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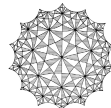


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Optimal measures for p -frame energies on spheres

Dmitriy Bilyk, Alexey Glazyrin, Ryan Matzke, Josiah Park and
Oleksandr Vlasiuk

Abstract. We provide new answers about the distribution of mass on spheres so as to minimize energies of pairwise interactions. We find optimal measures for the p -frame energies, i.e., energies with the kernel given by the absolute value of the inner product raised to a positive power p . Application of linear programming methods in the setting of projective spaces allows for describing the minimizing measures in full in several cases: we show optimality of tight designs and of the 600-cell for several ranges of p in different dimensions. Our methods apply to a much broader class of potential functions, namely, those which are absolutely monotonic up to a particular order.

1. Introduction

An intriguing natural phenomenon is the ubiquitous appearance of certain symmetric structures and configurations as solutions to optimization problems. In a number of spaces, highly symmetric configurations of points such as the vertices of the icosahedron on \mathbb{S}^2 or the minimal vectors of the Leech lattice Λ_{24} on \mathbb{S}^{23} are *optimal codes*, a type of best packing configuration [40]. First papers on spherical designs made important connections between symmetry and optimality through pioneering work on linear programming bounds [25]. Since these and new developments we now know several configurations, in addition to being spherical designs and optimal codes, that are also minimizers for a variety of harmonic energies [1, 37, 38, 65, 66].

For a finite configuration of points on the sphere $\mathcal{C} \subset \mathbb{S}^{d-1}$ (also known as a *code*), the discrete f -potential energies are defined as

$$(1.1) \quad E_f(\mathcal{C}) = \frac{1}{|\mathcal{C}|^2} \sum_{x, y \in \mathcal{C}} f(\langle x, y \rangle).$$

(The diagonal terms should be excluded if the kernel f is singular at 1, that is, when $x = y$.) *Universally optimal* point configurations, i.e., collections of points \mathcal{C} minimizing the discrete energies E_f among all point sets of fixed cardinality $|\mathcal{C}|$, for all absolutely

monotonic functions f on $[-1, 1]$, have been discovered through the linear programming approach of Cohn and Kumar in [21].

In contrast to the above setting, in the present paper, rather than considering configurations of fixed cardinality, we focus on the problem of minimizing energies over *all Borel probability measures*, discovering that surprisingly in many situations the minimizing measures are discrete. For a kernel function $f \in C[-1, 1]$ and a Borel measure μ on \mathbb{S}^{d-1} , we define the energy integral as

$$(1.2) \quad I_f(\mu) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} f(\langle x, y \rangle) d\mu(x) d\mu(y).$$

One is naturally interested in minimizing these energies over $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$, the set of all Borel probability measures on \mathbb{S}^{d-1} , i.e., finding the equilibrium distribution of unit mass under the interaction given by the potential function f . This definition is compatible with the discrete energy (1.1) in the sense that

$$(1.3) \quad E_f(\mathcal{C}) = I_f\left(\frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x\right),$$

and we shall repeatedly abuse the notation when saying that a configuration \mathcal{C} minimizes the energy I_f , to mean that the corresponding measure in the right-hand side of the above equation minimizes.

While many classical examples, such as the Riesz energy, feature increasing kernels f which give rise to energies with repulsive interactions (i.e., f is largest when $x = y$ and smallest when x and y are antipodal), we will concentrate on the *attractive-repulsive* potentials, which decrease at first, but increase eventually, as functions of the geodesic distance: in other words, a pair of points will repel when close together, but attract when far apart. Such potentials in \mathbb{R}^d appear naturally for self-assembly models in computational chemistry, emerging collective behavior in population biology, and in many other scientific models [5, 18, 19, 36, 48, 60, 64].

We will mostly consider attractive-repulsive potentials on the sphere which are symmetric and *orthogonalizing*, so that $f(t) = f(|t|)$, $f(t)$ is increasing for $t \in [0, 1]$, and f takes its minimal value at zero. For such potentials, the discrete energy for up to d particles is minimized by collections of orthogonal vectors. Since in this setting the energy does not change by replacing any x with λx , where $|\lambda| = 1$, its analysis naturally lends itself to the projective space $\mathbb{R}\mathbb{P}^{d-1}$, where the potential becomes repulsive, and we adopt this approach in the technical parts of the paper.

The main examples of the above potentials, which motivate the current paper, are of the form $f(t) = |t|^p$, $p > 0$, which yield the *p-frame energies*:

$$(1.4) \quad I_f(\mu) = \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} |\langle x, y \rangle|^p d\mu(x) d\mu(y),$$

where $\mathbb{S}_{\mathbb{F}}^{d-1} = \{x \in \mathbb{F}^d \mid \|x\| = 1\}$. For $\mathbb{F} = \mathbb{R}$ or \mathbb{C} this type of energy has a rich history.

When $p = 2$ and $\mathbb{F} = \mathbb{R}$, the discrete version of this energy, known simply as the *frame energy* or *frame potential*, has been introduced by Benedetto and Fickus [11]: they showed that global (as well as local) minimizers of this energy are precisely unit norm

tight frames. These configurations, which explain the nomenclature “frame energy”, play an important role in signal processing and other branches of applied mathematics and behave like overcomplete orthonormal bases. A finite collection of vectors $\mathcal{C} \subset \mathbb{F}^d$ is a tight frame, if for any $x \in \mathbb{F}^d$, and some constant $A > 0$, one has an analog of Parseval’s identity holding for \mathcal{C} ,

$$(1.5) \quad \sum_{y \in \mathcal{C}} |\langle x, y \rangle|^2 = A \|x\|^2.$$

These objects also minimize the continuous energy I_f for $p = 2$, but there are also other minimizers, such as the surface area, or Haar measure σ on $\mathbb{S}_{\mathbb{F}}^{d-1}$, and, more generally, *isotropic probability measures* on the sphere, i.e., those measures for which

$$\int_{\mathbb{S}_{\mathbb{F}}^{d-1}} |\langle x, y \rangle|^2 d\mu(y) = \frac{1}{d}$$

holds for all $x \in \mathbb{S}_{\mathbb{F}}^{d-1}$.

When $p = 4$, this energy plays an important role in connection to complex maximal *equiangular tight frames*, also known as *symmetric, informationally complete, positive operator-valued measures* (SIC-POVMs), i.e., unit norm tight frames in \mathbb{C}^d which satisfy $|\langle x, y \rangle| = \text{constant}$ for $x \neq y \in \mathcal{C}$ and $|\mathcal{C}| = d^2$, [49]. The existence of these objects is the subject of *Zauner’s conjecture* (see [67]), and much of the numerical evidence for this conjecture comes from the observation that they minimize the 4-frame energy among other energies, as projective 2-designs, see e.g. [53]. Since we will later work with minimizers over the skew field of quaternions, we mention that in that setting these equiangular tight frames are conjectured [22] to not always exist. In the real case, the existence of analogous objects (i.e., tight projective 2-designs) is also mysterious: they may exist only in dimensions $d = (2m - 1)^2 - 2$, [6, 7, 25, 39], but do not exist for infinitely many values of m , [9, 45]. In what follows, we demonstrate that when these objects do exist, they also minimize the p -frame energy for $2 \leq p \leq 4$.

More generally, for even integers p , these energies were considered in earlier works [55, 59, 62], and it is known that, for $\mathbb{F} = \mathbb{R}$ or \mathbb{C} , projective k -designs are precisely the finite configurations which minimize the $p = 2k$ energy. Unit norm tight frames are then in fact just equivalent to projective 1-designs (see Section 2.3 for precise definitions), while spherical 2-designs are exactly those unit norm tight frames, whose center of mass is at the origin. These were constructively shown to exist for $d \geq 2$ precisely when the number of points N satisfies $N \geq d + 1$ and $N \neq d + 2$ when d is odd [47]. The last restriction does not apply to unit norm tight frames, and these exist for all $N \geq d$, [11]. Surface measure is also known to be a minimizer for $p \in 2\mathbb{N}$: this can be seen either from the definition of k -designs, or from the fact that the function f is positive definite in this case (see Proposition 2.3), and was originally proved in the real case in [55].

For p not an even integer, optimal distributions of mass for p -frame energies are much less studied, to the point of there only being one result on these minimizing measures readily found in the literature. It states that distributing mass equally on the orthoplex or cross-polytope, an orthonormal basis and its antipodes, gives the unique symmetric minimizer, up to orthogonal transformations, for any energy with $p \in (0, 2)$. See [27].

This result (contained in our Theorem 1.1 below as a special case) points to an interesting distinction. When p is even, the p -frame energy has a multitude of both continuous, e.g. σ , and discrete minimizers. However, this is not the case when p is not an even integer: σ is no longer a minimizer, since the function $f(t) = |t|^p$ is not positive definite, and so the above result, along with our numerical studies, points to existence of discrete minimizers only.

In this paper we give a first description of minimizers for several dimensions and some ranges of p . The description relies on the notion of *tight designs*: designs of high strength, but with few distinct pairwise distances, see Definition 2.5. We show that if there exists a tight projective M -design (which in the real case is equivalent to a tight spherical $(2M + 1)$ -design), then it minimizes the p -frame energy for $p \in (2M - 2, 2M)$. The 600-cell, despite not being a tight design, minimizes the p -frame energy for $p \in (8, 10)$ among probability measures on \mathbb{S}^3 , as we show in Section 4.

Theorem 1.1. *Let $f(t) = |t|^p, t \in [-1, 1]$.*

(i) *If there exists a tight spherical $(2M + 1)$ -design $\mathcal{C} \subset \mathbb{S}^{d-1}$, then the measure*

$$\mu = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of the p -frame energy I_f with $2M - 2 \leq p \leq 2M$ over $\mu \in \mathcal{P}(\mathbb{S}^{d-1})$.

(ii) *Let $\mathbb{F} = \mathbb{R}, \mathbb{C}$ or \mathbb{H} . Assume that there exists a tight projective M -design $\tilde{\mathcal{C}} \subset \mathbb{F}\mathbb{P}^{d-1}$, and let the code $\mathcal{C} \subset \mathbb{S}_{\mathbb{F}}^{d-1}$ consist of the representers of $\tilde{\mathcal{C}}$ in $\mathbb{S}_{\mathbb{F}}^{d-1}$ according to (2.1). Then the measure*

$$\mu = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of the p -frame energy I_f with $2M - 2 \leq p \leq 2M$ over $\mu \in \mathcal{P}(\mathbb{S}_{\mathbb{F}}^{d-1})$.

(iii) *Let $\mathcal{C} \subset \mathbb{S}^3$ denote the 600-cell. Then the measure*

$$\mu = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of the p -frame energy I_f with $8 \leq p \leq 10$ over $\mu \in \mathcal{P}(\mathbb{S}^3)$.

For parts (i)–(ii) of the above theorem, we also prove a uniqueness statement: more precisely, whenever the corresponding statements hold, and additionally p is not an endpoint of the interval, i.e., $p \in (2M - 2, 2M)$, all minimizers have to be tight designs (although not necessarily coinciding with \mathcal{C}), in particular, they have to be discrete. Since tight $(2M + 1)$ -designs on the circle consist just of $2(M + 1)$ equally spaced points, the above result fully characterizes the minimizers for $d = 2$ (for both the sphere and the real projective space). See Section 3.5 for more details.

We observe that part (i) is essentially contained in part (ii) with $\mathbb{F} = \mathbb{R}$: indeed, odd-strength tight spherical designs are necessarily symmetric [25], and by taking one point in each antipodal pair one obtains a tight projective design (see Sections 2.3 and 2.4 for a more extensive discussion).

