ENERGY OPTIMIZATION ON THE SPHERE

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Abstract. In the present paper we discuss several issues connected by the common theme of optimizing energy integrals and discrete energy on the sphere. These include various versions, generalizations and applications of the Stolarsky identity, which relates optimal energy and discrepancy, Riesz-type energies based on geodesic distances, properties of minimizers of the p-frame energy, as well as a conjecture of Fejes Tóth on the sum of angles between lines.

1. Introduction

In the present paper we discuss optimization of some energy integrals and discrete energies on the unit sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$.

Let $\mathcal{B}$ and $\mathcal{M}$ denote the collection of all finite (signed) Borel measures and all Borel probability measures, respectively, on $\mathbb{S}^d$. Given a measure $\mu \in \mathcal{B}$, we define the energy integral $I_F(\mu)$ of a continuous function $F : [-1,1] \to \mathbb{R}$ by

$$I_F(\mu) := \int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} F(\langle x, y \rangle)\, d\mu(x)\, d\mu(y). \tag{1.1}$$

We are interested in finding the optimal (maximal or minimal, depending on F) values of $I_F(\mu)$ over $\mu \in \mathcal{M}$, as well as extremal measures μ for which these values are achieved, i.e. equilibrium distributions with respect to F.

A naturally related question is that of optimization of discrete energy. Consider a collection of N (not necessarily distinct) points $Z = \{z_1, \ldots, z_N\} \subset \mathbb{S}^d$. We define the discrete energy of Z with respect to F to be

$$E_F(Z) = \frac{1}{N^2} \sum_{i,j=1}^{N} F(\langle z_i, z_j \rangle). \tag{1.2}$$

Note that if $\mu = \frac{1}{N} \sum_{j=1}^{N} \delta_{z_j}$, then

$$E_F(Z) = I_F(\mu),$$

and due to the weak-* density of the linear span of Dirac masses in $\mathcal{M}$

$$\lim_{N\to\infty} \min_{\substack{Z \subset \mathbb{S}^d \\ \#Z = N}} E_F(Z) = \inf_{\mu \in \mathcal{M}} I_F(\mu). \tag{1.3}$$

Often one is interested in optimizing the discrete energy for a given N, analyzing extremal N-point configurations, comparing optimal values of the discrete energy to the optimal energy integral, and finding the asymptotic behavior of this difference. In the more general case of (bounded or non-negative) measureable functions $F : [-1,1] \to \mathbb{R} \cup \{\infty\}$, the diagonal terms $F(\langle z, z \rangle) = F(1)$ may not be defined and may have to be excluded from the sum.

Such problems arise naturally in various fields, e.g., in electrostatics, determining equilibrium distributions of charges which repel according to the law given by F. One of the most natural choices of the potential is the Riesz potential $F(\langle x, y \rangle) = ||x - y||^{-s}$, where $||x - y||$ is the Euclidean distance between x and y in $\mathbb{R}^{d+1}$. In the case that $d = 2$ and $s = 1$, minimization of the energy (1.2) (without the diagonal terms) is known as Thomson's problem and equates to finding the equilibrium distributions (according to Coulomb's Law) of N electrons on the sphere.

Let σ denote the standard (Lebesgue) uniform surface measure on the sphere, normalized so that $\sigma(\mathbb{S}^d) = 1$, i.e. $\sigma \in \mathcal{M}$. A natural question to ask is when σ, the normalized Lebesgue measure on $\mathbb{S}^d$, is a minimizer of I_F, and if so – whether it is unique. In plain words, this amounts to asking *whether minimizing energy imposes uniform distribution*. In section §2, we introduce Gegenbauer (ultraspherical) polynomials and discuss how minimizers of I_F relate to the Gegenbauer expansion of F. In particular, we show that σ is a minimizer if and only if F (modulo a constant) is positive definite on $\mathbb{S}^d$.

The problem of determining optimal discrete energy E_F for a fixed number N of points on the sphere is more delicate than finding optimal energy integral I_F. However, obviously, it is desirable to know minimizers of the energy integral in order to understand the distribution of optimal point sets for the discrete energy. In the case that σ is a minimizer of I_F, one might expect, according to (1.3), that as the number of points increases, minimizers of $E_F(Z)$ might be "uniformly distributed" in some sense, in order to approximate the Lebesgue measure. Discrepancy is a popular means of measuring uniformity of distribution of points on the sphere, and in §3, we show how it can be used to determine minimizers of I_F and E_F for positive definite functions F via a Generalized Stolarsky Principle. This section comes from previous work with Dmitriy Bilyk and Feng Dai [7].

In the remaining two sections, we deal with optimization problems that are noticeably different from many standard problems. In the vast majority of energy minimization problems, the potential $F(t)$ is maximized at $t = 1$ and minimized at $t = -1$, and often the potential is monotone (illustrated in Figure 1), as is the case for the Riesz potential. Interpreting points as electron and measures as charge distributions, this results in the strongest repulsion when the electrons are close to each other, and the weakest when they are far away. In this situation one often expects $E_F(Z)$ to be minimized by point configurations that are, in some sense, well distributed, perhaps maximizing the minimal distance between point or being a spherical design. Likewise, one would expect minimizers of $I_F(\mu)$ to spread out the charge, in some sense.

In §4 and §5, we deal with potentials that are even functions with $t = 0$ giving a minimum, illustrated in Figure 2. In these cases, the weakest repulsion occurs when two electrons are positioned orthogonally to each other. As a consequence, instead of expecting the charge to spread out, one might expect a certain amount of "orthogonality" to occur, although uniformity is still possible. Potential optimizers for such energies may include orthonormal bases, frames, or the uniform distribution σ, and well-distributed discrete sets, e.g. spherical designs. Technically speaking, a more appropriate setting for such problems would be the real projective space $\mathbb{RP}^d$, but we keep the current setup, i.e. $\mathbb{S}^d$, since it is more geometrically intuitive.

In §4, we discuss the p-frame potential, introduced by Ehler and Okoudjou in [23] as a generalization of the frame potential, which was used by Benedetto and Fickus in [5] to classify tight frames. We include new results found in collaboration with Dmitriy Bilyk, Alexey Glazyrin, Josiah Park, and Oleksandr Vlasuik [8]. Since this ongoing work has not been published yet (and even preprints do not yet exist), we include the proofs of our current results in this paper.

In §5, we discuss a conjecture of Fejes Tóth about the maximum sum of of acute angles of points on the sphere, and some of the new results in this direction obtained in collaboration with Dmitriy Bilyk [9].

In what follows, we can assume that $F \in C([-1, 1])$, unless stated otherwise, σ denotes the normalized Lebesgue surface measure on $\mathbb{S}^d$, i.e. $\sigma(\mathbb{S}^d) = 1$.

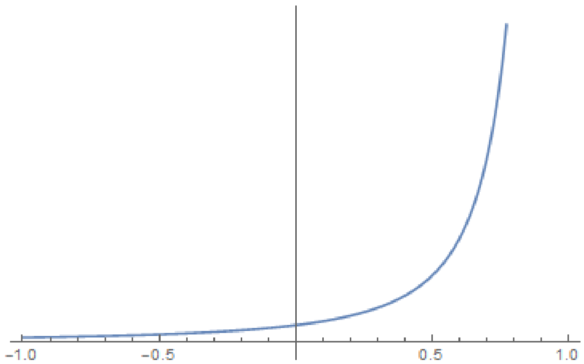

FIGURE 1. Graph of a "monotone potential"

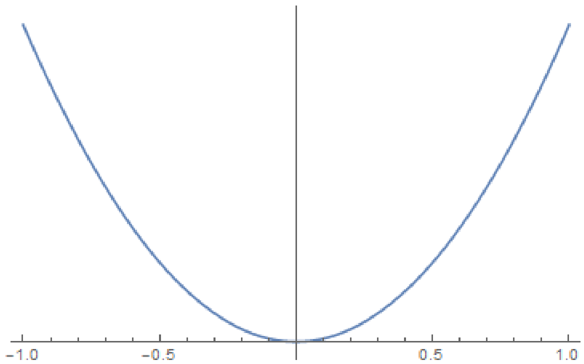

FIGURE 2. Graph of an "orthogonalizing potential"

1.1. **Ryan Matzke's work.** Since the current paper contains a number of preliminary and survey-style materials, we would like to emphasize the results that pertain directly to the author's work, which come from two published joint papers [7, 9] and a collaboration in progress [8], which will likely result in several papers. These results include a new simplified proof of the classical Stolarsky invariance principle (Theorem 3.1); generalized Stolarsky principle for positive definite kernels F (Theorem 3.2), characterizing measures maximizing the integral of the geodesic distance (Theorem 3.5, Corollary 3.6), as well as point configurations, which maximize the sum of geodesic distances (Theorem 3.9); characterizing maximizers of the Riesz-type energies with positive exponents based on geodesic distance (Theorem 3.7), a proof that tight designs are minimizers of the p-frame energy for appropriate ranges of p (Theorem 4.18), as well as a similar fact for the 600-cell modulo the positive definiteness of the interpolating polynomials, which has only been verified numerically (Proposition 4.19); a proof that the support of a minimizer of the p-frame energy, $p \notin 2\mathbb{N}$, has empty interior (Theorem 4.20); discreteness of minimizers for energies whose kernels have only finitely many positive Gegenbauer coefficients (Theorem 4.26); and the best known bound in the Fejes Tóth conjecture on the sum of angles between lines (Theorem 5.4) along with a new proof of the conjecture in the one-dimensional case (Theorem 5.3). The authorship of these results is clearly marked in the paper.

1.2. **Future directions.** All of the aforementioned research directions are very vital and ongoing. Perhaps, the most active is the work on the p-frame potentials, presented in §4. There are many components to this project, some of which, considering the recent breakthroughs may be quite within reach. One of the first problems along this lines is to prove the discreteness of minimizers of the p-frame potential, when p is not an even integer. More generally, one would like to understand for which potentials F the minimizers of the energy integral are necessarily discrete (or at least, for which F discrete minimizers exist). The next step is to understand the geometry of discrete minimizers: aside from the "tight designs" described in §4 there are no known configurations which are proven to be minimizers of the p-frame potential or other similar energies. There are however a number of putative candidates found mostly through computational experiments. We expect to prove minimality for these configurations and develop more general methods for finding minimizing configurations and proving their optimality. In particular, we strive to understand how one may "read" this information off of the function F or its Gegenbauer expansion. We also intend to explore the connections of the p-frame potential to other problems of discrete geometry, analysis, and approximation: e.g., the problem of mutually unbiased bases (MUBs), equiangular tight frames (ETFs), in particular, Zauner's conjecture. There are several current directions related to the material of §3: in particular, applying spectral theory to establish new versions of the Stolarsky principle on general metric spaces, finding new versions and applications of this principle as well as developing the theory of discrepancy and energy minimization on discrete spaces, such as the Hamming cube, graphs, etc. In addition, the author intends to write an extensive survey article (in collaboration with Bilyk and Skriganov) on various versions of the Stolarsky principle which have attracted considerable attention in the recent years. The author also plans to continue the work on Conjecture 5.1, as well as several other conjectures about point distributions and energy minimization on the sphere, which involve ideas from analysis, discrete and combinatorial geometry, and other areas of mathematics.

2. Gegenbauer Expansions and Positive Definite Kernels

In the present section we introduce some necessary background materials. We start by discussing Gegenbauer polynomials, spherical harmonics, and positive definite functions, as well as their connections to energy optimization. We also briefly discuss spherical designs.

2.1. **Gegenbauer polynomials.** Let $w_\lambda(t) = (1-t^2)^{\lambda-\frac{1}{2}}$ with $\lambda > 0$. Given $1 \le p < \infty$, we denote by $L^p_{w_\lambda}([-1,1])$ the space of all real integrable functions F on $[-1,1]$ with $\|F\|_{p,\lambda} := \left(\int_{-1}^1 |F(t)|^p w_\lambda(t)\,dt\right)^{1/p} < \infty$. Every function $F \in L^1_{w_\lambda}([-1,1])$ has a Gegenbauer (ultraspherical) polynomial expansion:

$$F(t) \sim \sum_{n=0}^{\infty} \widehat{F}(n;\lambda)\frac{n+\lambda}{\lambda}C_n^\lambda(t), \quad t\in[-1,1], \tag{2.1}$$

where C_n^λ are Gegenbauer polynomials and

$$\widehat{F}(n;\lambda) = \frac{\Gamma(\lambda+1)}{\Gamma(\lambda+\frac{1}{2})\Gamma(\frac{1}{2})C_n^\lambda(1)}\int_{-1}^{1} F(t)C_n^\lambda(t)w_\lambda(t)\,dt, \quad n\in\mathbb{N}_0.$$

For the rest of this paper, we use $\lambda = \frac{d-1}{2}$. Observe that this value corresponds to the weight w_λ which arises when integrating on $\mathbb{S}^d$ in cylindrical coordinates:

$$\int_{\mathbb{S}^d} F(\langle x,p\rangle)\,d\sigma(x) = \frac{\omega_{d-1}}{\omega_d}\int_{-1}^{1} F(t)(1-t^2)^{\frac{d-2}{2}}\,dt,$$

where p is an arbitrary pole on $\mathbb{S}^d$ and ω_d is the d-dimensional Lebesgue surface measure of $\mathbb{S}^d$.

In the special case $\lambda = 0$ (which corresponds to the circle $\mathbb{S}^1$) one obtains Chebyshev polynomials of the first kind, $T_n(t)$, which satisfy

$$\frac{1}{2}\lim_{\lambda\to 0}\frac{n+\lambda}{\lambda}C_n^\lambda(t) = T_n(t) = \cos\big(n\arccos t\big), \quad n\in\mathbb{N}.$$

Let $\{Y_{n,1},\cdots,Y_{n,a_n^d}\}$ denote a real orthonormal basis of $\mathcal{H}_n^d$, the space of all spherical harmonics of degree n on $\mathbb{S}^d$. The addition formula for spherical harmonics gives us ([22, 1.2.8])

$$\sum_{j=1}^{a_n^d} Y_{n,j}(x)Y_{n,j}(y) = \frac{n+\lambda}{\lambda}C_n^\lambda(\langle x,y\rangle) \quad \text{for all} \quad x,y\in\mathbb{S}^d, \tag{2.2}$$

with

$$a_n^d = \frac{n+\lambda}{\lambda}C_n^\lambda(1) = \dim\,\mathcal{H}_n^d = \binom{n+d}{n} - \binom{n+d-2}{n-2} = \frac{2n+d-1}{n+d-1}\binom{n+d-1}{d-1} \sim n^{d-1}.$$

When $F \in L^2_{w_\lambda}([-1,1])$, the series (2.1) naturally converges to F in the L^2 sense. However, more can be said in certain cases.

