The Coulomb energy of spherical designs on S^2

Kerstin Hesse* and Paul Leopardi†

The University of New South Wales

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Abstract

In this work we give upper bounds for the Coulomb energy of a sequence of well separated spherical n-designs, where a spherical n-design is a set of m points on the unit sphere $S^2 \subset \mathbb{R}^3$ that gives an equal weight cubature (or equal weight numerical integration) rule on S^2 which is exact for spherical polynomials of degree $\leqslant n$. (A sequence Ξ of m-point spherical n-designs X on S^2 is said to be well separated if there exists a constant $\lambda > 0$ such that for each m-point spherical n-design $X \in \Xi$ the minimum spherical distance between points is bounded from below by $\frac{\lambda}{\sqrt{m}}$.) In particular, if the sequence of well separated spherical designs is such that m and n are related by $m = O(n^2)$, then the Coulomb energy of each m-point spherical n-design has an upper bound with the same first term and a second term of the same order as the bounds for the minimum energy of point sets on S^2.

Keywords: acceleration of convergence, Coulomb energy, Coulomb potential, equal weight cubature, equal weight numerical integration, orthogonal polynomials, sphere, spherical designs, well separated point sets on sphere.

MSC2000: primary: 31C20, 42C10, secondary: 41A55, 42C20, 65B10, 65D32.

1   Introduction

This paper examines the (discrete) *Coulomb* (or r^{-1}) *energy* of spherical designs on the unit sphere $S^2 \subset \mathbb{R}^3$.

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*Corresponding author: School of Mathematics, The University of New South Wales, Sydney NSW 2052, Australia, phone: +61 2 938 57074, fax: +61 2 938 57123, email: k.hesse@unsw.edu.au

†School of Mathematics, The University of New South Wales, Sydney NSW 2052, Australia, email: paul.leopardi@unsw.edu.au

The Coulomb energy of a set of m distinct points (or m-point set) $X := \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$ on S^2 is defined as

$$E(X) := \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1, j\neq i}^{m} |\mathbf{x}_i - \mathbf{x}_j|^{-1},$$

where $|\mathbf{x}|$ denotes the Euclidean norm (in $\mathbb{R}^3$) of the vector $\mathbf{x}$.

There have been many equivalent definitions of spherical designs since the original one by Delsarte, Goethals, and Seidel [7]. The following is the most convenient one for our purposes.

Definition 1.1. *For $n \in \mathbb{N}_0$, a spherical n-design is a finite set of points $X \subset S^2$, such that the corresponding equal weight cubature rule Q_X is exact for $\mathbb{P}_n(S^2)$, the space of all spherical polynomials of degree up to and including n; that is, $X \subset S^2$ is a spherical n-design if it satisfies*

$$Q_X(p) = \int_{S^2} p(\mathbf{x}) \, d\omega(\mathbf{x}) \qquad \text{for all } p \in \mathbb{P}_n(S^2),$$

where

$$Q_X(f) := \frac{4\pi}{|X|} \sum_{\mathbf{x} \in X} f(\mathbf{x}), \qquad f \in C(S^2), \tag{1}$$

and where ω is the Lebesgue surface measure on S^2.

Noting that a spherical n-design is also a spherical k-design for all $k \in \mathbb{N}_0$ with $k < n$, we say that n is the strength of X if X is a spherical n-design but not a spherical $(n+1)$-design. By a spherical design we mean a spherical n-design without specifying n. The number $|X|$ denotes the cardinality of X. A spherical design of cardinality m is called an m-point spherical design.

Definition 1.2. *The spherical distance $d(\mathbf{x}, \mathbf{y}) \in [0, \pi]$ between two points $\mathbf{x}, \mathbf{y} \in S^2$ is the spherical angle between the two points, that is,*

$$d(\mathbf{x}, \mathbf{y}) := \cos^{-1}(\mathbf{x} \cdot \mathbf{y}),$$

where $\mathbf{x} \cdot \mathbf{y}$ denotes the Euclidean inner product of $\mathbf{x}$ and $\mathbf{y}$ in $\mathbb{R}^3$.

Our main result is Theorem 3.1, which yields the following special case.

Theorem 1.3. *Let Ξ be a sequence of spherical designs on S^2, with the following properties: there exist positive constants μ and λ, such that, if $X \in \Xi$ has cardinality $m \geqslant 2$ and strength n, then $m \leqslant \mu(n+1)^2$, and the minimum spherical distance between points of X is bounded from below by $\frac{\lambda}{\sqrt{m}}$. Then the Coulomb energy of each m-point spherical design $X \in \Xi$ is bounded from above by*

$$E(X) \leqslant \frac{1}{2} m^2 + C_{(\lambda,\mu)} \, m^{3/2}, \tag{2}$$

where the constant $C_{(\lambda,\mu)} > 0$ depends on λ and μ, but is independent of m.

The asymptotic behavior of the minimal Coulomb energy $\mathcal{E}_m$,

$$\mathcal{E}_m := \min_{X \subset S^2, |X|=m} E(X),$$

for a set of m points on S^2 has been investigated both theoretically and numerically.

In [25, Theorem 2] and [26, Theorem C] Wagner showed that there exist constants C_1 and C_2 such that

$$\frac{1}{2}m^2 + C_1 m^{3/2} \leqslant \mathcal{E}_m \leqslant \frac{1}{2}m^2 + C_2 m^{3/2} \qquad \text{for all } m \geqslant 2. \tag{3}$$

In [20, Corollary 2.6] Rakhmanov, Saff, and Zhou also give a proof of the upper bound in (3), and in [4] Brauchart proves the lower bound in (3). Both [20, Corollary 2.6] and [4] only verify the respective result for $m \geqslant m_0$ with m_0 large enough, but they obtain an explicit value for the constant C_2 and C_1, respectively.

Since the early 1990s there have been a number of conjectures concerning asymptotic behavior of the minimal energy: Erber and Hockney [8] conjectured that

$$\mathcal{E}_m \approx \frac{1}{2}m^2 - 0.5510\, m^{3/2}, \qquad m \to \infty.$$

Rakhmanov, Saff and Zhou gave numerical evidence (see [20, (4.5)] and [21, (4.4)]) that

$$\mathcal{E}_m \approx \frac{1}{2}m^2 - 0.55230\, m^{3/2} + 0.0689\, m^{1/2}, \qquad m \to \infty.$$

Kuijlaars and Saff [17, Conjecture 2] conjectured that

$$\mathcal{E}_m = \frac{1}{2}m^2 + c_1 m^{3/2} + o(m^{3/2}), \qquad m \to \infty,$$

where

$$c_1 := 3 \left(\frac{\sqrt{3}}{8\pi} \right)^{1/2} \zeta\left(\frac{1}{2}\right) L_{-3}\left(\frac{1}{2}\right) = -0.5530\ldots.$$

(Here L_{-3} is a Dirichlet L-function, and ζ is the Riemann zeta function.)

Comparing these theoretical results and conjectures with the bound for $E(X)$ given by the inequality (2), we find that the leading term coincides and the order of the second term is the same. This might seem remarkable, since we have made no explicit attempt to minimize the energy, but instead have imposed a separation constraint and restricted the point sets to be spherical designs.

The use of spherical designs in this work is suggested by a correspondence between energy and cubature, which is discussed in the next section.

Theorem 1.3 considers a sequence Ξ of spherical designs with the property that if a spherical design $X \in \Xi$ has strength n, then the cardinality m of X is bounded by $m \leqslant \mu(n+1)^2$. There is ample numerical evidence of m-point spherical n-designs with $m \leqslant (n+1)^2$ (up to at least strength $n = 13$ in [11], and up to strength $n = 50$ in [5]), but the existence of an infinite sequence of m-point spherical n-designs with

increasing n and with $m = O(n^2)$, though conjectured for at least ten years, has yet to be proved. If we use $M(n)$ to denote the minimum number of points for a spherical n-design, Korevaar and Meyers [16] proved by construction that $M(n) = O(n^3)$ and conjectured that $M(n) = O(n^2)$, and Hardin and Sloane [11] conjectured that $M(n) \leqslant \frac{1}{2} n^2 (1 + o(1))$.

