]$, the normalized counting measure σ_X of the spherical cap $S(x,R)$ satisfies*

$$\sigma_X\big(S(x,R)\big) = \frac{|X \cap S(x,R)|}{|X|} \leqslant 2^{5d/2-1} \left(\frac{R}{\Delta}\right)^d N^{-1}. \tag{18}$$

Proof For $\theta \in [0,\pi]$, define $\Upsilon(\theta) := 2\sin(\theta/2)$, to convert spherical to Euclidean distance. Now fix Δ and define

$$\varphi := \Upsilon^{-1}(\Delta)/2 = \sin^{-1}(\Delta/2).$$

The spherical distance φ is therefore less than or equal to the packing radius of X. This implies that we can place each point y of X in a spherical cap $S(y,\Upsilon(\varphi))$ with no two caps overlapping. This places an upper bound on σ_X, of the form

$$\sigma_X(R) \leqslant \frac{\mathscr{V}_d\big(\Upsilon(\Upsilon^{-1}(R)+\varphi)\big)}{\mathscr{V}_d\big(\Upsilon(\varphi)\big)}. \tag{19}$$

Since $\varphi \in (0,\pi/2]$, we have $\Upsilon(\varphi) = 2\sin(\varphi/2) > \sin\varphi = \Delta/2$, and since

$$\Upsilon^{-1}(R)+\varphi < \Upsilon^{-1}(R)+2\varphi = \Upsilon^{-1}(R)+\Upsilon^{-1}(\Delta) < \Upsilon^{-1}(R+\Delta), \quad \text{we see that}$$
$$\mathscr{V}_d\big(\Upsilon(\varphi)\big) > \mathscr{V}_d(\Delta/2), \quad \text{and} \quad \mathscr{V}_d\big(\Upsilon(\Upsilon^{-1}(R)+\varphi)\big) < \mathscr{V}_d(R+\Delta).$$

From (19) we therefore have $\sigma_X(R) \leqslant \mathscr{V}_d(R+\Delta)/\mathscr{V}_d(\Delta/2)$. Since $\Delta \leqslant \sqrt{2}$, (15) gives us

$$\sigma_X(R) \leqslant \frac{C_{H,d}\ (R+\Delta)^d}{C_{L,d}(\sqrt{2})(\Delta/2)^d} = 2^d \frac{C_{H,d}}{C_{L,d}(\sqrt{2})} \left(\frac{R+\Delta}{\Delta}\right)^d.$$

To obtain (18) we note that for $R > \Delta$, we have $2R > R+\Delta$ and so

$$\left(\frac{R+\Delta}{\Delta}\right)^d < 2^d \left(\frac{R}{\Delta}\right)^d. \quad \square$$

A simple packing argument for the whole sphere, when combined with the area estimate from Corollary 4.2 leads to a refinement of our bound (4).

Lemma 4.7 *Let X be a spherical code with cardinality $|X| = N > 2$ and minimum Euclidean distance bounded below by Δ. Then Δ must satisfy the bound*

$$\Delta^d N \leqslant 2^{3d/2-1}\ \frac{d}{C_{H,d}}, \tag{20}$$

where $C_{H,d}$ is defined by (15).

Proof Because Δ is a lower bound on the minimum Euclidean distance, we can use the same argument as in the proof of Lemma 4.6 to show that we can place a spherical cap of Euclidean radius $\Delta/2$ around each point of X, with no two caps overlapping. Using this observation, and applying the estimate from Corollary 4.2, we must therefore have

$$1 \geqslant N\ \mathscr{V}_d(\Delta/2) \geqslant N\ \left(1-\frac{T^2}{4}\right)^{d/2-1} C_{H,d}\ \frac{\Delta^d}{2^d\, d},$$

for any $T \in [\Delta/2, 2]$. Setting $T = \sqrt{2}$, which is always possible, we obtain

