Problems with a lot of Potential: Energy Optimization on Compact Spaces

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Dedication

To Angeliki, Mom, Dad, Jackie, and Ben,

You make the road rise up to meet my feet, make the wind always at my back, make the sun shine warm upon my face, make the rain fall soft upon my field, and bring equilibrium to my life.

Abstract

In this dissertation, we provide a survey of the author's work in energy optimization on compact spaces with continuous potentials. We present several new results relating the positive definiteness of a potential, convexity of its energy functional, and properties of the minimizing measures of the energy, first in general spaces, then specifically on two-point homogeneous spaces, and especially on spheres. We also obtain sufficient conditions for the existence, and in some cases uniqueness, of discrete minimizers for a large class of energies. We discuss the Stolarsky Invariance Principle, which connects discrepancy and energy, as well as some analogues and generalizations of this phenomenon. In addition, we investigate some particularly interesting optimization problems, such as determining the maximum sum of pairwise angles between N points on the sphere $\mathbb{S}^{d-1}$ and the maximum sum of angles between N lines passing through the origin, both of which are related to conjectures of Fejes Tóth. We also study the p-frame energies, which are related to signal processing and quantum mechanics. We show that on the sphere, the support of any minimizer of the p-frame energy has empty interior whenever p is not an even integer, and, moreover, that tight designs are the unique minimizers for certain values of p, among other results. We complete this paper by developing the theory of minimization for energies with multivariate kernels, i.e. energies for which pairwise interactions are replaced by interactions between triples, or more generally, n-tuples of particles. Such objects arise naturally in various fields and present subtle difference and complications when compared to the classical two-input case. We introduce appropriate analogues of conditionally positive definite kernels, establish a series of relevant results in potential theory, and present a variety of interesting examples, including some problems in probabilistic geometry which are related to multivariate versions of the Riesz s-energies.

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Chapter 1

Introduction

In numerous areas of mathematics and other sciences, one is faced with problems that can be reformulated as a question of minimizing the discrete or continuous pairwise interaction energy, i.e. expressions of the type

$$E_K(\omega_N) := \frac{1}{N^2} \sum_{x,y \in \omega_N} K(x,y) \text{ or } I_K(\mu) := \int_\Omega \int_\Omega K(x,y) d\mu(x) d\mu(y) \tag{1.1}$$

where ω_N is a discrete set of N (not necessarily distinct) points in Ω, μ is a Borel probability measure on the domain Ω, and K is the potential function describing the pairwise interaction. Perhaps one of the most famous examples of such a problem is the 1904 Thomson Problem, asking for the minimum electrostatic potential energy configuration(s), i.e. equilibrium distributions (according to Coulomb's Law), of N electrons on the unit sphere, which is notoriously still open for most values of N. Note that in this setting, where $K(x,y) = \frac{1}{\|x-y\|}$, as well as others where $K(x,x) = \infty$ for all $x \in \Omega$, we remove the diagonal terms from the sum in (1.1). In an abstract sense, one can generally view ω_N as a collection of particles (and μ as a charge distribution) which repel or attract according to the potential K.

The interactions described by (1.1) model many natural phenomena beyond electrostatics: swarm behavior, self-assembly in computational chemistry, patterns of pores on spherical pollen grains, and the structure of molecules, to name a few. The problem of determining optimal measures or point distributions for (1.1) also appears in a wide variety of more abstract settings, such as signal processing, coding theory, optimal transport, discrepancy theory, and discrete geometry, among others. In particular, energy optimization provides a method of distributing points on a manifold (i.e. the discretization of a manifold), which arises in several contexts that are of interest to the scientific community: quadrature rules, information theory, interpolation schemes, finite element tessellations, statistical sampling, etc. The vast quantity of applications and connections to other areas has stimulated much study into energy optimization, which has been developed into a full-blown theory whose state of the art is well presented in [BHS19].

In the present work, we add to the current theory by providing new methods to determine minimizers for certain classes of energies. While characterizing optimizers for energies (1.1) is of particular interest, this can often prove to be a difficult problem to address completely, so we also present methods to determine certain general properties, such as the discreteness or concentration of a minimizing measure's support. We also apply our methods to a number of interesting potentials.

We collect all of the necessary preliminary material in Chapter 2. In Chapter 3 we explore, and show connections between, a variety of properties of kernels K, their energy integrals I_K, and local and global minimizers of such energies. In particular, we provide numerous necessary and sufficient conditions in Section 3.3 to determine whether or not a measure μ with full support is a minimizer of I_K. In Sections 3.4 and 3.5, we provide some additional results specific to the compact, connected, two-point homogeneous spaces and the sphere, respectively. The new results in this chapter come predominantly from [BMV].

It shall be shown in Chapter 3 that if K is not positive definite (modulo an additive constant) on Ω then any minimizer of I_K cannot have full support. This naturally begs the question of what the support of minimizing measures could be in this situation. In Chapter 4, we provide some answers to this question, particularly on the compact, connected, two-point homogeneous spaces. Section 4.1 uses the structure of extreme points of sets of moment-constrained measures to provide a sufficient condition for I_K to have a discrete minimizer on the sphere. In Section 4.2, we show that for analytic kernels that are not positive definite (modulo a constant), the support of any minimizer must have empty interior. In Section 4.3, we make use of a linear programming method to show that tight designs are (possibly unique) minimizers of certain energies. This chapter is based on work from [BGM$^+$a, BGM$^+$b].

In Chapter 5, we present results that appear in [BDM18, BMV]. The problem of determining optimal configurations for E_K for a fixed number N of points on the sphere is often more delicate than finding the optimal measures for I_K. In the case that σ, the normalized Lebesgue measure on $\mathbb{S}^{d-1}$, is a minimizer of I_K, one might expect that as N increases, minimizers of E_K should be "uniformly distributed," in some sense, in order to approximate σ. Chapter 5 discusses using discrepancy, a popular means of measuring uniformity of distribution of points on the sphere, to determine minimizers of I_K and E_K for positive definite functions K via a Generalized Stolarsky Principle. Section 5.1 provides a simple proof of the classic Stolarsky Invariance Principle, and in Section 5.2, we present an analogue that addresses a conjecture of Fejes Tóth about the maximum sum of geodesic distances on the sphere. The Generalized Stolarsky Principle on spheres, and more generally in compact metric spaces, is then given in section 5.3 and 5.4, respectively.

In Chapter 6 we discuss the p-frame energies, introduced by Ehler and Okoudjou in [EO12] as a generalization of the frame energy, which Benedetto and Fickus used in [BF03] to classify finite unit norm tight frames (FUNTFs). We discuss the frame energy in Section 6.1 and the more general p-frame energy in Section 6.2, in particular applying the results of Section 4.3 to show that for some values of P, tight designs minimize the p-frame energy, when they exist. Section 6.3 shows that the 600-cell is also a minimizer for certain p-frame energies. In Section 6.2, we conjecture that for $p \notin 2\mathbb{N}$, all minimizers of the p-frame energy are discrete. Though a proof of this conjecture remains elusive, in Section 6.4, we show that for these p-frame energies on the real sphere, the support of any minimizer must have empty interior. Section 6.5 extends some of our results to a non-compact setting, and Section 6.6 connects our results to a problem from Convex Geometry. The results in this chapter are based on the work in [BGM^+a, BGM^+b].

In Chapter 7, we discuss a conjecture of Fejes Tóth about the maximum sum of acute angles of points on the sphere, and present new results in this direction in Section 7.1, as well as new proofs for the conjecture on $\mathbb{S}^1$ in Section 7.2. The results presented were obtained in [BM19].

Chapter 8 addresses a different type of problem than the other sections. In the last few decades, many-body interactions (i.e. kernels with three or more inputs instead of two) have become a greater subject of interest in material science, quantum mechanics, and discrete geometry. While a great deal of theory has been developed to address energy optimization problems that form from two-body interactions, i.e., those described in (1.1), very little exists for optimizing energies of the form

$$\frac{1}{N^n}\sum_{j_1=1}^{N}\cdots\sum_{j_n=1}^{N}K(x_{j_1},\dots,x_{j_n}) \text{ or } \int_{\Omega}\cdots\int_{\Omega}K(x_1,\dots,x_n)d\mu(x_1)\dots d\mu(x_n). \tag{1.2}$$

To address these deficiencies, we present the first steps in developing a general theory for such energies. In Section 8.1, we introduce some relevant notation and definitions, in particular defining n-positive definiteness, a generalization of positive definiteness. In Sections 8.2, 8.3, and 8.4, we provide various necessary and sufficient conditions for a measure μ to be a minimizer of the n-input energy. Many of these results are analogues, for our multivariate setting, of results in Chapter 3. In Sections 8.5 and 8.6, we present examples of n-input kernels which are (conditionally) n-positive definite and which are not, respectively. In Section 8.7, we adapt the semidefinite programming method from [BV08] to our setting, and apply that method, as well as others, to answer certain questions from probabilistic discrete geometry. This chapter is based on work from [BFG^+a, BFG^+b].

1.1 Summary of Main Results

The following is a list of the main results of this thesis.

- A list of properties equivalent to a kernel K being conditionally positive definite when there exists a K-invariant probability measure of full support (Theorem 3.3.1). Similar characterizations are provided for positive definiteness (Theorem 3.3.2) and conditionally strict positive definiteness (Theorem 3.3.3).

- The existence of discrete minimizers for the energy of any rotationally invariant kernel on the sphere with finitely many positive Gegenbauer coefficients (Theorem 4.1.3).

- A proof that the energy of a real-analytic kernel that is not positive definite (modulo a constant) on the sphere can only be minimized by a measure whose support has empty interior (Theorem 4.2.1).

- Characterizations of large classes of energies on spheres and projective spaces for which tight designs are minimizers (Theorem 4.3.1) and for which tight designs are unique minimizers (Theorem 4.3.12).

- An explicit connection between L^2 discrepancy with respect to hemisphere and the sum of geodesic distances of any point set on the sphere (Theorem 5.2.1). This is used to provide a complete solution of a conjecture of Fejes Tóth, which characterized all configurations on a sphere that maximize the sum of geodesic distances between points on the sphere (Theorem 5.2.10).

- Generalizations of the Stolarsky Invariance Principle for positive definite kernels on the sphere (Theorem 5.3.1) and positive definite kernels on general compact metric spaces (Theorem 5.4.1).

- A classification of p-frame energies for which tight designs are the unique minimizers (Theorem 6.2.3).
- A proof that the minimizers of the p-frame energy on the sphere necessarily have empty interior, whenever p is not a even integer (Theorem 6.4.1).
- The best known bound on the acute angle energy, which comes from a conjecture of Fejes Tóth (Theorem 7.1.1).
- Development of an initial theory for energy optimization with multivariate kernels (Chapter 8). In particular:
  - Necessary (Theorem 8.3.2) and sufficient (Theorem 8.3.3) conditions for a measure to minimize an multivariate energy.
  - The relationship between the local minimizers of a multivariate energy, and the corresponding two-input potential (Theorem 8.3.8).
  - The determination of a large class of multivariate energies on the sphere for which the uniform measure is a minimizer, based on a semidefinite programming method (Theorem 8.7.1).
  - A characterization of the maximizing measures of the expected value of the squared area of a triangle with i.i.d. vertices on the sphere (Theorem 8.8.4).

1.2 Notation

We shall use the following notation throughout the text.