The separation constraint is essential to the result (2). Since the Coulomb potential is unbounded as r approaches 0, and since spherical designs can have points arbitrarily close together, the separation constraint is needed to guarantee any asymptotic bounds on the energy. The separation constraint is also suggested by a result of Dahlberg [6], which states that the minimum energy point sets have this property.

The study of the potential energy and separation properties of spherical designs is relatively recent. For example, Bajnok et al. [3] constructed a sequence of 3-designs and numerically evaluated the energy and minimum Euclidean distance between points for a finite number of these 3-designs, but did not investigate the asymptotic properties of the sequence.

2 Preliminaries

In this section we give the necessary mathematical background and definitions for our results. In particular, we describe the correspondence between discrete energy and equal weight cubature, define spherical designs, the Coulomb potential and Coulomb energy, and the separation property.

2.1 Correspondence between discrete energy and cubature

The following definition of discrete energy will be used in this paper.

Definition 2.1. *For a point set* $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \subset S^2$, *the* discrete energy of a potential v *defined on* $(0, 2]$ *is given by the linear functional*

$$\mathfrak{E}_X(v) := \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1, \, j \neq i}^{m} v(|\mathbf{x}_i - \mathbf{x}_j|),$$

and the discrete energy of a function f *defined on* $[-1, 1)$ *is given by the linear functional*

$$E_X(f) := \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1, \, j \neq i}^{m} f(\mathbf{x}_i \cdot \mathbf{x}_j). \tag{4}$$

We observe that

$$|\mathbf{x} - \mathbf{y}| = \sqrt{(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})} = \sqrt{2 - 2\, \mathbf{x} \cdot \mathbf{y}} \qquad \text{for } \mathbf{x}, \mathbf{y} \in S^2. \tag{5}$$

Thus, given a potential v on $(0, 2]$, we can define a corresponding function f_v on $[-1, 1)$ by

$$f_v(z) := v\left(\sqrt{2 - 2z}\right), \qquad \text{so that} \qquad f_v(\mathbf{x} \cdot \mathbf{y}) = v(|\mathbf{x} - \mathbf{y}|), \tag{6}$$

and conversely, given a function f on $[-1, 1)$, we can define a corresponding potential v_f on $[0, 2)$ by

$$v_f(r) := f\left(1 - \frac{r^2}{2}\right), \qquad \text{so that} \qquad v_f(|\mathbf{x} - \mathbf{y}|) = f(\mathbf{x} \cdot \mathbf{y}).$$

We then have

$$\mathfrak{E}_X(v) = E_X(f_v) \qquad \text{and} \qquad E_X(f) = \mathfrak{E}_X(v_f). \tag{7}$$

We can now set out the correspondence between discrete energy and equal weight cubature.

For a bounded function f on $[-1, 1]$ and the m-point set $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \subset S^2$, if we define the functions $f_i : S^2 \to \mathbb{R}$ by $f_i(\mathbf{y}) := f(\mathbf{x}_i \cdot \mathbf{y})$, for $i \in \{1, \ldots, m\}$, we can express the discrete energy of f for the point set X as

$$E_X(f) = \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m f(\mathbf{x}_i \cdot \mathbf{x}_j) - \frac{m}{2} f(1)$$

$$= \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m f_i(\mathbf{x}_j) - \frac{m}{2} f(1).$$

We can now use the equal weight cubature rule Q_X defined by (1) to express the energy as

$$E_X(f) = \frac{1}{2} \frac{m}{4\pi} \sum_{i=1}^m Q_X(f_i) - \frac{m}{2} f(1).$$

By a suitable change of coordinates, we can show that for any $\mathbf{y} \in S^2$, we have

$$\int_{S^2} f(\mathbf{x} \cdot \mathbf{y}) \, d\omega(\mathbf{x}) = 2\pi \int_{-1}^1 f(z) \, dz.$$

If we define the error term $R(X, f)$ by

$$R(X, f) := \frac{1}{2} \frac{m}{4\pi} \sum_{i=1}^m \left(Q_X(f_i) - \int_{S^2} f_i(\mathbf{x}) \, d\omega(\mathbf{x}) \right)$$

$$= \frac{1}{2} \frac{m}{4\pi} \sum_{i=1}^m Q_X(f_i) - \frac{m^2}{4} \int_{-1}^1 f(z) \, dz,$$

then we obtain the representation

$$E_X(f) = \frac{m^2}{4} \int_{-1}^1 f(z) \, dz - \frac{m}{2} f(1) + R(X, f).$$

In particular, if X is a spherical n-design and if $p \in \mathbb{P}_n([-1, 1])$, where $\mathbb{P}_n([-1, 1])$ is the space of all polynomials on $[-1, 1]$ of degree $\leqslant n$, then $R(X, p) = 0$, and

$$E_X(p) = \frac{m^2}{4} \int_{-1}^1 p(z) \, dz - \frac{m}{2} p(1). \tag{8}$$

Therefore, for a spherical n-design X, if we can express a potential v on $(0, 2]$ as

$$v(|\mathbf{y} - \mathbf{x}|) = f_v(\mathbf{x} \cdot \mathbf{y}) = p(\mathbf{x} \cdot \mathbf{y}) + q(\mathbf{x} \cdot \mathbf{y}),$$

where p is a polynomial of degree at most n, then we have

$$\mathfrak{E}_X(v) = E_X(f_v) = E_X(p) + E_X(q).$$

From (8) we can compute $E_X(p)$ exactly. Thus if we can bound $E_X(q)$, we can bound the energy $\mathfrak{E}_X(v)$.

2.2   The Coulomb potential and the Coulomb energy

In this section we define the Coulomb potential and describe the Coulomb energy of a point set on S^2. The *Coulomb potential* is defined by $V(r) := r^{-1}$. In this paper we use the corresponding function $\Phi = \Phi_V$, defined on $[-1, 1)$ by

$$\Phi(z) := \frac{1}{\sqrt{2 - 2z}}.$$

By (5) we have $\Phi(\mathbf{x} \cdot \mathbf{y}) = V(|\mathbf{x} - \mathbf{y}|)$ for $\mathbf{x}, \mathbf{y} \in S^2$.

Definition 2.2. *The* Coulomb energy *of a finite point set* $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \subset S^2$ *is defined by*

$$E(X) := \mathfrak{E}_X(V) = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1, \, j \neq i}^{m} |\mathbf{x}_i - \mathbf{x}_j|^{-1}.$$

From (6) and (7) we also have

$$E(X) = E_X(\Phi) = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1, \, j \neq i}^{m} \Phi(\mathbf{x}_i \cdot \mathbf{x}_j). \tag{9}$$

This last representation is the starting point for the proof of our main result, which is given in Theorem 3.1.

2.3   Spherical designs and the separation property

The rest of this section is devoted to spherical n-designs and the separation property.

As we explain in Section 5, it is possible to construct an infinite sequence of spherical designs, with increasing strength, where the minimum distance between points decreases arbitrarily rapidly. Thus there can be no asymptotic upper bound on the Coulomb energy of a sequence of spherical designs without some further constraint of the minimum distance between points.

Therefore we restrict our attention in this work to sequences of spherical designs which are *well separated*. By this we mean the following:

Definition 2.3. *We say that a sequence Ξ of spherical designs is* well separated *or that Ξ has the* separation property*, if there exists a spherical separation constant $\lambda > 0$ such that for each m-point spherical design $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \in \Xi$, where $m \geqslant 2$, the spherical distance between the points satisfies the estimate*

$$d(\mathbf{x}_i, \mathbf{x}_j) \geqslant \frac{\lambda}{\sqrt{m}} \qquad \text{for all } i, j \in \{1, \ldots, m\} \text{ with } i \neq j. \tag{10}$$

Instead of the spherical distance, we could equivalently use the Euclidean distance $|\mathbf{x} - \mathbf{y}|$ and a Euclidean separation constant.

3   An upper bound for the Coulomb energy of a spherical design

As stated in the introduction, Theorem 1.3 is a special case of our main result, Theorem 3.1, given below. Theorem 3.1 gives upper bounds for the Coulomb energy of each spherical design of a sequence with the separation property, with no assumptions on the relationship between the number of points m and the strength n of each spherical design. Theorem 1.3 follows from Theorem 3.1 by imposing the additional assumption $m \leqslant \mu(n+1)^2$.