Lemma 2.1 (see, e.g. [6])**.** *Let $F \in C([-1,1])$ and assume that $\widehat{F}(n;\lambda) \geq 0$ for all $n \geq 1$. Then the series on the right hand side of (2.1) converges uniformly and absolutely to the function F on $[-1,1]$.*

This has the following immediate consequence:

Corollary 2.2. *Let $F \in C([-1,1])$ and assume that finitely many Gegenbauer coefficients are negative or finitely many are positive. Then the series on the right hand side of (2.1) converges uniformly and absolutely to the function F on $[-1,1]$.*

2.2. **Positive Definite Kernels.** A function $F \in C([-1,1])$ is called positive definite on the sphere $\mathbb{S}^d$ if for any set of points $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$, the Gram matrix $M = [F(\langle z_i, z_j \rangle)]_{i,j=1}^N$ is positive semidefinite, i.e.

$$u^T M u \geq 0, \quad \forall u \in \mathbb{R}^N. \tag{2.3}$$

We call F strictly positive definite if the inequality in (2.3) is strict for $x \neq 0$.

Theorem 2.3. *For a function $F \in C([-1,1])$ the following conditions are equivalent:*

(i) F is positive definite on $\mathbb{S}^d$.
(ii) For $\lambda = \frac{d-1}{2}$, all Gegenbauer coefficients of F are non-negative, i.e.

$$\widehat{F}(n,\lambda) \geq 0 \quad \text{for all } n \geq 0. \tag{2.4}$$

(iii) For any signed measure $\mu \in \mathcal{B}$ the energy integral is non-negative: $I_F(\mu) \geq 0$.
(iv) There exists a function $f \in L^2_{w_\lambda}([-1,1])$ such that

$$F(\langle x, y \rangle) = \int_{\mathbb{S}^d} f(\langle x, z \rangle) f(\langle z, y \rangle)\, d\sigma(z), \quad x, y \in \mathbb{S}^d, \tag{2.5}$$

i.e. F is the spherical convolution of f with itself.

The equivalence of (i) and (ii) was proven by Schoenberg in 1958 [36]. The equivalence of (iii) and (i) follows from (2.3), which states that $I_F\big(\sum u_i \delta_{z_i}\big) \geq 0$, and a standard argument based on the compactness of $\mathbb{S}^d$ and the weak-$*$ density of the linear span of Dirac masses in $\mathcal{B}$. Finally, the equivalence of (ii) and (iv) can be established by defining f through the relation $\big(\widehat{f}(n,\lambda)\big)^2 = \widehat{F}(n,\lambda)$. Lemma 2.1 guarantees the existance of $f \in L^2_{w_\lambda}([-1,1])$. The interested reader can find more details on spherical harmonics, ultraspherical polynomials, and positive definite functions in [22].

There is a strong connection between the Gegenbauer coefficients a function F and the minimizers of $I_F(\mu)$. For instance, one can determine that σ is a minimizer from the signs of the coefficients [6, 7].

Theorem 2.4. *If $F \in C([-1,1])$, then σ is a minimizer of $I_F(\mu)$ over $\mathcal{M}$ if and only if $F + C$ is positive definite for some constant $C \in \mathbb{R}$ or, equivalently, if $\widehat{F}(n,\lambda) \geq 0$ for all $n \geq 1$. The uniform measure σ is the unique minimizer of I_F if and only if $\widehat{F}(n,\lambda) > 0$ for all $n \geq 1$.*

Proof. Suppose first that $F + C$ is positive definite and let $\mu \in \mathcal{M}$. Using non-negativity of coefficients (Theorem 2.3, part ii) and absolute summability of the Gegenbauer series (Lemma 2.1), it follows from Fubini's theorem and the addition formula (2.2) that

$$\begin{aligned}
I_F(\mu) &= \sum_{n=0}^{\infty} \widehat{F}(n;\lambda) \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} \frac{n+\lambda}{\lambda} C_n^{\lambda}(\langle x,y\rangle)\, d\mu(x)\, d\mu(y) \\
&= \sum_{n=0}^{\infty} \widehat{F}(n;\lambda) \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} \sum_{j=1}^{a_n^d} Y_{n,j}(x) Y_{n,j}(y)\, d\mu(x) d\mu(y) \\
&= \widehat{F}(0;\lambda) + \sum_{n=1}^{\infty} \widehat{F}(n;\lambda) \sum_{j=1}^{a_n^d} \Big(\int_{\mathbb{S}^d} Y_{n,j}(x)\, d\mu(x) \Big)^2 \\
&\geq \widehat{F}(0;\lambda) = I_F(\sigma). \qquad (2.6)
\end{aligned}$$

(The last equality follows from the fact that spherical harmonics of nonzero degree vanish under the Lebesgue measure, i.e. $\int_{\mathbb{S}^d} Y_{n,j}(x)\, d\sigma(x) = 0$.)

Now suppose that $F + C$ was strictly positive definite, i.e. $\widehat{F}(n;\lambda) > 0$ for all $n \geq 1$. Then we could only have $I_F(\mu) = I_F(\sigma)$, with $\mu \in \mathcal{M}$ if

$$\int_{\mathbb{S}^d} Y(x)\, d\mu(x) = 0 = \int_{\mathbb{S}^d} Y(x)\, d\sigma(x)$$

for all $Y \in H_n^d$ and $n \geq 1$. The density of spherical polynomials in $C(\mathbb{S}^d)$ gives us that $d\mu = d\sigma$.

Now, suppose that $\widehat{F}(n;\lambda) \leq 0$ for some $n \geq 1$, and let $\mu \in \mathcal{B}$ be defined by $d\mu(x) = \big(1 + \varepsilon Y_{n,1}(x)\big) d\sigma(x)$, with $\varepsilon > 0$ small enough that $1 + \varepsilon Y_{n,1}(x) \geq 0$ on $\mathbb{S}^d$. The Funk-Hecke formula (Theorem 1.2.9 in [22]) states that for any spherical harmonic $Y \in \mathcal{H}_n^d$

$$\int_{\mathbb{S}^d} F(\langle x,y\rangle) Y(x) d\sigma(x) = \widehat{F}(n;\lambda) Y(y). \qquad (2.7)$$

Since $\int_{\mathbb{S}^d} Y_{n,1}(x) d\sigma(x) = 0$, we find that $\mu \in \mathcal{M}$ and

$$\begin{aligned}
I_F(\mu) &= \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} F(\langle x,y\rangle) \big(1 + \varepsilon Y_{n,1}(x)\big)\big(1 + \varepsilon Y_{n,1}(y)\big)\, d\sigma(x)\, d\sigma(y) \\
&= I_F(\sigma) + \varepsilon^2 \widehat{F}(n;\lambda) \int_{\mathbb{S}^d} Y_{n,1}^2(y) d\sigma(y) \\
&\leq I_F(\sigma),
\end{aligned}$$

so if σ is a minimizer of I_F, it is not unique. Note that if we restrict to the case $\widehat{F}(n;\lambda) < 0$, then we have $I_F(\mu) < I_F(\sigma)$, meaning that σ is not a minimizer of I_F.

□

2.3. **Other Minimizers.** This idea of using the Gegenbauer expansion to show existence of discrete minimizers can be extended to a large class of functions. In certain cases, such as for positive definite functions, explicit minimizers of functions are known based on their Gegenbauer expansion alone.

Proposition 2.5 (Bilyk, Dai [6])**.** *Let $F \in C([-1,1])$. Then we have the following:*

(1) If $\widehat{F}(n;\lambda) \leq 0$ for all $n \geq 1$, then any Dirac mass, δ_x, is a minimizer of I_F. If $\widehat{F}(n;\lambda) < 0$ for all $n \geq 1$, then all minimizers are Dirac masses.

(2) If $(-1)^n \widehat{F}(n;\lambda) \le 0$ for all $n \ge 1$, then

$$\min_{\mu\in\mathcal{B}} I_F(\mu) = \widehat{F}(0;\lambda) + \sum_{n=1}^{\infty} \widehat{F}(2n;\lambda) a_{2n}^d = \frac{F(1)+F(-1)}{2} = I_F\Big(\frac{\delta_p + \delta_{-p}}{2}\Big).$$

Moreover, if $(-1)^n \widehat{F}(n;\lambda) < 0$ for all $n \ge 1$, then any minimizer of I_F is of the form $\mu = \frac{1}{2}(\delta_p + \delta_{-p})$ for some $p \in \mathbb{S}^d$.

(3) If, for all $n \in \mathbb{N}$, $\widehat{F}(2n;\lambda) = 0$ and $\widehat{F}(2n-1;\lambda) \ge 0$, then any symmetric measure μ (i.e. such that $\mu(E) = \mu(-E)$ for all measurable $E \subset \mathbb{S}^d$) is a minimizer of I_F. If $\widehat{F}(2n-1;\lambda) > 0$ for all $n \in \mathbb{N}$, then all minimizers are symmetric.

We also refer the reader to §4.5 for more recent results in this vein: namely, existence of finitely supported minimizers for functions with only finitely many positive Gegenbauer coefficients.

2.4. **Spherical Designs.** A set of distinct points $Z = \{z_1, ..., z_n\} \subset \mathbb{S}^d$ is called a spherical t-design if

$$\int_{\mathbb{S}^d} P(x) d\sigma = \frac{1}{N} \sum_{j=1}^{N} P(x_j) \tag{2.8}$$

for all polynomials in $\mathbb{R}^{d+1}$ of total degree at most t. The strength of Z is the greatest $t \in \mathbb{N}$ such that Z is a spherical t-design. As an immediate consequence of Theorem 2.4, we see that if F is a positive definite polynomial of degree at most t and Z is a t-design, then $\frac{1}{N}\sum_{j=1}^N \delta_{z_j}$ is a minimizer of I_F, which also means that Z is a minimizer of E_F.

The concept of spherical designs was originally introduced in 1977 by Delsarte, Goethal, and Seidel in [20]. In the same paper, they found the following bound on $N(d,t)$, the minimum number of points needed in a spherical t-design in $\mathbb{S}^d$:

$$N(d,t) \ge \begin{cases} \binom{d+k}{d} + \binom{d+k-1}{d} & \text{if } t = 2k, \\ 2\binom{d+k}{k} & \text{if } t = 2k+1, \end{cases} \sim t^d. \tag{2.9}$$

Spherical designs attaining this bound are called tight. Tight designs are very symmetrical and optimal in many ways (see e.g. [2, 15, 17, 18, 42]), but also very rare. While the vertices of a regular $(t+1)$-gon form a tight t-design on $\mathbb{S}^1$, tight t-designs can only exist for $t = 1,2,3,4,5,7$ or 11 if $d \ge 2$.

Over the next few decades, proofs were given of the existence of spherical designs for all t and d, with better and better bounds on $N(d,t)$, culminating in the result of Bondarenko, Radchenko, and Viazovska that not only is $N(d,t)$ on the order of t^d, but for large enough N (relative to t and d), well-separated t-designs always exist [11, 12], which solved a long-standing conjecture of Korevaar and Meyers.

Theorem 2.6. *For all $d \in \mathbb{N}$ there exist $C_d > 0$ and $\lambda_d > 0$ such that for all $N \ge C_d t^d$, there exists a spherical t-design $\{z_1, ..., z_N\} \subset \mathbb{S}^d$ such that $||z_i - z_j|| > \lambda_d N^{-1/d}$ for $i \ne j$.*

Combining Theorems 2.4 and 2.6, we have

Corollary 2.7. *If F is a positive definite (modulo a constant) polynomial of degree t, then for $N \ge C_d t^d$, we have that spherical t-designs minimize the N-point energy and, moreover,*

$$\min_{\substack{Z\subset\mathbb{S}^d\\ \#Z=N}} E_F(Z) = I_F(\sigma) = \min_{\mu\in\mathcal{M}} I_F(\mu). \tag{2.10}$$

For a more detailed exposition on spherical designs, see [2].

3. Generalized Stolarsky Principle

In many areas of mathematics, one is often faced with the problem of distributing large sets of points as uniformly as possible. Two of the most popular ways to do this are through energy optimization and discrepancy. For positive definite functions F one may hope that point sets that minimize the discrete energy will in some sense approximate the uniform distribution σ, which minimizes the corresponding energy integral. Since discrepancy theory deals with approximating the uniform measure with discrete counting measures, it is natural to expect these two methods of distributing points to be connected. One of the first instances of such a connection was obtained in 1973 by Stolarsky [39], who proved that minimizing the L^2 discrepancy with respect to spherical caps is equivalent to maximizing the pairwise sum of Euclidean distances.

3.1. **Stolarsky Invariance Principle.** Let $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$ be an N-point configuration. For a given subset of the sphere, $A \subseteq \mathbb{S}^d$, we define the discrepancy of Z with respect to A as

$$D(Z, A) := \frac{1}{N} \sum_{k=1}^{N} \mathbb{1}_A(z_k) - \sigma(A). \tag{3.1}$$

In other words, $D(Z, A)$ indicates how well the counting measure $\frac{1}{N}\sum_{k=1}^{N} \delta_{z_k}$ approximates the Lebesgue measure of A. To obtain good finite distributions Z, one usually aims to minimize the supremum (extremal discrepancy) or average (e.g., L^2 discrepancy) of $|D(Z, A)|$ over some rich and well-structured collection of sets A such as spherical caps, slices, convex sets, etc (the specific choice depends on the problem at hand). Some good exposition of discrepancy theory in general can be found in [21, 35].

We consider spherical caps $C(x, t)$ with center $x \in \mathbb{S}^d$ and height $t \in [-1, 1]$,

$$C(x, t) := \{z \in \mathbb{S}^d : \langle z \cdot x\rangle > t\}. \tag{3.2}$$

We define the L^2 discrepancy of Z with respect to spherical caps:

$$[D_{L^2,\mathrm{cap}}(Z)]^2 := \int_{-1}^{1} \int_{\mathbb{S}^d} \left| \frac{1}{N} \sum_{j=1}^{N} \mathbb{1}_{C(x,t)}(z_j) - \sigma\big(C(x, t)\big) \right|^2 d\sigma(x)\, dt. \tag{3.3}$$

The following result was proved by Stolarsky in 1973 [39], after which the proof was simplified in [14] and [7]:

Theorem 3.1 (Stolarsky Invariance Principle)**.** *Let $Z = \{z_1, z_2, \ldots, z_N\} \subset \mathbb{S}^d$. Then*

$$[D_{L^2,\mathrm{cap}}(Z)]^2 = C_d \left(\int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\|\, d\sigma(x)\, d\sigma(y) \; - \; \frac{1}{N^2} \sum_{i,j=1}^{N} \|z_i - z_j\| \right), \tag{3.4}$$

where the constant C_d satisfies

$$C_d = \frac{1}{2} \int_{\mathbb{S}^d} |p \cdot z|\, d\sigma(z) = \frac{1}{d} \frac{\omega_{d-1}}{\omega_d} = \frac{v_d}{\omega_d} = \frac{1}{d} \frac{\Gamma\big((d+1)/2\big)}{\sqrt{\pi}\, \Gamma(d/2)} \sim \frac{1}{\sqrt{2\pi d}} \quad \text{as} \quad d \to \infty, \tag{3.5}$$

where ω_d is the surface area of $\mathbb{S}^d$, v_d is the volume of the unit ball in $\mathbb{R}^d$, and p is an arbitrary point on the sphere $\mathbb{S}^d$.