Minimizing the continuous energy (1.4) over all *measures* and obtaining discrete minimizers allows us to make new conclusions about the minimizing configurations of the discrete energies (1.1) for certain values of the cardinality N . One directly obtains the following corollary.

Corollary 1.2. *Let \mathbb{F} , d , p , and \mathcal{C} be as in any of the parts of Theorem 1.1, and let $N = k|\mathcal{C}|$, $k \in \mathbb{N}$. Then the N -point discrete p -frame energy is minimized by the configuration \mathcal{C} repeated k times, i.e.,*

$$(1.6) \quad \min_{\substack{\mathcal{C}' \subset \mathbb{S}_{\mathbb{F}}^{d-1} \\ |\mathcal{C}'|=N}} \frac{1}{N^2} \sum_{x,y \in \mathcal{C}'} |\langle x, y \rangle|^p = I_{|t|^p} \left(\frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x \right).$$

Thus, for example, if N is a multiple of 6, then repeated copies of a ‘‘half’’ of the icosahedron minimize the N -point p -frame energy on \mathbb{S}^2 for $p \in [2, 4]$. Some other results about the minima of discrete p -frame energies have been obtained in [20].

The arguments proving Theorem 1.1 are strongly reminiscent of those appearing in [21], and are based on the linear programming method which goes back to Delsarte and Yudin [24, 65]. Part (ii) of Theorem 1.1 is a consequence of the much more general Theorem 3.7. The latter theorem, in fact, demonstrates that tight M -designs possess a certain *universality* property: they minimize the energy for *all* strictly monotonic functions of degree exactly m over *all probability measures*, see Section 3 for details.

The proof of optimality for the 600-cell is computer assisted and makes use of the fact that the averages of spherical harmonics over the 600-cell vanish for a few orders above its maximal strength as a spherical design – the same idea was used in the proof of universal optimality of the 600-cell in [21], as well as earlier in [1, 2]. This allows us to construct a collection of interpolating polynomials h for each p which have the desired properties of lying below f , agreeing with f on the distances appearing in \mathcal{C} , and finally being positive definite, the last of which is checked using interval arithmetic. The details of the proof are taken up in Section 4.

We collect all the necessary preliminary material in Section 2: Section 2.1 contains the discussion of relevant properties of compact 2-point homogeneous connected spaces; Section 2.2 explains the specifics of minimizing energy functionals over probability measures on such spaces; Section 2.3 introduces designs, and, in particular, tight designs; and Section 2.4 describes the transference between energies on projective spaces and spheres, which connects Theorem 3.7 to Theorem 1.1.

Theorem 1.1 leads us to believe that clustering of minimizers is a general phenomenon when p is not an even integer and we will present our experimental evidence in favor of this conclusion in a separate publication [14].

Conjecture 1.3. *In all dimensions $d \geq 2$ and for all $p > 0$ such that $p \notin 2\mathbb{N}$, the minimizing measures of the p -frame energy (1.4) are discrete.*

This conjecture is additionally supported by the fact that discreteness of minimizers is known for certain attractive-repulsive potentials on \mathbb{R}^d , [18], and has been conjectured for some other potentials on the sphere, e.g. those appearing in [28], see also Section 7. It is worth noting that in the classical paper [15], it was shown that for $f(x, y) = -\|x - y\|^\alpha$ with $\alpha > 2$ and any compact domain $\Omega \subset \mathbb{R}^d$, the energy minimizers are discrete and

their support consists of at most $d + 1$ points (just two antipodal points if $\Omega = \mathbb{S}^{d-1}$). Moreover, in [18] discreteness has been established for mildly repulsive potentials, i.e., those that behave as $-\|x - y\|^\alpha$ with $\alpha > 2$ when $\|x - y\|$ is small. Observe that for the p -frame potential, we have $|\langle x, y \rangle|^p \approx 1 - \frac{p}{2}\|x - y\|^2$ when $x, y \in \mathbb{S}^{d-1}$ are close, hence the p -frame energy falls into the endpoint case $\alpha = 2$, and, according to the discussion above, this case is more subtle.

While we have yet to establish Conjecture 1.3 and prove discreteness, in our companion paper [13] we show that on \mathbb{S}^{d-1} , whenever p is not even, the support of the measure minimizing the p -frame potential necessarily has empty interior.

Section 5 extends some of our results to non-compact settings. In Section 6 we apply the results of Theorem 1.1 to the problems of minimizing mixed volumes of convex bodies, and in Section 7 we apply the methods of linear programming, similar to those employed in Theorems 1.1 and 3.7, to the optimization of energies related to *causal variational principles*, see [28].

We would like to point out that in many papers, the term *p-frame potential* is usually used to denote the p -frame energy (1.4) or its discrete counterpart. We find the term “energy” to be more appropriate in this context and reserve the term “potential” for the kernel $f(t)$ of the energy I_f .

2. Geometry and functions on 2-point homogeneous spaces

2.1. Two-point homogeneous spaces

For convenience, the above discussion mostly assumed the underlying space to be the unit sphere \mathbb{S}^{d-1} . This will no longer be the case, as our study concerns energy minimization on a broader class of spaces. A metric space (Ω, d) is said to be *two-point homogeneous* if, for every two pairs of points x_1, x_2 and y_1, y_2 such that $d(x_1, x_2) = d(y_1, y_2)$, there exists an isometry of Ω mapping x_i to $y_i, i = 1, 2$. It is known [61] that any such compact connected space is either a real sphere \mathbb{S}^{d-1} , a real projective space $\mathbb{R}\mathbb{P}^{d-1}$, a complex projective space $\mathbb{C}\mathbb{P}^{d-1}$, a quaternionic projective space $\mathbb{H}\mathbb{P}^{d-1}$, or the Cayley projective plane $\mathbb{O}\mathbb{P}^2$. Note that it suffices to consider $\mathbb{F}\mathbb{P}^{d-1}$ for $d > 2$ only, as $\mathbb{F}\mathbb{P}^1$ is just $\mathbb{S}^{\dim_{\mathbb{R}} \mathbb{F}}$ (see [4], p. 170), and so will not be separately considered in what follows.

Below, Ω always refers to a compact connected 2-point homogeneous space, equipped with the geodesic distance ϑ , normalized to take values in $[0, \pi]$. We let σ denote the unique probability measure invariant under the isometries of Ω .

The first three types of projective spaces $\{\mathbb{F}\mathbb{P}^{d-1} : \mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}\}$ have a simple description: they may be represented as the spaces of lines passing through the origin in \mathbb{F}^d ,

$$(2.1) \quad x\mathbb{F} = \{x\lambda \mid \lambda \in \mathbb{F} \setminus \{0\}\}.$$

Observe that the isometry groups $O(d)$, $U(d)$, and $Sp(d)$ of the corresponding vector spaces \mathbb{F}^d act transitively on each space, and that the stabilizers of a line represented by $x \in \mathbb{F}^d$ are $O(d - 1) \times O(1)$, $U(d - 1) \times U(1)$, and $Sp(d - 1) \times Sp(1)$, respectively. Thus

one has, [63], p. 28, the following quotient representations:

$$\begin{aligned} \mathbb{R}\mathbb{P}^{d-1} &= \mathrm{O}(d)/\mathrm{O}(d-1) \times \mathrm{O}(1), \\ \mathbb{C}\mathbb{P}^{d-1} &= \mathrm{U}(d)/\mathrm{U}(d-1) \times \mathrm{U}(1), \\ \mathbb{H}\mathbb{P}^{d-1} &= \mathrm{Sp}(d)/\mathrm{Sp}(d-1) \times \mathrm{Sp}(1), \end{aligned}$$

where we write $\mathrm{O}(d)$, $\mathrm{U}(d)$, and $\mathrm{Sp}(d)$ for the groups of matrices X over the respective algebra, satisfying $XX^* = I$.

Using the identification (2.1), one can associate each element of $\mathbb{F}\mathbb{P}^{d-1}$ ($\mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}$) with a unit vector $x \in \mathbb{F}^d$, $\|x\| = 1$, and we shall often abuse notation by doing so. This gives, in addition to the Riemannian metric ϑ , another metric, the *chordal distance* between points $x, y \in \Omega$, defined by

$$\rho(x, y) = \sqrt{1 - |\langle x, y \rangle|^2},$$

where $\langle x, y \rangle = \sum_{i=1}^d x_i \bar{y}_i$ is the standard inner product in \mathbb{F}^d . The chordal distance $\rho(x, y)$ is related to the geodesic distance $\vartheta(x, y)$ by the equation

$$\cos \vartheta(x, y) = 1 - 2\rho(x, y)^2 = 2|\langle x, y \rangle|^2 - 1.$$

Since the algebra of octonions is not associative, the line model of (2.1) fails, and instead a model given by Freudenthal [29] is used to describe $\mathbb{O}\mathbb{P}^{d-1}$. It is known [4] that only two octonionic spaces exist: $\mathbb{O}\mathbb{P}^1$ which is just \mathbb{S}^8 , as noted above, and $\mathbb{O}\mathbb{P}^2$ which can be described as the subset of 3×3 Hermitian matrices Π over \mathbb{O} , satisfying $\Pi^2 = \Pi$ and $\mathrm{Tr} \Pi = 1$, [4, 56]. We note that, while the definition of the p -frame energy does not extend to $\mathbb{O}\mathbb{P}^2$ (and thus Theorem 1.1 does not include this space), the more general Theorem 3.7 does apply to $\Omega = \mathbb{O}\mathbb{P}^2$.

One feature of spaces Ω that allows for the application of linear programming methods is the existence of a decomposition of $L^2(\Omega, \sigma)$, the space of complex-valued square-integrable functions on Ω :

$$L^2(\Omega, \sigma) = \bigoplus_{n \geq 0} V_n,$$

where V_n are finite-dimensional irreducible representations of the isometry group of Ω (see [40]). Moreover, these are in correspondence with the eigenspaces of the Laplace–Beltrami operator on Ω corresponding to the n -th eigenvalue in the increasing order. Let $Y_{n,k}$, $k = 1, \dots, \dim V_n$, be an orthonormal basis in V_n . Because of the invariance of V_n and due to the two-point homogeneity of Ω , the reproducing kernel for V_n only depends on the distance $\vartheta(x, y)$ between points [59]. Furthermore, as a function of

$$\tau(x, y) := \cos \vartheta(x, y),$$

the reproducing kernel is a polynomial C_n of degree n , which satisfies

$$(2.2) \quad C_n(\tau(x, y)) = \frac{1}{\dim V_n} \sum_{k=1}^{\dim V_n} Y_{n,k}(x) \overline{Y_{n,k}(y)}.$$

Formula (2.2) is known as the *addition formula*, and shows that functions C_n are *positive definite* on Ω , that is,

$$\sum_{1 \leq i, j \leq k} c_i \bar{c}_j C_n(\tau(x_i, x_j)) \geq 0$$

for all coefficients $c_1, \dots, c_k \in \mathbb{C}$, and all $x_1, \dots, x_k \in \Omega$.