The proof of Theorem 3.1 requires several lemmas, which we state in this section before we give the proof of the theorem. The proofs of the lemmas are deferred to Section 4.

Theorem 3.1. *Let Ξ be a sequence of spherical designs on S^2 which is well-separated with spherical separation constant λ. Then the Coulomb energy $E(X)$ of each spherical design $X \in \Xi$ of cardinality m and strength n is bounded from above by*

$$E(X) \leqslant \frac{1}{2}\, m^2 - \frac{1}{2}\, \frac{m(n+1)(n+2)}{2n+3} - \frac{1}{2}\, \frac{m^2}{2n+3} + c_\lambda \, \frac{m^{9/4}}{(n+1)^{3/2}}. \tag{11}$$

The constant $c_\lambda > 0$ depends on the separation constant λ, but is independent of m and n.

We now use Theorem 3.1 to prove Theorem 1.3.

Proof of Theorem 1.3. Any spherical design $X \in \Xi$ of cardinality 1 has a Coulomb energy of zero and so trivially satisfies (2).

Now consider a spherical design $X \in \Xi$ of cardinality $m \geqslant 2$ and strength n. The assumption $m \leqslant \mu(n+1)^2$ implies

$$n + 1 \geqslant \mu^{-1/2}\, m^{1/2},$$

and from (11) in Theorem 3.1 we have

$$\begin{aligned}
E(X) &\leqslant \frac{1}{2}\, m^2 - \frac{1}{2}\, \frac{m(n+1)(n+2)}{2n+3} - \frac{1}{2}\, \frac{m^2}{2n+3} + c_\lambda\, \mu^{3/4}\, m^{3/2} \\
&\leqslant \frac{1}{2}\, m^2 + c_\lambda\, \mu^{3/4}\, m^{3/2},
\end{aligned} \tag{12}$$

which yields (2) with $C_{(\lambda,\mu)} = c_\lambda \, \mu^{3/4}$. This concludes the proof. $\square$

Remark. In the proof of Theorem 1.3 we have left out the second and third term in the second line in (12), since they are negative. As these two terms are, due to the assumption $m \leqslant \mu \, (n+1)^2$, of the order $m^{3/2}$ they can be used to improve the value of the constant $C_{(\lambda,\mu)}$. In particular, when $m = (n+1)^2$, we have

$$E(X) \leqslant \frac{1}{2} \, m^2 - \frac{1}{2} \, m^{3/2} + c_\lambda \, m^{3/2},$$

so we can set $C_{(\lambda,\mu)} = c_\lambda - \frac{1}{2}$.

3.1   Lemmas needed for the proof of Theorem 3.1

For the proof of Theorem 3.1 we need several lemmas.

In this work P_k denotes the Legendre polynomial of degree $k \in \mathbb{N}_0$, and $P_k^{(\alpha,\beta)}$ is the Jacobi polynomial of degree $k \in \mathbb{N}_0$ with indices $\alpha > -1$ and $\beta > -1$, as defined in [24, Chapter II, 2.4, and Chapter IV]. The Legendre polynomial P_k is the Jacobi polynomial $P_k^{(0,0)}$ with indices $\alpha = \beta = 0$. The Jacobi polynomials $P_k^{(\alpha,\beta)}$ satisfy the orthogonality relation

$$\int_{-1}^{1} P_k^{(\alpha,\beta)}(z) \, P_\ell^{(\alpha,\beta)}(z) \, (1-z)^\alpha \, (1+z)^\beta \, dz = 0 \qquad \forall \, k, \ell \in \mathbb{N}_0 \text{ with } k \neq \ell.$$

Of particular interest for this work are the Legendre polynomials P_k and the Jacobi polynomials $P_k^{(1,0)}$. Both assume their maximum at $z = 1$, more precisely, we have $|P_k(z)| \leqslant P_k(1) = 1$ and $|P_k^{(1,0)}(z)| \leqslant P_k^{(1,0)}(1) = k+1$ for all $z \in [-1,1]$.

In the following we also use the Pochhammer symbol, defined by

$$(x)_0 := 1, \qquad (x)_n := \prod_{k=0}^{n-1} (x+k) \quad \text{for } n \in \mathbb{N}.$$

The first lemma (Lemma 3.2 below) splits the function $\Phi(z) = \frac{1}{\sqrt{2-2z}}$ into a polynomial part and a remainder. This split is based on the expansion of a function related to Φ in a Legendre series, as we will see in the proof in Subsection 4.1.

Lemma 3.2. *For $z \in [-1,1)$ and $n \in \mathbb{N}_0$*

$$\Phi(z) = s_n(z) + t_n(z), \qquad z \in [-1,1), \tag{13}$$

where s_n is a polynomial of degree n, given by

$$s_n(z) := \sum_{k=0}^{n} \frac{k+1}{2 \left(k + \frac{1}{2}\right)_2} P_k^{(1,0)}(z), \qquad z \in [-1,1], \tag{14}$$

and where $t_n := a_n + b_n$, with a_n and b_n given by

$$a_n(z) := \frac{n+2}{2\left(n+\frac{3}{2}\right)_2} \frac{P_{n+1}(z)}{1-z}, \qquad z \in [-1, 1), \tag{15}$$

$$b_n(z) := -\sum_{k=n+2}^{\infty} \frac{k+\frac{1}{2}}{2\left(k-\frac{1}{2}\right)_3} \frac{P_k(z)}{1-z}, \qquad z \in [-1, 1). \tag{16}$$

The equality (13) is pointwise on $[-1, 1)$, and the series b_n converges absolutely and uniformly in every closed interval contained in $[-1, 1)$.

We split off the polynomial term s_n because we can use the expression (8) to obtain its energy exactly, and because the 'tail' t_n and its corresponding energy are 'small', in a sense which is elaborated in the lemmas below. This splitting is one of the main ideas of the proof of Theorem 3.1.

The next lemma gives an estimate for t_n on the open interval $(-1, 1)$, and the subsequent lemma estimates the contribution of t_n to the energy sum.

Lemma 3.3. *For $\theta \in (0, \pi)$ the function t_n, as defined in Lemma 3.2, satisfies the estimate*

$$|t_n(\cos\theta)| \leqslant \frac{5}{3}\left(\frac{2}{\pi}\right)^{1/2} (n+1)^{-3/2} (\sin\theta)^{-5/2}. \tag{17}$$

Lemma 3.4. *Let Ξ be a well separated sequence of spherical designs with spherical separation constant λ. For a spherical design $X \in \Xi$ with cardinality $|X| = m$ and strength n, the estimate*

$$E_X(t_n) \leqslant c_\lambda \frac{m^{9/4}}{(n+1)^{3/2}} \tag{18}$$

is valid, where the constant $c_\lambda > 0$ depends only on the separation constant λ.

The proof of Lemma 3.4 requires the following three lemmas. The first of these gives an upper bound on the number of points of a point set X which can at most lie in an arbitrary spherical cap $S(\mathbf{x}, \theta)$ of center $\mathbf{x} \in S^2$ and angular radius $\theta \in (0, \pi]$. Such a *spherical cap* is defined by

$$S(\mathbf{x}, \theta) := \left\{ \mathbf{y} \in S^2 \,\middle|\, d(\mathbf{x}, \mathbf{y}) \leqslant \theta \right\}.$$

Lemma 3.5. *Let $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, $m \geqslant 2$, be a point set on S^2 with the property that the minimum spherical distance between points is bounded from below by $\delta = 2\rho$, that is*

$$\min\left\{ d(\mathbf{x}_i, \mathbf{x}_j) \mid i, j \in \{1, \ldots, m\} \text{ with } i \neq j \right\} \geqslant \delta. \tag{19}$$

Then $|X \cap S(\mathbf{x}, \theta)|$, the number of points of X which lie in the spherical cap $S(\mathbf{x}, \theta)$ with center $\mathbf{x} \in S^2$ and angular radius θ, where $\rho \leqslant \theta \leqslant \pi/2$, is bounded from above by

$$|X \cap S(\mathbf{x}, \theta)| \leqslant \frac{3\pi^2}{4} \rho^{-2} (\sin\theta)^2. \tag{20}$$

The next lemma gives an upper bound on the spherical separation constant for point sets on S^2.