This theorem states that the L^2 spherical cap discrepancy can be realized as the difference between the continuous and discrete energies, i.e. the error of numerical integration of the distance integral $\int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\|\, d\sigma(x)\, d\sigma(y)$ by the cubature formula with knots at the points of Z. It also has the immediate consequence that minimizing the L^2 spherical cap discrepancy of Z is equivalent to maximizing the sum of Euclidean distances between the points of Z.

The proof we have given in [7] is perhaps the most transparent and illuminating. The ideas is quite simple conceptually (with the devil, as usually, hiding in the details): one "squares out" the expression inside the integral in (3.3), and the "cross terms" yield an energy with pairwise point interactions. Naturally, integration over $\mathbb{S}^d$ then yields volumes of intersections of spherical caps $\sigma\big(C(z_i,t)\cap C(z_j,t)\big)$, and further averaging over $t\in[-1,1]$, turns this cumbersome object into the beautiful formula (3.4).

It was shown by Beck in 1984 [3, 4] that the optimal order of the L^2 spherical cap discrepancy is $N^{-\frac{1}{2}-\frac{1}{2d}}$, i.e.

$$c_d N^{-\frac{1}{2}-\frac{1}{2d}} \le \inf_{\#Z=N} D_{L^2,\mathrm{cap}}(Z) \le c_d' N^{-\frac{1}{2}-\frac{1}{2d}}, \tag{3.6}$$

which in turn bounds the difference of continuous and discrete energies in (3.4).

3.2. **Generalized Stolarsky Principle.** In [7], it was shown that this result of Stolarsky's could be extended to relate discrepancy and energy for all positive definite functions. For this Generalized Stolarsky Principle, we require a more general notion of discrepancy.

Given a positive definite function $F\in C([-1,1])$, we know from Theorem 2.3 (part iv) that there exists some $f\in L^2_{w_\lambda}([-1,1])$ such that F is the spherical convolution of f with itself. For any $\mu\in\mathcal{M}$, we define the L^2 discrepancy of μ with respect to f as

$$D_{L^2,f}(\mu) = \left(\int_{\mathbb{S}^d}\Big|\int_{\mathbb{S}^d} f(\langle x,y\rangle)\,d\mu(y) - \int_{\mathbb{S}^d} f(\langle x,y\rangle)\,d\sigma(y)\Big|^2 d\sigma(x)\right)^{\frac{1}{2}}. \tag{3.7}$$

We the define the L^2 discrepancy of a finite point-set $Z\subset\mathbb{S}^d$ with respect to f as

$$D_{L^2,f}(Z) := D_{L^2,f}\Big(\frac{1}{N}\sum_{j=1}^N \delta_{z_j}\Big) = \left(\int_{\mathbb{S}^d}\Big|\frac{1}{N}\sum_{i=1}^N f(\langle x,z_i\rangle) - \int_{\mathbb{S}^d} f(\langle x,y\rangle)\,d\sigma(y)\Big|^2 d\sigma(x)\right)^{\frac{1}{2}}. \tag{3.8}$$

Naturally, various choices of f recover different geometric notions of discrepancy. With this more general notion of discrepancy, we can now state the result of Bilyk, Dai, and Matzke in [7], which relates the minimization of energy to the minimization of discrepancy.

Theorem 3.2 (Generalized Stolarsky Principle)**.** *Let $\mu\in\mathcal{B}$ be a signed Borel probability measure on $\mathbb{S}^d$ and let $F\in C([-1,1])$ be positive definite with f as in (2.5). Then*

$$I_F(\mu) - I_F(\sigma) = D^2_{L^2,f}(\mu). \tag{3.9}$$

In particular, in the case of $\mu=\frac{1}{N}\sum_{i=1}^N\delta_{z_i}$, this relation becomes

$$\frac{1}{N^2}\sum_{i,j=1}^N F(\langle z_i,z_j\rangle) - \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} F(\langle x,y\rangle)d\sigma(x)d\sigma(y) = D^2_{L^2,f}(Z). \tag{3.10}$$

The proof of this theorem follows from a very important property of σ (Lemma 5.1 from [7]):

Lemma 3.3. *For any bounded or non-negative Borel measurable function F on $[-1,1]$ and any signed probability measure $\mu\in\mathcal{B}$, the following relation holds:*

$$I_F(\mu) - I_F(\sigma) = I_F(\mu-\sigma). \tag{3.11}$$

Proof of Theorem 3.2. According to (3.7), (2.5), and (3.11), we have

$$\begin{aligned} D^2_{L^2,f}(\mu) &= \int_{\mathbb{S}^d}\Big(\int_{\mathbb{S}^d} f(\langle x,y\rangle)\,d(\mu-\sigma)(y)\Big)^2\,d\sigma(x)\\ &= \int_{\mathbb{S}^d}\int_{\mathbb{S}^d}\int_{\mathbb{S}^d} f(\langle x,y\rangle)f(\langle x,z\rangle)d(\mu-\sigma)(y)d(\mu-\sigma)(z)d\sigma(x)\\ &= \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} F(\langle y,z\rangle)d(\mu-\sigma)(y)d(\mu-\sigma)(z)\\ &= I_F(\mu-\sigma)\\ &= I_F(\mu)-I_F(\sigma). \end{aligned}$$

□

In most contexts, the Stolarsky identity arises from the notion of the L^2 discrepancy, which in turn determines the specific form of the interaction potential F. Theorem 3.2 allows one to go in the opposite direction: starting with a positive definite potential F, one can produce a natural notion of discrepancy for which the Stolarsky principle holds. The precise form of the function f, defined through the identity $\big(\widehat{f}(n,\lambda)\big)^2=\widehat{F}(n,\lambda)$, cannot be made explicit in most cases (in fact, many different choices of f corresponding to the same F can be constructed by changing the signs of the coefficients $\widehat{f}(n,\lambda)$). However, this does not prevent one from being able to use information about either F or f to obtain a lower bound for the discrepancy, and consequently the energy, as shown in [6],

Proposition 3.4. *Let F be positive definite, and f as in (2.5). Then there exist positive constants c_d, c_d', and C_d such that for all $N\in\mathbb{N}$,*

$$C_d \min_{1\le k\le c_d N^{1/d}} \widehat{F}(k,\lambda) \le \min_{\substack{Z\subset\mathbb{S}^d\\ \#Z=N}} D^2_{L^2,f}(Z) \le N^{-1} \max_{0\le\theta\le c_d' N^{-1/d}}\big(F(1)-F(\cos(\theta))\big). \tag{3.12}$$

3.3. **Sum of Geodesic Distances.** We now discuss an application of Theorem 3.2, which we draw from [7, 37] (others can be found in [6, 7]). Let $F(t)=\frac{1}{\pi}\arccos(t)$, i.e., $d(x,y):=F(\langle x,y\rangle)$ is the normalized geodesic distance on $\mathbb{S}^d$. The function $G(t)=\frac12(1-F(t))$ is positive definite, with $g(t)=\mathbb{1}_{(0,1]}(t)$ satisfying relation (2.5). Our generalized Stolarsky principle then gives us

$$\begin{aligned} \frac12\big(I_F(\sigma)-I_F(\mu)\big) &= I_G(\mu)-I_G(\sigma)\\ &= D^2_{L^2,g}(\mu)\\ &= \int_{\mathbb{S}^d}\Big(\int_{\mathbb{S}^d} g(\langle x,y\rangle)\,d\mu(y)-\int_{\mathbb{S}^d} g(\langle x,y\rangle)\,d\sigma(y)\Big)^2\,d\sigma(x)\\ &= \int_{\mathbb{S}^d}\Big(\mu(H(x))-\sigma(H(x))\Big)^2\,d\sigma(x), \end{aligned}$$

where $H(x)=\{y\in\mathbb{S}^d:\ \langle x,y\rangle>0\}$ is the hemisphere on $\mathbb{S}^d$ centered at x. Naturally, $\sigma(H(x))=\frac12$ for any $x\in\mathbb{S}^d$. A quick computation shows that $I_F(\sigma)=\frac12$, and so we have the following:

Theorem 3.5 (Bilyk, Dai, Matzke, [7])**.** *If $\mu\in\mathcal{M}$ be a Borel measure on $\mathbb{S}^d$ with $\mu(\mathbb{S}^d)=1$, then the following relation holds*

$$\int_{\mathbb{S}^d}\left(\mu\big(H(x)\big)-\frac12\right)^2 d\sigma(x)=\frac12\cdot\left(\frac12-I_F(\mu)\right). \tag{3.13}$$

Consequently we have that $I_F(\mu) \le \frac{1}{2}$ for all $\mu \in \mathcal{M}$, with equality if and only if

$$\mu\big(H(x)\big) = \frac{1}{2} \quad \text{for } \sigma\text{-a.e.} \quad x \in \mathbb{S}^d. \tag{3.14}$$

A measure $\mu \in \mathcal{M}$ satisfies (3.14) if and only if μ is symmetric (Proposition 4.5 of [7]), i.e. $\mu(E) = \mu(-E)$ for every Borel set $E \subset \mathbb{S}^d$. Thus, we can classify all maximizers of I_F.

Corollary 3.6. *For a measure $\mu \in \mathcal{M}$,*

$$I_F(\mu) = \sup_{\gamma \in \mathcal{M}} I_F(\gamma) = \frac{1}{2}$$

if and only if μ is centrally symmetric.

This behavior of d, the geodesic distance, goes in sharp contrast with the behavior of the seemingly similar energy integral $\int\limits_{\mathbb{S}^d}\int\limits_{\mathbb{S}^d} \|x-y\|\, d\mu(x) d\mu(y)$. It is known [10] that the unique maximizer of this energy integral is σ. In this sense the behavior of

$$I_F(\mu) = \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} d(x,y) d\mu(x) d\mu(y)$$

is more similar (albeit still different) to that of $\int\limits_{\mathbb{S}^d}\int\limits_{\mathbb{S}^d} \|x-y\|^2\, d\mu(x) d\mu(y)$ which is maximized by any measure with center of mass at the origin, which follows from the relation

$$\int\limits_{\mathbb{S}^d}\int\limits_{\mathbb{S}^d} \|x-y\|^2\, d\mu(x) d\mu(y) = 2 - 2 \cdot \Bigg\| \int\limits_{\mathbb{S}^d} x d\mu(x) \Bigg\|^2. \tag{3.15}$$

Comparing positive powers of the Euclidean and geodesic distances, one finds that the energy integrals, as a function of the exponent δ, both have "breaking" points where the maximizer changes from being the uniform distribution σ to a pair of antipodal points. For the geodesic distance, this is $\delta = 1$, whereas for the Euclidean distance, this is $\delta = 2$.

Theorem 3.7 (Björck, [10])**.** *For $\delta > 0$, define the energy integral*

$$I_E(\mu) = \int\limits_{\mathbb{S}^d}\int\limits_{\mathbb{S}^d} \|x-y\|^\delta\, d\mu(x) d\mu(y). \tag{3.16}$$

The maximizers of this energy integral over $\mu \in \mathcal{M}$ can be characterized as follows:

(1) $0 < \delta < 2$: the unique maximizer of $I_E(\mu)$ is $\mu = \sigma$.
(2) $\delta = 2$: $I_E(\mu)$ is maximized if and only if the center of mass of μ is at the origin.
(3) $\delta > 2$: $I_E(\mu)$ is maximized if and only if $\mu = \frac{1}{2}(\delta_p + \delta_{-p})$, i.e. the mass is equally concentrated at two antipodal poles.

Theorem 3.8 (Bilyk, Dai, Matzke [6, 7])**.** *For $\delta > 0$, define the energy integral*

$$I_E(\mu) = \int\limits_{\mathbb{S}^d}\int\limits_{\mathbb{S}^d} \big(d(x,y)\big)^\delta\, d\mu(x) d\mu(y) \tag{3.17}$$

The maximizers of this energy integral over $\mu \in \mathcal{M}$ can be characterized as follows:

(1) $0 < \delta < 1$: the unique maximizer of $I_E(\mu)$ is $\mu = \sigma$ (the normalized surface measure).
(2) $\delta = 1$: $I_E(\mu)$ is maximized if and only if μ is centrally symmetric .
(3) $\delta > 1$: $I_E(\mu)$ is maximized if and only if $\mu = \frac{1}{2}(\delta_p + \delta_{-p})$, i.e. the mass is equally concentrated at two antipodal poles.

Now, let us turn our attention to the maximizers of the discrete energy. This then becomes a question, original posed by Fejes Tóth in [25], of maximizing the sum of geodesic distances of a point configuration, for any fixed number of points. Taking $\mu = \frac{1}{N}\sum_{i=1}^{N}\delta_{z_i}$, for some $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$, Stolarsky-type identity (3.13) gives us that

$$D^2_{L^2,g}(Z) = \int\limits_{\mathbb{S}^d} \left(\frac{\#\big(Z \cap H(x)\big)}{N} - \frac{1}{2} \right)^2 d\sigma(x) = \frac{1}{2} \cdot \left(\frac{1}{2} - \frac{1}{N^2} \sum_{i,j=1}^{N} d(z_i, z_j) \right). \tag{3.18}$$

This can then by used to prove the following:

Theorem 3.9 (Bilyk, Dai, Matzke [7]). *Let $d \geq 1$. Then the following holds:*

(1) For any point distribution $Z = \{z_1, \ldots, z_N\} \subset \mathbb{S}^d$,

$$\frac{1}{N^2} \sum_{i,j=1}^{N} d(z_i, z_j) \leq \frac{1}{2}. \tag{3.19}$$

(2) For a given $N \in \mathbb{N}$, the sum above is maximized if and only if the following condition holds: for any $x \in \mathbb{S}^d$, such that the hyperplane $x^\perp$ contains no points of Z, the numbers of points of Z on either side of $x^\perp$ differ by at most one, i.e.

$$\big|\#\big(Z \cap H(x)\big) - \#\big(Z \cap H(-x)\big)\big| \leq 1. \tag{3.20}$$

(3) If N is even,

$$\max_{\#Z=N} \frac{1}{N^2} \sum_{i,j=1}^{N} d(z_i, z_j) = \frac{1}{2},$$

and this maximum is achieved if and only if Z is a centrally symmetric set.

(4) If N is odd,

$$\max_{\#Z=N} \frac{1}{N^2} \sum_{i,j=1}^{N} d(z_i, z_j) = \frac{1}{2} - \frac{1}{2N^2},$$

and this maximum is achieved if and only if Z can be represented as a union $Z = Z_1 \cup Z_2$, where Z_1 is symmetric, while Z_2 lies on a two-dimensional hyperplane (i.e. on the same great circle) and satisfies $\frac{1}{M^2} \sum\limits_{z_i, z_j \in Z_2} d(z_i, z_j) = \frac{1}{2} - \frac{1}{2M^2}$ with $M = \#Z_2$, i.e. Z_2 is a maximizer of the sum of geodesic distances on $\mathbb{S}^1$.

Remark: Observe that the one-dimensional maximizers of odd cardinality N, which arise in part (4), are characterized by the condition that the sum of any $\lceil N/2 \rceil$ consecutive central angles defined by the points is at least π. In particular, any acute triangle is a maximizer for $d = 1$ and $N = 3$.