$\mathbb{R}$	The set of real numbers
$\mathbb{C}$	The set of complex numbers
$\mathbb{H}$	The set of quaternions

$\mathbb{O}$	The set of octonions
$\mathbb{F}$	$\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$, or $\mathbb{O}$
$\langle x,y\rangle_H$	The inner product for some Hilbert space H
$\langle\cdot,\cdot\rangle$	The inner product on $\mathbb{R}^d$, $\mathbb{C}^d$, or $\mathbb{H}^d$
$\|\|x\|\|_H$	The norm for some space H
$\|\|x\|\|$	The Euclidean norm on $\mathbb{R}^d$, $\mathbb{C}^d$, or $\mathbb{H}^d$
$\dim_{\mathbb{R}}(\mathbb{F})$	The dimension of $\mathbb{F}$ as a real manifold
$\mathbb{N}$	The set of positive integers
$\mathbb{N}_0$	The set of nonnegative integers
$\Omega=(\Omega,\rho)$	A metric space, compact unless stated otherwise
$\Phi=\Phi^{(\alpha,\beta)}$	A compact, connected, two-point homogeneous space
$\mathbb{FP}^{d-1}$	The projective space over $\mathbb{F}$
$\mathbb{S}^{d-1}$	The $(d-1)$-dimensional unit sphere in $\mathbb{R}^d$
α	For $\mathbb{S}^{d-1}$ or $\mathbb{FP}^{d-1}$, $\frac{(d-1)\dim_{\mathbb{R}}(\mathbb{F})}{2}-1$
β	α for $\Phi=\mathbb{S}^{d-1}$ and $\frac{\dim_{\mathbb{R}}(\mathbb{F})}{2}-1$ for $\Phi=\mathbb{FP}^{d-1}$
$\mathbb{S}^{d-1}_{\mathbb{F}}$	The $(d-1)$-dimensional unit sphere in $\mathbb{F}^d$
$L^2(\Omega,\mu)$	The space of real-valued square-integrable functions on Ω
$L^2(\Omega,\mu,\mathbb{C})$	The space of complex-valued square-integrable functions on Ω
$V_n=V_n^{(\alpha,\beta)}$	The eigenspaces of the Laplace-Beltrami operator on $\Phi^{(\alpha,\beta)}$
$Y_{n,k}=Y_{n,k}^{(\alpha,\beta)}$	The basis elements of $V_n^{(\alpha,\beta)}$
$\mathscr{H}_n^d$	The space of spherical harmonics of degree n on $\mathbb{S}^{d-1}$
λ	For the sphere $\mathbb{S}^{d-1}$, $\frac{d-2}{2}$
$\gamma_{\alpha,\beta}$	$2^{\alpha+\beta+1}B(\alpha+1,\beta+1)$, where B is the beta function
A_{d-1}	The surface area of $\mathbb{S}^{d-1}$
Vol_d	The volume of the unit ball in $\mathbb{R}^d$
η	The normalized uniform surface measure on Φ
σ	The normalized $(d-1)$-dimensional Hausdorff measure on $\mathbb{S}^{d-1}$

$d\nu^{(\alpha,\beta)}(t)$	$\frac{1}{\gamma_{\alpha,\beta}}(1-t)^{\alpha}(1+t)^{\beta}dt$
$dw_{\lambda}(t)$	$\frac{\Gamma(\lambda+1)}{\sqrt{\pi}\Gamma(\lambda+\frac{1}{2})}(1-t^2)^{\lambda-\frac{1}{2}}dt$
$\mathbb{P}(\Omega)$	The set of Borel probability measures on Ω
$\mathbb{P}^*(\Omega)$	The subset of $\mathbb{P}(\Omega)$ satisfying $\int_{\Omega} \lvert\lvert x\rvert\rvert^2 d\mu(x) = 1$
$\widetilde{\mathbb{P}}(\Omega)$	The set of signed probability measures on Ω
$\mathscr{M}(\Omega)$	The set of finite signed Borel measures on Ω
$\mathscr{Z}(\Omega)$	The set of finite signed Borel measures ν such that $\nu(\Omega) = 0$
$\mathscr{B}(\Omega)$	The set of finite positive Borel measures on Ω
ϑ	The geodesic (Riemannian) metric on Φ
ϑ^*	The normalization of ϑ, i.e. $\frac{\vartheta}{\pi}$
$\mathscr{D}$	The Euclidean metric, i.e. $\mathscr{D}(x,y) = \lVert x-y\rVert$
ρ	The chordal metric on Φ
$\tau(x,y)$	$\cos(\vartheta(x,y))$ for $x,y \in \Phi$
$\lvert Z\rvert$	The cardinality of a finite set Z
$P_n^{(\alpha,\beta)}$	The Jacobi polynomials, scaled so that $P_n^{(\alpha,\beta)}(1) = \dim(V_n^{(\alpha,\beta)})$
$C_n = C_n^{(\alpha,\beta)}$	The Jacobi polynomials, scaled so that $C_n(1) = 1$
$Q_n = Q_n^{(\alpha,\beta)}$	The monic Jacobi polynomials, i.e. scaled so the leading coefficient is 1
C_n^{λ}	The Gegenbauer polynomials
$\widehat{F}_n = \widehat{F}_n^{(\alpha,\beta)}$	The Jacobi coefficient of F with respect to $C_n^{(\alpha,\beta)}$
$\widehat{F}(n,\lambda)$	The Gegenbauer coefficients of F
$\mathscr{C}$	A code (finite point configuration) on Φ
$\mathscr{A}(\mathscr{C})$	The "distance set" of $\mathscr{C}$, $\{\tau(x,y) : x,y \in \mathscr{C}\}$
$C(z,h)$	The spherical cap of height h centered at z, i.e. $\{x \in \mathbb{S}^{d-1} : \langle x,z\rangle > h\}$
$p_{\mathbb{F}}$	The projection from the sphere $\mathbb{S}_{\mathbb{F}}^{d-1}$ to the projective space $\mathbb{FP}^{d-1}$
$e_1,\ldots,e_d$	The standard orthonormal basis in $\mathbb{R}^d$
$\overline{Y}$	The complex-conjugate of a function Y
$diam(\Omega)$	The diameter of Ω, i.e. $\sup_{x,y\in\Omega} \rho(x,y)$

$\text{supp}(\mu)$	The support of μ.
$\overline{A}$	The closure of a set A
U°	The interior of a set U

Chapter 2

Background

We begin with some important background material. Section 2.1 contains the discussion of background for our study of energy, including an introduction to the Riesz s-energies. Sections 2.2 and 2.3 introduce positive definiteness and various consequences of this property, including Mercer's Theorem and resulting characterization of positive definite kernels. In Section 2.4, we discuss compact, connected, two-point homogeneous spaces and covers the relevant properties of such spaces and the corresponding system of orthogonal, isometry invariant polynomials. Section 2.5 does the same for the real unit sphere. In Section 2.6, we provide an exposition on designs and, in particular, tight designs.

2.1 Energy

Unless otherwise noted, in what follows, we assume that (Ω, ρ) is a compact metric space and that the kernel (also referred to as potential) $K : \Omega^2 \to \mathbb{R}$ is continuous and symmetric, i.e. for all $x, y \in \Omega$, $K(x,y) = K(y,x)$. We denote by $\mathscr{M}(\Omega)$ the set of finite signed Borel measures on Ω, and by $\mathbb{P}(\Omega)$ the set of Borel probability measures on Ω.

Given $\mu, \nu \in \mathscr{M}(\Omega)$, we define their mutual/mixed K-energy as

$$I_K(\mu,\nu) = \int_\Omega \int_\Omega K(x,y)\,d\mu(x)\,d\nu(y), \tag{2.1}$$

and the (continuous) K-energy of μ to be

$$I_K(\mu) := I_K(\mu,\mu) = \int_\Omega \int_\Omega K(x,y)\,d\mu(x)\,d\mu(y). \tag{2.2}$$

We are interested in finding the optimal (maximal or minimal, depending on K) values of $I_K(\mu)$ over all $\mu \in \mathbb{P}(\Omega)$, as well as extremal measures for which these values are achieved, i.e. equilibrium measures with respect to K. Note that the minimization of I_K is equivalent to the maximization of I_{-K}, so we will often discuss optimization problems in terms of minimization, but switch to energy maximization when it is more convenient. In various parts of the text, we will be interested in local minimizers or global minimizers over different sets of measures, so it is worth specifying here that whenever we say a measure μ is a "minimizer" of I_K without any additional conditions, we mean that μ is a global minimizer of I_K over $\mathbb{P}(\Omega)$, i.e. for all $\nu \in \mathbb{P}(\Omega)$, $I_K(\mu) \le I_K(\nu)$. We denote the minimal continuous K-energy, i.e. the Wiener constant, by

$$\mathscr{I}_K(\Omega) = \inf_{\mu \in \mathbb{P}(\Omega)} I_K(\mu). \tag{2.3}$$

A naturally related question is that of discrete energy optimization. Let $\omega_N = \{z_1, z_2, \ldots, z_N\}$ be an N-point configuration (multiset) in Ω for $N \ge 2$. We define the discrete K-energy of ω_N to be

$$E_K(\omega_N) = \frac{1}{N^2} \sum_{x,y \in \omega_N} K(x,y) \tag{2.4}$$

and the minimal discrete N-point K-energy of Ω as

$$\mathscr{E}_K(\Omega,N) := \inf_{\omega_N \subseteq \Omega} E_K(\omega_N). \tag{2.5}$$

Note that since we are working with continuous K, the energy I_K is well-defined for all finite signed Borel measures. In addition, the compactness of Ω implies that $\mathbb{P}(\Omega)$ is weak* compact and guarantees the existence of global minimizers for both discrete and continuous energies.

The definitions of discrete (2.4) and continuous (2.2) energies are compatible in the sense that

$$E_K(\omega_N) = I_K(\mu_{\omega_N}), \quad \text{where } \mu_{\omega_N} = \frac{1}{N}\sum_{x\in\omega_N}\delta_x \tag{2.6}$$

and due to the weak* density of the linear span of Dirac masses in $\mathbb{P}(\Omega)$, we have the following lemma [Cho58, FN08].

Lemma 2.1.1. *For any continuous kernel K on Ω,*

$$\lim_{N\to\infty} \mathscr{E}_K(\Omega,N) = \mathscr{I}_K(\Omega). \tag{2.7}$$

Moreover, suppose that $\{\omega_N\}_{N=2}^{\infty}$ is a sequence of N-point configurations on Ω satisfying

$$\lim_{N\to\infty} E_K(\omega_N) = \mathscr{I}_K(\Omega),$$

and define, for each $N \geq 2$,

$$\mu_{\omega_N} = \frac{1}{N}\sum_{x\in\omega_N}\delta_x.$$

If $\mathscr{N} \subset \mathbb{N}$ is a sequence of integers such that μ_{ω_N} weak converges to a probability measure μ as $N\to\infty$, $N\in\mathscr{N}$, then*

$$I_K(\mu) = \mathscr{I}_K(\Omega)$$

i.e. μ is a minimizer of I_K.

For a measure $\mu \in \mathbb{P}(\Omega)$, we define the *potential* U_K^μ of μ with respect to K as

$$U_K^\mu(x) := \int_\Omega K(x,y)d\mu(y),\ x \in \Omega. \tag{2.8}$$

Notice that this meaning of the term "potential" is consistent with us calling K a potential, since the function $K(x,y)$ is simply the potential generated by a unit point charge at y, i.e. $K(x,y) = U_K^{\delta_y}(x)$.

Though this work predominantly focuses on energy minimization with compact domains Ω and continuous kernels K, energy optimization need not be restricted to such settings. For instance, if (Ω, ρ) is an arbitrary metric space, energy minimization is sensible so long as we can guarantee the existence of optimal discrete sets or probability measures. This clearly occurs when Ω is compact and K continuous, but for non-compact Ω, continuity of the kernel K is no longer sufficient. Instead, the compactness of the support of minimizers can be achieved by placing certain additional restrictions on our kernel K, as will be discussed in the introduction of Chapter 4, or by placing some conditions on the set of measures we optimize over, as will be discussed in Section 6.5.