Lemma 3.6. *If X is an m-point subset of S^2, with $m \geqslant 2$, such that the minimum spherical distance between any two distinct points of X is $\frac{\lambda}{\sqrt{m}}$, then*

$$\lambda \leqslant \pi \sqrt{2}.$$

A set consisting of two antipodal points of S^2 attains this bound.

The next lemma puts an upper bound on the strength of a spherical design on S^2.

Lemma 3.7. *If X is an m-point spherical n-design then*

$$n + 1 \leqslant 2\sqrt{m}. \tag{21}$$

Note that (21) in Lemma 3.7 tells us that for an infinite sequence Ξ of spherical designs of cardinality m and strict monotonically increasing strength n, the cardinality m can at best be of the order n^2. It is yet unknown (see Section 1) whether this order is achieved.

Lemma 3.2 is inspired by similar splitting lemmas in [12] and [13]. The papers [12] and [13] investigate the asymptotic behavior of the worst-case cubature error in the Sobolev space $H^s(S^2)$, with $s > 1$, of an infinite sequence of cubature rules with increasing degree of polynomial exactness, and with a regularity property. The worst-case cubature error in $H^s(S^2)$ has a representation which is essentially a double cubature sum applied to a kernel which is closely related to the reproducing kernel of $H^s(S^2)$. In [12] and [13], there is a lemma similar to our Lemma 3.2, which splits this kernel into a polynomial part which is integrated exactly by the double cubature sum, and a remaining part which can be estimated. The proof of the estimate of the energy $E_X(t_n)$ in Lemma 3.4 uses techniques similar to those used in [12] and [13] to deal with the double cubature sum applied to the remaining part.

We can use similar techniques for the estimation of the asymptotic behavior of the energy of a well separated sequence of spherical designs and for deriving upper bounds of the worst-case cubature error because in both cases we work with cubature rules that are exact up to a certain degree n.

We can now give the proof of Theorem 3.1.

Proof of Theorem 3.1. If the spherical design $X \in \Xi$ consists of only one point, then $E(X) = 0$. Since a spherical design of cardinality $m = 1$ has strength $n = 0$, the right hand side of (11) is in this case

$$\frac{1}{2} m^2 - \frac{1}{2} \frac{m(n+1)(n+2)}{2n+3} - \frac{1}{2} \frac{m^2}{2n+3} + c_\lambda \frac{m^{9/4}}{(n+1)^{3/2}} = \frac{1}{2} - \frac{1}{2} \frac{2}{3} - \frac{1}{2} \frac{1}{3} + c_\lambda = c_\lambda.$$

In this case the inequality (11) becomes $c_\lambda \geqslant 0$, which is automatically satisfied. Thus, in the remainder of the proof we assume that $X \in \Xi$ has cardinality $m \geqslant 2$.

Using (13) in Lemma 3.2, we split Φ into a polynomial part s_n and a 'well behaved' tail t_n. Correspondingly, we now split the energy (9) into two parts,

$$E(X) = E_X(s_n) + E_X(t_n). \tag{22}$$

The function s_n defined in Lemma 3.2 by (14) is a polynomial of degree n. Since X is a spherical n-design, we can use the expression (8) to obtain the energy $E_X(s_n)$ exactly. From (8), we have

$$E_X(s_n) = \frac{m^2}{4} \int_{-1}^1 s_n(z)\, dz - \frac{m}{2}\, s_n(1).$$

We now replace s_n by its definition (14) to obtain

$$\int_{-1}^1 s_n(z)\, dz = \sum_{k=0}^n \frac{k+1}{2\left(k+\frac{1}{2}\right)_2} \int_{-1}^1 P_k^{(1,0)}(z)\, dz = \sum_{k=0}^n \frac{1}{\left(k+\frac{1}{2}\right)_2} = 2\,\frac{n+1}{n+\frac{3}{2}}, \tag{23}$$

where we used (see [9, p. 284, (2)])

$$\int_{-1}^1 P_k^{(1,0)}(z)\, dz = \frac{2}{k+1}.$$

Also the identity $P_k^{(1,0)}(1) = k+1$ (see [24, (4.1.1)]) gives

$$s_n(1) = \sum_{k=0}^n \frac{k+1}{2\left(k+\frac{1}{2}\right)_2} P_k^{(1,0)}(1) = \sum_{k=0}^n \frac{(k+1)^2}{2\left(k+\frac{1}{2}\right)_2} = \frac{1}{2}\,\frac{(n+1)_2}{n+\frac{3}{2}}. \tag{24}$$

The two summation identities which have been used in the last step in (23) and (24) are easily proved by induction. Substituting back into the expression for $E_X(s_n)$, we obtain

$$\begin{aligned}
E_X(s_n) &= \frac{m^2}{2}\,\frac{n+1}{n+\frac{3}{2}} - \frac{m}{4}\,\frac{(n+1)_2}{n+\frac{3}{2}} \\
&= \frac{1}{2}\,m^2 - \frac{1}{4}\,\frac{m^2}{n+\frac{3}{2}} - \frac{1}{4}\,\frac{m\,(n+1)_2}{n+\frac{3}{2}}.
\end{aligned} \tag{25}$$

The estimate (18) from Lemma 3.4 gives

$$E_X(t_n) \leqslant c_\lambda\,\frac{m^{9/4}}{(n+1)^{3/2}}. \tag{26}$$

We thus obtain from (22), (25), and (26) the estimate

$$E(X) \leqslant \frac{1}{2}\,m^2 - \frac{1}{2}\,\frac{m\,(n+1)_2}{2n+3} - \frac{1}{2}\,\frac{m^2}{2n+3} + c_\lambda\,\frac{m^{9/4}}{(n+1)^{3/2}},$$

where the constant c_λ is given by (51) from the proof of Lemma 3.4. $\square$

4   Proofs of Lemmas

In this section we prove Lemmas 3.2 to 3.7.

4.1   Proof of Lemma 3.2

Before giving the proof of Lemma 3.2, we present some of the underlying ideas.

We start by noting that Φ is in $L^1([-1,1])$ and in $C([-1,1))$ but not in $L^2([-1,1])$ or $C([-1,1])$. The Legendre polynomials are a complete orthogonal system of continuous functions for $L^2([-1,1])$ (see [23, Chapter III, Section 9] and [24, Chapter II, 2.4, and Chapter IV]). Because Φ is in $L^1([-1,1])$, the coefficients of the formal Legendre series for Φ are well defined. We now determine the formal Legendre series for Φ and examine it for convergence.

For $f \in L^1([-1,1])$ and $g \in C([-1,1])$, we define the bilinear form

$$\langle f, g \rangle := \int_{-1}^{1} f(z)\, g(z)\, dz$$

If f and g are both in $L^2([-1,1])$, this coincides with the L^2 inner product. The formal Legendre series for Φ is then

$$S(\Phi) := \sum_{k=0}^{\infty} \widehat{\Phi}(k)\, P_k,$$

where the Legendre coefficients are given by

$$\widehat{\Phi}(k) := \frac{\langle \Phi, P_k \rangle}{\langle P_k, P_k \rangle}.$$

As a consequence of [9, p. 284, (2)] we have

$$\langle \Phi, P_k \rangle = \frac{1}{k + \frac{1}{2}}.$$

We also know from [24, (4.3.3)] that

$$\langle P_k, P_k \rangle = \frac{1}{k + \frac{1}{2}}, \tag{27}$$

so $\widehat{\Phi}(k) = 1$, and we have the formal Legendre series

$$S(\Phi) = \sum_{k=0}^{\infty} P_k.$$

The formal Legendre series expansion of Φ is a long known result, based on results of Neumann and Stieltjes and with a proof by Fejér as described in Sansone [23, Chapter III, Section 15]. Sansone gives a proof of uniform convergence for this series in any closed interval contained in $(-1, 1)$, based on Hobson's equiconvergence theorem [23, Chapter

III, Section 14], [14, pp. 388–395], [15], but Sansone does not give an estimate of the rate of convergence of $S(\Phi)$. In fact, this series converges too slowly for our purposes.