Parts (1) and (2) in $d = 1$ were proved by Fejes Tóth [25], who conjectured that the same holds for $d \geq 2$. Parts (1) and (3) follow immediately from Corollary 3.6. Part (2) follows from (3.18), in that to maximize $E_F(Z)$, one must minimize $\left| \frac{\#\left(Z \cap H(x)\right)}{N} - \frac{1}{2} \right|$ for x σ-a.e. Part (4) can be proved using part (2) and an interesting fact from combinatorial geometry known as the Sylvester–Gallai Theorem [1].

Theorem 3.9 demonstrates that the situation is drastically different from the spherical cap discrepancy and the sum of Euclidean distances, which is to be expected, given our earlier discussion on the related energy integrals. In the latter case, minimizing the L^2 spherical cap discrepancy (equivalently, maximizing the sum of Euclidean distances) leads to a rather uniform distribution of Z. In particular, for $d = 1$ the sum is maximized by the vertices of a regular N-gon [24], and in higher dimensions maximizing distributions have to be well-separated [39]. The sum of *geodesic* distances, however, may be maximized by very non-uniform sets, e.g. $N/2$ points in two antipodal poles.

4. p-Frame Potentials

4.1. **Frame Potential.** The energy with the potential $F(t) = t^2$ arises naturally in functional analysis and signal processing. In [5], Benedetto and Fickus defined the discrete "frame potential", which up to normalization is equal to $E_F(Z)$, and proved that the minimizers of E_F were a generalization of an orthonormal basis. An N-point configuration $Z \subset \mathbb{S}^d$ is a tight frame exactly when one has an analogue of Parseval's identity for each $x \in \mathbb{R}^{d+1}$, i.e. there exists some constant $\lambda > 0$ such that

$$\sum_{z \in Z} \langle x, z \rangle^2 = \lambda ||x||^2, \quad \forall x \in \mathbb{R}^{d+1},$$

or, equivalently,

$$x = \frac{1}{\lambda} \sum_{z \in Z} \langle x, z \rangle z, \quad \forall x \in \mathbb{R}^{d+1}.$$

These objects also have a strong connection to energy minimization.

Proposition 4.1 (Benedetto, Fickus [5])**.** *Let $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$.*

(1) If $N \le d+1$, then

$$\min_{\substack{Z \subset \mathbb{S}^d \\ \#Z = N}} E_F(Z) = \frac{1}{N},$$

and the minimizers are exactly the orthonormal sequences in $\mathbb{R}^{d+1}$.

(2) If $N \ge d+1$, then

$$\min_{\substack{Z \subset \mathbb{S}^d \\ \#Z = N}} E_F(Z) = \frac{1}{d+1},$$

and the minimizers are exactly the N-element tight frames in $\mathbb{S}^d$.

This result can be easily extended to continuous energy, e.g. [9, 23]. A probability measure $\mu \in \mathcal{M}$ is a tight frame (isotropic measure) if there exists some $\lambda > 0$ such that

$$\int_{\mathbb{S}^d} \langle x, y \rangle^2 d\mu(y) = \lambda ||x||^2, \quad \forall x \in \mathbb{R}^{d+1}.$$

Combining the results of [9] and [23], we have

Theorem 4.2. *For any $\mu \in \mathcal{M}$, we have*

$$I_F(\mu) \ge \frac{1}{d+1}. \tag{4.1}$$

Equality above is achieved precisely when μ is a tight frame, which is equivalent to the second moment matrix of μ being a multiple of the identity, i.e. $\left[\int_{\mathbb{S}^d} x_i x_j \, d\mu(x) \right]_{i,j=1}^{d+1} = c\, \mathbf{I}_{d+1}$.

4.2. **p-Frame Potential.** The concept of frame potential and tight frames was generalized by Ehler and Okoudjou in [23], where they introduced the p-frame potential, i.e. the energy with the following kernel: $F(t) = |t|^p$, for $0 < p < \infty$. A measure $\mu \in \mathcal{M}$ is a tight p-frame if there exists some $\lambda > 0$ such that

$$\int_{\mathbb{S}^d} |\langle x, y \rangle|^p d\mu(y) = \lambda ||x||^p, \quad \forall x \in \mathbb{R}^{d+1}.$$

Moreover, they were able to generalize the results of Theorem 4.2 to the case where p is an even integer:

Theorem 4.3 (Ehler, Okoudjou [23]). *Let $F(t) = t^{2k}$, with $k \in \mathbb{N}$. Then*

$$I_F(\mu) \geq \frac{1 \cdot 3 \cdot 5 \cdots (2k-1)}{(d+1)(d+3)\cdots(d+2k-1)},$$

with equality if and only if μ is a tight $2k$-frame.

This is somewhat intuitive, as when p is an even integer, $F(t) = t^p$, which is a positive definite polynomial. Theorem 2.4, along with (2.8), quickly gives us σ and spherical p-designs as a minimizers of I_F, and the expression on the right-hand side of the estimate above is precisely the value of $I_{t^{2k}}(\sigma)$. Since

$$\int_{\mathbb{S}^d} \langle x, y\rangle^p d\sigma(y) = ||x||^p \int_{\mathbb{S}^d} \langle x/||x||, y\rangle^p d\sigma(y) = C_{d,p}||x||^p, \quad \forall x \in \mathbb{R}^{d+1} \setminus \{0\}, \tag{4.2}$$

we have that σ is a tight p-frame for all p, which means that for even p, spherical p-designs are also tight p-frames.

This result of Ehler and Okoudjou holds only when p is an even integer. When p is not an even integer, F is not positive definite, so σ, a tight p-frame, is not a minimizer, and in some cases we have found minimizers, described in the next subsection, that are not tight p-frames.

A large amount of examples and numerical experiments lead us to conjecture that for $p > 0$, $p \notin 2\mathbb{N}$, the minimizers of the p-frame potential are necessarily finitely supported discrete measures. While we cannot yet prove this in full generality, we present the proof of some special cases, namely, that tight designs are minimizers for appropriate ranges of p, §4.3, as well as the proof that minimizers are supported on sets with empty interior, §4.4.

4.3. **Universally optimal sets.** One possible way of finding minimizers of a kernel F is through interpolation. If $\mu \in \mathcal{M}$ is a minimizer of I_G, where $G \in C([-1,1])$ is such that $G \leq F$, and $F(\langle x, y\rangle) = G(\langle x, y\rangle)$ for all $x, y \in \operatorname{supp}(\mu)$, then μ is a minimizer of I_F, since for each $\nu \in \mathcal{M}$

$$I_F(\nu) \geq I_G(\nu) \geq I_G(\mu) = I_F(\mu). \tag{4.3}$$

The results in this section are an analouge of the results of Cohn and Kumar on sharp designs [15]. While we only need the result of Corollaries 4.10 and 4.15 for projective real spaces, we will prove the general result for all two-point compact homogeneous spaces.

A metric space (Ω, ρ) 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 $\rho(x_1, x_2) = \rho(y_1, y_2)$ there exists an isometry of Ω, mapping x_i to y_i, $i = 1, 2$. It is known [43] that any such compact connected space is either a real sphere $\mathbb{S}^d$, a real projective space $\mathbb{RP}^d$, a complex projective space $\mathbb{CP}^d$, a quaternion projective space $\mathbb{HP}^d$, or the Cayley projective plane $\mathbb{OP}^2$. For each of these spaces, there is a unique probability measure σ_Ω invariant under the isometry group on Ω (the Haar measure of Ω). In the case of $\Omega = \mathbb{S}^d$, σ_Ω is the normalized Lebesgue measure. In what follows, we let $\mathbb{F}$ denote the field over which the respective linear spaces are considered: $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}, \mathbb{H}, \mathbb{O}\}$.

Let Ω be a compact, connected two-point homogeneous set with convex metric ρ (the geodesic distance with respect to the Riemannian metric) normalized so that the greatest distance between points in Ω is π. In the case when $\Omega = \mathbb{RP}^d$, this distance can be represented through

$$\cos \rho(x, y) = 2|\langle x, y\rangle|^2 - 1, \tag{4.4}$$

where the points of $\mathbb{RP}^d$ are (non-uniquely) associated with points of $\mathbb{S}^d$ through the projective quotient map, which maps the points x and $-x \in \mathbb{S}^d$ into the same point of $\mathbb{RP}^d$.

Let $\alpha = \frac{d'}{2} - 1$, where d' is the dimension of Ω as a real manifold, and let

$$\beta = \begin{cases} \frac{d}{2} - 1 & \text{if } \Omega = \mathbb{S}^d; \\ \dim_{\mathbb{R}}(\mathbb{F})/2 - 1 & \text{if } \Omega = \mathbb{FP}^d. \end{cases} \tag{4.5}$$

The sequence of Jacobi polynomials $P_n^{(\alpha,\beta)}(t)$, $n \in \mathbb{N}_0$ is an orthogonal basis in the space $L^1_{w_{\alpha,\beta}}([-1,1])$ with the weight $w_{\alpha,\beta}(t) = (1-t)^\alpha(1+t)^\beta$, i.e. the space of functions F on $[-1,1]$ satisfying

$$\int_{-1}^{1} |F(t)|(1-t)^\alpha(1+t)^\beta dt < \infty.$$

On the sphere $\mathbb{S}^d$, these are the Gegenbauer polynomials:

$$P_n^{\left(\frac{d}{2}-1,\frac{d}{2}-1\right)}(t) = C_n^{\frac{d-1}{2}}(t). \tag{4.6}$$

Note that the weight $w_{\alpha,\beta}(t)$ arises when integrating on Ω, i.e.

$$\int_\Omega F(\cos(\rho(x,p)))d\sigma_\Omega(x) = c_\Omega \int_{-1}^{1} F(t) w_{\alpha,\beta}(t)dt,$$

where p is an arbitrary point in Ω and c_Ω is a constant depending only on Ω [29].

A function $F \in C([-1,1])$ is positive definite on Ω if for any set of points $Z = \{z_1, ..., z_N\} \subset \Omega$, the Gram matrix

$$(F(\cos(\rho(z_i, z_j))))_{i,j=1}^N$$

is positive semidefinite. As was the case on the sphere, a polynomial is positive definite on Ω if and only if it can be written as a nonnegative linear combination of the corresponding Jacobi polynomials [15, 34]. An argument similar to Theorem 2.4, in turn, implies that if F is a polynomial, then σ_Ω is a minimizer of the energy integral

$$I_{F,\Omega}(\mu) = \int_\Omega \int_\Omega F(\cos(\rho(x,y)))d\mu(x)d\mu(y)$$

over $\mathcal{M}(\Omega)$, the set of probability measures on Ω, if and only if $F + C$ is positive definite on Ω for some constant $C > 0$. For a fixed Ω, we write simply

$$P_n(t) := P_n^{(\alpha,\beta)}(t).$$

4.3.1. *Tight designs.* We call a finite subset $\mathcal{C} \subset \Omega$ an *M-design* if

$$\sum_{x,y\in\mathcal{C}} P_k(\cos(\rho(x,y))) = I_{P_k,\Omega}(\sigma_\Omega) = 0$$

for $1 \le k \le M$. As in the spherical case, this means M-designs give minimizers of $I_{F,\Omega}$ for positive definite polynomials of degree up to M. For any $\mathcal{C} \subseteq \Omega$, we define the distance set of $\mathcal{C}$ as

$$A(\mathcal{C}) := \{\rho(x,y) : x, y \in C\}.$$

Clearly $A(\mathcal{C})$ is finite if and only if $\mathcal{C}$ is finite and $0 \in A(\mathcal{C})$ if $\mathcal{C} \neq \emptyset$.

We call $\mathcal{C}$ tight if it satisfies one of the following conditions:

(1) $\mathcal{C}$ is a $(2m-1)$-design, $\#A(\mathcal{C}) = m+1$, and $\pi \in A(\mathcal{C})$;
(2) $\mathcal{C}$ is a $2m$-design and $\#A(\mathcal{C}) = m+1$.

We note that this definition of a tight design is equivalent to our previous definition on the sphere, see [20]. A slight relaxation on these conditions gives us so-called *sharp* designs. We call $\mathcal{C}$ sharp if it satisfies one of the following:

(1) $\mathcal{C}$ is a $(2m-2)$-design, $\#A(\mathcal{C}) = m+1$, and $\pi \in A(\mathcal{C})$;
(2) $\mathcal{C}$ is a $(2m-1)$-design and $\#A(\mathcal{C}) = m+1$.

In [15], Cohn and Kumar proved that if $\mathcal{C} = \{z_1, ..., z_N\} \subset \Omega$ is a sharp M-design and $F \in C([-1,1])$ is absolutely monotone, then $\mathcal{C}$ is a minimizer of the discrete energy

$$E_{F,\Omega}(Z) = \frac{1}{N^2} \sum_{i,j=1}^{N} F(\cos(\rho(z_i, z_j)))$$

over all N point configurations on Ω. Following their methods allows one to show that in certain cases, tight designs give minimizers of the continuous energy $I_{F,\Omega}$.

4.3.2. *Hermite interpolation.* Suppose, for some $K \in \mathbb{N}_0$, we are given a function $F \in C^K([-1,1])$, and a collection $t_1 < \ldots < t_m \in [-1,1]$, as well as positive integers $k_1, \ldots, k_m$, with

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

We wish to find a polynomial 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 polynomial always exists and is unique, because the linear map that takes a polynomial p of degree less than D to

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

is bijective.

In order to know if our polynomial bounds our function F from below, we will need the following fact about Hermite interpolation [19]:

Lemma 4.4. *Under the hypotheses above, for each $t \in [-1,1]$ there exists $\xi \in (-1,1)$ such that $\min(t, t_1) < \xi < \max(t, t_m)$ and*

$$F(t) - p(t) = \frac{F^{(D)}(\xi)}{D!} \prod_{i=1}^{m} (t - t_i)^{k_i}.$$

Given a polynomial g with $\deg(g) \geq 1$, let $H(F,g)$ denote the polynomial of degree less than $\deg(g)$ that agrees with F at each root of g to the order of that root and let

$$Q(F,g)(t) = \frac{F(t) - H(F,g)(t)}{g(t)}.$$

We call $F \in C^M([-1,1])$ absolutely monotonic of degree M if $F^{(n)}(t) \geq 0$ for $0 \leq n \leq M$ and $t \in [-1,1]$, and we call a nonconstant polynomial g on $[-1,1]$ conductive if for all functions F absolutely monotonic of degree $\deg(g)$, $H(F,g)$ is positive definite. Note that $t - s$ is conductive for all $s \in [-1,1]$. Cohn and Kumar give us the following two lemmas [15]:

Lemma 4.5. *Let g_1, g_2 be polynomials on $[-1,1]$. If $F \in C^{\deg(g_1)+\deg(g_2)-1}([-1,1])$, then*

$$H(F, g_1 g_2) = H(F, g_1) + g_1 H(Q(F, g_1), g_2). \tag{4.7}$$

Lemma 4.6. *If g_1 and g_2 are conductive, and g_1 is positive definite, then $g_1 g_2$ is conductive.*

Let Ω be a compact, connected two-point homogeneous set and let ρ and $P_0, P_1, \ldots$ be the appropriate metric and system of orthogonal polynomials. We shall prove that tight M-designs yield minimizers of energy integrals for M-absolutely monotonic functions with negative $(M+1)^{st}$ derivative. We treat the cases of even and odd M separately.