The polynomials C_n given by (2.2) satisfy $C_n(1) = 1$ and are orthogonal with respect to the probability measure

$$d\nu^{(\alpha, \beta)} = \frac{1}{\gamma_{\alpha, \beta}} (1 - t)^\alpha (1 + t)^\beta dt,$$

where $\alpha = (d - 1) \dim_{\mathbb{R}}(\mathbb{F})/2 - 1$ and

$$(2.3) \quad \beta = \begin{cases} \alpha, & \text{if } \Omega = \mathbb{S}^{d-1}, \\ \dim_{\mathbb{R}}(\mathbb{F})/2 - 1, & \text{if } \Omega = \mathbb{F}\mathbb{P}^{d-1}, \end{cases}$$

and the normalization factor is given by

$$\gamma_{\alpha, \beta} = 2^{\alpha + \beta + 1} B(\alpha + 1, \beta + 1),$$

where B is the beta function. These polynomials, known as Jacobi polynomials (Gegenbauer polynomials in the special case when $\Omega = \mathbb{S}^{d-1}$), form an orthogonal basis in $L^2([-1, 1], d\nu^{(\alpha, \beta)})$; equivalently, the span of $C_n(\tau(x, y))$, $n \geq 0$, is dense in the subset of $L^2(\Omega \times \Omega, \sigma \otimes \sigma)$ consisting of functions that depend only on the distance between x and y .

This allows for expanding functions from $L^2([-1, 1], d\nu^{(\alpha, \beta)})$ in terms of C_n :

$$f(t) = \sum_{n=0}^{\infty} \hat{f}_n C_n(t), \quad \text{where } \hat{f}_n = \dim V_n \int_{-1}^1 f(t) C_n(t) d\nu^{(\alpha, \beta)}(t).$$

As we have already done above, for a fixed space Ω we will not indicate the dependence of polynomials $C_n = C_n^{(\alpha, \beta)}$ on the indices α, β . We refer to \hat{f}_n as the Jacobi coefficients of the function f ; the normalization $C_n(1) = 1$ used here is common in the coding theory community [40, 58].

2.2. Energies on 2-point homogeneous spaces

For the space of probability measures $\mathcal{P}(\Omega)$ supported on Ω , and for a lower semi-continuous function $f: [-1, 1] \rightarrow \mathbb{R} \cup \infty$, the f -energy integral is defined as the functional mapping μ to

$$I_f(\mu) = \int_{\Omega} \int_{\Omega} f(\tau(x, y)) d\mu(x) d\mu(y).$$

Observe that when $\Omega = \mathbb{S}^{d-1}$, we have $\tau(x, y) = \cos \vartheta(x, y) = \langle x, y \rangle$ and the definition above coincides with (1.2).

We start by introducing the notion of positive definite functions, which plays an important role in energy minimization and for the linear programming bounds we derive later. Below, $C[-1, 1] = C_{\mathbb{R}}[-1, 1]$ denotes the space of continuous real valued functions on the interval $[-1, 1]$.

Definition 2.1. Let $f \in C[-1, 1]$. We say that f is *positive definite* on Ω if for any $x_1, \dots, x_N \in \Omega$, the matrix $[f(\tau(x_i, x_j))]_{i,j=1}^N$ is positive semidefinite, i.e., if for every collection $c_1, \dots, c_N \in \mathbb{C}$, we have

$$\sum_{1 \leq i, j \leq N} f(\tau(x_i, x_j)) c_i \bar{c}_j \geq 0.$$

We have already seen that the Jacobi polynomials C_n are positive definite on Ω , and so their positive linear combinations must also be. It is a classical fact that this implication can be reversed:

Proposition 2.2 ([16, 30, 52]). *A function $f \in C[-1, 1]$ is positive definite on Ω if and only if $\hat{f}_n \geq 0$ for all $n \geq 0$.*

Next we show that positive definite functions f give rise to f -energy integrals which are minimized over probability measures by the surface (or Haar) measure σ on Ω . This result appears in a number of papers, see for instance [12, 23]. We adapt the proof given in [12] to our purposes.

Proposition 2.3. *Let $f \in C[-1, 1]$, $f(t) = \sum_{n=0}^{\infty} \hat{f}_n C_n(t)$, and $\mu \in \mathcal{P}(\Omega)$. Then, the following are equivalent:*

- (i) $\hat{f}_n \geq 0$ for all $n \geq 1$,
- (ii) the surface measure σ is a minimizer of I_f .

Moreover, σ is the unique minimizer of I_f if and only if $\hat{f}_n > 0$ for all $n \geq 1$.

To prove this statement we use the following lemma, generalizing the behavior of Fourier expansions with positive coefficients [30, 44] to Jacobi expansions with the same property.

Lemma 2.4. *Assume that $f \in C[-1, 1]$ has the Jacobi expansion $f(t) = \sum_{n=0}^{\infty} \hat{f}_n C_n(t)$ with $\hat{f}_n \geq 0$ for all $n \geq 1$. Then this expansion converges uniformly and absolutely to f on $[-1, 1]$.*

Proof of Proposition 2.3. We first show that σ is a minimizer of I_f . Assume that $\hat{f}_n \geq 0$ for all $n \geq 1$. Then by the lemma above, the Fubini theorem, and the addition formula, we have

$$\begin{aligned} I_f(\mu) &= \sum_{n=0}^{\infty} \hat{f}_n \int_{\Omega} \int_{\Omega} C_n(\tau(x, y)) d\mu(x) d\mu(y) \\ &= \sum_{n=0}^{\infty} \frac{1}{\dim V_n} \sum_{k=1}^{\dim V_n} \hat{f}_n \int_{\Omega} \int_{\Omega} Y_{n,k}(x) \overline{Y_{n,k}(y)} d\mu(x) d\mu(y) \\ &= \hat{f}_0 + \frac{1}{\dim V_n} \sum_{n=1}^{\infty} b_{n,\mu} \hat{f}_n \geq \hat{f}_0 = I_f(\sigma). \end{aligned}$$

The last inequality holds since $b_{n,\mu} = \sum_{k=1}^{\dim V_n} |\int_{\Omega} Y_{n,k}(x) d\mu(x)|^2 \geq 0$. If $\hat{f}_n > 0$ for all $n \geq 1$, then equality can be achieved above only if μ is orthogonal to all spaces $V_n, n \geq 1$, which directly implies that $\mu = \sigma$.

Let us assume that for some $m \in \mathbb{N}_0$, $\widehat{f}_n < 0$. For a fixed point $p \in \Omega$, we see that $Y_{n,1}(x) := C_n(\tau(x, p))$ is in V_n and real-valued. Set $d\mu(x) = (1 + \varepsilon Y_{n,1}(x))d\sigma(x)$, where $\varepsilon > 0$ is sufficiently small so that $(1 + \varepsilon Y_{n,1}(x)) \geq 0$ on Ω . Orthogonality and the addition formula (or the Funk–Hecke formula) give that for $Y \in V_n$,

$$\int_{\Omega} f(\tau(x, y)) Y(x) d\sigma(x) = \frac{1}{\dim(V_n)} \widehat{f}_n \overline{Y(y)} \quad \text{and} \quad \int_{\Omega} Y(x) d\sigma = 0.$$

Thus,

$$\begin{aligned} I_f(\mu) &= \int_{\Omega} \int_{\Omega} f(\tau(x, y)) (1 + \varepsilon Y_{n,1}(x)) (1 + \varepsilon Y_{n,1}(y)) d\sigma(x) d\sigma(y) \\ &= I_f(\sigma) + \frac{1}{\dim(V_n)} \int_{\Omega} \varepsilon^2 \widehat{f}_n Y_{n,1}^2(x) d\sigma(x) < I_f(\sigma), \end{aligned}$$

implying that σ is not a minimizer for I_f . If $\widehat{f}_n = 0$ for some $n \geq 1$, the same argument shows that $I_f(\mu) = I_f(\sigma)$, i.e., σ is not the unique minimizer. ■

The p -frame energies correspond to taking $\Omega = \mathbb{F} \mathbb{P}^{d-1}$ ($\mathbb{F} = \mathbb{R}, \mathbb{C}$, or \mathbb{H}) and f of the form

$$(2.4) \quad f(t) = \left(\frac{1+t}{2}\right)^{p/2},$$

because in this case, since $\tau(x, y) = \cos \vartheta(x, y) = 2|\langle x, y \rangle|^2 - 1$, we have

$$f(\tau(x, y)) = f(2|\langle x, y \rangle|^2 - 1) = |\langle x, y \rangle|^p.$$

We shall now prove that, whenever p is an even integer, these energies are minimized by the uniform measure on Ω .

When $p = 2k$ and $\Omega = \mathbb{F} \mathbb{P}^{d-1}$ ($\mathbb{F} = \mathbb{R}, \mathbb{C}$, or \mathbb{H}), we have that $f(t) = 2^{-k} \cdot (1+t)^k$ is a polynomial. It is standard to check that this polynomial is positive definite on Ω : this could be done by checking that the coefficients in its Jacobi expansion are non-negative, but it would be perhaps simpler to prove it as follows. Observe that, since $C_0^{(\alpha, \beta)}(t) = 1$ and $C_1^{(\alpha, \beta)}(t) = \frac{\alpha - \beta}{2(\alpha + 1)} + \frac{\alpha + \beta + 2}{2(\alpha + 1)} \cdot t$, we have that

$$1 + t = \frac{2(\alpha + 1)}{(\alpha + \beta + 2)} C_1^{(\alpha, \beta)}(t) + \frac{2(\beta + 1)}{\alpha + \beta + 2} C_0^{(\alpha, \beta)}(t).$$

Since $\alpha + 1 = \frac{d-1}{2} \cdot \dim_{\mathbb{R}}(\mathbb{F}) > 0$ and $\beta + 1 = \frac{1}{2} \cdot \dim_{\mathbb{R}}(\mathbb{F}) > 0$, we see that the function $1 + t$ is positive definite on Ω . The well known Schur theorem on Hadamard (element-wise) products of positive semidefinite matrices implies that if g and h are positive definite on Ω , then so is their product gh , and, in particular, all integer powers g^n are positive definite. Hence, the function $f(t) = 2^{-k} \cdot (1+t)^k$ is positive definite on Ω , and therefore I_f is minimized by the uniform surface measure σ .

The minimal values of the $p = 2k$ energy may be expressed in terms of elementary functions for each \mathbb{F} . These constants, $c_{\mathbb{F}}(d, k)$, are given below:

$$\begin{aligned}
 c_{\mathbb{F}}(d, k) &= \frac{1 \cdot 3 \cdot 5 \cdots (2k - 1)}{d \cdot (d + 2) \cdots (d + 2(k - 1))}, & \mathbb{F} &= \mathbb{R}, \\
 c_{\mathbb{F}}(d, k) &= \frac{1}{\binom{d+k-1}{k}}, & \mathbb{F} &= \mathbb{C}, \\
 c_{\mathbb{F}}(d, k) &= \frac{k + 1}{\binom{2d+k-1}{k}}, & \mathbb{F} &= \mathbb{H}.
 \end{aligned}$$

When p is not an even integer, the p -frame energies are not positive definite, due to the appearance of negative terms in the Jacobi polynomial expansion of f , hence σ does not minimize the p -frame energy for $p \notin 2\mathbb{N}$, see Lemma 6.2.2 in [46].

2.3. Designs

We now treat the topic of designs in compact connected two-point homogeneous spaces Ω . A finite, nonempty set (code) $\mathcal{C} \subset \Omega$ is called an M -design if

$$(2.5) \quad \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} p(x) = \int_{\Omega} p(x) d\sigma(x)$$

holds for all polynomials p of degree at most M . A relaxation of the above identity allows the configuration to be weighted, so that the equality

$$(2.6) \quad \sum_{x \in \mathcal{C}} \omega_x p(x) = \int_{\Omega} p(x) d\sigma(x),$$

holds for some weights $\{\omega_x\}_{x \in \mathcal{C}} \subset \mathbb{R}_{\geq 0}$, satisfying $\sum_{x \in \mathcal{C}} \omega_x = 1$, and for all polynomials p of degree at most M . Such weighted formulas are called *cubature formulas* or *weighted designs*. In both of the above equations, it is understood that polynomials p may be given explicitly as complex-valued functions which are polynomials in coordinates of \mathbb{F}^d , satisfying additionally $p(\alpha x) = p(x)$, for $|\alpha| = 1, \alpha \in \mathbb{F}$, in the projective case.