To accelerate convergence, we use a known method of approximation of an integrable function f, which replaces the series $S(f)$ with a series which has faster convergence at the expense of a higher order of singularity as z approaches 1. This technique was employed in 1954 by Yennie, Ravenhall and Wilson [27, p. 505] and is sometimes called 'YRW resummation' [1].

We apply YRW resummation to Φ. Thus instead of expanding Φ into the formal Legendre series $S(\phi)$, we define $w(z) := 1 - z$, and expand $w\Phi$, where

$$(w\Phi)(z) = (1 - z)\,\Phi(z) = \sqrt{\frac{1 - z}{2}},$$

into the formal Legendre series

$$S(w\Phi) := \sum_{k=0}^{\infty} \widehat{(w\Phi)}(k)\, P_k, \tag{28}$$

with

$$\widehat{(w\Phi)}(k) := \frac{\langle w\Phi, P_k \rangle}{\langle P_k, P_k \rangle},$$

and examine (28) for convergence. We then use the series expansion

$$W(\Phi)(z) := \frac{S(w\Phi)(z)}{w(z)} = \frac{1}{1 - z} \sum_{k=0}^{\infty} \widehat{(w\Phi)}(k)\, P_k(z) \tag{29}$$

as a representation of Φ.

The function $w\Phi$ is continuous on $[-1, 1]$ and hence in $L^2([-1, 1])$. This means that the series $S(w\Phi)$ as defined by (28) converges to $w\Phi$ in the L^2 sense, since the Legendre polynomials form a complete orthogonal system for $L^2([-1, 1])$. To prove Lemma 3.2 we need to examine $S(w\Phi)$ with respect to pointwise and uniform convergence. As a result of [9, p. 284, (2)] we have

$$\langle w\Phi, P_k \rangle = -\frac{1}{2\left(k - \frac{1}{2}\right)_3}.$$

Using (27) we have

$$\widehat{(w\Phi)}(k) = -\frac{k + \frac{1}{2}}{2\left(k - \frac{1}{2}\right)_3},$$

and therefore

$$S(w\Phi)(z) = -\sum_{k=0}^{\infty} \frac{k + \frac{1}{2}}{2\left(k - \frac{1}{2}\right)_3}\, P_k(z). \tag{30}$$

The simple estimate $|P_k(z)| \leqslant 1$ for $z \in [-1, 1]$ (see [24, (7.21.1)]) now implies that the series $S(w\Phi)$ converges uniformly and absolutely on this interval. Since the uniform limit and the L^2 limit have the same Legendre coefficients they coincide in the L^2 sense.

Furthermore $w\Phi$ and the uniform limit are both continuous on $[-1, 1]$, and therefore we conclude that they are identical: the series $S(w\Phi)$ converges uniformly to the function $w\Phi$.

Now that we have a well behaved series, we can concentrate on splitting off an appropriate polynomial s_n. We use the identity

$$(1 - z)\, P_k^{(1,0)}(z) = P_k(z) - P_{k+1}(z), \qquad k \in \mathbb{N}_0, \tag{31}$$

(see [24, (4.5.4)]) and summation by parts to derive the following lemma on finite Legendre sums.

Lemma 4.1. *For any sequence* $(u_n)_{n\in\mathbb{N}_0} \subset \mathbb{R}$, *we have*

$$\sum_{k=0}^{n+1} u_k\, P_k(z) = v_{n+1}\, P_{n+1}(z) + (1 - z) \sum_{k=0}^{n} v_k\, P_k^{(1,0)}(z),$$

where

$$v_k := \sum_{\ell=0}^{k} u_\ell.$$

Proof. We have $u_0 = v_0$ and $u_k = v_k - v_{k-1}$ for $k > 0$. Therefore, with the help of (31),

$$
\begin{aligned}
\sum_{k=0}^{n+1} u_k\, P_k(z) &= v_0\, P_0(z) + \sum_{k=1}^{n+1} (v_k - v_{k-1})\, P_k(z) \\
&= v_0\, P_0(z) + \sum_{k=1}^{n+1} v_k\, P_k(z) - \sum_{k=0}^{n} v_k\, P_{k+1}(z) \\
&= v_{n+1}\, P_{n+1}(z) + \sum_{k=0}^{n} v_k\big(P_k(z) - P_{k+1}(z)\big) \\
&= v_{n+1}\, P_{n+1}(z) + (1 - z) \sum_{k=0}^{n} v_k\, P_k^{(1,0)}(z).
\end{aligned}
$$

This concludes the proof. $\square$

After these preparations we can now prove Lemma 3.2.

Proof of Lemma 3.2. From (29), the discussion of the convergence of $S(w\Phi)$, and (30), we have for $z \in [-1, 1)$,

$$\Phi(z) = W(\Phi)(z) = \frac{S(w\Phi)(z)}{w(z)} = -\frac{1}{1-z} \sum_{k=0}^{\infty} \frac{k + \frac{1}{2}}{2\left(k - \frac{1}{2}\right)_3}\, P_k(z).$$

We can now split $W(\Phi)$ into a partial sum and a well behaved tail.

$$W(\Phi) = W_{(n+1)}(\Phi) + W^{(n+1)}(\Phi),$$

where

$$W_{(n+1)}(\Phi)(z) := -\frac{1}{1-z} \sum_{k=0}^{n+1} \frac{k+\frac{1}{2}}{2\left(k-\frac{1}{2}\right)_3} P_k(z),$$

$$W^{(n+1)}(\Phi)(z) := -\sum_{k=n+2}^{\infty} \frac{k+\frac{1}{2}}{2\left(k-\frac{1}{2}\right)_3} \frac{P_k(z)}{1-z}.$$

We see that $W^{(n+1)}(\Phi)(z) = b_n(z)$ where b_n is defined by (16).

We now apply Lemma 4.1 to $W_{(n+1)}(\Phi)$ to split a polynomial from the partial sum,

$$\begin{aligned}
W_{(n+1)}(\Phi)(z) &= \left(-\sum_{\ell=0}^{n+1} \frac{\ell+\frac{1}{2}}{2\left(\ell-\frac{1}{2}\right)_3}\right) \frac{P_{n+1}(z)}{1-z} + \sum_{k=0}^{n} \left(-\sum_{\ell=0}^{k} \frac{\ell+\frac{1}{2}}{2\left(\ell-\frac{1}{2}\right)_3}\right) P_k^{(1,0)}(z) \\
&= \frac{n+2}{2\left(n+\frac{3}{2}\right)_2} \frac{P_{n+1}(z)}{1-z} + \sum_{k=0}^{n} \frac{k+1}{2\left(k+\frac{1}{2}\right)_2} P_k^{(1,0)}(z) \\
&= a_n(z) + s_n(z),
\end{aligned}$$

where we have used the identity

$$-\sum_{\ell=0}^{n} \frac{\ell+\frac{1}{2}}{2\left(\ell-\frac{1}{2}\right)_3} = \frac{n+1}{2\left(n+\frac{1}{2}\right)_2}$$

in the second step. So, we have $\Phi(z) = s_n(z) + a_n(z) + b_n(z)$ pointwise on $[-1,1)$. The uniform convergence of b_n on every closed interval contained in $[-1,1)$ follows from the uniform convergence of $S(w\Phi)$ on $[-1,1]$. $\square$

Remark. The function Φ is in the weighted L^2 space $L^2(w,[-1,1])$ with weight function $w(z) = 1-z$, and the Jacobi polynomials $P_k^{(1,0)}$, $k \in \mathbb{N}_0$, are a complete orthogonal system for this space. Using [9, p. 284, (2)] and [24, (4.3.3)] it is possible to show that s_n is the partial sum up to degree n of the Jacobi series expansion of Φ with respect to the Jacobi polynomials $P_k^{(1,0)}$, $k \in \mathbb{N}_0$. We could have used this orthogonal expansion as the basis of an alternative (but not easier) proof of Lemma 3.2.