4.3.3. *Optimality of tight 2m-designs.* Suppose that $\mathcal{C} \subset \Omega$ is a tight $2m$-design. Let $t_1 < \cdots < t_m < t_{m+1} = 1$ be the cosines of distances occurring in $\mathcal{C}$. Let

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

and

$$g(t) = (t-1) f(t)^2.$$

Theorem 4.7. *Let $\mathcal{C} \subset \Omega$ be a tight $2m$-design and let F be absolutely monotonic of degree $2m$, with $F^{(2m+1)}(t) \le 0$ for $t \in (-1,1)$. Then*

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

is a minimizer of $I_{F,\Omega}(\mu)$ over $\mathcal{M}(\Omega)$.

To prove Theorem 4.7 we must prove that $F(t) \ge H(F,g)(t)$ for $t \in [-1,1]$, and that $H(F,g)(t)$, which is a degree $2m$ polynomial, is positive definite. Then μ is a minimizer of $I_{H(F,g),\Omega}$ (see e.g. Corollary 2.7 in the case of $\mathbb{S}^d$ and the discussion in the beginning of §4.3.1 for the more general case), and since $H(F,g)(t) = F(t)$ on $A(\mathcal{C})$, it is also a minimizer of $I_{F,\Omega}$, as shown in (4.3).

Lemma 4.8. *For $t \in [-1,1]$, $F(t) \ge H(F,g)(t)$.*

Proof. By Lemma 4.4, we know that for all $t \in [-1,1]$ there exists a point $\xi \in (-1,1)$ such that

$$F(t) - H(F,g)(t) = \frac{F^{(2m+1)}(\xi)}{(2m+1)!} g(t).$$

The right side is nonnegative, so $F(t) \ge H(F,g)(t)$. □

For $n \in \mathbb{N}_0$, let $p_n = P_n^{(\alpha+1,\beta)}$. These polynomials are orthogonal with respect to the measure

$$dw_{\alpha+1,\beta}(t) = (1-t)dw_{\alpha,\beta}.$$

Lemma 4.9. *For $k \le m$, $\prod_{j=1}^{k}(t-t_j)$ is positive definite.*

Proof. For $n < m$, the degree of $(1-t)f(t)p_n(t)$ is at most $2m$, so for any $y \in \mathcal{C}$, there exist positive constants $a_1, \dots, a_m, c$ such that

$$\begin{aligned}
\int_{-1}^{1} f(t)p_n(t)dw_{\alpha+1,\beta}(t) &= \int_{-1}^{1}(1-t)f(t)p_n(t)dw_{\alpha,\beta}(t) \\
&= c\sum_{x\in\mathcal{C}}(1-\cos(\rho(x,y)))f(\cos(\rho(x,y)))p_n(\cos(\rho(x,y))) \\
&= c\sum_{j=1}^{m} a_j(1-t_j)f(t_j)p_n(t_j) = 0.
\end{aligned}$$

Since f is a degree m polynomial with 1 as its leading coefficient $f = p_m$. This means that for $k \le m$, $\prod_{j=1}^{k}(t-t_j)$ is linear combination of $p_0, \dots, p_k$ with nonnegative coefficients [15]. For all $k \in \mathbb{N}_0$, p_k is a linear combination of $P_0, \dots, P_k$ with nonnegative coefficients, meaning that all the p_k are positive definite. □

Lemmas 4.6 and 4.9 imply that f is conductive, and thus f^2 is positive definite and conductive. Lemmas 4.4 and 4.5 then tell us that there exists $\xi \in (-1,1)$ such that

$$\begin{aligned}
H(F,g)(t) &= H(F,f^2)(t) + f(t)^2 H(Q(F,f^2), \frac{g}{f^2})(t) \\
&= H(F,f^2)(t) + f(t)^2 \frac{F(1) - H(F,f^2)(1)}{f(1)^2} \\
&= H(F,f^2)(t) + f(t)^2 \frac{F^{(2m)}(\xi)}{(2m)!},
\end{aligned}$$

and this proves our theorem.

Now, if $F^{(2m+1)}(t) < 0$ for $t \in (-1,1)$, then $F(t) = H(F,g)(t)$ at exactly $t_1, ..., t_{m+1}$, meaning that if $A(\mathrm{supp}(\nu)) \not\subseteq A(\mathcal{C})$, then

$$I_{F,\Omega}(\nu) > I_{H(F,g),\Omega}(\nu) \geq I_{H(F,g),\Omega}(\mu) = I_{F,\Omega}(\mu),$$

so ν cannot be a minimizer. This gives us the following:

Corollary 4.10. *Suppose that there exists a tight $2m$-design, $\mathcal{C} \subset \Omega$, and F is absolutely monotonic of degree $2m$, with $F^{(2m+1)}(t) < 0$ for $t \in (-1,1)$. Then if ν is a minimizer of $I_{F,\Omega}$ over $\mathcal{M}(\Omega)$, then ν has finite support. In particular,*

$$A(supp(\nu)) \subseteq A(\mathcal{C}).$$

4.3.4. *Optimality of tight (2m-1)-designs.* Suppose that $\mathcal{C} \subset \Omega$ is a tight $(2m-1)$-design. Let $-1 = t_1 < \cdots < t_m < t_{m+1} = 1$ be the cosines of the distances between points in $\mathcal{C}$. Let

$$f(t) = \prod_{i=2}^{m}(t - t_i),$$

$$g_1(t) = (t+1)f(t)^2.$$

and

$$g(t) = (t^2-1)f(t)^2.$$

Theorem 4.11. *Let $\mathcal{C} \subset \Omega$ be a tight $(2m-1)$-design and let F be absolutely monotonic of degree $2m-1$, with $F^{(2m)}(t) \leq 0$ for $t \in (-1,1)$. Then*

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

is a minimizer of

$$I_F(\mu) = \int_\Omega \int_\Omega F(\cos(\rho(x,y))d\mu(x)d\mu(y)$$

over $\mathcal{M}(\Omega)$.

The proof of Theorem 4.11 is very similar to the proof of Theorem 4.7. However, in order to ensure that $\deg(H(F,g)) \leq 2m-1$, as opposed to $2m$ in the previous case, and $H(F,g)(t) \leq F(t)$, with equality at $t_1, ..., t_{m+1}$, one must make $t_1 = -1$ a root of order one in g. Since $\frac{g(t)}{t-1}$ is no longer a square of some polynomial, we require a slightly different proof that it is conductive and positive definite.

Lemma 4.12. *For $t \in [-1,1]$, $F(t) \geq H(F,g)(t)$.*

Proof. By Lemma 4.4, we know that for all $t \in [-1,1]$ there exists a point $\xi \in (-1,1)$ such that

$$F(t) - H(F,g)(t) = \frac{F^{(2m)}(\xi)}{(2m)!}g(t).$$

The right side is nonnegative, so $F(t) \geq H(F,g)(t)$. □

For $n \in \mathbb{N}_0$, let $q_n = P_n^{(\alpha+1,\beta+1)}$. These polynomials are orthogonal with respect to the measure

$$dw_{\alpha+1,\beta+1}(t) = (1-t^2)dw_{\alpha,\beta}(t).$$

Lemma 4.13. *The polynomial $(t+1)q_k(t)$ is positive definite for all $k \in \mathbb{N}_0$.*

Proof. For all $k \in \mathbb{N}_0$, $(t+1)q_k(t)$ is orthogonal to all polynomials of degree less than k with respect to the measure $(t-1)dw_{\alpha,\beta}(t)$, so $(t+1)q_k(t) = p_{k+1}(t) + bp_k(t)$ for some constant b. Since $p_{k+1}(-1) + bp_k(-1) = 0$, and $p_j(-1)$ has sign $(-1)^j$, we have that $b \geq 0$. Since each p_j is positive definite, $(t+1)q_k(t)$ is positive definite. □

Lemma 4.14. *For $1 \le k \le m$, $(t+1)\prod_{j=2}^{k}(t-t_j)^2$ and $(t+1)(t-t_k)\prod_{j=2}^{k-1}(t-t_j)^2$ are positive definite.*

Proof. For $n < m-1$, the degree of $(1-t^2)f(t)q_n(t)$ is at most $2m-1$, so for any $y \in \mathcal{C}$, there exist positive constants $a_2, \dots, a_{m-1}, c$ such that

$$\begin{aligned}\int_{-1}^{1} f(t)q_n(t)dw_{\alpha+1,\beta+1}(t) &= \int_{-1}^{1}(1-t^2)f(t)q_n(t)dw_{\alpha,\beta}(t)\\ &= c\sum_{x\in\mathcal{C}}(1-\cos^2(\rho(x,y)))f(\cos(\rho(x,y)))q_n(\cos(\rho(x,y)))\\ &= c\sum_{j=2}^{m} a_j(1-t_j^2)f(t_j)q_n(t_j) = 0.\end{aligned}$$

Since f is a degree $m-1$ polynomial with 1 as its leading coefficient, $f = q_{m-1}$. This means that for $k \le m$, $\prod_{j=2}^{k}(t-t_j)$ is linear combination of $q_0, \dots, q_k$ with nonnegative coefficients.

The set of linear combinations of $q_0, q_1, \dots$ with nonnegative coefficients is closed under multiplication. This, combined with Lemma 4.13, gives us our claim.

□

Combining this with Lemma 4.6, we see that g_1 is conductive and positive definite. Lemmas 4.4 and 4.5 then tell us that there exists some $\xi \in (-1,1)$ such that

$$\begin{aligned}H(F,g)(t) &= H(F,g_1)(t) + g_1(t)H(Q(F,g_1),\frac{g}{g_1})(t)\\ &= H(F,g_1)(t) + g_1(t)\frac{F(1)-H(F,g_1)(1)}{g_1(1)}\\ &= H(F,g_1)(t) + g_1(t)\frac{F^{(2m-1)}(\xi)}{(2m)!}\end{aligned}$$

and this proves our theorem. As in the previous section, we immediately have the following corollary:

Corollary 4.15. *Suppose that there exists a tight $(2m-1)$-design, $\mathcal{C} \subset \Omega$, and F is absolutely monotonic of degree $2m-1$, with $F^{(2m)}(t) < 0$ for $t \in (-1,1)$. Then if ν is a minimizer of $I_{F,\Omega}$ over $\mathcal{M}(\Omega)$, then ν has finite support. In particular,*

$$A(supp(\nu)) \subseteq A(\mathcal{C}).$$

4.3.5. *Application to p-frame potential.* Now, when F is an even function $F(t) = F(|t|)$, it suffices to minimize I_F over centrally-symmetric probability measures on $\mathbb{S}^d$. Indeed, we have

$$I_F\left(\frac{\mu(x)+\mu(-x)}{2}\right) = \frac{1}{4}\left[I_F(\mu(x)) + 2\int_{\mathbb{S}^d}\int_{\mathbb{S}^d} F(\langle x,y\rangle)d\mu(x), d\mu(-y)) + I_F(\mu(-x))\right] = I_F(\mu)$$

By identifying centrally-symmetric measures on $\mathbb{S}^d$ with the measures on $\mathbb{RP}^d$, it is therefore possible to consider this an energy minimization problem on on $\mathbb{RP}^d$.

Defining the standard metric ρ on $\mathbb{RP}^d$ as above, so that $\operatorname{diam}_\rho \mathbb{RP}^d = \pi$, we have

$$\cos(\rho(x,y)) = 2\langle x,y\rangle^2 - 1. \tag{4.8}$$

We then have $-1 \le \cos(\rho(x,y)) \le 1$, and the function F can be expressed as $F(\langle x,y\rangle) = G(\cos(\rho(x,y)))$, where

$$G(s) := F\left(\sqrt{(s+1)/2}\right) \quad \text{or, equivalently,} \quad F(t) = G(2t^2-1).$$

Minimization of $I_{G,\mathbb{RP}^d}$ is then equivalent minimization of $I_{F,\mathbb{S}^d}$. For any $\mu \in \mathcal{M}(\mathbb{S}^d)$, let $\tilde{\mu} \in \mathcal{M}(\mathbb{RP}^d)$ be the pushforward measure of the projective quotient mapping, i.e., slightly abusing notation:

$$\tilde{\mu}(E) = \mu((-E) \cup E), \ \ \forall E \subseteq \mathbb{S}^d.$$

The above discussion can be summarized in the following

Proposition 4.16. *Let $F : [-1, 1] \to \mathbb{R}$ be a continuous function such that $F(t) = F(|t|)$ and let $G(s) = F\left(\sqrt{\frac{s+1}{2}}\right)$. Then μ is a minimizer of*

$$\int_{\mathbb{S}^d}\int_{\mathbb{S}^d} F(\langle x, y\rangle) d\mu(x) d\mu(y)$$

over $\mathcal{M}(\mathbb{S}^d)$ if and only if $\tilde{\mu}$ is a minimizer of

$$\int_{\mathbb{RP}^d}\int_{\mathbb{RP}^d} G(\cos(\rho(x, y))) d\tilde{\mu}(x) d\tilde{\mu}(y)$$

over $\mathcal{M}(\mathbb{RP}^d)$.

Observe that G is a polynomial of degree k if and only if the corresponding even function F is a polynomial of degree $2k$. Proposition 4.16 tells us that $\sigma_{\mathbb{S}^d}$ is a minimizer of I_F if and only if $\sigma_{\mathbb{RP}^d} = \widetilde{\sigma}_{\mathbb{S}^d}$ is a minimizer of $I_{G,\Omega}$. Thus, G is a positive definite polynomial on $\mathbb{RP}^d$ if and only if F is a positive definite polynomial on $\mathbb{S}^d$. Alternatively, this could be seen through the identity [38]:

$$C^{\lambda}_{2n}(t) = P_n^{\left(\lambda-\frac{1}{2},\lambda-\frac{1}{2}\right)}(t) = \frac{\Gamma\left(2n+\lambda+\frac{1}{2}\right)\Gamma\left(n+1\right)}{\Gamma\left(n+\lambda+\frac{1}{2}\right)\Gamma\left(2n+1\right)} P_n^{\left(\lambda-\frac{1}{2},-\frac{1}{2}\right)}(2t^2-1),$$

which implies that $F(t) = G(2t^2-1)$ is a positive linear combination of the Gegenbauer polynomials $C_{2n}^{\frac{d-1}{2}}(t)$ if and only if $G(s)$ is a positive linear combination of the Jacobi polynomials $P_n^{\left(\frac{d}{2}-1,-\frac{1}{2}\right)}(s)$, corresponding to the real projective space $\mathbb{RP}^d$.