The *strength* of a (weighted) design is the maximum value of M for which identity (2.5) (accordingly, (2.6)) holds. An M -design can be equivalently defined as a configuration $\mathcal{C} \subset \Omega$, for which

$$\sum_{x, y \in \mathcal{C}} C_n(\tau(x, y)) = 0 \quad \text{for } 1 \leq n \leq M.$$

Equivalently, \mathcal{C} is an M -design in Ω if and only if it satisfies

$$\sum_{x \in \mathcal{C}} Y(x) = 0 \quad \text{for } Y \in \bigoplus_{n=1}^M V_n.$$

Similar definitions can be given for weighted designs.

Linear programming bounds [25] imply exact constraints on the size of *tight designs*, configurations which, in addition to being M -designs, have the smallest possible number of pairwise distances between their elements, for a design of strength M . The exact definition may be given as follows.

Definition 2.5. A discrete set $\mathcal{C} \subset \Omega$ is called a *tight M -design* if one of the following conditions is satisfied.

- (i) \mathcal{C} is a design of strength $M = 2m - 1$ and there are m distances between its distinct elements, including at least one pair diameter apart;
- (ii) \mathcal{C} is a design of strength $M = 2m$ and there are m distances between its distinct elements.

Table 1 provides a list of known tight spherical designs (see, e.g., [21]), as well as the 600-cell, which is not a tight design, but will be of interest in Section 4. Each arrangement labeled ‘kissing’ is the kissing configuration of a set. By centering non-overlapping congruent spherical caps of maximal radius at each point in a given code, the resulting points of tangency on a given cap form a spherical code in a lower dimensional space which we call the kissing configuration for that set.

Tight spherical designs with $d \geq 3$ and $M \geq 4$ may only exist for $M = 4, 5,$ and 7 with the one exception of the spherical 11-design formed by the Leech lattice minimal vectors [6, 7]. The problem of finding tight spherical 5-designs is the same as that of finding maximal equiangular tight frames, and it is known that existence of a tight spherical 5-design in \mathbb{S}^{d-1} is possible only for $d = 1, 2, 3$ and for dimensions of the form $d = (2k + 1)^2 - 2$, where $k \geq 1$; see [6, 7, 25, 39] for details on how these conditions arise. A direct correspondence with such spherical designs and regular graphs has long been recognized [54], and, in connection, it is known that for infinitely many values of k , a tight spherical 5-design cannot exist in dimension $d = (2k + 1)^2 - 2$ [9, 45].

d	N	M	Inner products	Name
d	2	1	± 1	two antipodal points
d	$d + 1$	2	$-1/d, 1$	regular simplex
d	$2d$	3	$0, \pm 1$	cross-polytope
2	N	$N - 1$	$\cos(2j\pi/N), 0 \leq j \leq N/2$	regular N -gon
3	12	5	$\pm 1/\sqrt{5}, \pm 1$	icosahedron
4	120	11	$0, (\pm 1 \pm \sqrt{5})/4, \pm 1/2, \pm 1$	600-cell
6	27	4	$-1/2, 1/4, 1$	Schläfli config.
7	56	5	$\pm 1/3, \pm 1$	kissing configuration for E_8
8	240	7	$0, \pm 1/2, \pm 1$	E_8 root system
22	275	4	$-1/4, 1/6, 1$	McLaughlin configuration
23	552	5	$\pm 1/5, \pm 1$	equiangular lines
23	4600	7	$0, \pm 1/3, \pm 1$	kissing configuration for Λ_{24}
24	196560	11	$0, \pm \frac{1}{4}, \pm \frac{1}{2}, \pm 1$	Leech lattice Λ_{24} minimal vectors

Table 1. A list of known tight spherical designs (with the 600-cell). Here M denotes the strength of the design, d the dimension of the ambient space \mathbb{R}^d , and N is the size of the design.

Table 2 lists all known tight projective designs (see [22]), except those for the spaces $\mathbb{F}\mathbb{P}^1$, which are congruent to real spheres. Identifying tight projective designs is simple in the real setting. Tight spherical designs of odd strength must be centrally symmetric [25], and by choosing points from each antipode in an odd tight design, one arrives at a real projective tight design. Thus, all tight designs of odd strength in Table 1 correspond to entries in Table 2.

For the other projective spaces, the vertices of a cross-polytope (i.e., an orthonormal basis in the projective space) always provide a tight 1-design, as they did in $\mathbb{R}\mathbb{P}^{d-1}$. However, unlike the real case, it is known that no tight t -designs exist in the complex or quaternionic setting whenever $M \geq 4$ and $d \geq 3$, [8, 33, 44]. In the complex setting, tight 2-designs, also known as *symmetric, informationally complete, positive operator-valued measures (SIC-POVMs)*, are known to exist for $d \leq 16$, $d = 19, 24, 28, 35, 48$, and numerical experiments suggest that they may exist in every dimension [3, 49, 53, 67]. With the exception of the (3, 15) quaternionic and (3, 27) octonionic designs from [22], explicit constructions are readily found in [32] for the other designs mentioned in Table 2.

d	N	M	$ (x, y) ^2$	\mathbb{F}	Name
d	$d + 1$	1	0, 1	\mathbb{R}	cross-polytope/ONB
2	N	$N - 1$	$\cos^2(\pi j/N), 1 \leq j \leq N$	\mathbb{R}	regular $2N$ -gon
3	6	2	1/5, 1	\mathbb{R}	icosahedron
7	28	2	1/9, 1	\mathbb{R}	kissing configuration for E_8
8	120	3	0, 1/4, 1	\mathbb{R}	roots of E_8 lattice
23	276	2	1/25, 1	\mathbb{R}	equiangular lines
23	2300	3	0, 1/9, 1	\mathbb{R}	kissing configuration for Λ_{24}
24	98280	5	0, 1/16, 1/4, 1	\mathbb{R}	minimal vectors of Λ_{24}
d	$d + 1$	1	0, 1	\mathbb{C}	cross-polytope/ONB
d	d^2	2	$1/(d + 1), 1$	\mathbb{C}	SIC-POVM
4	40	3	0, 1/3, 1	\mathbb{C}	Eisenstein structure on E_8
6	126	3	0, 1/4, 1	\mathbb{C}	Eisenstein structure on K_{12}
d	$d + 1$	1	0, 1	\mathbb{H}	cross-polytope/ONB
3	15	2	2/7, 1	\mathbb{H}	equiangular lines
5	165	3	0, 1/4, 1	\mathbb{H}	quaternionic reflection group
3	$d + 1$	1	0, 1	\mathbb{O}	cross-polytope/ONB
3	27	2	2/13, 1	\mathbb{O}	equiangular lines
3	819	5	0, 1/4, 1/2, 1	\mathbb{O}	generalized hexagon of order (2, 8)

Table 2. A list of parameters for which projective tight designs are known to exist (besides designs in $\mathbb{F}\mathbb{P}^1$ for $\mathbb{F} \neq \mathbb{R}$). Here M denotes the strength of the design, d the dimension of the ambient space \mathbb{F}^d , and N is the size of the design. For SIC-POVMs, these configurations exist for certain values of d , and may or may not exist for all values.

A weaker property of a design is sharpness, which will not play a role here. The paper [21] proves that sharp designs, and tight designs in particular, are minimizers for discrete minimization problems with absolutely monotone kernels. A similar approach allows us to show that tight designs are optimal for the continuous p -frame energy.

2.4. Antipodal symmetry

We observe that the energy I_f on the sphere $\mathbb{S}_{\mathbb{F}}^{d-1}$, $\mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}$, for the kernels f with $f(\langle x, y \rangle) = f(|\langle x, y \rangle|)$ remains the same after averaging over unit multiples of vectors in the support of μ . Let $U(\mathbb{F})$ be the set of units in \mathbb{F} , $U(\mathbb{F}) = \{c \in \mathbb{F} : |c| = 1\}$, and let η be the uniform measure on $U(\mathbb{F})$. If one defines, for a positive Borel measure μ on the sphere $\mathbb{S}_{\mathbb{F}}^{d-1}$ and Borel sets $B \subset \mathbb{S}_{\mathbb{F}}^{d-1}$,

$$v(B) = \frac{1}{\eta(U(\mathbb{F}))} \int_{U(\mathbb{F})} \mu(cB) d\eta(c),$$

then $I_f(v) = I_f(\mu)$ for potential functions f as above. This is the primary reason it is natural to consider projective spaces $\mathbb{F}\mathbb{P}^{d-1}$ as the optimization spaces for p -frame energies, as opposed to the spheres, in the cases when the elements $x \in \mathbb{F}\mathbb{P}^{d-1}$ may be represented by unit vectors in \mathbb{F}^d .

This discussion shows that a minimizing measure on the sphere for I_f , with f as above, can be taken to be symmetric, and that the problem of minimizing over symmetric measures on spheres is equivalent to minimizing energy over projective spaces. In particular, this explains part (i) of Theorem 1.1, since tight spherical $(2M + 1)$ -designs are necessarily symmetric [25] and hence correspond to tight real projective M -designs.

3. Optimality of tight designs for kernels absolutely monotonic to degree M

3.1. Linear programming

The main goal of this section is to show that for those dimensions and values of t for which tight designs exist, they are the global minimizers of the p -frame energies for intervals of p between consecutive even integers. We will use linear programming bounds to this end.

The linear programming method provides bounds for optima in various optimization problems, and its use is often aided by computational tools, where a problem is approximated by a finite-dimensional or discretized counterpart, then solved with a computer. It is surprising that this simple method often provides optimal bounds. This technique applies to all the 2-point homogeneous spaces Ω described above.

Our application of the method can be summed up in the following lemma, which is a measure-theoretic counterpart of the linear programming bound of Delsarte and Yudin, see [24, 65].

Lemma 3.1. *Let $h \in C[-1, 1]$ be a positive-definite function, i.e., $h(t) = \sum_{n=0}^{\infty} \hat{h}_n C_n(t)$ and $\hat{h}_n \geq 0$ for all $n \geq 0$.*

- (i) *Assume that $h(t) \leq f(t)$ for all $t \in [-1, 1]$. Then for any $\mu \in \mathcal{P}(\Omega)$,*

$$I_f(\mu) \geq \hat{h}_0 = I_h(\sigma).$$

- (ii) Assume further that h is a polynomial of degree k and that there exists a k -design $\mathcal{C} \subset \Omega$ such that $h(t) = f(t)$ for each $t \in \{\tau(x, y) : x, y \in \mathcal{C}\}$. Then for any $\mu \in \mathcal{P}(\Omega)$,

$$I_f(\mu) \geq I_f\left(\frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x\right),$$

i.e., I_f is minimized by the uniform distribution on \mathcal{C} .

Proof. For the first part, observe that

$$I_f(\mu) \geq I_h(\mu) \geq I_h(\sigma) = \hat{h}_0,$$

where the first inequality follows from the fact that $f \geq h$, while the second one is due to Proposition 2.3, since h is positive definite.