Another, more common, generalization is to consider lower semi-continuous kernels $K : \Omega^2 \to (-\infty, \infty]$. In this setting, one often removes the diagonal terms from 2.4 (and must if $K(x,x) = \infty$ for all $x \in \Omega$), and can only consider the mutual energy of finite signed measures $\mu, \nu \in \mathscr{M}(\Omega)$ if $I_K(\mu, \nu)$ is well-defined. Many of the results we present in Section 3.3 have analogues or generalizations to lower semi-continuous kernels, though the proofs are often more technically demanding, by necessity.

The most famous family of lower semi-continuous kernels in Potential Theory are known as the Riesz s-kernels, defined by

$$D_s(x,y) = ||x-y||^{-s} \quad s \in \mathbb{R} \setminus \{0\}. \tag{2.9}$$

The optimization of Riesz s-energies is related to several other well-known problems in mathematics and other sciences and has been the subject of study for over a century, with the physicist J.J. Thomson posing the problem of finding the minimizers of E_{D_1} on $\mathbb{S}^2$ in 1904. Though exact minimizing configurations for the Thompson problem are known only for a few values of N [And96, Föp12, Sch, Sch20, Yud92], the asymptotic behavior of minimizers of the discrete Riesz s-energies are better understood. In particular, on the sphere $\mathbb{S}^{d-1}$, it is known that for all $s > 0$, minimizing point configurations are asymptotically uniformly distributed with respect to the normalized $(d-1)$-dimensional Hausdorff measure on the sphere, σ [KS98, Lan72]. For $s \geq d$, this result, known as the "Poppy-Seed Bagel Theorem," has been generalized to d-rectifiable manifolds [HS05]. This is a natural consequence of the fact that as $s \to \infty$ with N fixed, the discrete Riesz s-energy is increasingly dominated by the term(s) involving the smallest pairwise distances, a property that, on the sphere, leads to the limiting case (i.e. $s = \infty$) being the best-packing problem [CS99, BHS19].

In the case where $s < 0$, we see that the Riesz s-kernels are continuous, and the optimization problem becomes one of maximization instead of minimization. The maximum value of I_{D_s} for $s < 0$ was first studied by Pólya and Szegö on spheres and balls in [PS31]. In [Bjö56], Björck determined properties of maximizing measures on general compact sets.

Theorem 2.1.2. *Let $d \geq 1$, $s < 0$, and $\Omega \subseteq \mathbb{R}^d$ be compact. If μ is a maximizer of I_{D_s} over $\mathbb{P}(\Omega)$, then the following hold:*

1. $\mathrm{supp}(\mu)$ *is a subset of the boundary of Ω, i.e. $\overline{\Omega} \setminus \Omega^{\circ}$, where $\overline{\Omega}$ and Ω° are the closure and interior of Ω in $\mathbb{R}^d$, respectively.*

2. *if $s < -1$, then* $\mathrm{supp}(\mu)$ *is a subset of the extreme points of the convex hull of Ω.*

3. *If $s < -2$, then μ is a discrete measure consisting of no more than $d+1$ point masses.*

4. *If $0 > s > -2$, then μ is the unique maximizer of I_{D_s}.*

Moreover, on the sphere, Björck was able to completely characterize the maximizer of these Riesz s-energies on the unit sphere $\mathbb{S}^d$, see Theorem 5.2.9.

We finish this section with a fairly basic and intuitive idea, but one which will play an important role in our results.

Lemma 2.1.3. *If $\mu \in \mathbb{P}(\Omega)$ is a minimizer of I_K, then for all $C \in \mathbb{R}$, μ is a minimizer of I_{K+C}. Likewise, if ω_N is a minimizer of E_K over all N-point configurations in Ω then for all $C \in \mathbb{R}$, ω_N is also a minimizer of E_{K+C}*

Proof. Let $C \in \mathbb{R}$. For all $\nu \in \mathbb{P}(\Omega)$,

$$I_{K+C}(\nu) = I_K(\nu) + (\nu(\Omega))^2 C = I_K(\nu) + C \geq I_K(\mu) + C = I_{K+C}(\mu).$$

The discrete case follows immediately from the continuous case. □

For a more comprehensive exposition on Energy Optimization, especially one that discusses lower semi-continuous kernels and Riesz s-energy in greater detail, we refer the reader to [BHS19].

2.2 Positive Definite Kernels

We now recall the classical notion of positive definite kernels, which play an extremely important role in various areas of mathematics, such as Partial Differential Equations, Machine Learning, and Probability. Here, we will focus on their relation to energy minimization problems, but an exposition on their role in other areas can be found in [Fas11]. We state the definition in the form most relevant to our work.

Definition 2.2.1. *A kernel $K : \Omega^2 \to \mathbb{R}$ is called* ***conditionally positive definite*** *if for every $\nu \in \mathscr{Z}(\Omega)$ (i.e. finite signed Borel measures satisfying $\nu(\Omega) = 0$), $I_K(\nu) \geq 0$.*

If, moreover, $I_K(\nu) \geq 0$ for every finite signed Borel measure, i.e. $\nu \in \mathscr{M}(\Omega)$, then we call K ***positive definite***.

We call a ***kernel strictly positive definite*** *or* ***conditionally strictly positive definite*** *if it is positive definite or conditionally positive definite, respectively, and* $I_K(\nu) = 0$ *only if* $\nu(A) = 0$ *for all Borel sets* $A \subseteq \Omega$*.*

If there exists some $C \in \mathbb{R}$ *such that* $K + C$ *is a (strictly) positive definite kernel, we call* K ***(strictly) positive definite modulo an additive constant*** *(or up to an additive constant).*

A more standard way of defining positive definiteness of a kernel $K : \Omega^2 \to \mathbb{R}$ is by requiring, for every $n \in \mathbb{N}$ and $\{z_i\}_{i=1}^N \subset \Omega$, the matrix $\left[K\left(z_i, z_j\right)\right]_{i,j=1}^N$ is positive semidefinite, i.e. for any sequence $\{c_i\}_{i=1}^N \subset \mathbb{R}$, the kernel K satisfies the inequality

$$\sum_{i,j=1}^{N} c_i c_j K\left(z_i, z_j\right) \geq 0. \tag{2.10}$$

Since our kernel K is continuous, this is clearly equivalent to Definition 2.2.1 due to the weak* density of discrete measures in $\mathscr{M}(\Omega)$.

Occasionally in this text, especially when focusing on energy maximization, we will also want to make use of the negative definiteness of a kernel. We shall call a kernel K *negative definite* if the kernel $-K$ is positive definite.

A constant, positive kernel, i.e. $K(x,y) = c > 0$ for all $x, y \in \Omega$, is clearly positive definite, so it is clear such kernels always exist. Moreover, we can construct continuous positive definite kernels in the following way:

Lemma 2.2.2. *For* $j \in \mathbb{N}_0$*, let* $\lambda_j \geq 0$ *and* $\phi_j : \Omega \to \mathbb{R}$ *be continuous. Then if the series converges absolutely and uniformly, the kernel*

$$K(x,y) = \sum_{j=0}^{\infty} \lambda_j \phi_j(x) \phi_j(y) \tag{2.11}$$

(which is continuous, due to uniform convergence) is positive definite.

Proof. Let $\mu \in \mathscr{M}(\Omega)$. Then

$$\begin{aligned} I_K(\mu) &= \sum_{j=0}^{\infty} \lambda_j \int_\Omega \int_\Omega \phi_j(x)\phi_j(y)d\mu(x)d\mu(y) \\ &= \sum_{j=0}^{\infty} \lambda_j \Big(\int_\Omega \phi_j(x)d\mu(x) \Big)^2 \\ &\geq 0. \end{aligned}$$

□

In Section 2.3, we will show that this actually provides a characterization of positive definite kernels.

In addition to a relatively simple characterization, positive definite kernels have several other useful properties, many of which will be discussed in Chapter 3. To begin with, they are closed under addition, multiplication (a result known as the Schur product theorem), and limits of uniformly convergent sequences.

Lemma 2.2.3. *If K and L are positive definite kernels on Ω, then so are $K+L$ and KL. If $K_1, K_2, \ldots,$ are positive definite and $\lim_{n\to\infty} K_n = K$ uniformly, then K is positive definite. The statements regarding the sum and limit (but not the product) hold if we replace positive definiteness with conditional positive definiteness.*

Though the theory tends to focus on the (strict) positive definiteness of kernels, Lemma 2.1.3 shows us that adding a constant does not affect the minimizer, so we often consider kernels that are (strictly) positive definite modulo a constant. However, adding a constant never changes conditional (strict) positive definiteness, as for all $C \in \mathbb{R}$ and $\nu \in \mathscr{Z}(\Omega)$,

$$I_{K+C}(\nu) = I_K(\nu) + (\nu(\Omega))^2 C = I_K(\nu).$$

Since (strict) positive definiteness implies conditional (strict) positive definiteness, we arrive at the following lemma.

Lemma 2.2.4. *If K is (strictly) positive definite modulo a constant, then K is conditionally (strictly) positive definite.*

In Section 3.3, we will demonstrate that the converse of Lemma 2.2.4 can hold under certain conditions. However, it does not hold in general:

Example 2.2.5. *Consider $K : \left(\mathbb{S}^{d-1}\right)^2 \to \mathbb{R}$ defined by $K(x,y) = x_1 + y_1$, where $x_1 = \langle x, e_1 \rangle$ here. Then K is conditionally positive definite, but not positive definite modulo a constant.*

Proof. For all $\nu \in \mathscr{Z}(\mathbb{S}^{d-1})$,

$$I_K(\nu) = 2 \int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} x_1 d\nu(x) d\nu(y) = 0,$$

so K is conditionally positive definite.

Now we show there is no constant C such that $K + C$ is positive definite. If $C < 0$, then

$$I_{K+C}(\sigma) = 2 \int\limits_{\mathbb{S}^{d-1}} x_1 d\sigma(x) + C = C < 0.$$

Suppose that $C \geq 0$ and let $\mu = (C+1)\delta_{-e_1} - C\delta_{e_1} \in \mathscr{M}(\mathbb{S}^{d-1})$. Then

$$\begin{aligned} I_{K+C}(\mu) &= 2\mu(\mathbb{S}^{d-1}) \int\limits_{\mathbb{S}^{d-1}} x_1 d\mu(x) + C(\mu(\mathbb{S}^{d-1}))^2 \\ &= 2(-2C-1) + C \\ &= -3C - 2 < 0. \end{aligned}$$

Our proof is now complete. □

We complete this section by presenting an interesting result that allows one to construct positive definite kernels from conditionally positive definite ones, a result we shall use in Chapter 8.

Lemma 2.2.6 (Chp. 3, Lemma 2.1, [BCR84]). *Let $x_0 \in \Omega$, $K : \Omega^2 \to \mathbb{R}$ be a kernel, define*

$$K'(x,y) := K(x,y) + K(x_0,x_0) - K(x,x_0) - K(x_0,y).$$

Then K' is positive definite if and only if K is conditionally positive definite. If $K(x_0,x_0) \leq 0$ and

$$K'_0(x,y) := K(x,y) - K(x,x_0) - K(x_0,y),$$

then K'_0 is positive definite if and only if K is conditionally positive definite.