$$1 \geqslant N\ 2^{1-d/2} C_{H,d}\ \frac{\Delta^d}{2^d\, d},$$

which leads directly to the bound (20). $\square$

5 Proof of Theorem 1.1

We fix d and drop all subscripts d where this does not cause confusion. We fix $s \in (0,d)$, fix a sequence $\mathscr{X}$ having the required properties. We also fix ℓ, drop all subscripts ℓ, and examine the spherical code $X := \{x_1, \ldots, x_N\}$. We use the abbreviations $\mathrm{E} := \mathrm{E}(X)$, $U := U_s$, $\Delta := \Delta(N)$, $\delta := \delta(N)$.

We calculate the normalized energy $\mathrm{E}U$ using a sum of Riemann-Stieltjes integrals, one for each of the N nodes. We have

$$\mathrm{E}U = \frac{1}{N} \sum_{k=1}^{N} \mathrm{E}_k U$$

where for any integrable function $u : (0,2] \to \mathbb{R}$,

$$\mathrm{E}_k u := \frac{1}{N} \sum_{\substack{j=1 \\ j \neq k}}^{N} u\left(\left\|x_k - x_j\right\|\right).$$

We use the punctured normalized counting function g_k defined by

$$g_k(r) := \sigma_X\left(S(x_k, r) \backslash \{x_k\}\right) = \frac{|X \cap S(x_k, r)| - 1}{N}.$$

This gives us

$$\mathrm{E}_k u = \int_0^2 u(r)\, dg_k(r) = \int_\Delta^2 u(r)\, dg_k(r),$$

where the last equation is a result of the separation condition (3). If u is differentiable on $(\Delta, 2]$ we can integrate by parts to obtain

$$\mathrm{E}_k u = [u(r) g_k(r)]_\Delta^2 - \int_\Delta^2 g_k(r)\, du(r) = u(2)\,(1 - N^{-1}) - \int_\Delta^2 g_k(r)\, du(r).$$

Since $U(r) = r^{-s}$, we have $dU(r) = -sr^{-s-1}\, dr$, and so

$$\mathrm{E}_k U = 2^{-s}(1 - N^{-1}) + \int_\Delta^2 sr^{-s-1}\, g_k(r)\, dr. \tag{21}$$

Upper bound

We use the packing argument of Lemma 4.6 to show that

$$g_k(r) \leqslant C_1\, \Delta^{-d} N^{-1} r^d - N^{-1}, \quad \text{where} \quad C_1 := 2^{5d/2-1}.$$

From the normalized spherical cap discrepancy δ and Corollary 4.2 we also know that

$$g_k(r) \leqslant \mathscr{V}(r) + \delta - N^{-1} \leqslant C_2\, r^d + \delta - N^{-1}, \quad \text{where} \quad C_2 := \frac{C_{H,d}}{d}.$$

We now find the Euclidean radius ρ where these two upper bounds are equal. This is given by

$$\rho = \left(\frac{1}{C_1 - C_2\,\Delta^d N}\right)^{1/d} \delta^{1/d}\,\Delta N^{1/d}. \tag{22}$$

Using Lemma 4.7, we see that $C_2\,\Delta^d N \leqslant 2^{3d/2-1}$, so that

$$C_1 - C_2\,\Delta^d N \geqslant 2^{5d/2-1} - 2^{3d/2-1} > 0.$$

Therefore

$$\rho = \mathrm{O}\left(\delta^{1/d}\,\Delta\,N^{1/d}\right). \tag{23}$$

Since $C_1 - C_2\,\Delta^d N < C_1$, we also have

$$\rho = \Omega\left(\delta^{1/d}\,\Delta\,N^{1/d}\right). \tag{24}$$

Since $\Delta\,N^{1/d} = \mathrm{O}(1)$ and since $\delta \to 0$, we must therefore have $\rho \to 0$. We also know from (8) that $\delta\,N$ is at least $\Omega(1)$. Therefore $0 < \Delta < \rho < 2$, for N sufficiently large.