For the second part, one can continue as follows:

$$I_h(\sigma) = I_h\left(\frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x\right) = I_f\left(\frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x\right).$$

The first equality follows from the fact that \mathcal{C} is a k -design, and the second one from the fact that f and h coincide on the set $\{\tau(x, y) : x, y \in \mathcal{C}\}$. Together with part (i), this proves the statement in part (ii). ■

This lemma provides insights in two different ways for how the linear programming method can be applied.

If a candidate \mathcal{C} is available, one can apply part (ii) of Lemma 3.1 by constructing a polynomial $h \leq f$ as a Hermite interpolant of the function f at the points of $\{\tau(x, y) : x, y \in \mathcal{C}\}$. This reasoning, which lies behind the proof of Theorems 3.7 and 1.1, explains the appearance of tight designs: indeed, the number of elements in the set of interpolation points (i.e., distinct distances between the points of \mathcal{C}) determines the degree of the interpolant h – hence one wants a design of high strength, but with few mutual distances.

The same reasoning as above applies to the emergence of sharp designs as universally optimal sets in [21], and it also explains why this slightly weaker notion does not suffice for our purposes: since we are working with general measures rather than point sets with fixed cardinality, we cannot avoid interpolating at the point $t = 1$, which requires a design of higher strength. The main technical difficulty in this setting is proving positive definiteness of the Hermite interpolating polynomial h . We take this approach to Theorem 3.7 and carry out the technicalities in Sections 3.2–3.4.

If a suitable candidate is not available, one can still rely on part (i) of Lemma 3.1 and attempt to optimize the value of the energy $I_h(\sigma)$ over auxiliary positive definite polynomials h , obtaining a lower bound for the energy over all probability measures. If the degree of an auxiliary function h is bounded by D , we have $D + 1$ non-negative variables $\hat{h}_i, 0 \leq i \leq D$, and infinitely many linear constraints $h(t) \leq f(t)$ for all $t \in [-1, 1]$. In order to get the best possible lower bound, we need to maximize \hat{h}_0 given these linear conditions.

3.2. Properties of orthogonal polynomials

Recall that, for fixed Ω , we write simply $C_n(t) = C_n^{(\alpha,\beta)}(t)$ with $C_n(1) = 1$. In some of the arguments in Section 3.4 we will instead use the monic polynomials proportional to C_n ; we therefore introduce notation $Q_n(t) = Q_n^{(\alpha,\beta)}(t)$ for these Jacobi polynomials.

In this subsection we collect several results about orthogonal polynomials relevant to the proof of our main theorem. Fix a space Ω , and let α and β be the corresponding parameters of the associated Jacobi polynomials. According to Proposition 2.3, a function being positive definite on Ω is equivalent to having positive coefficients in the Jacobi expansion in terms $Q_n^{(\alpha,\beta)}$.

It will be useful to consider *adjacent* Jacobi polynomials, defined as one of the three sequences $Q_n^{k,l} = Q_n^{(\alpha+k,\beta+l)}$ with $k, l \in \{0, 1\}$, $k + l > 0$. Specifically, we will need the following corollary, which comes out of representing $Q_n^{1,0}$ through $Q_n^{0,0}$ (see equation (3.4) in [40]):

Proposition 3.2. *Adjacent Jacobi polynomials $Q_n^{1,0}$ are positive definite on Ω .*

On the other hand, adjacent polynomials $Q_n^{1,1}$, defined as orthogonal with respect to the measure $(1 - t^2) d\nu^{(\alpha,\beta)}$, are not positive definite. The following property, a special case of the strengthened Krein condition [41], Lemma 3.22, can serve as a substitute.

Lemma 3.3. *$(t + 1)Q_n^{1,1}(t)$ are positive definite on Ω for $n \geq 0$.*

Proof. For all $n \in \mathbb{N}_0$, $(t + 1)Q_n^{1,1}$ is orthogonal to all polynomials of degree less than n with respect to the measure $(1 - t) d\nu^{(\alpha,\beta)} = c_{\alpha,\beta} d\nu^{(\alpha+1,\beta)}$, so it can be expressed through the orthogonal polynomials corresponding to $d\nu^{(\alpha+1,\beta)}$ as

$$(t + 1)Q_n^{1,1}(t) = Q_{n+1}^{1,0}(t) + bQ_n^{1,0}(t),$$

for some constant b . Since all the roots of $Q_n^{1,0}$ lie in $(-1, 1)$, $\text{sgn } Q_n^{1,0}(-1) = (-1)^n$. Substituting $t = -1$ in the last equation gives $Q_{n+1}^{1,0}(-1) + bQ_n^{1,0}(-1) = 0$, and so $b \geq 0$. By Proposition 3.2, each $Q_n^{1,0}(t)$ is positive definite, and thus $(t + 1)Q_n^{1,1}(t)$ is also positive definite. ■

Lastly, we will need the strict positive-definiteness of polynomials annihilated by subsets of roots of $p_n + \gamma p_{n-1}$. We recall the following result.

Proposition 3.4 ([21], Theorem 3.1). *Consider a sequence of orthogonal monic polynomials $p_0(t), p_1(t), p_2(t), \dots$, such that $\deg p_k = k$ for all $k \in \mathbb{N}_0$, and let $t_1 < \dots < t_n$ be the zeros of $p_n + \gamma p_{n-1}$ for some fixed γ . Then the polynomials*

$$\prod_{i=1}^k (t - t_i), \quad 1 \leq k < n,$$

can be represented as a linear combination of $p_0(t), p_1(t), \dots, p_n(t)$ with positive coefficients.

3.3. Hermite interpolation

Let $f \in C^K[a, b]$, for some $K \in \mathbb{N}_0$, and let one be given a collection $t_1 < \dots < t_m \subset [a, b]$, as well as positive integers k_1, \dots, k_m with

$$\max\{k_1, \dots, k_m\} \leq K + 1.$$

There exists a polynomial p of degree less than $D = \sum_{i=1}^m k_i$, such that for $1 \leq i \leq m$ and $0 \leq k < k_i$,

$$p^{(k)}(t_i) = f^{(k)}(t_i).$$

Such a p is called the *Hermite interpolating polynomial* of f ; it always exists and is unique because the linear map that takes a polynomial p of degree less than D to

$$(p(t_1), p'(t_1), \dots, p^{(k_1-1)}(t_1), p(t_2), p'(t_2), \dots, p^{(k_m-1)}(t_m))$$

is bijective.

It is convenient to organize both the collection $t_1 < \dots < t_m$ and the orders of derivatives k_1, \dots, k_m into a polynomial $g(t)$. Given such a polynomial

$$g(t) = \prod_{i=1}^m (t - t_i)^{k_i},$$

where $D = \deg(g) \geq 1$, we write $H[f, g]$ for the interpolating polynomial of degree less than D that agrees with f at each t_i to the order k_i . Similarly, we let

$$Q[f, g](t) = \frac{f(t) - H[f, g](t)}{g(t)}$$

be the *divided difference* associated with the polynomial g . Under the above hypotheses, for every $t \in [a, b]$ and a collection $t_1 < t_2 < \dots < t_m$ as above, there exists $\xi \in (a, b)$ such that $\min(t, t_1) < \xi < \max(t, t_m)$, and

$$(3.1) \quad Q[f, g](t) = \frac{f^{(D)}(\xi)}{D!}.$$

Enumerate the roots of g with multiplicities in increasing order, and denote these by s_j , $1 \leq j \leq D$, where $s_j \leq s_{j+1}$. Let g_n be the polynomial annihilated on the first n elements of the sequence s_1, \dots, s_D :

$$g_n(t) = \prod_{j=1}^n (t - s_j), \quad 1 \leq n \leq D.$$

The usual assignment of the empty product applies here: $g_0(t) = 1$.

By Newton's formula, see [26], Chapter 4.6-7, the Hermite interpolating polynomial $H[f, g]$ can be represented as

$$(3.2) \quad H[f, g](t) = f(s_1) + \sum_{j=1}^{D-1} g_j(t) Q[f, g_j](s_{j+1}).$$

The relevant property of the p -frame kernel $(\frac{s+1}{2})^{p/2}$ considered on a projective space $\mathbb{F}P^{d-1}$ (for $\mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}$), is that its first several derivatives are nonnegative on $(-1, 1)$, followed by a negative one. The positivity of the derivatives implies, due to (3.1), that the

divided differences in formula (3.2) for the p -frame kernel are nonnegative. It will be convenient to introduce notation for this number of nonnegative derivatives of a function.

Definition 3.5. Let $f \in C^M(a, b)$. We say that f is *absolutely monotonic of degree M* if $f^{(k)}(t) \geq 0$ for $0 \leq k \leq M$ and $t \in (a, b)$. If these derivatives are positive, we say that f is *strictly absolutely monotonic of degree M* .

The usefulness of this new class of functions lies in that the Hermite interpolant of an absolutely monotonic function f of degree M with $(M + 1)$ st derivative negative, will stay below f , as shown in the following observation [65].

Lemma 3.6. Let $f : [-1, 1] \rightarrow \mathbb{R}$ be absolutely monotonic of degree M , with $f^{(M+1)}(t) \leq 0$ for all $t \in (-1, 1)$. If the roots of a polynomial g of degree $M + 1$ are contained in $[-1, 1]$, and in addition $g(t) \leq 0$ for $t \in [-1, 1]$, then

$$f(t) \geq H[f, g](t), \quad t \in [-1, 1].$$

Proof. According to (3.1), there exists $\xi \in (-1, 1)$ such that $\min(t, t_0) < \xi < \max(t, t_M)$, where the roots of g are $t_0 \leq \dots \leq t_M$, and

$$f(t) - H[f, g](t) = \frac{f^{(M+1)}(\xi)}{(M + 1)!} g(t).$$

The expression on the right is nonnegative, so the conclusion of the lemma follows. ■

3.4. Optimality of tight designs

As above, Ω is a compact, connected two-point homogeneous space and Q_0, Q_1, Q_2, \dots are the corresponding orthogonal polynomials. Recall that Q_n are orthogonal with respect to the measure $dv^{(\alpha, \beta)} = \frac{1}{\gamma_{\alpha, \beta}}(1 - t)^\alpha(1 + t)^\beta dt$, where the parameters α, β are chosen as in Section 2.1. The main result of this section is the following.

Theorem 3.7. Let f be absolutely monotonic of degree M , with $f^{(M+1)}(t) \leq 0$ for $t \in (-1, 1)$. Then for a tight M -design \mathcal{C} ,

$$\mu_{\mathcal{C}} = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of

$$I_f(\mu) = \int_{\Omega} \int_{\Omega} f(\tau(x, y)) d\mu(x) d\mu(y)$$

over $\mathcal{P}(\Omega)$, the set of probability measures on Ω .

First of all, we show that this statement implies part (ii) of Theorem 1.1.

Proof of part (ii) of Theorem 1.1. Recall that, according to (2.4), the p -frame energy on $\mathbb{S}_{\mathbb{F}}^{d-1}$ corresponds to the kernel $f(t) = (\frac{1+t}{2})^{p/2}$ in the projective setting $\Omega = \mathbb{F}\mathbb{P}^{d-1}$. One can easily check that $f^{(\lceil p/2 \rceil + 1)}(t) \leq 0, -1 < t < 1$, and that all derivatives of smaller order are nonnegative. Thus Theorem 3.7 applies with $M = \lceil p/2 \rceil$, i.e., tight projective

M -designs minimize I_f on $\mathbb{F}\mathbb{P}^{d-1}$ for $2M - 2 < p \leq M$ (the case $p = 2M - 2$ is easy, since f is a positive definite polynomial, so σ is a minimizer and hence so are tight designs). Transferring the problem back to the sphere $\mathbb{S}_{\mathbb{F}}^{d-1}$, as explained in Section 2.4, finishes the proof of part (ii) of Theorem 1.1. ■

In what follows we give a proof of Theorem 3.7, splitting it into two separate cases, depending on whether the design \mathcal{C} contains two points separated by the diameter of Ω ; equivalently, depending on the parity of the strength M of \mathcal{C} .