2.3 Mercer's Theorem

Let μ be a Borel probability measure on Ω and let K be a continuous kernel on Ω. We shall consider the operator $T_{K,\mu}$ associated to K on the space of real-valued functions on Ω that are square-integrable with respect to μ, $L^2(\Omega,\mu)$. This is a linear integral operator, with kernel K, defined by

$$T_{K,\mu}\psi(x) = \int_{\Omega} K(x,y)\psi(y)d\mu(y). \tag{2.12}$$

Lemma 2.3.1. *Let $\widetilde{\Omega} = \mathrm{supp}(\mu)$. The operator $T_{K,\mu}$ is self-adjoint and Hilbert-Schmidt, and the eigenfunctions of $T_{K,\mu}$ corresponding to non-zero eigenvalues are continuous on $\widetilde{\Omega}$. The kernel K is positive definite on $\widetilde{\Omega}$ if and only if $T_{K,\mu}$ is a positive operator on $L^2(\Omega,\mu)$.*

Proof. Self-adjointedness immediately follows from $K(x,y)$ being symmetric. Since Ω is compact (and hence $\widetilde{\Omega}$ is also) and K continuous, we know that

$$\int_{\Omega}\int_{\Omega} |K(x,y)|^2 d\mu(x)d\mu(y) < \infty,$$

which implies that $T_{K,\mu}$ is Hilbert-Schmidt.

Now, suppose that $T_{K,\mu}\phi = \lambda\phi$ for $\lambda \neq 0$. Then the representation

$$\phi(x) = \frac{1}{\lambda}\int_{\Omega} K(x,y)\phi(y)d\mu(y)$$

implies that ϕ is continuous on $\widetilde{\Omega}$.

We now show that the positive definiteness of K and the positivity of $T_{K,\mu}$ are equivalent. If K is positive definite on $\widetilde{\Omega}$, then for any $\psi \in L^2(\Omega,\mu)$,

$$\langle \psi, T_{K,\mu}\psi\rangle_{L^2(\Omega,\mu)} = \int_{\Omega}\int_{\Omega} K(x,y)\psi(x)\psi(y)d\mu(x)d\mu(y) = I_K(\psi(\cdot)\mu) \geq 0,$$

so $T_{K,\mu}$ is indeed positive.

Assume instead that $T_{K,\mu}$ is positive. Observe that measures, which are absolutely continuous with respect to μ and have bounded density, i.e. measures of the form $d\nu = f\,d\mu$, where f is a bounded Borel measurable function on $\widetilde{\Omega}$, are weak* dense in $\mathscr{M}(\widetilde{\Omega})$. To show this, notice that for each ball $B(z,r)$ of radius $r > 0$ centered at the point $z \in \widetilde{\Omega}$, we have $\mu(B(z,r)) \neq 0$, and therefore, the functions $f_r(x) = \frac{1}{\mu(B(z,r))}\mathbb{1}_{B(z,r)}(x)$ are well-defined and bounded. Obviously, the measures ν_r defined by $d\nu_r = f_r\,d\mu$ converge weak* to δ_z as $r \to 0$, which suffices due to weak* density of discrete measures.

Then for all such measures of the form $d\nu = f\,d\mu$, since bounded functions are in $L^2(\Omega,\mu)$, we have

$$I_K(\nu) = \langle T_{K,\mu}f, f\rangle \geq 0,$$

and by weak* density, it follows that K is positive definite on $\widetilde{\Omega}$. □

Moreover, since $T_{K,\mu}$ is a Hilbert-Schmidt operator, it is in fact a compact operator. Hence, we may apply the Spectral Theorem.

Theorem 2.3.2 (Spectral Theorem for Compact Operators)**.** *Suppose that H is a Hilbert space and $T : H \to H$ is a compact, self-adjoint operator. Then there exists an orthonor-*

mal basis $\{\phi_j\}_{j=1}^{\dim(H)}$ *of* H *consisting of eigenvectors of* T *and corresponding eigenvalues* $\{\lambda\}_{j=1}^{\dim(H)}$ *such that* $|\lambda_j| \geq |\lambda_{j+1}|$ *for* $1 \leq j < \dim(H)$*. If* $\dim(H) = \infty$*, then* $\lim_{j\to\infty} \lambda_j = 0$*.*

Thus, there exists an orthonormal basis $\{\phi_j\}_{j=1}^{\dim(L^2(\Omega,\mu))}$ of $L^2(\Omega,\mu)$ consisting of eigenfunctions of $T_{K,\mu}$, i.e. $T_{K,\mu}\phi_j = \lambda_j \phi_j$, where the sequence of eigenvalues satisfies $|\lambda_j| \geq |\lambda_{j+1}|$ and $\lim_{j\to\infty} \lambda_j = 0$ if $\dim(L^2(\Omega,\mu)) = \infty$. Moreover, the Spectral Theorem tells us that, in the L^2 sense,

$$K(x,y) = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \lambda_j \phi_j(x)\phi_j(y).$$

For the rest of this section, we will assume that $\operatorname{supp}(\mu) = \Omega$, in other words, every non-empty open subset of Ω has strictly positive measure (if $\operatorname{supp}(\mu) \neq \Omega$, then the results of this section apply for $\widetilde{\Omega} = \operatorname{supp}(\mu)$), and that K, $\{\phi_j\}_{j=1}^{\dim(L^2(\Omega,\mu))}$, and $\{\lambda\}_{j=1}^{\dim(L^2(\Omega,\mu))}$ are as above. If K is positive definite, we know that $T_{K,\mu}$ is a positive operator, so for each $j \geq 1$,

$$\lambda_j = \langle \phi_j, \lambda_j \phi_j \rangle_{L^2(\Omega,\mu)} = \langle \phi_j, T_{K,\mu}\phi_j \rangle_{L^2(\Omega,\mu)} \geq 0.$$

Mercer's theorem then provides a series representation for any positive definite kernel K.

Theorem 2.3.3 (Mercer's Theorem)**.** *If* $K(x,y)$ *is positive definite, then*

$$K(x,y) = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \lambda_j \phi_j(x)\phi_j(y), \tag{2.13}$$

where the sum converges absolutely and uniformly.

It is worth noting that it would suffice to assume that K is continuous and that all eigenvalues of $T_{K,\mu}$ are nonnegative (which is in fact equivalent to K being positive definite).

Proof. As mentioned above, the fact that (2.13) holds in the L^2 sense follows from the Spectral Theorem for compact operators, hence, only uniform and absolute convergence need to be proven. They immediately follow if $\dim(L^2(\Omega,\mu)) < \infty$, so we assume that $L^2(\Omega,\mu)$ is infinite dimensional.

Consider the remainder of the series, i.e. the continuous function

$$R_N(x,y) = K(x,y) - \sum_{j=1}^{N} \lambda_j \phi_j(x)\phi_j(y).$$

The corresponding Hilbert-Schmidt operator defined by $T_{R_N,\mu}\psi(x) = \int_{\Omega} R_N(x,y)\psi(y)d\mu(y)$ is clearly bounded and positive: if $\psi = \sum_{j=1}^{\infty} \widehat{\psi}_j \phi_j$, then

$$\langle T_{R_N,\mu}\psi, \psi\rangle = \sum_{j=N+1}^{\infty} \lambda_j \left|\widehat{\psi}_j\right|^2 \geq 0.$$

For a positive Hilbert-Schmidt operator, the kernel is non-negative on the diagonal, i.e. $R_N(x,x) \geq 0$ for each $x \in \Omega$. Indeed, assume that for some $x \in \Omega$ we have $R_N(x,x) < 0$. Then we can choose a neighborhood U of x so that R_N is negative on $U \times U$, so

$$\langle T_{R_N,\mu}\mathbb{1}_U, \mathbb{1}_U\rangle = \int_U \int_U R_N(x,y)d\mu(x)d\mu(y) < 0,$$

which is a contradiction.

Thus, $R_N(x,x) \geq 0$ for each $x \in \Omega$, i.e. for any $N \geq 1$ we have $\sum_{j=1}^{N} \lambda_j \phi_j^2(x) \leq K(x,x)$, and thus

$$\sum_{j=1}^{\infty} \lambda_j \phi_j^2(x) \leq K(x,x).$$

Invoking the Cauchy–Schwarz inequality, we find that

$$\begin{aligned}\left|\sum_{j=1}^{\infty} \lambda_j \phi_j(x)\phi_j(y)\right| &\leq \sum_{j=1}^{\infty} \lambda_j \left|\phi_j(x)\phi_j(y)\right| \leq \left(\sum_{j=1}^{\infty} \lambda_j \phi_j^2(x)\right)^{1/2} \left(\sum_{j=1}^{\infty} \lambda_j \phi_j^2(y)\right)^{1/2} \\ &\leq K^{1/2}(x,x)K^{1/2}(y,y) \leq \sup_{x\in\Omega} K(x,x) < \infty.\end{aligned}$$

Therefore, the series in (2.13) converges absolutely. Combining this with the Cauchy Criterion for Uniform Convergence (which we may use, since Ω is compact, and therefore complete), we find that the series converges uniformly. □

We now provide a few simple corollaries of Mercer's Theorem. From the absolute convergence, we obtain

$$\int_{\Omega} K(x,x)d\mu(x) = \sum \lambda_j \int \phi_j^2 d\mu = \sum \lambda_j,$$

and thus

$$\sum_{j=1}^{\dim(L^2(\Omega,\mu))} \lambda_j < \infty. \tag{2.14}$$

By combining Mercer's Theorem with Lemma 2.2.2 we arrive at a characterization of all positive definite kernels.

Corollary 2.3.4. *The kernel K is positive definite if and only if for some orthonormal basis $\{\psi_j\}_{j=1}^{\dim(L^2(\Omega,\mu))}$ of $L^2(\Omega,\mu)$ and sequence of nonnegative real numbers $\{\kappa_j\}_{j=1}^{\dim(L^2(\Omega,\mu))}$,*

$$K(x,y) = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \kappa_j \psi_j(x)\psi_j(y)$$

where the sum converges absolutely and uniformly, $\kappa_j \geq 0$ for each j, and ψ_j is continuous whenever $\kappa_j > 0$.

We can also obtain a clear generalization of Mercer's Theorem. Consider the sets $N_+(K) = \{n \geq 1 : \lambda_j > 0\}$ and $N_-(K) = \{n \geq 1 : \lambda_j < 0\}$. If $|N_-(K)| < \infty$, then the kernel

$$K(x,y) - \sum_{n \in N_-(K)} \lambda_j \phi_j(x)\phi_j(y)$$

is continuous and positive definite. The absolute and uniform convergence of this new kernel then guarantees the following Corollary.

Corollary 2.3.5. *Suppose the operator $T_{K,\mu}$ has finitely many negative eigenvalues. Then* (2.13) *holds, with the series converging uniformly and absolutely.*

Finally, we supply another way to characterize positive definite functions.

Proposition 2.3.6. *A kernel K is positive definite if and only if there exists some $k \in L^2(\Omega \times \Omega, \mu \times \mu)$ such that k can be represented as*

$$k(x,y) = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \kappa_j \phi_j(x) \phi_j,$$

in the L^2 sense, and for all $x, y \in \Omega$,

$$K(x,y) = \int_{\Omega} k(x,z) k(z,y) d\mu(z). \tag{2.15}$$

As will be shown in the proof below, the coefficients κ_j satisfy $\kappa_j^2 = \lambda_j$ for all j.

Proof. For any choices of real κ_j's, we have, in the L^2 sense, the following equalities:

$$\int_{\Omega} k(x,z) k(z,y) d\mu(z) = \langle k(x,\cdot), k(y,\cdot) \rangle_{L^2(\Omega,\mu)} = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \kappa_j^2 \phi_j(x) \phi_j(y).$$

If we assume that K is positive definite, and choose $\kappa_j = \sqrt{\lambda_j}$ for each j, then clearly $k \in L^2(\Omega \times \Omega, \mu \times \mu)$, and, since

$$\int_{\Omega} k(x,z) k(z,y) d\mu(z) = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \lambda_j \phi_j(x) \phi_j(y) = K(x,y)$$

in the L^2 sense, we have pointwise equality due to Mercer's Theorem.