4.2 Proofs of remaining lemmas

Proof of Lemma 3.3. To estimate $|t_n(\cos\theta)|$ for $\theta \in (0,\pi)$, we start with

$$|t_n(\cos\theta)| \leqslant |a_n(\cos\theta)| + |b_n(\cos\theta)|, \qquad \theta \in (0,\pi), \tag{32}$$

and then treat each term on the right-hand side separately.

We use Antonov and Holševnikov's sharpened Bernstein inequality (see [2], [18], [19])

$$|P_k(\cos\theta)| < \left(\frac{2}{\pi}\right)^{1/2} \left(k+\frac{1}{2}\right)^{-1/2} (\sin\theta)^{-1/2} \qquad \text{for } \theta \in (0,\pi),$$

and the estimate

$$\frac{1}{1 - \cos\theta} = \frac{1 + \cos\theta}{(\sin\theta)^2} \leqslant 2\,(\sin\theta)^{-2} \qquad \text{for } \theta \in (0, \pi).$$

These result in the estimate

$$\left| \frac{P_k(\cos\theta)}{1 - \cos\theta} \right| < \left(\frac{8}{\pi}\right)^{1/2} \left(k + \frac{1}{2}\right)^{-1/2} (\sin\theta)^{-5/2} \qquad \text{for } \theta \in (0, \pi). \tag{33}$$

Using this estimate we obtain, for $\theta \in (0, \pi)$,

$$
\begin{aligned}
|a_n(\cos\theta)| &\leqslant \frac{n + 2}{2\left(n + \frac{3}{2}\right)_2} \left| \frac{P_{n+1}(\cos\theta)}{1 - \cos\theta} \right| \\
&\leqslant \left(\frac{8}{\pi}\right)^{1/2} \left(n + \frac{3}{2}\right)^{-1/2} \frac{n + 2}{2\left(n + \frac{3}{2}\right)_2} (\sin\theta)^{-5/2} \\
&\leqslant \left(\frac{2}{\pi}\right)^{1/2} (n + 1)^{-3/2} (\sin\theta)^{-5/2}.
\end{aligned}
\tag{34}
$$

We use (33) again to estimate $b_n(\cos\theta)$ for $\theta \in (0, \pi)$

$$
\begin{aligned}
|b_n(\cos\theta)| &\leqslant \sum_{k=n+2}^{\infty} \frac{\left(k + \frac{1}{2}\right)}{2\left(k - \frac{1}{2}\right)_3} \left| \frac{P_k(\cos\theta)}{1 - \cos\theta} \right| \\
&\leqslant \left(\frac{8}{\pi}\right)^{1/2} (\sin\theta)^{-5/2} \sum_{k=n+2}^{\infty} \frac{\left(k + \frac{1}{2}\right)^{1/2}}{2\left(k - \frac{1}{2}\right)_3} \\
&\leqslant \left(\frac{2}{\pi}\right)^{1/2} (\sin\theta)^{-5/2} \sum_{k=n+2}^{\infty} k^{-5/2} \\
&\leqslant \left(\frac{2}{\pi}\right)^{1/2} (\sin\theta)^{-5/2} \int_{n+1}^{\infty} t^{-5/2}\, dt \\
&\leqslant \frac{2}{3} \left(\frac{2}{\pi}\right)^{1/2} (n + 1)^{-3/2} (\sin\theta)^{-5/2}.
\end{aligned}
\tag{35}
$$

Combining (32), (34), and (35), we obtain the estimate (17) for $\theta \in (0, \pi)$. $\square$

Proof of Lemma 3.4. By definition (4) we have

$$E_X(t_n) := \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1,\, j \neq i}^{m} t_n(\mathbf{x}_i \cdot \mathbf{x}_j). \tag{36}$$

If $m = 1$ then the inner sum in (36) is empty, thus $E_X(t_n) = 0$, and (17) is automatically satisfied. In what follows, we can therefore assume that $m \geqslant 2$.

Let now $m \geqslant 2$. The separation property (10) then implies that

$$\frac{\lambda}{\sqrt{m}} \leqslant \pi. \tag{37}$$

We split the inner sum in (36) into a sum over all points in the northern hemisphere with respect to $\mathbf{x}_i$ as north pole and a sum over all points in the corresponding southern hemisphere. The equator is arbitrarily included in the northern hemisphere. Then

$$E_X(t_n) = E^+ + E^-, \tag{38}$$

where

$$E^\pm := \frac{1}{2} \sum_{i=1}^m \sum_{j=1, \, j\neq i}^m \chi(H_i^\pm)(\mathbf{x}_j) \, t_n(\mathbf{x}_i \cdot \mathbf{x}_j),$$

with

$$H_i^+ := \left\{ \mathbf{x} \in S^2 \, \big| \, 0 \leqslant \mathbf{x}_i \cdot \mathbf{x} \leqslant 1 \right\},$$
$$H_i^- := \left\{ \mathbf{x} \in S^2 \, \big| \, -1 \leqslant \mathbf{x}_i \cdot \mathbf{x} < 0 \right\} = S^2 \setminus H_i^+,$$

for $i \in \{1, \ldots, m\}$, and where $\chi(H_i^\pm)$ is the characteristic function of $H_i^\pm$.

The estimate for t_n given in Lemma 3.3 has singularities at $\theta \in \{0, \pi\}$. Therefore for each $i \in \{1, \ldots, m\}$ we split the inner sum in $E^\pm$ further into a sum over those points in the closed spherical cap $S(\pm\mathbf{x}_i, \rho)$, where

$$\rho = \rho(m) := \frac{\lambda}{2\sqrt{m}},$$

and a sum over the remaining points in $H_i^\pm$. From (37) we have $\rho \leqslant \frac{\pi}{2}$. Thus

$$E^\pm = D^\pm + R^\pm, \tag{39}$$

with the in-cap contribution

$$D^\pm := \frac{1}{2} \sum_{i=1}^m \sum_{j=1, j\neq i}^m \chi\left(S(\pm\mathbf{x}_i, \rho) \cap H_i^\pm\right)(\mathbf{x}_j) \, t_n(\mathbf{x}_i \cdot \mathbf{x}_j),$$

and the out-of-cap contribution

$$R^\pm := \frac{1}{2} \sum_{i=1}^m \sum_{j=1, j\neq i}^m \chi\left(H_i^\pm \setminus S(\pm\mathbf{x}_i, \rho)\right)(\mathbf{x}_j) \, t_n(\mathbf{x}_i \cdot \mathbf{x}_j).$$

It remains to estimate $D^\pm$ and $R^\pm$. First we examine the in-cap part $D^\pm$.

We have $D^+ = 0$, since (due to the separation property) there are no points of the point set X in $S(\mathbf{x}_i, \rho)$ other than $\mathbf{x}_i$ itself, and $\mathbf{x}_i$ is excluded from the sum.

For each fixed $i \in \{1, \ldots, m\}$, in the inner sum of D^- we are summing only over points of X in $S(-\mathbf{x}_i, \rho) \cap H_i^-$, and because of the separation property (10) there are at

most two such points. If there are two points in the spherical cap $S(-\mathbf{x}_i, \rho)$ they are on the boundary opposite each other along a diameter. Because $\rho \in (0, \frac{\pi}{2}]$ we know that for each point $\mathbf{x}_j \in S(-\mathbf{x}_i, \rho) \cap H_i^-$ we have $\mathbf{x}_i \cdot \mathbf{x}_j < 0$. Because this is well away from the singularity of t_n at 1, we can use the definitions (15) and (16) of a_n and b_n from Lemma 3.2, with $|P_k(z)| \leqslant 1$, to estimate $|t_n(\mathbf{x}_i \cdot \mathbf{x}_j)|$. For each point $\mathbf{x}_j \in S(-\mathbf{x}_i, \rho)$ we have

$$
\begin{aligned}
|t_n(\mathbf{x}_i \cdot \mathbf{x}_j)| &\leqslant |a_n(\mathbf{x}_i \cdot \mathbf{x}_j)| + |b_n(\mathbf{x}_i \cdot \mathbf{x}_j)| \\
&\leqslant \frac{n+2}{2\left(n+\frac{3}{2}\right)_2} + \sum_{k=n+2}^{\infty} \frac{k+\frac{1}{2}}{2\left(k-\frac{1}{2}\right)_3} \\
&\leqslant \frac{1}{2(n+1)} + \sum_{k=n+2}^{\infty} \frac{1}{2k^2} \\
&\leqslant \frac{1}{2(n+1)} + \frac{1}{2}\int_{n+1}^{\infty} t^{-2}\, dt \\
&= (n+1)^{-1},
\end{aligned}
\tag{40}
$$

where we have used the estimate $1 - \mathbf{x}_i \cdot \mathbf{x}_j > 1$. From (40) we obtain

$$
D^- \leqslant \frac{1}{2}\sum_{i=1}^{m} \frac{2}{n+1} = \frac{m}{n+1}.
\tag{41}
$$