We now have

$$g_k(r) \leqslant h(r) := \begin{cases} 0, & r \in [0, \Delta] \\ C_1\,\Delta^{-d} N^{-1} r^d - N^{-1}, & r \in (\Delta, \rho) \\ \mathscr{V}(r) + \delta - N^{-1}, & r \in [\rho, 2]. \end{cases}$$

On substitution back into (21) we obtain

$$\begin{aligned} \mathrm{E}_k\,U &= 2^{-s}(1 - N^{-1}) + \int_\Delta^\rho s r^{-s-1}\,g_k(r)\,dr + \int_\rho^2 s r^{-s-1}\,g_k(r)\,dr \\ &\leqslant 2^{-s}(1 - N^{-1}) + C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,(\rho^{d-s} - \Delta^{d-s}) \\ &\qquad + \int_\rho^2 s r^{-s-1}\,\mathscr{V}(r)\,dr + \delta\,(\rho^{-s} - 2^{-s}) - N^{-1}\,(\Delta^{-s} - 2^{-s}). \end{aligned}$$

We see that this upper bound is independent of our code point index k and therefore we have

$$\begin{aligned} \mathrm{E}U &\leqslant 2^{-s}(1 - N^{-1}) + C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,(\rho^{d-s} - \Delta^{d-s}) \\ &\qquad + \int_\rho^2 s r^{-s-1}\,\mathscr{V}(r)\,dr + \delta\,(\rho^{-s} - 2^{-s}) - N^{-1}\,(\Delta^{-s} - 2^{-s}). \end{aligned}$$

Using (16), we have

$$\mathscr{I}\,U = \int_0^2 U(r)\,d\mathscr{V}(r) = U(2) - \int_0^2 DU(r)\,\mathscr{V}(r)\,dr = 2^{-s} + \int_0^2 s r^{-s-1}\,\mathscr{V}(r)\,dr.$$

Using (22), and integrating by parts, we therefore obtain

$$\begin{aligned} \mathrm{E}U - \mathscr{I}\,U &\leqslant -2^{-s} N^{-1} + C_1\,\frac{s}{d-s}\Delta^{-d} N^{-1}\,(\rho^{d-s} - \Delta^{d-s}) + \rho^{-s}\,\mathscr{V}(\rho) \\ &\qquad - \int_0^\rho r^{-s}\,d\mathscr{V}(r) + \delta\,(\rho^{-s} - 2^{-s}) - N^{-1}\,(\Delta^{-s} - 2^{-s}). \end{aligned}$$

We now use the estimate (17) to obtain

$$\begin{aligned}\mathrm{E}U - \mathscr{I}U &\leqslant C_1 \frac{s}{d-s}\Delta^{-d}N^{-1}\rho^{d-s} + C_2\rho^{d-s} + \delta\rho^{-s}\\ &\quad - (C_1 \frac{s}{d-s}+1)\Delta^{-s}N^{-1} - C_3 \frac{1}{d-s}\rho^{d-s} - 2^{-s}\delta\,.\end{aligned}$$

where $C_3 := C_{L,d}(\sqrt{2})$. Substituting the order estimate for ρ from (23), we obtain

$$\mathrm{E}U - \mathscr{I}U \leqslant \mathrm{O}\left(\delta^{1-s/d}\Delta^{-s}N^{-s/d}\right) + \mathrm{O}\left(\delta^{1-s/d}\Delta^{d-s}N^{1-s/d}\right).$$

Since $\Delta^d N$ is at most $\mathrm{O}(1)$, we obtain our upper bound (5).