Alternatively, if we assume that

$$K(x,y) = \int_{\Omega} k(x,z) k(z,y) d\mu(z),$$

then for any finite point configuration $\omega_N = \{z_1, ..., z_N\}$ in Ω and $c_1, ..., c_N \in \mathbb{R}$, we have

$$\begin{aligned}\sum_{j=1}^{N}\sum_{i=1}^{N} K(z_j, z_i) c_j c_i &= \sum_{j=1}^{N}\sum_{i=1}^{N} c_j c_i \int_{\Omega} k(z_j, z) k(z, z_i) d\mu(z) \\ &= \int_{\Omega} \Big(\sum_{j=1}^{N} c_j k(z_j, z)\Big)^2 d\mu(z) \geq 0.\end{aligned}$$

Thus, K is clearly positive definite. □

2.4 Two-Point Homogeneous Spaces

In this paper, we will predominantly focus on energy optimization problems for compact, connected, two-point 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 [Wan52] that any such compact connected space is either a real sphere $\mathbb{S}^{d-1}$, a real projective space $\mathbb{RP}^{d-1}$, a complex projective space $\mathbb{CP}^{d-1}$, a quaternionic projective space $\mathbb{HP}^{d-1}$, or the Cayley projective plane $\mathbb{OP}^2$. Note that it suffices to consider $\mathbb{FP}^d$ for $d > 2$ only, as $\mathbb{FP}^1$ is isomorphic to the sphere $\mathbb{S}^{\dim_{\mathbb{R}}(\mathbb{F})}$ [Bae02, p. 170], and so it will not be separately considered in what follows. Naturally, other two-point homogeneous spaces exist, such as the Euclidean spaces $\mathbb{R}^d$, which are not compact, and the Hamming Cube, which is not connected, but here we will only consider the spaces listed above.

Below, Φ always refers to a compact connected two-point homogeneous space, equipped with the geodesic distance ϑ, normalized to take values in $[0, \pi]$. We let η denote the unique probability measure invariant under the isometries of Φ, i.e. the normalized uniform surface measure.

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

$$x\mathbb{F} = \{x\lambda \mid \lambda \in \mathbb{F} \setminus \{0\}\}. \tag{2.16}$$

Observe that the isometry groups $O(d)$, $U(d)$, $Sp(d)$ of the corresponding vector spaces $\mathbb{F}^d$ act transitively on each space, and that the stabilizers of a line represented by $x \in \mathbb{F}^d$ are $O(d-1) \times O(1)$, $U(d-1) \times U(1)$, and $Sp(d-1) \times Sp(1)$, respectively. Thus one has [Wol07, p. 28] the following quotient representations:

$$\begin{aligned}
\mathbb{RP}^{d-1} &= O(d)/\Big(O(d-1) \times O(1)\Big), \\
\mathbb{CP}^{d-1} &= U(d)/\Big(U(d-1) \times U(1)\Big), \\
\mathbb{HP}^{d-1} &= Sp(d)/\Big(Sp(d-1) \times Sp(1)\Big),
\end{aligned}$$

where we write $O(d)$, $U(d)$, $Sp(d)$ for the groups of matrices X, over the respective algebras, satisfying $XX^* = I$.

Using the identification (2.16), one can associate each element of $\mathbb{FP}^{d-1}$ ($\mathbb{F} = \mathbb{R}, \mathbb{C}, \mathbb{H}$) with a unit vector $x \in \mathbb{F}^d$, $\|x\| = 1$, and we shall at times abuse notation by doing so. In addition to the Riemannian metric ϑ, this gives us the *chordal distance* between points $x, y \in \Phi$, defined by

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

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

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

Since the algebra of octonions is not associative, the line model of (2.16) fails, and instead a model given by Freudenthal [Fre53] is used to describe $\mathbb{OP}^{d-1}$. It is known [Bae02] that only two octonionic spaces exist: $\mathbb{OP}^1$ and $\mathbb{OP}^2$, however $\mathbb{OP}^1$ is just $\mathbb{S}^8$, as noted above.

$\mathbb{OP}^2$ can be described as the subset of 3×3 Hermitian matrices Π over $\mathbb{O}$, satisfying $\Pi^2 = \Pi$ and Tr $\Pi = 1$ (see, e.g.,[CKM16, Skr17]). A metric for $\mathbb{OP}^2$ is then given by the Frobenius product,

$$\rho(\Pi_1, \Pi_2) = \frac{1}{\sqrt{2}} \|\Pi_1 - \Pi_2\|_F = \sqrt{1 - \langle \Pi_1, \Pi_2 \rangle},$$

where $\langle \Pi_1, \Pi_2 \rangle = \text{Re Tr } \frac{1}{2}(\Pi_1 \Pi_2 + \Pi_2 \Pi_1)$. This is the chordal distance on $\mathbb{OP}^2$ whereas the geodesic distance can be defined through $\sin \frac{\vartheta(x,y)}{2} = \rho(x,y)$, as in the above projective spaces. All Π given as above may be written in the form

$$\begin{pmatrix} |a|^2 & a\overline{b} & a\overline{c} \\ b\overline{a} & |b|^2 & b\overline{c} \\ c\overline{a} & c\overline{b} & |c|^2 \end{pmatrix},$$

where $|a|^2 + |b|^2 + |c|^2 = 1$ and $(ab)c = a(bc)$. This gives a representation of $\mathbb{OP}^2$ as the quotient $F_4/\text{Spin}(9)$ [Bae02, p. 189].

One feature of spaces Φ that allows for the application of linear programming methods is the existence of a decomposition of $L^2(\Phi, \eta, \mathbb{C})$, the space of complex-valued square-integrable functions on Φ. Consider the representation $L(g)$, of the isometry group G of Φ, for $L^2(\Phi, \eta, \mathbb{C})$, defined by

$$L(g)\phi(x) = \phi(g^{-1}x).$$

This representation is decomposable into an orthogonal direct sum of pairwise non-equivalent irreducible representations $L_n(g)$ acting on isometry invariant finite dimensional subspaces $V_n^{(\alpha,\beta)}$, of continuous functions (see [Lev98, Vil]), with $V_0^{(\alpha,\beta)}$ being the space of constant functions, where $\alpha = (d-1)\frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1$ and

$$\beta = \begin{cases} \alpha, & \text{if } \Phi = \mathbb{S}^{d-1}; \\ \frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1, & \text{if } \Phi = \mathbb{FP}^{d-1} \end{cases}. \tag{2.17}$$

These subspaces $V_n^{(\alpha,\beta)}$, which satisfy

$$L^2(\Phi, \eta, \mathbb{C}) = \overline{\bigoplus_{n \geq 0} V_n^{(\alpha,\beta)}}, \tag{2.18}$$

can be chosen as the eigenspaces of the Laplace–Beltrami operator on Φ corresponding to the n-th eigenvalue in the increasing order [Skr, Wol07]. Let $Y_{n,k} = Y_{n,k}^{(\alpha,\beta)}$, for $k = 1, \ldots, \dim(V_n^{(\alpha,\beta)})$, be an orthonormal basis in $V_n^{(\alpha,\beta)}$. Because of the invariance of $V_n^{(\alpha,\beta)}$ and the two-point homogeneity of Φ, the reproducing kernel for $V_n^{(\alpha,\beta)}$ only depends on the distance $\vartheta(x,y)$ between points [CS99, Ven01]. Furthermore, as a function of

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

the reproducing kernel is a polynomial $P_n^{(\alpha,\beta)}$ of degree n, which satisfies

$$P_n^{(\alpha,\beta)}(\tau(x,y)) = \sum_{k=1}^{\dim(V_n^{(\alpha,\beta)})} Y_{n,k}(x)\overline{Y_{n,k}(y)}. \tag{2.19}$$

Formula (2.19) is known as the *addition formula*, and a slight alteration of the proof of 2.2.2 tells us that the $P_n^{(\alpha,\beta)}$ are positive definite on Φ. We note that on the sphere, $\tau(x,y) = \langle x,y \rangle$. For any kernel K that depends only on the distance between points $\vartheta(x,y)$, there is a corresponding function $F : [-1,1] \to \mathbb{R}$ defined by

$$F(\tau(x,y)) := K(x,y). \tag{2.20}$$

We call F positive definite if and only if K is positive definite, and may replace K with F in definitions such as the energy integral.

For more details on compact, connected, two-point homogeneous spaces, particularly projective spaces, we refer the reader to [Bes78, Hel78, Hel84, Lev92, Sha01, Skr20, Skr, Wol11, Wol07].

Jacobi Polynomials

The polynomials $C_n = C_n^{(\alpha,\beta)} = \frac{P_n^{(\alpha,\beta)}}{\dim(V_n^{(\alpha,\beta)})}$ satisfy $C_n(1) = 1$ and are orthogonal with respect to the probability measure on $[-1,1]$,

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

where, as above, $\alpha = (d-1)\frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1$,

$$\beta = \begin{cases} \alpha, & \text{if } \Phi = \mathbb{S}^{d-1}; \\ \frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1, & \text{if } \Phi = \mathbb{FP}^{d-1}, \end{cases}$$

and the normalization factor is given by

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

where B is the beta function. The weight measure $\nu^{(\alpha,\beta)}$ is related to integration on Φ in the following way: for any $p \in \Phi$,

$$\int_{\Phi} F(\tau(x,p))d\eta(x) = I_F(\eta) = \int_{-1}^{1} F(t)d\nu^{(\alpha,\beta)}(t). \tag{2.21}$$

The *normalized Jacobi polynomials*, C_n, form an orthogonal basis in $L^2([-1,1], \nu^{(\alpha,\beta)})$; equivalently, the span of $C_n(\tau(x,y))$, $n \geq 0$, is dense in the subset of $L^2(\Phi \times \Phi, \eta \otimes \eta)$

consisting of functions that depend only on the distance between x and y. In the case that Φ is the sphere, i.e. $\alpha = \beta = \frac{d-3}{2}$, then these polynomials are known as the (normalized) Gegenbauer/ultraspherical polynomials.

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

$$F(t) = \sum_{i=0}^{\infty} \widehat{F}_n C_n(t), \quad \text{where} \quad \widehat{F}_n = \dim(V_n^{(\alpha,\beta)}) \int_{-1}^{1} F(t) C_n(t)\, d\nu^{(\alpha,\beta)}(t). \tag{2.22}$$

For a fixed space Φ we will not indicate the dependence of polynomials $C_n = C_n^{(\alpha,\beta)}$, the spaces $V_n = V_n^{(\alpha,\beta)}$, and the functions $Y_{n,k} = Y_{n,k}^{(\alpha,\beta)}$ on the indices α, β. We refer to $\widehat{F}_n$ as the Jacobi coefficients of the function F; the normalization $C_n(1) = 1$ used here is common in the coding theory community [Sze75, Lev92].

We have already seen that Jacobi polynomials C_n are positive definite on Φ, so uniformly convergent series with nonnegative coefficients must be as well. Fortunately, similar to the result of Mercer's Theorem, if $F \in C([-1,1])$ has a Jacobi expansion with nonnegative coefficients, then the sum is uniformly convergent [BD19, Gan67, Lyu09].

Lemma 2.4.1. *Let $F \in C([-1,1])$, $F(t) = \sum_{n=0}^{\infty} \widehat{F}_n C_n(t)$ with $\widehat{F}_n < 0$ for finitely many $n \in \mathbb{N}_0$. Then the Jacobi expansion of F converges uniformly and absolutely to F on $[-1,1]$.*

With this lemma, we now have the following analogue of Corollary 2.3.4 [Boc41, Gan67, Sch42].