Now we examine the out-of-cap part $R^\pm$. With the estimate (17) for t_n from Lemma 3.3, we can estimate $R^\pm$ as

$$
R^\pm \leqslant \frac{5}{3\sqrt{2}\sqrt{\pi}}\, (n+1)^{-3/2} \sum_{i=1}^{m} R_i^\pm,
\tag{42}
$$

with

$$
R_i^\pm := \sum_{j=1, j\neq i}^{m} \chi\left(H_i^\pm \setminus S(\pm\mathbf{x}_i, \rho)\right)(\mathbf{x}_j)\,(\sin\theta_{ij}^\pm)^{-5/2},
\tag{43}
$$

where $\theta_{ij}^\pm \in [0, \pi]$ is determined by $\cos\theta_{ij}^\pm = \pm\mathbf{x}_i \cdot \mathbf{x}_j$, $i, j = 1, \ldots, m$. Note that in the sum $R_i^\pm$ in (43) we only count points for which $\theta_i^\pm$ is in $(\rho, \frac{\pi}{2}]$, since we only count points in the forward hemisphere with respect to $\pm\mathbf{x}_i$ without the spherical cap $S(\pm\mathbf{x}_i, \rho)$. (To obtain (43) from (17) we have also made use of $\sin\theta = \sin(\pi - \theta)$ for $\theta \in [0, \pi]$, and thus $\sin\theta_{ij}^+ = \sin\theta_{ij}^-$.)

Define the counting function $g_i^\pm : [\rho, \frac{\pi}{2}] \to \mathbb{R}$ which counts the number of points $\mathbf{x}_j$ which lie in $H_i^\pm \cap (S(\pm\mathbf{x}_i, \theta) \setminus S(\pm\mathbf{x}_i, \rho))$, by

$$
g_i^\pm(\theta) := \sum_{j=1}^{m} \chi\left(H_i^\pm \cap \left(S(\pm\mathbf{x}_i, \theta) \setminus S(\pm\mathbf{x}_i, \rho)\right)\right)(\mathbf{x}_j).
$$

Then $g_i^\pm(\rho) = 0$, and $g_i^\pm$ is monotonically increasing and therefore of bounded variation.

Also, for $\theta \in [\rho, \frac{\pi}{2}]$ define $h(\theta) := (\sin \theta)^{-5/2}$. This function is continuous and strictly monotonically decreasing, and therefore we can express $R_i^{\pm}$ as a Riemann-Stieltjes integral, as in Reimer [22],

$$R_i^{\pm} = \int_{\rho}^{\pi/2} h(\theta) \, dg_i^{\pm}(\theta).$$

Integration by parts gives

$$
\begin{aligned}
R_i^{\pm} &= h\left(\frac{\pi}{2}\right) g_i^{\pm}\left(\frac{\pi}{2}\right) - h(\rho) \, g_i^{\pm}(\rho) - \int_{\rho}^{\pi/2} g_i^{\pm}(\theta) \, dh(\theta) \\
&= g_i^{\pm}\left(\frac{\pi}{2}\right) + \frac{5}{2} \int_{\rho}^{\pi/2} g_i^{\pm}(\theta) \, (\sin \theta)^{-7/2} \cos \theta \, d\theta.
\end{aligned}
\tag{44}
$$

Since $g_i^{\pm}$ counts points of X, we know that $g_i^{\pm}(\frac{\pi}{2}) \leqslant m$. From (20) of Lemma 3.5 we have, for $\theta \in [\rho, \frac{\pi}{2}]$, the estimate

$$g_i^{\pm}(\theta) \leqslant \frac{3\pi^2}{4} \, \rho^{-2} \, (\sin \theta)^2. \tag{45}$$

Thus, using (45) to estimate $g_i^{\pm}$ in (44), we obtain

$$
\begin{aligned}
R_i^{\pm} &\leqslant m + \frac{15\pi^2}{8\rho^2} \int_{\rho}^{\pi/2} (\sin \theta)^{-3/2} \cos \theta \, d\theta \\
&= m - \frac{15\pi^2}{4\rho^2} \left[(\sin \theta)^{-1/2} \right]_{\rho}^{\pi/2} \\
&= m + \frac{15\pi^2}{4\rho^2} \left((\sin \rho)^{-1/2} - 1 \right).
\end{aligned}
\tag{46}
$$

With the estimate

$$\sin \theta \geqslant \frac{2\theta}{\pi}, \qquad \theta \in \left[0, \frac{\pi}{2}\right],$$

we can eliminate the sine function from (46). Thus

$$R_i^{\pm} \leqslant m + \frac{15\pi^2}{4\rho^2} \left(\sqrt{\frac{\pi}{2\rho}} - 1 \right).$$

We now substitute $2\rho = \frac{\lambda}{\sqrt{m}}$ to obtain

$$
\begin{aligned}
R_i^{\pm} &\leqslant m + \frac{15\pi^2}{\lambda^2} \left(m^{1/4} \sqrt{\frac{\pi}{\lambda}} - 1 \right) m \\
&\leqslant 15 \left(\frac{\pi}{\lambda}\right)^{5/2} m^{5/4} + \left(1 - 15 \left(\frac{\pi}{\lambda}\right)^2 \right) m \\
&\leqslant 15 \left(\frac{\pi}{\lambda}\right)^{5/2} m^{5/4}.
\end{aligned}
\tag{47}
$$

In the last step we have used Lemma 3.6 to bound λ, which makes the second term in the second line of (47) negative.

Combining (47) with (42) yields

$$R^{\pm} \leqslant \frac{25\pi^2}{\sqrt{2}\,\lambda^{5/2}}\,\frac{m^{9/4}}{(n+1)^{3/2}}. \tag{48}$$

The equations and estimates (38), (39), (41), and (48), together with $D^+ = 0$ yield

$$E_X(t_n) \leqslant \frac{25\sqrt{2}\,\pi^2}{\lambda^{5/2}}\,\frac{m^{9/4}}{(n+1)^{3/2}} + \frac{m}{n+1}. \tag{49}$$

We can now eliminate the second term of (49) by increasing the constant in the first term. Using (21) from Lemma 3.7 and recalling that $m \geqslant 2$, we have

$$\frac{m^{9/4}}{(n+1)^{3/2}} = \frac{m^{5/4}}{(n+1)^{1/2}}\,\frac{m}{n+1} \geqslant 2\,\frac{m^{1/4}}{(n+1)^{1/2}}\,\frac{m}{n+1} \geqslant \sqrt{2}\,\frac{m}{n+1}.$$

Thus,

$$\frac{m}{n+1} \leqslant \frac{1}{\sqrt{2}}\,\frac{m^{9/4}}{(n+1)^{3/2}}. \tag{50}$$

Using (50), we can simplify our estimate (49) into the final form

$$E_X(t_n) \leqslant c_\lambda\,\frac{m^{9/4}}{(n+1)^{3/2}},$$

with the constant c_λ given by

$$c_\lambda := \frac{25\sqrt{2}\,\pi^2}{\lambda^{5/2}} + \frac{1}{\sqrt{2}}. \tag{51}$$

This concludes the proof. $\square$

Proof of Lemma 3.5. The spherical separation (19) puts a bound on the number of points within a spherical cap. It is equivalent to a result on spherical cap packing in the following sense.