Proposition 3.8. *Theorem 3.7 holds when $M = 2m, m \geq 1$.*

Proof. Let $t_1 < \dots < t_m < t_{m+1} = 1$ be the values of $\tau(x, y) = \cos(\vartheta(x, y))$ occurring in \mathcal{C} . Let further

$$g_k(t) = \prod_{i=1}^k (t - t_i), \quad 1 \leq k \leq m + 1.$$

and

$$(3.3) \quad g(t) = g_m(t) g_{m+1}(t) = (t - 1) g_m^2(t).$$

To prove the statement of the theorem, we verify the following chain of inequalities, satisfied for arbitrary $\mu \in \mathcal{P}(\Omega)$, similar to the proof of Lemma 3.1:

$$(3.4) \quad I_f(\mu) \geq I_{H[f,g]}(\mu) \geq I_{H[f,g]}(\sigma) = I_{H[f,g]}(\mu_{\mathcal{C}}) = I_f(\mu_{\mathcal{C}}).$$

Since $g(t) \leq 0$ for $t \in [-1, 1]$, Lemma 3.6 implies that $f(t) \geq H[f, g](t), t \in [-1, 1]$, which gives the first inequality. The equality $I_{H[f,g]}(\sigma) = I_{H[f,g]}(\mu_{\mathcal{C}})$ is satisfied since \mathcal{C} is a design of strength $2m \geq \deg H[f, g]$. The last equality holds since the interpolant $H[f, g]$ agrees with f at the cosines of distances occurring in \mathcal{C} . All that remains to show is the second inequality: by Proposition 2.3, it will follow from the positive definiteness of $H[f, g]$, which we will now demonstrate.

For any $n < m$, the degree of $g_{m+1}(t)Q_n(t)$ is at most $2m$. As \mathcal{C} is a $2m$ -design, for every fixed $y \in \mathcal{C}$ there holds

$$\begin{aligned} \int_{-1}^1 g_{m+1}(t) Q_n(t) d\nu^{(\alpha,\beta)} &= \int_{\Omega} g_{m+1}(\tau(x, y)) Q_n(\tau(x, y)) d\sigma(x) \\ &= \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} g_{m+1}(\tau(x, y)) Q_n(\tau(x, y)) = \frac{1}{|\mathcal{C}|} \sum_{i=1}^{m+1} c_i g_{m+1}(t_i) Q_n(t_i) = 0, \end{aligned}$$

since, by construction, g_{m+1} is annihilated on all the t_i . The constants c_i are given by, for any fixed $y \in \mathcal{C}$,

$$c_i = |\{x \in \mathcal{C} \mid \tau(x, y) = t_i\}|.$$

Both g_{m+1} and Q_{m+1} are monic, so we conclude that

$$g_{m+1}(t) = Q_{m+1}(t) + \gamma Q_m(t),$$

for some $\gamma \in \mathbb{R}$. By Proposition 3.4, subproducts of zeros of g_{m+1} , which we denote by $g_k, 1 \leq k \leq m$, can be expressed as linear combinations of Q_n with positive coefficients, and therefore are positive definite.

According to the Newton formula (3.2), the Hermite interpolant of f can be expressed as the sum of partial products of factors of g multiplied by the appropriate divided difference. We will use this formula to show that $H[f, g]$ is positive definite. Indeed, (3.2) gives

$$(3.5) \quad H[f, g](t) = f(t_1) + \sum_{k=1}^m (g_k(t)g_{k-1}(t) Q[f, g_k g_{k-1}](t_k) + g_k^2(t) Q[f, g_k^2](t_{k+1})),$$

where as usual, $g_0 = 1$. Observe that the divided differences in the last equation are non-negative due to (3.1), as the function f is absolutely monotonic of degree $2m$. Since we have shown that each g_k is positive definite, Schur’s theorem implies that so are g_k^2 and $g_k g_{k-1}$, and it follows that $H[f, g]$ is positive definite as well. ■

Before turning to the proof of Theorem 3.7 for tight designs of odd strength, recall the definition of the adjacent polynomials $Q_n^{1,1} = Q_n^{(\alpha+1, \beta+1)}$ for $n \geq 0$. They are monic, orthogonal with respect to the measure

$$d\nu^{(\alpha+1, \beta+1)}(t) = \frac{1}{\gamma_{\alpha+1, \beta+1}} (1-t)^{\alpha+1} (1+t)^{\beta+1} dt = \frac{\gamma_{\alpha, \beta}}{\gamma_{\alpha+1, \beta+1}} (1-t^2) d\nu^{(\alpha, \beta)}(t),$$

since the polynomials $Q_n^{(\alpha, \beta)}(t)$ are orthogonal with respect to measure $d\nu^{(\alpha, \beta)}$.

Proposition 3.9. *Theorem 3.7 holds when $M = 2m - 1$, $m \geq 1$.*

Proof. Suppose that $\mathcal{C} \subset \Omega$ is a tight $(2m - 1)$ -design. As discussed in Section 2.3, tight designs of odd strength necessarily contain antipodal points, i.e., there exist $x, y \in \mathcal{C}$ such that $\vartheta(x, y) = \pi$ and thus $-1 \in \mathcal{A}(\mathcal{C}) = \{\tau(x, y) \mid x, y \in \mathcal{C}\}$. Let $-1 = t_1 < \dots < t_m < t_{m+1} = 1$ be the values of $\tau(\vartheta(x, y))$ for $x, y \in \mathcal{C}$, and set

$$(3.6) \quad w(t) = \prod_{j=2}^m (t - t_j) \quad \text{and} \quad g(t) = w^2(t)(t^2 - 1).$$

As in the proof of Proposition 3.8, we need to verify the inequalities (3.4). Applying Lemma 3.6 to $H[f, g]$ gives the first inequality; it remains to show positive-definiteness of $H[f, g]$.

For $n < m - 1$, the degree of $(1 - t^2)w(t)Q_n^{1,1}(t)$ is at most $2m - 1$, so for any $y \in \mathcal{C}$ there holds

$$\begin{aligned} & \frac{\gamma_{\alpha+1, \beta+1}}{\gamma_{\alpha, \beta}} \int_{-1}^1 w(t) Q_n^{1,1}(t) d\nu^{(\alpha+1, \beta+1)} \\ &= \int_{\Omega} (1 - \tau^2(x, y)) w(\tau(x, y)) Q_n^{1,1}(\tau(x, y)) d\sigma(x) \\ &= \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} (1 - \tau^2(x, y)) w(\tau(x, y)) Q_n^{1,1}(\tau(x, y)) \\ &= \frac{1}{|\mathcal{C}|} \sum_{j=1}^{m+1} c_j (1 - t_j^2) w(t_j) Q_n^{1,1}(t_j) = 0, \end{aligned}$$

as $(1 - t^2)w(t)$ is annihilated on the cosines of distances from \mathcal{C} . Because $w(t)$ is a degree $m - 1$ monic polynomial, the above implies $w(t) = Q_{m-1}^{1,1}(t)$. By Proposition 3.4, this also means that for $2 \leq k \leq m - 1$, the polynomials $\prod_{j=2}^k (t - t_j)$ are linear combinations of $Q_n^{1,1}$ with nonnegative coefficients. Since the cone of functions with nonnegative Jacobi coefficients with respect to $Q_n^{1,1}$ is closed under multiplication, the polynomials $\prod_{j=2}^k (t - t_j)^2$ and $(t - t_k) \prod_{j=2}^{k-1} (t - t_j)^2$ also have nonnegative Jacobi coefficients in $Q_n^{1,1}$. Due to Lemma 3.3, since $t - t_1 = t + 1$, we obtain that

$$(3.7) \quad a_k(t) := (t - t_1)(t - t_l) \prod_{j=2}^{k-1} (t - t_j)^2 \quad \text{and} \quad b_k(t) := (t - t_1) \prod_{j=2}^k (t - t_j)^2$$

are linear combinations of $Q_n^{(\alpha,\beta)}$ with positive coefficients, that is, they are positive definite on Ω for $1 \leq k \leq m$.

We conclude by the same observations as in the proof of Proposition 3.8; in particular, the positive definiteness of the Hermite interpolant $H[f, g]$ follows from the representation

$$(3.8) \quad H[f, g](t) = f(t_1) + b_1(t) Q[f, b_1](t_2) + \sum_{k=2}^m (a_k(t) Q[f, a_k](t_k) + b_k(t) Q[f, b_k](t_{k+1})),$$

combined with the absolute monotonicity of f to degree $2m - 1$, which implies positivity of the divided differences Q . ■

3.5. Uniqueness of minimizers supported on tight designs

The proofs in the last section left the question of uniqueness of minimizers open. Are there any other minimizers for p -frame energies when tight designs minimize and p is not an even integer? The answer, as this section details, is no.

In general, whenever a tight design minimizes I_f for some kernel f that is strictly absolutely monotonic of degree M and which satisfies $f^{(M+1)}(t) < 0, t \in (-1, 1)$, the energy is minimized only by a tight design, although such designs are not necessarily unique up to equivalence, as mentioned in Section 2.3. Before stating our result in full, we introduce a couple standard lemmas (in slightly simplified form adapted to our needs).

Let N_M denote the cardinality of a tight M -design in Ω or, more precisely, the linear programming lower bound on the cardinality of M -designs [25, 32], which is well-defined even if tight M -designs do not exist and coincides with the cardinality of a tight design when they do. In fact, tight designs are often equivalently defined in terms of this quantity.

The first lemma, which can be found in [41], Theorem 4.4, states that tight designs have the smallest cardinality among all *weighted* designs of given strength.

Lemma 3.10. *Let (\mathcal{B}, w) be a weighted M -design in Ω . Then $|\mathcal{B}| \geq N_M$, and equality holds if and only if $w(x) = 1/|\mathcal{B}|$ for all $x \in \mathcal{B}$ and \mathcal{B} is a tight M -design.*

The second lemma shows that tight designs have the largest cardinality among all sets with a given number of distinct distances.

Lemma 3.11. *Let $\mathcal{B} \subset \Omega$ be an m -distance set, i.e., $|\mathcal{A}(\mathcal{B})| = m$. Then $|\mathcal{B}| \leq N_{2m}$. Moreover, if \mathcal{B} is antipodal (contains a pair of points diameter apart), then $|\mathcal{B}| \leq N_{2m-1}$.*

This lemma was proved in [25] for the sphere, and in [32] for projective spaces. We are now ready for the uniqueness result.

Theorem 3.12. *Suppose that a tight M -design \mathcal{C} minimizes the f -energy integral, for f strictly absolutely monotonic of degree M and such that $f^{(M+1)}(t) < 0$, $t \in (-1, 1)$. Then any minimizer of I_f must be a tight M -design.*

Proof. The argument developed to prove Theorem 3.7 may be described concisely through the following string of inequalities:

$$I_f(\mu) \geq I_{H[f,g]}(\mu) \geq I_{H[f,g]}(\sigma) = I_{H[f,g]}(\mu_{\mathcal{C}}) = I_f(\mu_{\mathcal{C}}),$$

where g is of the form (3.3) or (3.6), as is appropriate. In order for $I_f(\mu) = I_f(\mu_{\mathcal{C}})$ to hold, the inequalities must be equalities. The first inequality can only be an equality in the case that $\mathcal{A}(\text{supp}(\mu)) \subseteq \mathcal{A}(\mathcal{C})$. This follows from the fact that $H[f, g](t) < f(t)$ for all $t \notin \mathcal{A}(\mathcal{C})$ by the remainder formula from Lemma 3.6. In particular, this shows that $|\text{supp}(\mu)|$ is finite. Moreover, Lemma 3.11 then guarantees that $|\text{supp}(\mu)| \leq N_M = |\mathcal{C}|$, since N_M is increasing with M .