Proposition 2.4.2. *A function $F \in C([-1,1])$ is positive definite on Φ if and only if $\widehat{F}_n \geq 0$ for all $n \geq 0$.*

Proof. One direction is clear. For the other, let us assume that for some $m \in \mathbb{N}_0$, $\widehat{F}_m < 0$. For a fixed point $p \in \Phi$, we see that $Y_m(x) := C_m(\tau(x,p))$ is in V_m and real-valued. By orthogonality of the spaces V_n in (2.18) and the fact that $P_m(\tau(x,y)) = \dim(V_m) C_m(\tau(x,y))$

is the reproducing kernel of V_m, we have that, for $d\mu(x) = Y_m(x)d\eta(x)$,

$$I_F(\mu) = \int_\Phi \int_\Phi F(\tau(x,y))Y_m(x)Y_m(y)d\eta(x)d\eta(y)$$
$$= \frac{\widehat{F}_m}{\dim(V_m)} \int_\Phi Y_m(y)^2 d\eta(y) < 0,$$

so F is not positive definite. □

Antipodal Symmetry

Let us consider the kernels of the form $K(x,y) = G(\langle x,y \rangle)$ on the unit sphere $\mathbb{S}_{\mathbb{F}}^{d-1}$ for $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}, \mathbb{H}\}$, where $\langle x,y \rangle$ is the inner product in the ambient space. We observe that if $G(t) = G(|t|)$, the energy I_G remains the same after averaging over unit multiples of vectors in the support of a measure μ. Let $U(\mathbb{F})$ be the set of units in $\mathbb{F}$, $U(\mathbb{F}) = \{c \in \mathbb{F} : |c| = 1\}$, and ζ be the uniform measure on $U(\mathbb{F})$. If one defines, for Borel sets $B \subset \mathbb{S}_{\mathbb{F}}^{d-1}$,

$$\mu_{U(\mathbb{F})}(B) = \frac{1}{\zeta(U(\mathbb{F}))} \int_{U(\mathbb{F})} \mu(cB)d\zeta(c) \tag{2.23}$$

then

$$I_G(\mu_{U(\mathbb{F})}) = \frac{1}{\zeta(U(\mathbb{F}))^2} \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} \int_{U(\mathbb{F})} \int_{U(\mathbb{F})} G(|\langle cx, by \rangle|)d\mu(x)d\mu(y)d\zeta(c)d\zeta(b)$$
$$= \frac{1}{\zeta(U(\mathbb{F}))^2} \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} \int_{U(\mathbb{F})} \int_{U(\mathbb{F})} G(|\langle x, y \rangle|)d\mu(x)d\mu(y)d\zeta(c)d\zeta(b)$$
$$= \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} G(|\langle x, y \rangle|)d\mu(x)d\mu(y) = I_G(\mu).$$

Moreover, this tells us that for any $\mu, \nu \in \mathbb{P}(\mathbb{S}_{\mathbb{F}}^{d-1})$, $I_G(\mu) = I_G(\nu)$ whenever $I_G(\mu_{U(\mathbb{F})}) = I_G(\nu_{U(\mathbb{F})})$.

Now, let $p_{\mathbb{F}} : \mathbb{S}_{\mathbb{F}}^{d-1} \to \mathbb{FP}^{d-1}$ be the projection of the sphere onto the projective space, i.e.

$$p_{\mathbb{F}}(x) = x\mathbb{F}$$

as defined by (2.16). Defining $F : [-1,1] \to \mathbb{R}$ by

$$F(\tau(p_{\mathbb{F}}(x), p_{\mathbb{F}}(y))) = F(\tau(x\mathbb{F}, y\mathbb{F})) = F(2|\langle x,y\rangle|^2 - 1) = G(|\langle x,y\rangle|) = G(\langle x,y\rangle),$$

for $x, y \in \mathbb{S}_{\mathbb{F}}^{d-1}$ we then see that for any $\mu \in \mathscr{B}(\mathbb{S}_{\mathbb{F}}^{d-1})$,

$$\begin{aligned}\int_{\mathbb{FP}^{d-1}} \int_{\mathbb{FP}^{d-1}} F(\tau(x,y)) d((p_{\mathbb{F}})_* \mu)(x) d((p_{\mathbb{F}})_* \mu)(y) &= \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} F(\tau(p_{\mathbb{F}}(x), p_{\mathbb{F}}(y))) d\mu(x) d\mu(y) \\ &= \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} \int_{\mathbb{S}_{\mathbb{F}}^{d-1}} G(\langle x,y\rangle) d\mu(x) d\mu(y),\end{aligned}$$

where $(p_{\mathbb{F}})_*\mu$ is the push-forward measure defined by $(p_{\mathbb{F}})_*\mu(B) = \mu(p_{\mathbb{F}}^{-1}(B))$ for all Borel subsets of $\mathbb{FP}^{d-1}$.

This discussion shows that for G as above, a minimizing measure on the sphere for I_G, can be taken to be symmetric, and that the problem of minimizing over symmetric measures on spheres is equivalent to minimizing energy over measures on the projective spaces. In Chapters 6 and 7 we will use these relations in order to address optimization problems for kernels G of this form.

2.5 The Sphere

Of the compact, connected two-point homogeneous spaces, real unit spheres $\mathbb{S}^{d-1}$ are by far the most well studied, and will be the space we work in most often in this paper. When specifically working on the sphere, we will use σ, instead of η, to denote the surface measure, i.e. the normalized $(d-1)$-dimensional Lebesgue/Hausdorff measure on the sphere.

Like the other compact, connected, two-point homogeneous spaces, the sphere $\mathbb{S}^{d-1}$

may be represented as a quotient space [Wol11]. For $d > 2$, $SO(d)$ acts transitively on $\mathbb{S}^{d-1}$ and $SO(d-1)\times\{1\}$ is the stabilizer of any point $x \in \mathbb{S}^{d-1}$, whereas for $d = 2$, these groups are $O(2)$ and $O(1)\times\{1\}$ so

$$\mathbb{S}^{d-1} = SO(d)/\Big(SO(d-1)\times\{1\}\Big) \quad d > 2$$
$$\mathbb{S}^{2} = O(2)/\Big(O(1)\times\{1\}\Big).$$

On the sphere, the chordal metric is simply the Euclidean metric, i.e. $\rho(x,y) = \|x-y\|$, and the geodesic distance is $\vartheta(x,y) = \arccos(\langle x,y\rangle)$, meaning that on the sphere

$$\tau(x,y) = \cos(\vartheta(x,y)) = \langle x,y\rangle.$$

Since $\mathbb{S}^{d-1}$ is a two-point homogeneous space, $L^2(\mathbb{S}^{d-1},\sigma,\mathbb{C})$ has a decomposition of the form (2.18). In this setting the space $V_n^{(\frac{d-3}{2},\frac{d-3}{2})}$ is exactly the space of *spherical harmonics* of degree n (i.e. the restrictions to $\mathbb{S}^{d-1}$ of homogeneous polynomials, of degree n, on $\mathbb{R}^d$ that are in the kernel of the Euclidean Laplacian) [Sha01]. Clearly, any complex-valued spherical harmonic of degree n must be of the form $p(x)+iq(x)$, where p and q are real-valued spherical harmonics of degree n. Thus, each $V_n^{(\frac{d-3}{2},\frac{d-3}{2})}$, and thereby $L^2(\mathbb{S}^{d-1},\sigma,\mathbb{C})$, has an orthonormal basis of real-valued spherical harmonics. Denoting the space of real-valued spherical harmonics of degree n on $\mathbb{S}^{d-1}$ by $\mathscr{H}_n^d$, we see that this means that

$$L^2(\mathbb{S}^{d-1},\sigma) = \bigoplus_{n\geq 0}\mathscr{H}_n^d$$

and that for all $n \in \mathbb{N}_0$ and $d \geq 2$,

$$\dim(V_n^{(\frac{d-3}{2},\frac{d-3}{2})}) = \dim(\mathscr{H}_n^d) = \binom{n+d-1}{n} - \binom{n+d-3}{n-2}.$$

Our addition formula (2.19) now tells us that for all $n \in \mathbb{N}_0$, if $Y_{n,1},\ldots,Y_{n,\dim(\mathscr{H}_n^d)}$ is an orthonormal basis of $\mathscr{H}_n^d$, then

$$C_n^{(\frac{d-3}{2},\frac{d-3}{2})}(\langle x,y\rangle) = \frac{1}{\dim(\mathscr{H}_n^d)} \sum_{j=1}^{\dim(\mathscr{H}_n^d)} Y_{n,j}(x)Y_{n,j}(y).$$

In certain instances, it will be more convenient to use the standard Gegenbauer/ultraspherical polynomials instead of the normalized ones.

Gegenbauer Polynomials

For a parameter $\lambda > 0$, consider the measure

$$dw_\lambda(t) = d\nu^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(t) = \frac{\Gamma(\lambda+1)}{\sqrt{\pi}\Gamma(\lambda+\frac{1}{2})}(1-t^2)^{\lambda-\frac{1}{2}}dt$$

on the interval $[-1,1]$. For the rest of this text, we will assume that $\lambda = \frac{d-2}{2}$, so that

$$dw_\lambda(t) = \frac{A_{d-2}}{A_{d-1}}(1-t^2)^{\frac{d-3}{2}}dt,$$

where $A_{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the $(d-1)$-dimensional Hausdorff surface measure of $\mathbb{S}^{d-1}$. The weighted measure w_λ is related to integration on the sphere $\mathbb{S}^{d-1}$ in the following way: for a unit vector $p \in \mathbb{S}^{d-1}$,

$$\int_{\mathbb{S}^{d-1}} F(\langle x,p\rangle)d\sigma(x) = I_F(\sigma) = \int_{-1}^{1} F(t)dw_\lambda(t) \tag{2.24}$$

where, as before, σ is the normalized surface measure on the sphere $\mathbb{S}^{d-1}$.

The Gegenbauer polynomials C_n^λ, $n \geq 0$, as a special case of the Jacobi polynomials, clearly form an orthogonal basis of $L^2([-1,1],\nu^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}) = L^2([-1,1],w_\lambda)$. However, in this instance, we are not normalizing these polynomials, which means that we must properly adjust our formulae from Section 2.4. Every function $F \in L^1\big([-1,1],w_\lambda\big)$ has a

Gegenbauer (ultraspherical) expansion

$$F(t) \sim \sum_{n=0}^{\infty} \widehat{F}(n,\lambda) \frac{n+\lambda}{\lambda} C_n^{\lambda}(t) \quad t \in [-1,1] \tag{2.25}$$

where

$$\widehat{F}(n,\lambda) := \frac{1}{C_n^{\lambda}(1)} \int_{-1}^{1} F(t) C_n^{\lambda}(t) dw_{\lambda}(t). \tag{2.26}$$

For $F \in L^2\big([-1,1], w_\lambda\big)$ this expansion converges to F in the L^2 sense.

In the case of $\mathbb{S}^1$, when $\lambda = 0$, the relevant polynomials are the Chebyshev polynomials of the first kind

$$T_n(t) = \cos\big(n \arccos(t)\big) = \frac{1}{2} \lim_{\lambda \to 0} \frac{n+\lambda}{\lambda} C_n^{\lambda}(t), \tag{2.27}$$

and for $\mathbb{S}^2$, the polynomials are appropriately scaled Legendre polynomials [Sze75].