First we observe that $m \geqslant 2$ implies that $\delta \leqslant \pi$ and hence that $\rho \leqslant \frac{\pi}{2}$. As the minimum spherical distance between points of X is bounded from below by $\delta = 2\rho$, each point is contained in a spherical cap of angular radius ρ, and the caps do not overlap. This implies that for a spherical cap $S(\mathbf{x}, \theta)$, of angular radius $\theta \in (0, \frac{\pi}{2}]$ and center $\mathbf{x}$, the number of points of X within this spherical cap is bounded from above by the number of spherical caps of angular radius ρ which can be packed into the spherical cap $S(\mathbf{x}, \theta + \rho)$. The total area covered by these small spherical caps of angular radius ρ is bounded from above by the area $|S(\mathbf{x}, \theta + \rho)|$.

For any $\mathbf{x} \in S^2$, it is well-known that the area of a spherical cap $S(\mathbf{x}, r)$ for $r \in [0, \pi]$ is given by

$$|S(\mathbf{x}, r)| = 2\pi(1 - \cos r) = 4\pi \left(\sin \frac{r}{2}\right)^2, \tag{52}$$

where the second equality is a trigonometric identity. Thus,

$$2\pi(1 - \cos \rho) \, |X \cap S(\mathbf{x}, \theta)| \leqslant 2\pi(1 - \cos(\theta + \rho)),$$

or equivalently

$$|X \cap S(\mathbf{x}, \theta)| \leqslant \frac{1 - \cos(\theta + \rho)}{1 - \cos \rho}. \tag{53}$$

From the trigonometric identities, the estimate

$$\sin \frac{\rho}{2} \geqslant \frac{\sin \frac{\pi}{4}}{\frac{\pi}{4}} \frac{\rho}{2} = \frac{2\sqrt{2}}{\pi} \frac{\rho}{2} = \frac{\sqrt{2}}{\pi} \rho,$$

and the estimates $\sin \rho \leqslant \sin \theta$ and $1 + \cos \theta \geqslant 1$ for $\rho \leqslant \theta \leqslant \frac{\pi}{2}$ we obtain

$$
\begin{aligned}
\frac{1 - \cos(\theta + \rho)}{1 - \cos \rho} &= \frac{\cos \rho - \cos(\theta + \rho)}{1 - \cos \rho} + 1 \\
&= \frac{\cos \rho \, (1 - \cos \theta)}{1 - \cos \rho} + \frac{\sin \rho \sin \theta}{1 - \cos \rho} + 1 \\
&= \frac{\cos \rho \, (\sin \theta)^2}{2(1 + \cos \theta) \left(\sin \frac{\rho}{2}\right)^2} + \frac{\sin \rho \sin \theta}{2 \left(\sin \frac{\rho}{2}\right)^2} + 1 \\
&\leqslant \frac{\pi^2 \, \cos \rho \, (\sin \theta)^2}{4 \, (1 + \cos \theta) \, \rho^2} + \frac{\pi^2 \, \sin \rho \sin \theta}{4\rho^2} + 1 \\
&\leqslant \frac{\pi^2 (\sin \theta)^2}{4\rho^2} + \frac{\pi^2 \, (\sin \theta)^2}{4\rho^2} + 1.
\end{aligned} \tag{54}
$$

The last term in (54) can be estimated by

$$1 = \frac{(\sin \theta)^2}{(\sin \theta)^2} \leqslant \frac{(\sin \theta)^2}{(\sin \rho)^2} \leqslant \frac{\pi^2 (\sin \theta)^2}{4\rho^2}, \tag{55}$$

where we have used the estimate $\sin \theta \geqslant \sin \rho \geqslant \frac{2\rho}{\pi}$, since $\rho \leqslant \theta \leqslant \frac{\pi}{2}$. Combination of (53), (54), and (55) yields

$$|X \cap S(\mathbf{x}, \theta)| \leqslant \frac{3\pi^2}{4} \rho^{-2} (\sin \theta)^2.$$

This completes the proof. $\square$

Proof of Lemma 3.6. The maximum spherical distance between any two points of S^2 is π, which is attained by two antipodal points. For X consisting of two antipodal points, we have

$$\frac{\lambda}{\sqrt{m}} = \frac{\lambda}{\sqrt{2}} = \pi,$$

so that $\lambda = \pi\sqrt{2}$.

For the general case we use an area argument similar to that in the proof of Lemma 3.5. As the minimum spherical distance between points of X is $\delta = \delta(m) := \frac{\lambda}{\sqrt{m}} \leqslant \pi$, each point is contained in a spherical cap of angular radius $\rho = \rho(m) := \frac{\lambda}{2\sqrt{m}}$, where $\rho \leqslant \frac{\pi}{2}$, and the caps do not overlap. For a set X containing $m \geqslant 2$ points of S^2, the total area of these spherical caps must not exceed the area of S^2. Thus, using (52), we must have

$$m\, 4\pi \left(\sin\frac{\rho}{2}\right)^2 \leqslant 4\pi,$$

that is,

$$\sin\frac{\rho}{2} \leqslant \frac{1}{\sqrt{m}}.$$

Since $\frac{\rho}{2} \in (0, \frac{\pi}{4}]$, we must have

$$\sin\frac{\rho}{2} \geqslant \frac{\sin\frac{\pi}{4}}{\frac{\pi}{4}} \frac{\rho}{2} = \frac{\sqrt{2}}{\pi}\rho$$

and so

$$\frac{\sqrt{2}}{\pi}\rho \leqslant \frac{1}{\sqrt{m}}.$$

Substituting $\rho = \frac{\lambda}{2\sqrt{m}}$ yields

$$\frac{\sqrt{2}}{\pi}\frac{\lambda}{2\sqrt{m}} \leqslant \frac{1}{\sqrt{m}},$$

and so $\lambda \leqslant \pi\sqrt{2}$. $\square$

Remark. For $m \geqslant 3$, L. Fejes Tóth [10] states that the minimum spherical distance $\delta(m)$ of m points on S^2 satisfies the inequality

$$\delta(m) \leqslant \Delta(m) := \cos^{-1}\left(\frac{\left(\cot\left(\frac{m}{m-2}\frac{\pi}{6}\right)\right)^2 - 1}{2}\right),$$

and that this bound is attained for $m = 3, 4, 6, 12$ and is an exact asymptotic estimate as $m \to \infty$. This estimate should give a tighter bound on λ than Lemma 3.6.

Proof of Lemma 3.7. The bounds given in [7, Theorem 5.11, Theorem 5.12] imply that

$$m \geqslant (k+1)^2 \geqslant \frac{1}{4}(n+1)^2, \qquad \text{for } n = 2k, \text{ and}$$

$$m \geqslant (k+1)(k+2) \geqslant \frac{1}{4}(n+1)^2, \qquad \text{for } n = 2k+1.$$

Thus $n + 1 \leqslant 2\sqrt{m}$. $\square$

5   The separation property is necessary

It has been known since the original paper of Delsarte, et al. [7] that any disjoint union of spherical n-designs is a spherical n-design. This leads to the following classification of spherical n-designs.

- Compound. A disjoint union of two or more spherical n-designs.

- Degenerate. A cubature rule with less than m points, where each weight is a positive integer multiple of $4\pi/m$, which can be considered as an m point spherical n-design with a number of coincident points.

- Simple. Neither compound nor degenerate.

We can use this classification to examine the separation condition more closely. We first note that any sequence of spherical designs with a degenerate member is not well-separated.

Any finite sequence of non-degenerate spherical designs is trivially well-separated.

With infinite sequences of spherical designs, the separation property is no longer trivial. Many such infinite sequences do not have the separation property. This is because a compound spherical design can have points which are arbitrarily close together.

Given any compound spherical n-design, where n is now fixed, it is easy to construct an infinite sequence of spherical n-designs such that the number of points remains constant, but the minimum distance approaches zero. This can be done by rotating one component of the compound spherical design with respect to the other components, in such a way that two of the points approach each other. Specific examples of starting points for such a sequence are any compound spherical 1-design consisting of two pairs of opposite points, and any compound spherical 3-design consisting of the vertices of two cubes. (It is known that any pair of antipodal points is a simple 1-design, and that the points of a cube form a simple 3-design (see [7, 11]).)

Using a similar principle of construction, it is possible to construct an infinite sequence of compound spherical designs, with increasing strength (and hence increasing cardinality), such that the minimum distance between points decreases arbitrary rapidly. Clearly such a sequence does not have the separation property.

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