This in turn means that a centrally symmetric set $\mathcal{C} \subset \mathbb{S}^d$ is a $2k$-design (and therefore also a $(2k+1)$-design) on $\mathbb{S}^d$ if and only if $\tilde{\mathcal{C}} := q(\mathcal{C})$ is a k-design on $\mathbb{RP}^d$, where q is the standard quotient map from $\mathbb{S}^d$ to $\mathbb{RP}^d$. If $\mathcal{C}$ is a tight $(2k+1)$-design on $\mathbb{S}^d$, then $\mathcal{C}$ is centrally symmetric [20] and $\#A(\mathcal{C}) = k+2$. The symmetry of $\mathcal{C}$ implies that

$$\#A(\tilde{\mathcal{C}}) = \begin{cases} \frac{k+3}{2} = \ell + 1, & \text{if } k = 2\ell - 1 \text{ is odd,} \\ \frac{k}{2} + 1 = \ell + 1, & \text{if } k = 2\ell \text{ is even.} \end{cases}$$

Observe that if $k = 2\ell - 1$ is odd, then $\#A(\mathcal{C}) = k + 2$ is also odd, therefore $\frac{\pi}{2} \in A(\mathcal{C})$, and hence $\pi \in A(\tilde{\mathcal{C}})$ if k is odd, implying that $\tilde{\mathcal{C}}$ is a tight k-design.

Conversely, if $\tilde{\mathcal{C}}$ is a tight k-design in $\mathbb{RP}^d$, let $\mathcal{C}$ be its centrally symmetric preimage in $\mathbb{S}^d$ under q. Then $\mathcal{C}$ is a $(2k+1)$-design in $\mathbb{S}^d$, and the condition $\pi \in A(\mathcal{C})$ is satisfied automatically. Notice that $\#A(\mathcal{C}) = 2 \cdot \#A(\tilde{\mathcal{C}})$ or $\#A(\mathcal{C}) = 2 \cdot \#A(\tilde{\mathcal{C}}) - 1$.

If $k = 2\ell - 1$, then $\#A(\tilde{\mathcal{C}}) = \ell + 1$ and $\pi \in A(\tilde{\mathcal{C}})$, and hence $\frac{\pi}{2} \in A(\mathcal{C})$, i.e., $\#A(\mathcal{C})$ is odd. Thus $\#A(\mathcal{C}) = A(\tilde{\mathcal{C}}) - 1 = 2\ell + 1 = k + 2$. Hence, C is a tight $(2k+1)$-design.

If $k = 2\ell$, we have $\#A(\tilde{\mathcal{C}}) = \ell + 1$. Hence, $\#A(\mathcal{C})$ is either $2\ell + 2 = k + 2$ or $2\ell + 1 = k - 1$. But a spherical $(2k+1)$-design cannot have fewer than $k + 2$ distances (see the observation after Definition 1.1 in [15]), thus $\#A(\mathcal{C}) = k + 2$, and $\mathcal{C}$ is a tight $(2k+1)$-design in $\mathbb{S}^d$. This can be summarized as follows:

Proposition 4.17. *Let $\mathcal{C} \subset \mathbb{S}^d$ be a centrally symmetric set. The set $\mathcal{C}$ is a tight $(2k+1)$-design in $\mathbb{S}^d$ if and only if its image $\tilde{\mathcal{C}} = q(\mathcal{C})$ is a tight k-design in $\mathbb{RP}^d$.*

We see that if $F(t) = |t|^p$, then the corresponding function G is $G(s) := \left(\frac{1+s}{2}\right)^{\frac{p}{2}}$, which is absolutely monotonic of degree $\lceil \frac{p}{2} \rceil$, with $G^{(\lceil \frac{p}{2} \rceil + 1)}(s) < 0$ on $(-1, 1)$. By our discussion above, we have the following:

Theorem 4.18 (Bilyk, Glazyrin, Matzke, Park, Vlasiuk, [8])**.** *Suppose there exists a tight spherical $(2k+1)$-design, $\mathcal{C} \subset \mathbb{S}^d$, and let $F(t) = |t|^p$, with $2k-2 < p < 2k$. Then*

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

is a minimizer of I_F. In addition, if ν is a minimizer of I_F, then $A(supp(\nu)) \subseteq A(\mathcal{C})$, so $supp(\nu)$ is finite.

Finally, in this section, we want to consider the 600-cell, $\mathcal{C}_{600}$, – a highly symmetrical four-dimensional regular polytope, see e.g. [15]. It is almost a 9-design in $\mathbb{RP}^3$ in that

$$\sum_{x \in \mathcal{C}_{600}} P_n(x) = 0$$

for $n \in \{1, 2, 3, 4, 5, 7, 8, 9\}$, but not for $n = 6$. Since $\#A(\mathcal{C}_{600}) = 5$ and $\pi \in A(\mathcal{C}_{600})$, we cannot use the method above, as that would require $\mathcal{C}_{600}$ to be a 7-design in $\mathbb{RP}^3$. However, this can be remedied by adjusting our polynomial. Let $G(t) = \left(\frac{t+1}{2}\right)^{p/2}$ for some $8 < p < 10$, and let $t_1 = -1$, $t_2 = \frac{-\sqrt{5}-1}{4}$, $t_3 = -\frac{1}{2}$, $t_4 = \frac{\sqrt{5}-1}{4}$, and $t_5 = 1$. Let $h(t)$ be the unique 8^{th} degree polynomial, with Jacobi expansion $\sum_{n=0}^{8} a_n P_n^{\left(\frac{1}{2}, -\frac{1}{2}\right)}(t)$, such that $a_6 = 0$, $h(t_i) = p(t_i)$ for $1 \leq i \leq 5$, and $h'(t_i) = p'(t_i)$ for $2 \leq i \leq 4$.

Numerical results seem to indicate that the coefficients in the Jacobi expansion of $h(t)$ are all nonnegative for $p \in [8, 10]$, i.e. $h(t)$ is positive definite (see, e.g., Figures 3 and 4). This would mean that that the 600-cell is a minimizer of $I_{h,\mathbb{RP}^3}$.

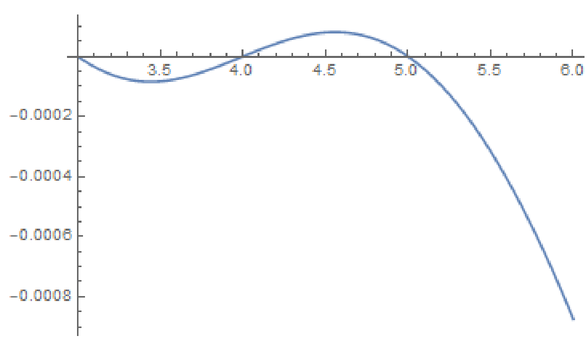

FIGURE 3. Graph of a_7 as a function of $p/2$

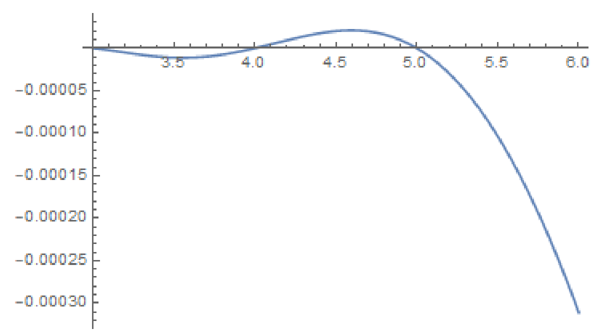

FIGURE 4. Graph of a_8 as a function of $p/2$

Assuming that h is indeed positive definite, it remains to show that $h(t)$ bounds $G(t)$ from below. Let $g(t) = (t^2 - 1)\prod_{i=2}^{4}(t - t_i)^2$ and $\tilde{h}(t) = H(G, g)(t)$. Since $h(t) = G(t)$ at the points of interpolation, we also have $\tilde{h}(t) = H(h, g)(t)$. Lemma 4.4 shows us that, for all $t \in [-1, 1]$, there exists some $\xi, \lambda \in (-1, 1)$ such that

$$G(t) - \tilde{h}(t) = \frac{G^{(8)}(\xi)}{8!} g(t) \geq 0,$$

with the inequality being strict off of the points of interpolation, and

$$h(t) - \tilde{h}(t) = \frac{h^{(8)}(\lambda)}{8!} g(t) \leq 0.$$

We thus have

$$G(t) - h(t) = G(t) - \tilde{h}(t) + \tilde{h}(t) - h(t) \geq 0,$$

with the inequality being strict off of the points of interpolation. Thus, we arrive at the following *conditional result*, supported by numerical evidence.

Proposition 4.19 (Bilyk, Glazyrin, Matzke, Park, Vlasiuk, [8])**.** *Let $F(t) = |t|^p$, with $8 < p < 10$ and $\mathcal{C}$ be the 600-cell in $\mathbb{S}^3$. If the function h as described above is positive definite, then*

$$\mu = \frac{1}{120} \sum_{x \in \mathcal{C}} \delta_x$$

is a minimizer of I_F. In addition, if h is positive definite, then if ν is a minimizer of I_F, then $A(supp(\nu)) \subseteq A(\mathcal{C})$, so $supp(\nu)$ is finite.

The table below shows all known tight spherical designs of odd strength, as well as the 600-cell [15].

d	$\#\mathcal{C}$	Strength	inner products	configuration/origin
d	$2d+2$	3	$0, \pm 1$	Cross polytope in $\mathbb{R}^{d+1}$
1	$2k$	$2k-1$	$\cos\left(\frac{j\pi}{N}\right)$, $0 \leq j \leq k$	regular polygon
2	12	5	$\pm\frac{1}{\sqrt{5}}, \pm 1$	Icosahedron
3	120	11	$0, \frac{\pm 1 \pm \sqrt{5}}{4}, \pm\frac{1}{2}, \pm 1$	600-cell
6	56	5	$\pm\frac{1}{3}, \pm 1$	Equiangular lines, kissing configuration of E_8
7	240	7	$0, \pm\frac{1}{2}, \pm 1$	E_8 root system
22	552	5	$\pm\frac{1}{5}, \pm 1$	Equiangular Lines
22	4600	7	$0, \pm\frac{1}{3}, \pm 1$	Kissing configuration of Leech Lattice
23	196560	11	$0, \pm\frac{1}{4}, \pm\frac{1}{2}, \pm 1$	Leech Lattice minimal vectors

4.4. **Support of Minimizers.** Outside of the cases in the previous section, we have not been able to prove finite support for minimizers of the p-frame energy. However, inspired by some of the ideas from the work of Finster and Schiefeneder on minimizers of causal variation [26], we were able to prove a somewhat weaker statement in this direction – that the support of the minimizers cannot have interior points.

Theorem 4.20 (Bilyk, Glazyrin, Matzke, Park, Vlasiuk, [8])**.** *Let $F(t) = |t|^p$, for $p > 0$ and $p \notin 2\mathbb{N}$. Let μ be a minimizer of the p-frame energy I_F. Then* $\mathrm{supp}(\mu)$ *has empty interior.*

To prove this theorem, we first need two results. One standard fact from potential theory ([10, 13, 26]), and the second was proven by Finster and Schiefeneder in [26].

Lemma 4.21. *If $F \in C([-1,1])$ and μ is a minimizer of I_F, the the potential,*

$$f_\mu(x) := \int_{\mathbb{S}^d} F(\langle x, y \rangle) d\mu(y), \tag{4.9}$$

is constant on the support of μ:

$$f_\mu \big|_{\mathrm{supp}(\mu)} = \inf_{x \in \mathbb{S}^{d-1}} f_\mu(x) = I_F(\mu). \tag{4.10}$$

Lemma 4.22. *If $F \in C([-1,1])$ is nonnegative and μ is a minimizer of I_F, then the function F must be positive definite on* $\mathrm{supp}(\mu)$*, in other words for any $Z = \{z_1, \ldots, z_N\} \subset$* $\mathrm{supp}(\mu)$ *the matrix*

$$\left[F(\langle z_i, z_j \rangle)\right]_{i,j=1}^N$$

is positive semidefinite.

The proof of Theorem 4.20 is based on two mutually exclusive propositions concerning interior points of $\operatorname{supp}(\mu)$. In what follows, the value of $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$ is fixed, $F(t) = |t|^p$, and μ is assumed to be a minimizer of I_F.

Proposition 4.23. *Let $z \in \big(\operatorname{supp}(\mu)\big)^\circ$. Then*

$$\operatorname{supp}(\mu) \cap z^\perp = \emptyset. \tag{4.11}$$

Proposition 4.24. *Let $z \in \big(\operatorname{supp}(\mu)\big)^\circ$. Then*

$$\operatorname{supp}(\mu) \cap z^\perp \neq \emptyset. \tag{4.12}$$

Since these two propositions clearly cannot hold simultaneously, their validity proves Theorem 4.20, i.e. that there are no interior points in the support of a minimizer. The remainder of this section is dedicated to the proof of the propositions.

Proof of Proposition 4.23. We prove that if z is an interior point of a minimizer's support, then the orthogonal hyperplane $z^\perp$ does not intersect the support of μ. In short, the idea of the proof is the following. Assume that there exists a point $y \in \operatorname{supp}(\mu)$ such that $\langle y, z\rangle = 0$. We shall construct a finite set of points $Z = \big\{x_i\big\} \subset \operatorname{supp}(\mu)$, such that the matrix $\big[F(\langle x_i, x_j\rangle)\big]$ is not positive semidefinite, thus violating Lemma 4.22. The set Z will consist of the points z, y, and a number (depending on p) of points, equidistantly spaced around z on the great circle connecting y and z. We now make this precise.

Fix z in the interior of $\operatorname{supp}(\mu)$ and let $y \in \mathbb{S}^d$ be any point such that $\langle y, z\rangle = 0$. Setting $k \in \mathbb{N}$ so that $2k-2 < p < 2k$, we shall construct a set $\{x_0, \dots, x_{N-1}\}$ of $N = 2k+2$ points, all of which lie on the great circle connecting z and y. The points $x_0, \dots, x_{2k}$ are chosen in such a way that the angle between x_j and z is $(j-k)\varepsilon$ for some small $\varepsilon > 0$. Thus $x_k = z$, and the points x_0 and x_{2k} make angles $-k\varepsilon$ and $k\varepsilon$ with z, respectively. Observe that when ε is small enough, all of these points $x_0, \dots, x_{2k}$ belong to $\operatorname{supp}(\mu)$, since z is an interior point. Finally, we set $x_{2k+1} = y$. Then the angle between $x_{2k+1} = y$ and x_j, $j = 0, \dots, 2k$, is $\frac{\pi}{2} - (j-k)\varepsilon$. In order to apply Lemma 4.22 we consider the matrix

$$A := \big[F(\langle x_i, x_j\rangle)\big]_{i,j=0}^{2k+1} = \begin{pmatrix} F(\langle x_0, x_0\rangle) & F(\langle x_0, x_1\rangle) & \cdots & F(\langle x_0, x_{2k}\rangle) & F(\langle x_0, x_{2k+1}\rangle) \\ F(\langle x_1, x_0\rangle) & F(\langle x_1, x_1\rangle) & \cdots & F(\langle x_1, x_{2k}\rangle) & F(\langle x_1, x_{2k+1}\rangle) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ F(\langle x_{2k}, x_0\rangle) & F(\langle x_{2k}, x_1\rangle) & \cdots & F(\langle x_{2k}, x_{2k}\rangle) & F(\langle x_{2k}, x_{2k+1}\rangle) \\ F(\langle x_{2k+1}, x_0\rangle) & F(\langle x_{2k+1}, x_1\rangle) & \cdots & F(\langle x_{2k+1}, x_{2k}\rangle) & F(\langle x_{2k+1}, x_{2k+1}\rangle) \end{pmatrix}.$$

We intend to show that the matrix A is not positive semidefinite. To this end, we first construct an auxiliary vector $v \in \mathbb{R}^{2k+1} \setminus \{0\}$ such that for $m \in \{0, 1, ..., 2k-1\}$,

$$\sum_{j=0}^{2k} j^m v_j = 0, \tag{4.13}$$

i.e. this vector must be in the (right) kernel of the Vandermonde matrix

$$\begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 2 & 3 & \cdots & 2k \\ 0 & 1 & 2^2 & 3^2 & \cdots & (2k)^2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & 2^{2k-1} & 3^{2k-1} & \cdots & (2k)^{2k-1} \end{pmatrix}.$$

We can take the entries of v to be

$$v_j = \prod_{\substack{i=0\\ i\neq j}}^{2k} \frac{1}{j-i} = \frac{(-1)^j}{(2k-j)!j!}. \tag{4.14}$$

This can be shown by finding the inverse of the square Vandermonde matrix using a Lagrange interpolation argument, see, e.g. [44].