For any $n \in \mathbb{N}_0$ and $d \geq 2$, let $\{Y_{n,j}\}_{j=1}^{\dim(\mathscr{H}_n^d)}$ be any orthonormal basis in $\mathscr{H}_n^d$. The Gegenbauer polynomials are related to the spherical harmonics by the following *addition formula*

$$\sum_{j=1}^{\dim(\mathscr{H}_n^d)} Y_{n,j}(x) Y_{n,j}(y) = \frac{n+\lambda}{\lambda} C_n^{\lambda}(\langle x,y \rangle) \quad \text{for all } x,y \in \mathbb{S}^{d-1}. \tag{2.28}$$

Comparing this to the normalized Gegenbauer polynomials $C_n^{(\frac{d-3}{2},\frac{d-3}{2})}$, we see that for all $n \in \mathbb{N}_0$ and $d \geq 2$,

$$\widehat{F}_n C_n^{(\frac{d-3}{2},\frac{d-3}{2})}(t) = \widehat{F}(n,\lambda) \frac{n+\lambda}{\lambda} C_n^{\lambda}(t) \quad t \in [-1,1],$$

as one would expect. Thus, Lemma 2.4.1 and Proposition 2.4.2 hold with the Gegenbauer expansion (2.25). Likewise, all results in this text that are given for general compact, connected, two-point homogeneous spaces using Jacobi expansions (with normalized Jacobi polynomials) hold on the sphere with the standard Gegenbauer polynomials.

Expanding in terms of standard Gegenbauer polynomials will be more convenient for formulating various results in this text when working on the sphere, such as the Funk-Hecke formula, which clearly follows from orthogonality, (2.25), and the addition formula (2.28).

Theorem 2.5.1. *Let $F \in L^2([-1,1], w_\lambda)$. Then for every $Y_n \in \mathscr{H}_n^d$,*

$$\int_{\mathbb{S}^{d-1}} F(\langle x,y\rangle) Y_n(y) d\sigma(y) = \widehat{F}(n,\lambda) Y_n(x). \tag{2.29}$$

We complete this section with the following corollary of Proposition 2.3.6, where our decision to use standard Gegenbauer polynomials simplifies the result.

Corollary 2.5.2. *Let $F \in C([-1,1])$. Then F is positive definite on $\mathbb{S}^{d-1}$ if and only if there exists some $f \in L^2([-1,1], w_\lambda)$ such that*

$$F(\langle x,y\rangle) = \int_{\mathbb{S}^{d-1}} f(\langle x,z\rangle) f(\langle z,y\rangle) d\sigma(z). \tag{2.30}$$

If such a function f exists, then for all $n \in \mathbb{N}_0$, $\widehat{F}(n,\lambda) = \left(\widehat{f}(n,\lambda)\right)^2$.

Proof. For each $n \in \mathbb{N}_0$, let $Y_{n,1}, \ldots, Y_{n,\dim(\mathscr{H}_n^d)}$ be an orthonormal basis of $\mathscr{H}_n^d$. Then we know that $\{Y_{n,k} : n \in \mathbb{N}_0, k \in \{1, \ldots, \dim(\mathscr{H}_n^d)\}\}$ forms an orthonormal basis of $L^2(\mathbb{S}^{d-1}, \sigma)$ which consists of continuous eigenfunctions of the linear integral operator $T_{K,\sigma}$, with $K(x,y) = F(\langle x,y\rangle)$ for all $x,y \in \mathbb{S}^{d-1}$. From (2.25) and (2.28), we know that

$$F(\langle x,y\rangle) = \sum_{n=0}^{\infty} \widehat{F}(n,\lambda) \sum_{k=1}^{\dim(\mathscr{H}_n^d)} Y_{n,k}(x) Y_{n,k}(y).$$

Proposition 2.3.6 then tells us that F is positive definite if and only if there exists some $k \in L^2(\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}, \sigma \times \sigma)$ such that

$$F(\langle x,y\rangle) = \int_{\mathbb{S}^{d-1}} k(x,z) k(z,y) d\sigma(z), \tag{2.31}$$

and that if such a k exists, then

$$k(x,y)=\sum_{n=0}^{\infty}\sum_{k=1}^{\dim(\mathscr{H}_n^d)}\kappa_{n,k}Y_{n,k}(x)Y_{n,k}(y),$$

with $\kappa_{n,k}^2=\widehat{F}(n,\lambda)$. Moreover, if such a k exists, then there are infinitely many choices of k satisfying (2.31), as we may change the sign of each $\kappa_{n,k}$. Thus, if there exists some k satisfying (2.31), then we may choose its coefficients such that

$$k(x,y)=\sum_{n=0}^{\infty}\sqrt{\widehat{F}(n,\lambda)}\frac{n+\lambda}{\lambda}C_n^{\lambda}(\langle x,y\rangle)$$

meaning that k only depends on the distance between x and y, and so can be expressed by a function $f\in L^2([-1,1],w_\lambda)$, i.e. $f(t)=\sum_{n=0}^{\infty}\sqrt{\widehat{F}(n,\lambda)}\frac{n+\lambda}{\lambda}C_n^{\lambda}(t)$. Our claim now follows. □

For more background information on spherical harmonics, Gegenbauer polynomials, and harmonic analysis on the sphere, we refer the reader to [DX13, Mül66, Gro96].

2.6 Designs

We now treat the topic of designs in the compact, connected, two-point homogeneous spaces Φ. Any finite (non-empty) set, also known as a *code*, $\mathscr{C}\subset\Omega$ is characterized by its distance set

$$\mathscr{A}(\mathscr{C})=\{\tau(x,y):x,y\in\mathscr{C}\}. \tag{2.32}$$

We note that $\mathscr{A}$ is the set of cosines of geodesic distances between points, rather than the distances themselves, which is more convenient for our purposes. The *degree* of $\mathscr{C}$ is the number of distinct distances that occur between distinct elements of $\mathscr{C}$, i.e. $|\mathscr{A}(\mathscr{C})\setminus\{1\}|$. Codes in two-point homogeneous spaces, particularly the sphere, have a rich history, and have been the basis of several famous optimization problems. For instance, for any $A\subseteq$

$[-1,1)$, we call $\mathscr{C} \subset \Phi$ an A-code if $\mathscr{A}(\mathscr{C}) \subseteq A \cup \{1\}$. Often, one is interested in finding upper bounds of the cardinality $|\mathscr{C}|$ of A-codes, and determining extremal configurations with respect to such bounds. On $\mathbb{S}^{d-1}$, for $A = [-1,b]$, for some $b < 1$, this is equivalent to the classical problem of placing non-overlapping spherical caps of angular radius $\frac{1}{2}\arccos(b)$ on the sphere [DGS77, Ran55]. In particular, when $A = [-1,\pi/3]$, this becomes a problem of finding the *kissing number* of the sphere, i.e. the maximum number of non-overlapping balls in $\mathbb{R}^d$ of radius r that can all touch a single ball of radius r, which is only known for $d \in \{1,2,3,4,8,24\}$ [SvdW53, Lev79, OS79, Mus08]. Another famous optimization problem is the classification of tight designs.

A code $\mathscr{C} \subset \Phi$ is called a *t-design* if

$$\frac{1}{|\mathscr{C}|}\sum_{x\in\mathscr{C}} p(x) = \int_{\Omega} p(x)\, d\eta(x) = 0 \quad \forall p \in \bigcup_{n=1}^{t} V_n. \tag{2.33}$$

A relaxation of the above identity allows the configuration to be weighted, so that the equality

$$\sum_{x\in\mathscr{C}} w(x)p(x) = \int_{\Omega} p(x)\, d\eta(x) = 0 \quad \forall p \in \bigcup_{n=1}^{t} V_n \tag{2.34}$$

holds for some weights $\{w(x)\}_{x\in\mathscr{C}} \subset \mathbb{R}_{\geq 0}$, satisfying $\sum_{x\in\mathscr{C}} w(x) = 1$. Such weighted formulas are called *cubature formulas* or *weighted t-designs*. We will make a slight abuse of terminology, and refer to the measure

$$\mu_{\mathscr{C},w} = \sum_{x\in\mathscr{C}} w(x)\delta_x \tag{2.35}$$

as a weighted t-design if $\mathscr{C}$, with weight function w, is a weighted t-design. If $w(x) = \frac{1}{|\mathscr{C}|}$ for all $x \in \mathscr{C}$, i.e. $\mathscr{C}$ is a t-design, we shall denote our measure $\mu_{\mathscr{C}} := \mu_{\mathscr{C},w}$, and refer to it as a t-design. We note that our definition implies that if $\mathscr{C}$ is a weighted t-design with weight function w, then

$$\sum_{x,y\in\mathscr{C}} w(x)w(y)C_n(\tau(x,y)) = 0 \quad \text{for } 1 \le n \le t.$$

The *strength* of a (weighted) design is the maximum value of t for which identity (2.33) (or (2.34), accordingly) holds.

The concept of spherical designs was originally introduced in 1977 by Delsarte, Goethal, and Seidel in [DGS77], in which they determined a lower bound on $N(\mathbb{S}^{d-1},t)$, the minimum number of points necessary to construct a spherical t-design, and provided several important examples of designs. The existence of spherical t-designs for any $d \ge 2$ and $t \in \mathbb{N}$ was proved in 1984 by Seymour and Zaslavsky in [SZ84]. However, this proof is nonconstructive, and gives no indication of the size of $N(\mathbb{S}^{d-1},t)$. Various upper bounds of $N(\mathbb{S}^{d-1},t)$ were given in [WV91, Baj92, KM93, BV10], culminating in the results of Bondarenko, Radchenko, and Viazovska in [BRV13, BRV15]. In their works, they showed that not only is $N(\mathbb{S}^{d-1},t)$ on the order of t^{d-1} (the lower bound given in Lemma 2.6.4), but for large enough N, relative to t and d, well separated spherical t-designs of size N always exist. This solved a long-standing conjecture of Korevaar and Meyers [KM93].

Theorem 2.6.1 ([BRV13, BRV15])**.** *For all $d \ge 2$ there exists some $C_d > 0$ and $b_d > 0$ such that for all $N \ge C_d t^{d-1}$, there exists a spherical t-design $\mathscr{C} = \{z_1, ..., z_N\} \subset \mathbb{S}^{d-1}$ such that $||z_i - z_j|| > b_d N^{-1/(d-1)}$ for $i \ne j$.*

The concept of codes and designs was generalized to projective spaces (as well as other spaces) in the 1980's by Neumaier, Bannai, and Hoggar [BH85, BH89, Hog82a, Hog82b, Neu81], among others, though they were studied previously (see, e.g., [DGS75]). In the following decades, a general theory was developed, a good overview of which, as well as additional background, can be found in, for instance [BB09, Lev92, Lev98, Lev98]. Concerning the relationship between t-designs and classical designs in ranked partially ordered sets, see [Del76, Sta81, Sta86].

The equalities (2.33) and (2.34) show that (weighted) designs can provide a good approximation to the whole space Φ, and the strength of the design characterizes the degree of such an approximation. This makes the problem of finding the minimum cardinality of a (weighted) design of a certain strength of significant interest in factorial experiments, cryptography, complexity theory, and calculation theory [AGHP92, CS99, GMS74, Rao47, Sti93].

Linear programming bounds imply exact constraints on the size of designs, in particular giving the cardinality of *tight t-designs*, which have the smallest possible number of pairwise distances between their elements, for a design of strength t. The exact definition may be given as follows.

Definition 2.6.2. *A code $\mathscr{C} \subset \Omega$ is called a **tight** t**-design** if one of the following conditions is satisfied.*

(i) $\mathscr{C}$ is a design of strength $t = 2m-1$ and degree m, and $-1 \in \mathscr{A}(\mathscr{C})$, i.e. there is at least one pair of points diameter apart;

(ii) $\mathscr{C}$ is a design of strength $t = 2m$ and degree m.