Lower bound

We define the Euclidean radius τ by $\mathscr{V}(\tau) = \delta + N^{-1}$. Using (8), we see that

$$\tau = \mathrm{O}\left(\delta^{1/d}\right) \quad \text{and} \quad \tau = \Omega\left(\delta^{1/d}\right). \tag{25}$$

Since $\Delta = \mathrm{O}(N^{-1/d})$ and since $\delta \to 0$, we must therefore have $0 < \Delta < \tau < 2$, for N sufficiently large.

Using arguments similar to those for the upper bound, we obtain

$$g_k(r) \geqslant \lambda(r) := \begin{cases} 0, & r \in [0,\tau] \\ \mathscr{V}(r) - \delta - N^{-1}, & r \in [\tau, 2]. \end{cases}$$

On substituting back into (21), we obtain

$$\begin{aligned}\mathrm{E}_k U &= 2^{-s}(1-N^{-1}) + \int_\Delta^2 sr^{-s-1}\, g_k(r)\, dr\\ &\geqslant 2^{-s}(1-N^{-1}) + \int_\tau^2 sr^{-s-1}\,\mathscr{V}(r)\, dr - (\delta + N^{-1})(\tau^{-s} - 2^{-s}).\end{aligned}$$

We see that this lower bound is independent of our code point index k and we therefore have

$$\mathrm{E}U \geqslant 2^{-s}(1-N^{-1}) + \int_\tau^2 sr^{-s-1}\,\mathscr{V}(r)\, dr - (\delta + N^{-1})(\tau^{-s} - 2^{-s}).$$

Similarly to the argument for the upper bound, we obtain

$$\begin{aligned}\mathscr{I}U - \mathrm{E}U &\leqslant 2^{-s}N^{-1} + \int_0^\tau sr^{-s-1}\,\mathscr{V}(r)\, dr + (\delta + N^{-1})(\tau^{-s} - 2^{-s})\\ &\leqslant \mathrm{O}\left(N^{-1}\right) + \mathrm{O}\left(\tau^{d-s}\right) + \mathrm{O}\left(\delta\,\tau^{-s}\right) + \mathrm{O}\left(N^{-1}\tau^{-s}\right).\end{aligned}$$

Using (25) we now have

$$\mathscr{I}U - \mathrm{E}U \leqslant \mathrm{O}\left(N^{-1}\right) + \mathrm{O}\left(\delta^{1-s/d}\right) + \mathrm{O}\left(N^{-1}\,\delta^{-s/d}\right),$$

yielding our lower bound (6). □

Further remarks

1. The spherical cap discrepancy has been well studied [1] [2, Chapters 7 and 8] [10, 18, 29]. The papers [5, 7] explore some relationships between spherical cap discrepancy and energy, in relation to generalizations of the Erdős-Turán inequality [18] and Stolarky's invariance principle [37], treating the energy as the limit of a continuous energy functional.
   Other relationships between discrepancy and energy can be found if the notion of discrepancy is generalized. Stolarky's original invariance principle [37, Theorem 2] is expressed in terms of a discrepancy defined in terms of a kernel function.
   Damelin et al. [9, 12] generalize discrepancy and energy results on the sphere to compact symmetric spaces. Their main result is that if the discrepancy and energy are defined in terms of the same positive definite kernel, then the discrepancy is the square root of the energy. To apply the result to spherical codes, the kernel must be a reproducing kernel, and therefore continuous. This rules out the Riesz s-energy considered in the current paper, since for $0 < s < d$ the corresponding kernel has a singularity on the diagonal. The paper of Levesley and Sun [28] gives closely related results. In another closely related recent paper [8], Brauchart and Dick re-examine Stolarky's invariance principle in terms of reproducing kernel Hilbert spaces and L^2 spherical cap discrepancy.
2. In view of Blümlinger's results [3], and the results mentioned in the previous remark, the techniques used to prove Theorem 1.1 might be generalized to treat compact connected Riemannian manifolds. In this case, the potential would be a function of geodesic distance in the manifold, rather than Euclidean distance in some embedding space, and the discrepancy would be based on geodesic balls.

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