Now assume that the second inequality above is an equality. We first note that since f is strictly absolutely monotonic of degree M , $f(t_1) \geq 0$, and the divided differences appearing in (3.5) or (3.8) are all positive due to (3.1). Thus, $H[f, g]$ is a linear combination (possibly modulo a constant), with positive coefficients, of positive definite polynomials of degrees $1, \dots, M$, so $H[f, g] = a_0 + \sum_{j=1}^M a_j C_j$, where $a_j > 0$ for $j > 1$ and $a_0 \geq 0$. We see that μ must then be a weighted M -design, and due to Lemma 3.10, we have $|\text{supp}(\mu)| \geq N_M = |\mathcal{C}|$.

Therefore, $|\text{supp}(\mu)| = N_M = |\mathcal{C}|$, and the second part of Lemma 3.10 implies that $\text{supp}(\mu)$ is a tight M -design and μ has equal weights. ■

4. Optimality of the 600-cell

This section concerns only the p -frame kernels; it will be shown here that the 600-cell minimizes the p -frame energy on \mathbb{S}^3 for a certain range of p . The 600-cell is one of the six 4-dimensional convex regular polytopes; it has 600 tetrahedral faces, which explains the origin of its name. When its 120 vertices are identified with unit quaternions, they give a representation of the elements of a group known as the binary icosahedral group [57].

As discussed above (2.4), optimization of p -frame energy on the sphere \mathbb{S}^3 is equivalent to optimization of the expression $\iint_{(\mathbb{R}\mathbb{P}^3)_2} f(\tau(x, y)) d\mu(x) d\mu(y)$ over measures μ on $\mathbb{R}\mathbb{P}^3$, where the kernel f is given by

$$f(t) = \left(\frac{1+t}{2}\right)^{p/2}.$$

We therefore assume for the rest of this section the underlying space to be $\mathbb{R}\mathbb{P}^3$, and use the corresponding Jacobi polynomials $C_n^{(-1/2, 1/2)}(t)$. Following the approach of the previous section, we will establish a sequence of inequalities similar to (3.4).

The 600-cell is only a projective 5-design and therefore not tight. The authors in [21], motivated by an approach found in the paper [1], found means to prove universal optimality of the 600-cell by using a higher degree interpolating polynomial. The 600-cell has the notable property that the 7th, 8th, and 9th degree harmonic averages over it vanish, although the 6th degree average does not. This allows for constructing a degree 8 polynomial h which is less than or equal to f , positive definite, and agrees with f at the distances appearing in the 600-cell, and which finally has the property that its 6th Jacobi coefficient vanishes.

For a polynomial h of the form

$$(4.1) \quad h = \sum_{n \in \{0, \dots, 8\}, n \neq 6} \hat{h}_n C_n^{(1/2, -1/2)}(t),$$

the coefficients \hat{h}_n can be uniquely determined as functions of p by setting

$$h(t_i) = f(t_i), \quad 1 \leq i \leq 5, \quad \text{and} \quad h'(t_i) = f'(t_i), \quad 2 \leq i \leq 4,$$

where $-1 = t_1 < t_2 < \dots < t_5 = 1$ are the values of $\tau(x, y)$ when vectors x, y vary over the vertices of the 600-cell, see the proof of Theorem 4.2 below. It turns out that for all $p \in [8, 10]$, $\hat{h}_n(p) \geq 0$ when $0 \leq n \leq 8, n \neq 6$. We apply a computer-assisted approach to verify this positivity; specifically, using interval arithmetic, we compute values of $\hat{h}_n(p)$ on a grid fine enough to guarantee that $\hat{h}_n(p) \geq 0$. The details of this computation are available in the auxiliary files of the arXiv submission of this paper. Even though the computations performed are carried out in finite floating point precision, interval arithmetic guarantees that the results of these computations lie in precisely defined intervals (using libraries [34, 50, 68]). The computer-assisted argument yields the following.

Lemma 4.1. *If $p \in [8, 10]$ and the polynomial h is constructed as above, the coefficients \hat{h}_n in the Jacobi expansion (4.1) satisfy $\hat{h}_n(p) \geq 0$.*

Using this fact, we show optimality of the 600-cell on the range $p \in [8, 10]$.

Theorem 4.2. *The 600-cell minimizes the p -frame energy for $p \in [8, 10]$ over Borel probability measures on S^3 or $\mathbb{R}P^3$.*

Proof. Let $f(t) = ((t + 1)/2)^{p/2}$ for some $8 < p < 10$, $t_1 = -1$, $t_2 = (-\sqrt{5} - 1)/4$, $t_3 = -1/2$, $t_4 = (\sqrt{5} - 1)/4$, and $t_5 = 1$. Let $h(t)$ be the 8th degree polynomial given by (4.1), such that $h(t_i) = p(t_i)$ for $1 \leq i \leq 5$, and $h'(t_i) = p'(t_i)$ for $2 \leq i \leq 4$. By Lemma 4.1, the coefficients \hat{h}_n are non-negative for $p \in [8, 10]$.

Let $p(t) = (t^2 - 1) \prod_{i=2}^4 (t - t_i)^2$ and $\tilde{h}(t) = H[f, p](t)$. Then we also have $\tilde{h}(t) = H[h, p](t)$. This gives

$$f(t) - \tilde{h}(t) = \frac{f^{(8)}(\xi)}{8!} p(t) \geq 0 \quad \text{and} \quad h(t) - \tilde{h}(t) = \frac{h^{(8)}(v)}{8!} p(t) \leq 0.$$

We thus have $f(t) - h(t) = f(t) - \tilde{h}(t) + \tilde{h}(t) - h(t) \geq 0$. Since $h(t)$ is positive definite and $\hat{h}_6 = 0$, for the 600-cell \mathcal{C}_{600} , we have the following sequence of inequalities:

$$I_f(\mu) \geq I_h(\mu) \geq I_h(\sigma) = I_h(\mu_{\mathcal{C}_{600}}) = I_f(\mu_{\mathcal{C}_{600}}),$$

implying that equally weighted vertices of \mathcal{C}_{600} minimize p -frame energy. ■

5. p -frame energies in non-compact spaces

In the previous sections, we used linear programs to bound energies on compact two-point homogeneous spaces. This approach can be extended to p -frame energies in non-compact spaces as well. Just as above, we consider $\mathbb{F} = \mathbb{R}, \mathbb{C},$ or \mathbb{H} . In this setting, we consider the set of probability measures $\mathcal{P}(\mathbb{F}^d)$ with the additional restriction

$$(5.1) \quad \int_{\mathbb{F}^d} |x|^2 d\mu(x) = 1$$

for each $\mu \in \mathcal{P}(\mathbb{F}^d)$. This normalization allows us to obtain a direct extension of above results for the spherical case, and by scaling, solutions to more general problems can be obtained from these results. A similar problem of finding maximizers for p -frame energies for $p \leq 2$, subject to the condition that measures be isotropic, was investigated in [31].

For a potential function $f = f(\tau(x, y)) = f(2|\langle x, y \rangle|^2 - 1)$, we define the energy with respect to a measure $\mu \in \mathcal{P}(\mathbb{F}^d)$ as

$$I_f(\mu) = \int_{\mathbb{F}^d} \int_{\mathbb{F}^d} f(\tau(x, y)) d\mu(x) d\mu(y).$$

We will be concerned in this section only with the case that $f(\tau(x, y)) = |\langle x, y \rangle|^p$. The Jacobi polynomials for the projective spaces $\mathbb{F}\mathbb{P}^{d-1}$, as above, are denoted C_m .

Lemma 5.1. *For $p \geq 2$, assume $f(t) = (\frac{t+1}{2})^{p/2} \geq h(t) = \sum_{m=0}^{\infty} \hat{h}_m C_m(t)$ for all $t \in [-1, 1]$, where $\hat{h}_m \geq 0$ for all $m \geq 0$. Then $I_f(\mu) \geq \hat{h}_0$ for all $\mu \in \mathcal{P}(\mathbb{F}^d)$ satisfying (5.1).*

Proof. Since discrete masses are weak- $*$ dense in $\mathcal{P}(\mathbb{F}^d)$, it is sufficient to prove the inequality for them only. Let μ take the form $\mu = \frac{1}{N} \sum_{i=1}^N \delta_{x_i}$, $x_i \in \mathbb{F}^d$, and set $y_i = x_i/|x_i|$. (Note that if x_i is 0 then we can assign an arbitrary unit vector for y_i). Then,

$$\begin{aligned} I_f(\mu) &= \frac{1}{N^2} \sum_{i,j=1}^N |\langle x_i, x_j \rangle|^p = \frac{1}{N^2} \sum_{i,j=1}^N |x_i|^p |x_j|^p |\langle y_i, y_j \rangle|^p \\ &= \frac{1}{N^2} \sum_{i,j=1}^N |x_i|^p |x_j|^p f(\tau(y_i, y_j)) \geq \frac{1}{N^2} \sum_{i,j=1}^N |x_i|^p |x_j|^p h(\tau(y_i, y_j)) \\ &= \frac{1}{N^2} \sum_{m=0}^{\infty} \hat{h}_m \sum_{i,j=1}^N |x_i|^p |x_j|^p C_m(\tau(y_i, y_j)). \end{aligned}$$

For any $m \geq 1$, C_m is positive definite on $\mathbb{F}\mathbb{P}^{d-1}$, and so we have that each sum $\sum_{i,j=1}^N |x_i|^p |x_j|^p C_m(\tau(y_i, y_j))$ is non-negative. Thus,

$$I_f(\mu) \geq \hat{h}_0 \frac{1}{N^2} \sum_{i,j=1}^N |x_i|^p |x_j|^p C_0(\tau(y_i, y_j)) = \hat{h}_0 \left(\frac{1}{N} \sum_{i=1}^N |x_i|^p \right)^2.$$

Since $p \geq 2$,

$$\frac{1}{N} \sum_{i=1}^N |x_i|^p \geq \left(\frac{1}{N} \sum_{i=1}^N |x_i|^2 \right)^{p/2}$$

holds by Jensen’s inequality. The constraint 5.1 is equivalent to $\frac{1}{N} \sum_{i=1}^N |x_i|^2 = 1$, and by combining all inequalities, we complete the proof of the lemma. ■

Lemma 5.1 gives that any linear programming bounds for p -frame energies applicable to the spherical/projective case will work in the non-compact setting as well. As a consequence of this approach, we obtain the following result.

Theorem 5.2. *Let \mathcal{C} be a set of arbitrary unit representatives of a tight projective M -design, $M \geq 2$, in $\mathbb{F}\mathbb{P}^{d-1}$ and let $f(\tau(x, y)) = |\langle x, y \rangle|^p$ with $p \in [2M - 2, 2M]$. Then*

$$\mu_{\mathcal{C}} = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of

$$I_f(\mu) = \int_{\mathbb{F}^d} \int_{\mathbb{F}^d} f(\tau(x, y)) d\mu(x) d\mu(y)$$

over the set of probability measures on \mathbb{F}^d satisfying the constraint (5.1).