Consider a vector $u = [\alpha v_0, \alpha v_1, ..., \alpha v_{2k}, \beta]^T \in \mathbb{R}^{2k+2}$, where α, $\beta \in \mathbb{R}$. Then we have

$$\langle Au, u\rangle = \alpha^2 \left(\sum_{i,j=0}^{2k} v_i v_j F(\langle x_i, x_j\rangle)\right) + 2\alpha\beta \left(\sum_{j=0}^{2k} v_j F(\langle x_{2k+1}, x_j\rangle)\right) + \beta^2. \tag{4.15}$$

We shall show that the real numbers α and β can be chosen in such a way that the expression above is negative, for ε sufficiently small.

Observe that for i, $j = 0, \dots, 2k$ we have

$$F(\langle x_i, x_j\rangle) = \cos^p\big((i-j)\varepsilon\big).$$

Since $\cos^p(t)$ is even, smooth near zero, and $\cos^p(0) = 1$, we can use its Taylor expansion to estimate the first term of (4.15) as follows

$$\begin{aligned}
\sum_{i,j=0}^{2k} v_i v_j F(\langle x_i, x_j\rangle) &= \sum_{i,j=0}^{2k} v_i v_j \cos^p\big((i-j)\varepsilon\big) \\
&= \sum_{i,j=0}^{2k} v_i v_j \left(1 + \sum_{m=1}^{2k-1} a_m \varepsilon^{2m} (i-j)^{2m} + O(\varepsilon^{4k})\right) \\
&= \left(\sum_{j=0}^{2k} v_j\right)\left(\sum_{i=0}^{2k} v_i\right) + \sum_{m=1}^{2k-1} a_m \varepsilon^{2m} \left(\sum_{i,j=0}^{2k} v_i v_j (i-j)^{2m}\right) + O(\varepsilon^{4k}) \\
&= \sum_{m=1}^{2k-1} a_m \varepsilon^{2m} \sum_{i,j=0}^{2k} v_i v_j \sum_{l=0}^{2m} \binom{2m}{l} i^l j^{2m-l} + O(\varepsilon^{4k}) \\
&= \sum_{m=1}^{2k-1} a_m \varepsilon^{2m} \sum_{l=0}^{2m} \binom{2m}{l} \left(\sum_{i=0}^{2k} v_i i^l\right)\left(\sum_{j=0}^{2k} v_j j^{2m-l}\right) + O(\varepsilon^{4k}) \\
&= O(\varepsilon^{4k}),
\end{aligned} \tag{4.16}$$

where we have used the fact that for all values of $l = 0, 1, \dots, 2m$, either $l \leq 2k-1$ or $2m-l \leq 2k-1$.

We now turn to the second term of (4.15). Observe that for $j = 0, \dots, 2k$ we have

$$F(\langle x_{2k+1}, x_j\rangle) = F(\langle y, x_j\rangle) = \cos^p\left(\frac{\pi}{2} - (j-k)\varepsilon\right) = \big|\sin\big((j-k)\varepsilon\big)\big|^p. \tag{4.17}$$

We then find that

$$\begin{aligned}
\sum_{j=0}^{2k} v_j F(\langle y, x_j\rangle) &= \sum_{j=0}^{2k} v_j \sin^p(|k-j|\varepsilon) = \sum_{j=0}^{2k} v_j \big(|k-j|\varepsilon + O(\varepsilon^3)\big)^p \\
&= \sum_{j=0}^{2k} v_j (|k-j|\varepsilon)^p \big(1 + O(\varepsilon^2)\big)^p = \varepsilon^p \sum_{j=0}^{2k} v_j |k-j|^p + O(\varepsilon^{p+2}).
\end{aligned} \tag{4.18}$$

We now analyze the coefficient of ε^p in the above expression using (4.14)

$$\sum_{j=0}^{2k} v_j|k-j|^p = \sum_{j=0}^{2k}(-1)^j \frac{|k-j|^p}{(2k-j)!j!} = 2\sum_{j=0}^{k-1}(-1)^j \frac{(k-j)^p}{(2k-j)!j!}.$$

Since the above is a sum of k exponential functions of p, we know that $\sum_{j=0}^{k-1}(-1)^j \frac{(k-j)^p}{(2k-j)!j!}$ has at most $k-1$ zeros, see e.g. [41]. We shall demonstrate that these zeros are exhausted by the even integer values $p = 2, 4, \ldots, 2k-2$. Indeed, assume indirectly, that

$$2\sum_{j=0}^{k-1}(-1)^j \frac{(k-j)^p}{(2k-j)!j!} = b \neq 0$$

for some even integer $0 < p \leq 2k-2$. Then according to (4.15), (4.16), and (4.18) we would have

$$\langle Au, u\rangle = \alpha^2 O(\varepsilon^{4k}) + 2\alpha\beta\left(b\varepsilon^p + O(\varepsilon^{p+2})\right) + \beta^2.$$

Since $p < 2k$, for ε sufficiently small, the discriminant of this quadratic form is negative, hence we can choose α and β so that $\langle Au, u\rangle < 0$. However, since F is a positive definite function for even p, this is a contradiction, as the matrix A must be positive semidefinite for any collection $\{x_i\}$. Therefore

$$2\sum_{j=0}^{k-1}(-1)^j \frac{(k-j)^p}{(2k-j)!j!} = 0$$

for all $p \in \{2, 4, ..., 2k-2\}$. Since there are at most $k-1$ zeros of this function, we then know that

$$b_p := 2\sum_{j=0}^{k-1}(-1)^j \frac{(k-j)^p}{(2k-j)!j!} \neq 0$$

for all other values of p. Let $p \in (0, 2k) \setminus \{2, 4, ..., 2k-2\}$, then

$$\langle Au, u\rangle = \alpha^2 O(\varepsilon^{4k}) + 2\alpha\beta\left(b_p\varepsilon^p + O(\varepsilon^{p+2})\right) + \beta^2,$$

and by the previous argument, for ε sufficiently small, we could choose α and β so that $\langle Au, u\rangle < 0$, i.e. A is not positive definite. Thus, according to Lemma 4.22, the set $\{x_0, x_1, ..., x_{2k}, y\} \not\subseteq \operatorname{supp}(\mu)$. Since, by assumption, for small $\varepsilon > 0$ the points $x_0, x_1, \ldots, x_{2k}$ all lie in a neighborhood of z and hence in $\operatorname{supp}(\mu)$, it implies that $y \notin \operatorname{supp}(\mu)$. Thus $\operatorname{supp}(\mu) \cap z^\perp = \emptyset$.

□

Remark: The argument above obviously fails if p is an even integer, since then F is positive definite on the whole sphere. We note that for other values of p the number of points, required to disprove positive definiteness of $F(t) = |t|^p$ in our argument, is of the order p. Some restriction of this type is actually necessary. Indeed, according to the result of Fitzgerald and Horn [27], for any positive definite matrix $A = \left[a_{ij}\right]_{i,j=1}^N$ with non-negative entries $a_{ij} \geq 0$, its Hadamard powers $A^{(\alpha)} = \left[a_{ij}^\alpha\right]_{i,j=1}^N$ are also positive definite when $\alpha \geq N-2$. Let $G = \left[\langle z_i, z_j\rangle\right]_{i,j=1}^N$ be the Gram matrix of the set $Z = \{z_1, \ldots, z_N\} \subset \mathbb{S}^d$. Since the matrix $G^{(2)} = \left[|\langle z_i, z_j\rangle|^2\right]_{i,j=1}^N$ is positive definite and has non-negative entries, we have that the matrix

$$G^{(p)} = \left[|\langle z_i, z_j\rangle|^p\right]_{i,j=1}^N = \left(G^{(2)}\right)^{(p/2)}$$

is positive definite whenever $p/2 \geq N-2$. Therefore, to obtain a non-positive definite matrix $G^{(p)}$, we must take $N \geq 2 + p/2$ points.

The proof of Proposition 4.24. Let $z \in \mathbb{S}^d$ be an interior point of the support of μ. We shall demonstrate that $\operatorname{supp}(\mu)$ must intersect the hyperplane $z^\perp$.

Let us assume the contrary, i.e. $\operatorname{supp}(\mu) \cap z^\perp = \emptyset$. We first move all the mass of μ to the hemisphere centered at z by defining a new measure $\mu_z \in \mathcal{M}$ such that

$$\mu_z(E) = \begin{cases} \mu(-E \cup E), & \text{if } E \subseteq \{x \in \mathbb{S}^{d-1} : \langle z, x\rangle > 0\}, \\ \mu(E), & \text{if } E \subseteq z^\perp, \\ 0, & \text{if } E \subseteq \{x \in \mathbb{S}^{d-1} : \langle z, x\rangle < 0\}. \end{cases}$$

Since $F(\langle z, y\rangle) = F(\langle z, -y\rangle)$ for all $y \in \mathbb{S}^d$, this obviously doesn't change the energy, i.e. $I_F(\mu_z) = I_F(\mu)$, meaning that μ_z is also a minimizer.

Since $\operatorname{supp}(\mu) \cap z^\perp = \emptyset$, we also have that $\operatorname{supp}(\mu_z) \cap z^\perp = \emptyset$, i.e. $\operatorname{supp}(\mu_z) \subset \{x \in \mathbb{S}^d : \langle z, x\rangle > 0\}$. Compactness of the support of μ_z then implies that it is separated from $z^\perp$, i.e. for some $\delta > 0$ we have $\langle y, z\rangle > \delta$ for each $y \in \operatorname{supp}(\mu_z)$. Let us choose an open neighborhood U_z of z, small enough so that $U_z \subset \operatorname{supp}(\mu_z)$ and such that for each $x \in U_z$ and each $y \in \operatorname{supp}(\mu_z)$ we have $\langle y, x\rangle > \delta > 0$.

We can now write the potential (4.9) of μ_z at the point $x \in U_z$ as

$$f_{\mu_z}(x) = \int\limits_{\mathbb{S}^d} |\langle x, y\rangle|^p \, d\mu_z(y) = \int\limits_{\operatorname{supp}(\mu_z)} \langle x, y\rangle^p \, d\mu_z(y). \tag{4.19}$$

The discussion above implies that the last expression is well-defined (even for negative exponents). According to Lemma 4.21 $f_{\mu_z}(x)$ is constant on $U_z \subset \operatorname{supp}(\mu_z)$.

When p is an odd integer, the proof can be finished very quickly. Indeed, in this case the expression

$$g(x) = \int\limits_{\operatorname{supp}(\mu_z)} \langle x, y\rangle^p \, d\mu_z(y)$$

is well defined for each $x \in \mathbb{S}^d$ and yields an analytic function on the sphere (actually, a polynomial). Hence, being constant on an open set, implies that it is is constant on all of $\mathbb{S}^d$, which is not possible since, obviously, $g(-z) = -g(z) = -f_{\mu_z}(z) = -I_F(\mu_z) \neq 0$.

However, we shall present an approach which works for all $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$. Assume that there exists a differential operator D acting on functions on the sphere with the following two properties:

(i) D locally annihilates constants, i.e. if $u(x)$ is constant on some open set Ω, then $D_x u = 0$ on Ω;

(ii) $D_x\left(\langle x, y\rangle^p\right) < 0$ for all $x \in U_z$ and $y \in \operatorname{supp}(\mu_z)$.

Existence of such an operator would finish the proof since we would then have for each $x \in U_z$

$$0 = D_x f_{\mu_z}(x) = \int\limits_{\operatorname{supp}(\mu_z)} D_x\left(\langle x, y\rangle^p\right) d\mu_z(y) < 0, \tag{4.20}$$

which is a contradiction. Note that that switching to $D_x\left(\langle x, y\rangle^p\right) > 0$ in condition (ii) does not affect the proof.

We now construct such an operator D. Let Δ denote the Laplace–Beltrami operator on $\mathbb{S}^d$. Writing it in the standard spherical coordinates $\theta_1, \ldots, \theta_d$ one obtains (see, e.g., equation (2.2.4) in [33])

$$\Delta = \sum_{j=1}^{d} \frac{1}{q_j (\sin\theta_j)^{d-j}} \frac{\partial}{\partial\theta_j}\left((\sin\theta_j)^{d-j} \frac{\partial}{\partial\theta_j}\right), \tag{4.21}$$

where $q_1 = 1$ and $q_j = (\sin\theta_1 \dots \sin\theta_{j-1})^2$ for $j > 1$.

For fixed $y \in \mathbb{S}^d$, choose the coordinates so that $\cos\theta_1 = \langle y, x\rangle$. Then $\langle y, x\rangle^p = \cos^p\theta_1$, effectively leaving just one term in the formula above, and a direct computation shows that

$$\Delta_x\left(\langle x, y\rangle^p\right) = p(p-1)\langle x, y\rangle^{p-2} - p(p+d-1)\langle x, y\rangle^p. \tag{4.22}$$

Observe that if $p \in (0,1]$, then the operator Δ_x satisfies conditions (i) and (ii), hence completing the proof for this range of p.

Now consider the operator $D = \Delta\big(\Delta + p(p+d-1)\big)$. It is easy to see that

$$\begin{aligned}\Delta_x\big(\Delta_x + p(p+d-1)\big)\left(\langle x, y\rangle^p\right) &= \Delta_x\left(p(p-1)\langle x, y\rangle^{p-2}\right)\\ &= p(p-1)\cdot\big((p-2)(p-3)\langle x, y\rangle^{p-4} - (p-2)(p+d-3)\langle x, y\rangle^{p-2}\big)\\ &= p(p-1)(p-2)\langle x, y\rangle^{p-4}\cdot\big((p-3) - (p+d-3)\langle x, y\rangle^2\big).\end{aligned} \tag{4.23}$$

If $p \in (2,3]$, then $p-3 \le 0$ and $p+d-3 > d-1 \ge 0$, so the expression above is strictly negative. Hence this operator satisfies conditions (i) and (ii) for $2 < p \le 3$.