Proof. For the proof, we take $f(t) = (\frac{t+1}{2})^{p/2}$, h to be the interpolating polynomial $H[f, g]$ used in the proof of Theorem 3.7 or the h used in the proof of Theorem 4.2, and $h^*(x, y) = |x|^p |y|^p h(\tau(x/|x|, y/|y|))$ for all $x, y \in \mathbb{F}^d$. We follow the same line of reasoning as before to find

$$(5.2) \quad I_f(\mu) \geq I_{h^*}(\mu) \geq I_{h^*}(\sigma^*) = I_{h^*}(\mu_{\mathcal{C}}) = I_f(\mu_{\mathcal{C}}),$$

where σ^* is the uniform probability measure on the unit sphere in \mathbb{F}^d (and so projects to the Haar measure on $\mathbb{F}\mathbb{P}^{d-1}$).

All inequalities are verified in a similar manner as in the previous section, except for $I_{h^*}(\mu) \geq I_{h^*}(\sigma^*)$. This part follows from Lemma 5.1 applied to h^* because $I_{h^*}(\sigma^*) = I_h(\sigma)$ is precisely \hat{h}_0 for positive definite functions h . ■

Note: A similar result may be derived in the same manner as above for \mathcal{C} , a set of arbitrary unit representatives of the 600-cell in $\mathbb{R}\mathbb{P}^3$ and $p \in [8, 10]$, in light of Theorem 4.2.

6. Mixed volume inequalities

In this section we demonstrate an intriguing connection between the p -frame energy and convex geometry. We begin by briefly recalling some of the basic notions from convex geometry. See [35], Chapter 2, for a more thorough development.

Let K be a convex body and let $\sigma_K(u)$ be the surface measure of K , that is, a measure supported on the unit sphere S^{d-1} satisfying, for all Borel sets $B \subset S^{d-1}$,

$$\sigma_K(B) = |\{x \in \partial K, \text{ the outer unit normal to } K \text{ at } x \text{ belongs to } B\}|_{d-1},$$

where $|\cdot|_{d-1}$ denotes the $(d - 1)$ -dimensional Hausdorff measure.

For example, if K is a polytope with faces $\{K_i\}_{i=1}^m$ and normals $\{n_i\}_{i=1}^m$, σ_K is atomic with mass $|K_i|_{d-1}$ at each n_i ,

$$\sigma_K = \sum_{i=1}^m |K_i|_{d-1} \delta_{n_i},$$

and if $K = \mathbb{B}$ is the d -dimensional unit ball, then σ_K simply coincides with the standard (unnormalized) uniform surface area measure $\sigma_K(B) = |B|_{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)} \sigma(B)$.

Recall that for a convex body, $K \subset \mathbb{R}^d$, the *support function* $h_K(u)$ of K takes the form

$$h_K(u) = \sup_{v \in K} \langle u, v \rangle.$$

Given two convex bodies K and L , and $p \geq 1$, define

$$V_p(K, L) = \frac{p}{d} \lim_{\varepsilon \rightarrow 0} \frac{|K +_p \varepsilon L| - |K|}{\varepsilon},$$

where $K +_p \varepsilon L$ is the convex body with support function $h_{K+_p \varepsilon L}(u)$ satisfying

$$h_{K+_p \varepsilon L}(u)^p = h_K(u)^p + \varepsilon h_L(u)^p.$$

Note that for $L = \mathbb{B}_d$ is the unit ball and $p = 1$, the above quantity is just the definition of the surface area of K . In general, $V_p(K, L)$ is known as the L_p -mixed volume of K and L . The following alternative integral representation for $V_p(K, L)$ is known:

$$V_p(K, L) = \frac{1}{d} \int_{\mathbb{S}^{d-1}} h_L(u)^p d\sigma_K^p(u),$$

where $d\sigma_K^p(u) = h_K(u)^{1-p} d\sigma_K(u)$, so that in particular $d\sigma_K^1(u) = d\sigma_K(u)$.

Now, call a probability measure μ supported on \mathbb{S}^{d-1} *admissible* if it is symmetric and not concentrated on a subspace. A classical result, which follows from Minkowski's theorem, says that any admissible measure can be realized as the surface area measure of a symmetric convex body; see more in Chapter 7 of [51].

The *projection body* ΠK of a convex body K is defined to be a body such that for each $u \in \mathbb{S}^{d-1}$,

$$h_{\Pi K}(u) = |K|u^\perp|_{d-1},$$

that is, the support function of ΠK equals the volume of the projection of K onto the hyperplane orthogonal to u , [17]. Since

$$|K|u^\perp|_{d-1} = \frac{1}{2} \int_{\mathbb{S}^{d-1}} |\langle u, v \rangle| d\sigma_K(v),$$

the identities

$$\begin{aligned} I_{| \cdot |}(\sigma_K) &= \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} |\langle u, v \rangle| d\sigma_K(u) d\sigma_K(v) = 2 \int_{\mathbb{S}^{d-1}} |K|u^\perp|_{d-1} d\sigma_K(u) \\ &= 2 \int_{\mathbb{S}^{d-1}} h_{\Pi K}(u) d\sigma_K(u) = 2d V_1(K, \Pi K) \end{aligned}$$

finally establish the connection between L_1 -mixed volumes and 1-frame energies.

Our main theorem, Theorem 1.1, shows that all minimizers of $I_{|t|^p}(\mu)$ over probability measures are admissible when a corresponding tight design exists, as this measure is both discrete and can be taken to be symmetric. From this, we obtain what appears to be a new observation, namely the following.

Proposition 6.1. *The minimum of the quantity*

$$\frac{V_1(K, \Pi K)}{|\partial K|^2}$$

over all symmetric convex bodies in \mathbb{R}^d is achieved when K is a cube.

Indeed, it is easy to see that, when K is a cube, the surface measure σ_K is equally distributed on the vertices of a cross-polytope, which minimizes the p -frame energy for $p = 1$.

One may also define L^p -intersection bodies $\Pi_p K$, [42, 43], in a similar fashion and obtain analogous relations for $V_p(K, \Pi_p K)/|\partial K|^2$ for the several dimensions and ranges of p considered in this manuscript (for which tight designs exist), as well as pose conjectures corresponding to the numerically obtained minimizers. We anticipate, in particular, in accordance with Conjecture 1.3, that whenever p is not an even integer, this quantity is always minimized by a convex body which is polyhedral (with discrete surface measure).

7. Causal variational principle

We now turn to another application of the linear programming method. Define the kernel

$$(7.1) \quad F(t) = F_\tau(t) := \max\{0, 2\tau^2(1+t)(2-\tau^2(1-t))\}$$

for $\tau > 0$. The minimization problem for the energy

$$(7.2) \quad I_F(\mu) = \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} F(\langle x, y \rangle) d\mu(x) d\mu(y)$$

is known as the *causal variational principle* on the sphere and is connected to relativistic quantum field theory. It is conjectured in [28] that there exist discrete minimizers for $\tau \geq 1$ and, moreover, that all the minimizers of (7.2) are discrete whenever $\tau > \sqrt{2}$. The background on this problem can be found in [10, 28].

Here we confirm this conjecture for two values of $\tau > 0$, for which we can show that the cross-polytope (or orthoplex) and the icosahedron indeed minimize the energy, which was suggested by numerical experiments in [28]. The proofs are another application of the linear programming framework. In this instance, Hermite interpolation is unavailable to us as F is not differentiable on $(-1, 1)$. However, since we are dealing with a single kernel, instead of a class of them as in the previous section, we need only construct the correct auxiliary function.

We address the cross-polytope first. When $\tau = \sqrt{2}$, we have

$$F_\tau(t) = \max\{0, 8t^2 + 8t\},$$

and thus $F_\tau(0) = 0$. Setting the measure

$$\nu_{\text{cross}} = \frac{1}{6} \sum_{i=1}^3 (\delta_{e_i} + \delta_{-e_i}),$$

where $\{e_1, e_2, e_3\}$ is an orthonormal basis of \mathbb{R}^3 , i.e., ν_{cross} is a measure whose mass is equally concentrated in the vertices of a cross-polytope, we have the following.

Proposition 7.1. *The measure ν_{cross} is a minimizer for the energy $I_{F_{\sqrt{2}}}$ over $\mathbb{P}(\mathbb{S}^2)$.*

Proof. The function

$$h(t) = 8t^2 + 8t.$$

is positive definite on \mathbb{S}^2 (hence, I_h is minimized by σ) and clearly satisfies $h(t) \leq F_{\sqrt{2}}(t)$ for all $t \in [-1, 1]$, and $h(-1) = F_{\sqrt{2}}(-1) = 0, h(0) = F_{\sqrt{2}}(0) = 0, h(1) = F_{\sqrt{2}}(1) = 16$. so that $I_h(\nu_{\text{cross}}) = I_{F_{\sqrt{2}}}(\nu_{\text{cross}})$. Moreover, $I_h(\sigma) = I_h(\nu_{\text{cross}})$, since the cross-polytope is a 3-design. Therefore, for any measure $\mu \in \mathbb{P}(\mathbb{S}^2)$,

$$I_{F_{\sqrt{2}}}(\mu) \geq I_h(\mu) \geq I_h(\sigma) = I_h(\nu_{\text{cross}}) = I_{F_{\sqrt{2}}}(\nu_{\text{cross}}),$$

which finishes the proof. ■

We now focus on the case of the icosahedron. Here we set $\tau = \sqrt{2\sqrt{5}/(\sqrt{5}-1)}$ so that $F_\tau(1/\sqrt{5}) = 0$. Let $\mathcal{C} \subset \mathbb{S}^2$ consist of the vertices of a regular icosahedron and let $\nu_{\text{icos}} = \frac{1}{12} \sum_{x \in \mathcal{C}} \delta_x$ be the uniform measure on the vertices of the icosahedron.

Proposition 7.2. *The measure ν_{icos} minimizes the energy I_{F_τ} over $\mathbb{P}(\mathbb{S}^2)$ for $\tau = \sqrt{\frac{2\sqrt{5}}{\sqrt{5}-1}}$.*

Proof. The proof is almost identical to that of Proposition 7.1, except h is instead taken to be

$$\begin{aligned} h(t) &= \frac{5(5-\sqrt{5})}{32} t^4 + \frac{5}{8} t^3 + \frac{3\sqrt{5}-5}{16} t^2 - \frac{1}{8} t + \frac{1-\sqrt{5}}{32} \\ &= \frac{5-\sqrt{5}}{28} C_4(t) + \frac{1}{4} C_3(t) + \frac{20+3\sqrt{5}}{84} C_2(t) + \frac{1}{4} C_1(t) + \frac{1}{12} C_0(t), \end{aligned}$$

where C_k are the standard Legendre polynomials (i.e., the Gegenbauer polynomials $C_k^{1/2}$). One may verify that h is positive definite and satisfies $h(t) \leq F(t)$ for $-1 \leq t \leq 1$ with equality for $t \in \{\pm 1/\sqrt{5}, \pm 1\}$, so that $I_h(\nu_{\text{icos}}) = I_{F_\tau}(\nu_{\text{icos}})$. Since the icosahedron is a 5-design, the same argument as in the proof of Proposition 7.1 finally shows that

$$I_{F_\tau}(\nu_{\text{icos}}) = \inf_{\mu \in \mathbb{P}(\mathbb{S}^2)} I_{F_\tau}(\mu),$$

i.e., the icosahedron minimizes the energy I_{F_τ} for $\tau^2 = \frac{2\sqrt{5}}{\sqrt{5}-1}$. ■

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