Moreover, if $p \in (1,2)$, the expression above is strictly positive. Indeed, the function $g_p(t) = (p-3) - (p+d-3)t$ is monotone on $[0,1]$ with $g_p(0) = p-3 < 0$ and $g_p(1) = -d < 0$. Therefore, condition (ii) holds with an opposite inequality sign, so the case $1 < p < 2$ is also covered.

It is now clear how to iterate this process. Define the operator $D^{(0)} = \Delta$, $D^{(1)} = \Delta\big(\Delta + p(p+d-1)\big)$, and, more generally, for $k \in \mathbb{N}$, define the differential operator of order $2k+2$

$$D^{(k)} = \Delta\left(\Delta + (p+d-2k+1)\prod_{j=0}^{2k-2}(p-j)\right)\cdots\Big(\Delta + p(p-1)(p-2)(p+d-3)\Big)\big(\Delta + p(p+d-1)\big). \tag{4.24}$$

Let $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$ and choose $k \in \mathbb{N}_0$ so that $2k-1 < p \le 2k+1$. An iterative computation akin to (4.23) shows that

$$\begin{aligned}D_x^{(k)}\left(\langle x, y\rangle^p\right) &= \left(\prod_{j=0}^{2k+1}(p-j)\right)\langle x, y\rangle^{p-2k-2} - \left(\prod_{j=0}^{2k}(p-j)\right)(p+d-2k-1)\langle x, y\rangle^{p-2k}\\ &= \left(\prod_{j=0}^{2k}(p-j)\right)\langle x, y\rangle^{p-2k-2}\cdot\big((p-2k-1) - (p+d-2k-1)\langle x, y\rangle^2\big).\end{aligned} \tag{4.25}$$

For $p \in (2k, 2k+1]$, the expression above is strictly negative, since $p-2k-1 \le 0$ and $p+d-2k-1 > d-1 \ge 0$.

At the same time, for $p \in (2k-1, 2k)$, this expression is strictly positive, because $\prod_{j=0}^{2k}(p-j) < 0$ and the monotone function $g_p(t) = (p-2k-1) - (p+d-2k-1)t$ takes values $g_p(0) = p-2k-1 < 0$ and $g_p(1) = -d < 0$. Thus, operator $D^{(k)}$ allows us to prove the statement of Proposition 4.24 for p in the range $(2k-1, 2k) \cup (2k, 2k+1]$. ☐

4.5. **Discrete minimizers for some energies.** While we cannot yet prove the conjectured discreteness of minimizers for the p-frame potential, we can prove that discrete minimizers exist for another class of energies.

Let E be a compact metric space and fix the functions $f_0 \equiv 1$, $f_1, \dots, f_n \in C(E)$, and constants $c_0 = 1$, $c_1, \dots, c_n \in \mathbb{R}$. Consider the set

$$K = \left\{\mu \in \mathcal{M}(E) : \int_E f_i\, d\mu = c_i, i = 0, 1, \dots, n\right\}, \tag{4.26}$$

which consists of (probability) measures whose moments with respect to f_i are fixed. It is easy to see that K is convex, bounded, and weak-$*$ closed, and therefore weak-$*$ compact. Thus, by the Krein-Milman theorem, K is the weak-$*$ closure of $\operatorname{ext}(K)$, the set of extreme points of K. We then have the following result of Karr, which demonstrates the discreteness of the elements of $\operatorname{ext}(K)$.

Theorem 4.25 (Karr, [32]). *Let $\mu \in K$. Then the following statements are equivalent:*

(1) $\mu \in \operatorname{ext}(K)$.

(2) The cardinality of $\operatorname{supp}\mu$ is at most $n+1$. Moreover, if we denote $\operatorname{supp}\mu = \{x_1, \dots, x_k\}$, then the vectors $v_j = \big(1, f_1(x_j), \dots, f_n(x_j)\big)$, $j = 1, 2, \dots, k$, are linearly independent.

We apply this theorem to energy minimization on the sphere. Let $E = \mathbb{S}^d$ and denote $N_+(F) = \{n \in \mathbb{N}_0 : \widehat{F}(n;\lambda) > 0\}$ and $N_-(F) = \{n \in \mathbb{N}_0 : \widehat{F}(n;\lambda) < 0\}$. We have the following result:

Theorem 4.26 (Bilyk, Glazyrin, Matzke, Park, Vlasiuk, [8]). *Assume that $F \in C[-1,1]$ and*

$$\# N_+(F) < \infty,$$

i.e. there are only finitely many positive definite terms in the Gegenbauer expansion. Then there exists a measure $\mu^* \in \mathcal{M}$ such that

$$\# \operatorname{supp}\mu^* \le \sum_{n \in N_+ \cup \{0\}} \dim \mathcal{H}_n^d, \tag{4.27}$$

and μ^* minimizes I_F.

Proof. Let $\mu \in \mathcal{M}$ be any minimizer of I_F and set $M = \inf\limits_{\nu \in \mathcal{M}} I_F(\nu) = I_F(\mu)$. Using the summation formula (2.2) and the absolute convergence of the Gegenbauer series (2.1), which we have from Corollary 2.2, we see that, for $\nu \in \mathcal{B}$,

$$\begin{aligned}
I_F(\nu) &= \sum_{n=0}^{\infty} \widehat{F}(n;\lambda)\frac{n+\lambda}{\lambda} \int\limits_{\mathbb{S}^d}\int\limits_{\mathbb{S}^d} C_n^\lambda(\langle x,y\rangle)\,d\nu(x)d\nu(y) \\
&= \sum_{n=0}^{\infty} \widehat{F}(n;\lambda)\frac{n+\lambda}{\lambda}\left(\sum_{k=1}^{\dim \mathcal{H}_n^d}\Big(\int\limits_{\mathbb{S}^d} Y_{n,k}(x)d\nu(x)\Big)^2\right) \\
&= \sum_{n \in N_+} \widehat{F}(n;\lambda)\frac{n+\lambda}{\lambda}\left(\sum_{k=1}^{\dim \mathcal{H}_n^d}\Big(\int\limits_{\mathbb{S}^d} Y_{n,k}(x)d\nu(x)\Big)^2\right) - \sum_{n \in N_-}\Big(-\widehat{F}(n;\lambda)\frac{n+\lambda}{\lambda}\Big)\left(\sum_{k=1}^{\dim \mathcal{H}_n^d}\Big(\int\limits_{\mathbb{S}^d} Y_{n,k}(x)d\nu(x)\Big)^2\right) \\
&=: \mathcal{F}(\nu) - \mathcal{G}(\nu).
\end{aligned}$$

It is easy to see that $\mathcal{G}$ is convex with respect to ν since it is a positive linear combination of squares of linear functionals of ν.

Let us set

$$K = \left\{\nu \in \mathcal{B} : \int\limits_{\mathbb{S}^d} Y_{n,k}\,d\nu(x) = \int\limits_{\mathbb{S}^d} Y_{n,k}\,d\mu(x),\ n \in N_+,\ k = 1, 2, \dots, \dim \mathcal{H}_n^d\right\}.$$

Without loss of generality, we shall assume that $0 \in N_+$. This guarantees that $\nu \in K$ is a probability measure.

Since $\mathcal{G}$ is convex in ν and K is a convex weak-$*$ closed subset of $\mathcal{M}$, $\mathcal{G}(\nu)$ achieves its maximum on K at a point of $\operatorname{ext}(K)$. Hence, there exists a measure $\mu^* \in \operatorname{ext}(K)$ such that $\mathcal{G}(\mu^*) = \sup\limits_{\mu \in K} \mathcal{G}(\mu)$.

We then find that

$$M = \inf_{\nu\in\mathcal{M}} I_F(\nu) = I_F(\mu) = \mathcal{F}(\mu) - \mathcal{G}(\mu) = \mathcal{F}(\mu^*) - \mathcal{G}(\mu) \geq \mathcal{F}(\mu^*) - \mathcal{G}(\mu^*) = I_F(\mu^*) \geq M,$$

i.e. μ^* is also a minimizer of I_F. Applying Karr's Theorem, we obtain the above result on the existence of discrete minimizers of I_F. ☐

We observe that, when F is a positive definite polynomial of degree n, the result of Theorem 4.26 immediately implies the existence of weighted spherical n-designs of cardinality

$$\sum_{k=0}^{n} \dim \mathcal{H}_k^d = \sum_{k=0}^{n} \left(\binom{d+k}{k} - \binom{d+k-2}{k-2} \right) = \binom{d+k}{k} + \binom{d+k-1}{k-1}.$$

5. Fejes Tóth Conjecture of sum of acute angles

In 1959, Fejes Tóth posed a conjecture that the sum of pairwise non-obtuse angles between N unit vectors in $\mathbb{S}^d$ (i.e., angles between lines generated by these vectors) is maximized by periodically repeated elements of the standard orthonormal basis. In terms of energy optimization, this can be phrased as

Conjecture 5.1 (Fejes Tóth [24])**.** *Let $d \geq 1$, $N = m(d+1) + k$ with $m \in \mathbb{N}_0$ and $0 \leq k \leq d$, and $F(t) = \arccos(|t|)$. Then the discrete energy $E_F(Z)$ on $\mathbb{S}^d$ is maximized by the point set $Z = \{z_1, \ldots, z_N\} \subset \mathbb{S}^d$ with $z_{p(d+1)+i} = e_i$, where $\{e_i\}_{i=1}^{d+1}$ is the standard orthonormal basis of $\mathbb{R}^{d+1}$. In this case,*

$$E_F(Z) = \frac{\pi}{2N^2} \left(k(k-1)(m+1)^2 + 2km(d+1-k)(m+1) + (d-k)(d+1-k)m^2 \right). \tag{5.1}$$

In particular, if $N = m(d+1)$, the sum is maximized by m copies of the orthonormal basis:

$$\max_{\substack{Z\subset\mathbb{S}^d \\ \#Z=N}} = \frac{\pi}{2} \cdot \frac{d}{d+1}. \tag{5.2}$$

This conjecture has been independently stated in [31] for all $d \geq 1$ (Fejes Tóth originally formulated it just for $\mathbb{S}^2$, and provided a solution for $N = 4, 5, 6$ points).

This naturally leads to a continuous version of the conjecture:

Conjecture 5.2. *The energy integral $I_F(\mu)$ is maximized by $\frac{1}{d+1}\sum_{i=1}^{d+1} \delta_{e_i}$:*

$$\max_{\mu\in\mathcal{M}} I_F(\mu) = I_F\left(\frac{1}{d+1} \sum_{i=1}^{d+1} \delta_{e_i} \right) = \frac{\pi}{2} \cdot \frac{d}{d+1}. \tag{5.3}$$

The case of $d = 1$ been settled in [9, 28] in several ways: one proof is purely geometric, two are based on orthogonal expansions, and the final one is using the Generalized Stolarsky Principle since F is negative definite on $\mathbb{S}^1$. Moreover, the geometric and discrepancy methods characterize all possible maximizers:

Proposition 5.3 (Bilyk, Matzke [9])**.** *For $x \in \mathbb{S}^1$, let us define the antipodal quadrants in the direction of x as $Q(x) = \{y \in \mathbb{S}^1 : |\langle x, y\rangle| > \frac{\sqrt{2}}{2}\}$. Then we have the following:*

(1) An N-point configuration $Z \subset \mathbb{S}^1$ is a maximizer of $E_F(Z)$ if and only if for every $x \in \mathbb{S}^1$, such that the boundary of $Q(x)$ does not contain any points of Z, i.e. $\partial Q(x) \cap Z = \emptyset$, the number of points of Z in $Q(x)$ and in its complement $\big(Q(x)\big)^c$ differ by at most one.

(2) A measure $\mu \in \mathcal{C}$ is a maximizer of $I_F(\mu)$ if and only if, for σ-almost everywhere $\mu\big(Q(x)\big) = \mu\big(Q(x)^c\big) = \frac{1}{2}$.

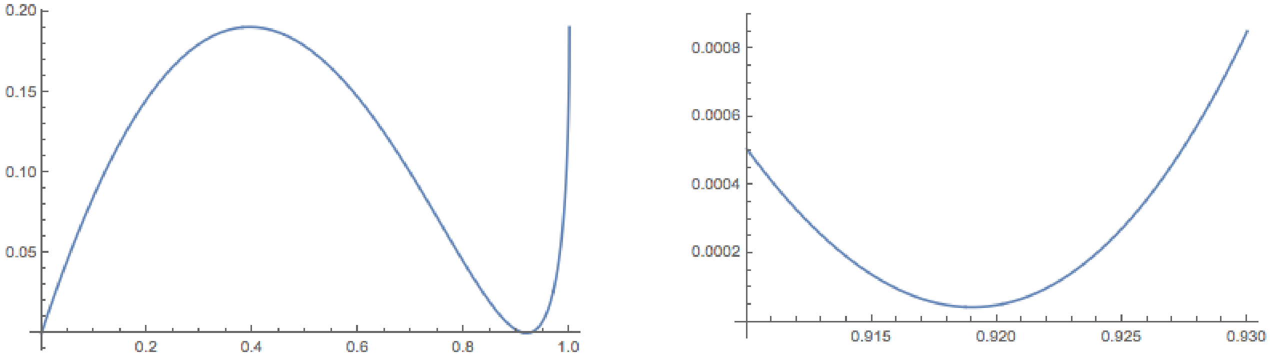

FIGURE 5. An illustration to inequality (5.5): the graph of the function $f(t) = \frac{\pi}{2} - \frac{69}{50}t^2 - \arccos|t|$ for $0 \le t \le 1$.

Unfortunately, none of these approaches immediately extends to higher dimensions: for $d \ge 2$ the function $F(t) = \arccos(|t|)$ is not negative definite, and one cannot obtain a Stolarsky principle. In dimension $d = 2$, Fejes Tóth confirmed Conjecture 5.1 for $N \le 6$ in [25]. Currently, the best known bound, from [9], on I_F is the following:

Theorem 5.4 (Bilyk, Matzke [9]). *In all dimensions $d \ge 2$*

$$\max_{\mu \in \mathcal{M}} I(\mu) \le \frac{\pi}{2} - \frac{69}{50(d+1)}. \tag{5.4}$$

The proof of this result, which improves the best previously known bound on $\mathbb{S}^2$ [28], is surprisingly simple. A simple calculus exercise shows that

$$\arccos(|t|) \le \frac{\pi}{2} - \frac{69}{50}t^2 \tag{5.5}$$

holds for all $t \in [-1, 1]$, which we illustrate with Figure 5. The bound on the frame potential, (4.1), then implies that for all $\mu \in \mathcal{B}(\mathbb{S}^d)$,

$$I(\mu) \le \frac{\pi}{2} - \frac{69}{50} I_{t^2}(\mu) \le \frac{\pi}{2} - \frac{69}{50(d+1)}, \tag{5.6}$$

proving Theorem 5.4.

It is easy to see that there is very little room for improvement via this method, and it will definitely not yield Conjecture 5.2. It seems, however, that it may be possible to adjust the methods of §4.4 to show that the support of any maximizer of I_F must have empty interior.

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