Often, tight designs are defined by their cardinality rather than their degree. Though the latter is of greater use for our needs in this paper, it is worth connecting the two definitions and showing the bounds on cardinality. Let $\mathscr{C} \subset \Phi$ be code of degree m. Set $e = |\mathscr{A}(\mathscr{C}) \setminus \{-1\}| - 1$. The annihilating polynomial of a configuration is defined by $Ann(\mathscr{C}) := \Pi_{a\in\mathscr{A}(\mathscr{C})\setminus\{1\}}(x-a)$. For a positive number t, let $(t)^{\overline{k}} = t(t+1)\dots(t+k-1)$ be the rising factorial and $(t)^{\underline{k}} = t(t-1)\dots(t-k+1)$ be the falling factorial. We define, for $k \in \mathbb{N}$

$$R_{k,\lambda}(x) := \sum_{j=0}^{k} \frac{j+\lambda}{\lambda} C_j^{\lambda}(x), \tag{2.36}$$

$$Q_{k,\lambda}(x) := \sum_{j=0}^{\lfloor k/2 \rfloor} \frac{k-2j+\lambda}{\lambda} C_{k-2j}^{\lambda}(x), \tag{2.37}$$

and

$$T_{m,e}^{(\alpha,\beta)} := \frac{(\alpha+\beta+2)^{\overline{m+e}}}{(\beta+1)^{\overline{m}}e!}\sum_{j=0}^{e}(-1)^j\frac{(m+\beta)^{\underline{j}}}{(m+e+\alpha+\beta+1)^{\underline{j}}}\left(\frac{x+1}{2}\right)^{e-j}. \tag{2.38}$$

The following lemmas from [DGS77] now let us relate the degree, strength, and cardinality of spherical designs, and provide us with information about the distance set $\mathscr{A}(\mathscr{C})$ of tight designs.

Lemma 2.6.3. *Let $\mathscr{C} \subset \mathbb{S}^{d-1}$ be code of degree m such that $|\mathscr{C}| = N$.*

(i) If $\mathscr{C}$ is a design of strength t, then $t \leq 2m$ and $N \leq R_{m,\lambda}(1)$. Equality holds in either of these inequalities if and only if $\mathscr{C}$ is a tight $2m$-design

(ii) If $\mathscr{C}$ is an antipodal design of strength t, then $t \leq 2m-1$, and $N \leq 2Q_{m-1,\lambda}(1)$. Equality holds in either of these inequalities if and only if $\mathscr{C}$ is a tight $(2m-1)$-design.

Lemma 2.6.4. *Let $\mathscr{C} \subset \mathbb{S}^{d-1}$ be a t-design such that $|\mathscr{C}| = N$.*

(i) If $t = 2k$, then

$$N \geq R_{k,\lambda}(1) = \binom{d-k-1}{d-1} + \binom{d-k-2}{d-1}. \tag{2.39}$$

Equality holds (i.e. $\mathscr{C}$ is a tight spherical $(2k)$-design) if and only if $\mathscr{A}(\mathscr{C})$ is exactly the set of roots of $(1-x)R_{k,\lambda}(x)$.

(ii) If $t = 2k-1$, then

$$N \geq 2Q_{k-1,\lambda}(1) = 2\binom{d-k-2}{d-1}. \tag{2.40}$$

Equality holds (i.e. $\mathscr{C}$ is a tight spherical $(2k-1)$-design) if and only if $\mathscr{A}(\mathscr{C})$ is exactly the set of roots of $(1-x^2)C_{k-1,\lambda}(x)$.

Similar results exist for the projective settings [Hog82a].

Lemma 2.6.5. *Let $\mathscr{C} \subset \mathbb{FP}^{d-1}$ be a code of degree m such that $|\mathscr{C}| = N$.*

(i) We have

$$N \leq T_{m,e}^{(\alpha,\beta)}(1) = \frac{(\alpha+\beta+2)^{\overline{m}}(\alpha+2)^{\overline{e}}}{(\beta+1)^{\overline{m}}e!} \tag{2.41}$$

with equality if and only if $Ann(\mathscr{C})(x) = \left(\frac{x+1}{2}\right)^{m-e} T_{m,e}^{(\alpha,\beta)}(x)$.

(ii) If $\mathscr{C}$ *is a design of strength* t*, then* $t \leq m+e$*, and equality holds (i.e.* $\mathscr{C}$ *is a tight* t*-design) if and only if equality holds in* (2.41).

The bounds on cardinality one achieves from these results were generalized to weighted designs by Levenshtein in [Lev98].

Theorem 2.6.6. *Let* $(\mathscr{C}, w)$ *be a weighted* t*-design in* Φ*. Then with* $k = \lfloor \frac{t+1}{2} \rfloor$ *and* $\varepsilon = 2k - t$*, we have the following:*

1. *If* $\Phi = \mathbb{S}^{d-1}$*, then*

$$|\mathscr{C}| \geq \binom{d+k-1-\varepsilon}{d-1} + \binom{d+k-2}{d-1}. \tag{2.42}$$

2. *If* $\Phi = \mathbb{FP}^{d-1}$*, then*

$$|\mathscr{C}| \geq \frac{(\alpha+\beta+2)^{\overline{k}}(\alpha+2)^{\overline{k-\varepsilon}}}{(\beta+1)^{\overline{k}}(k-\varepsilon)!}. \tag{2.43}$$

In both cases, equality holds if and only if $w(x) = \frac{1}{|\mathscr{C}|}$ *for all* $x \in \mathscr{C}$ *and* $\mathscr{C}$ *is a tight* t*-design.*

Note that this means that any weighted tight design is a design (known also as a "simple" design), a result that was shown for the sphere in [Tay95]. In addition, observe that from our above lemmas, it is clear that if $\mathscr{C}_1$ and $\mathscr{C}_2$ are tight t-designs on Φ, then $\mathscr{A}(\mathscr{C}_1) = \mathscr{A}(\mathscr{C}_2)$ and $|\mathscr{C}_1| = |\mathscr{C}_2|$. However, tight designs, generally, are not unique (not even up to unitary equivalence). This is known to be true in particular for the tight projective 2-designs on $\mathbb{CP}^2$, through the characterization of all such designs in [Szö].

Table 2.1 provides a list of known tight spherical designs, as well as the 600-cell, which is not a tight design, but will be of interest in Section 6.3. Tight spherical 1-designs are clearly just pairs of antipodal points, and tight 2-designs and 3-designs are precisely the vertices of regular simplices and cross polytopes, respectively. On the circle $\mathbb{S}^1$, tight t-designs exist for all $t \in \mathbb{N}$: they are simply the vertices of the regular $(t+1)$-gon. For $d \geq 3$ and $t \geq 4$ there are eight tight spherical designs known. Aside from the icosahedron, these designs do not come from regular polytopes. Instead, several are derived from the E_8 root lattice in $\mathbb{R}^8$ and the Leech Lattice Λ_{24} in $\mathbb{R}^{24}$, objects that provide optimal spherical packings in their respective dimensions [Via17, CKM$^+$17]. The 240-point and 196560-point configurations are the minimal (nonzero) vectors in those lattices. Each arrangement labeled "kissing" is the kissing configuration of the set below it: by centering non-overlapping congruent spherical caps of maximal height at each of the points in a given configuration, one arrives at a "sphere packing" on the sphere, and the resulting points of tangency on a given cap form a spherical code in a lower dimensional space. Some of the kissing configurations are of independent interest. The configuration of 240 points produces a set of 120 equiangular lines passing though the origin in $\mathbb{R}^7$, and the configuration of 27 points forms the Schläfli arrangement. The remaining two designs are the configuration of 552 points in $\mathbb{R}^{23}$ which comes from an equiangluar arrangement of 276 lines described by the unique regular two-graph on 276 vertices, and the resulting kissing configuration, which is a 275 point arrangement associated with the McLaughlin group in $\mathbb{S}^{21}$.

Tight spherical designs with $d \geq 3$ and $t \geq 4$ may only exist for $t = 4, 5$, and 7 with the one exception of the spherical 11-design formed by the Leech lattice minimal vectors [BD79, BD80]. The problem of finding tight spherical 5-designs is the same as that of finding maximal equiangular tight frames, and it is known that existence of a tight spherical 5-design in $\mathbb{S}^{d-1}$ is possible only for $d = 1, 2, 3$ and for dimensions of the form $d = (2k+1)^2 - 2$, where $k \geq 1$; see [BD79, BD80, DGS77, LS73] for details on how these conditions arise. A direct correspondence with such spherical designs and regular graphs has long been recognized [Sei73], and, in connection, it is known that for infinitely many values of

k, a tight spherical 5-design cannot exist in dimension $d = (2k+1)^2 - 2$ [BMV04, Mak02].

Table 2.1: A list of known tight spherical designs (with the 600-cell). Here M denotes the strength of the design, d the dimension of the ambient space $\mathbb{R}^d$, and N is the size of the design.

d	N	M	Inner products	Name
d	2	1	± 1	Pair of antipodal points
d	$d+1$	2	$-1/d, 1$	Regular simplex
d	$2d$	3	$0, \pm 1$	Cross-polytope
2	N	$N-1$	$\cos(2j\pi/N), 0 \leq j \leq N/2$	Regular N-gon
3	12	5	$\pm 1/\sqrt{5}, \pm 1$	Icosahedron
4	120	11	$0, (\pm 1 \pm \sqrt{5})/4, \pm 1/2, \pm 1$	600-cell
6	27	4	$-1/2, 1/4, 1$	Kissing/Schläfli
7	56	5	$\pm 1/3, \pm 1$	Kissing/Equiangular lines
8	240	7	$0, \pm 1/2, \pm 1$	E_8 root system
22	275	4	$-1/4, 1/6, 1$	Kissing/McLaughlin
23	552	5	$\pm 1/5, \pm 1$	Equiangular lines
23	4600	7	$0, \pm 1/3, \pm 1$	Kissing
24	196560	11	$0, \pm\frac{1}{4}, \pm\frac{1}{2}, \pm 1$	Leech Lattice minimal vectors

Table 2.2 lists all known tight projective designs, except those for the spaces $\mathbb{FP}^1$, as those are congruent to real spheres. Identifying tight projective designs is simple in the real setting. Tight spherical designs of odd strength must be centrally symmetric [DGS77], and by choosing points from each antipode in an odd tight design, one arrives at a real projective tight design. Thus, all tight designs of odd strength in Table 2.1 correspond to entries in Table 2.2.

For the other projective spaces, the vertices of a cross-polytope (i.e. an orthonormal basis in the projective space) always provide a tight 1-design, as they did in $\mathbb{RP}^{d-1}$. However, unlike the real case, it is known that no tight t-designs exist in the complex or quaternionic setting whenever $t \geq 4$ and $d \geq 3$ [BH89, Hog89, Lyu09]. In the complex setting, tight 2-designs, also known as *symmetric, informationally complete, positive operator-valued measures (SIC-POVMs)*, are known to exist for $d \leq 16$, $d = 19, 24, 28, 35, 48$, and numerical experiments suggest that they may exist in every dimension [ABB$^+$14, RBKSC04, SG10, Zau11]. With exception of the $(3,15)$ quaternionic and $(3,27)$ octonionic designs from [CKM16], explicit constructions are readily found for the other designs mentioned in Table 2.2 [Hog82a].

Table 2.2: A list of parameters for the known to exist projective tight designs (besides designs in $\mathbb{FP}^1$ for $\mathbb{F} \neq \mathbb{R}$). Here M denotes the strength of the design, d the dimension of the ambient space $\mathbb{F}^d$, and N is the size of the design. For SIC-POVMs, the $(*)$ indicates that these exist for certain values of d, and may or may not exist for all values.

d	N	M	$\lvert\langle x,y\rangle\rvert^2$	$\mathbb{F}$	Name
d	$d+1$	1	$0,1$	$\mathbb{R}$	Cross-polytope/ONB
2	N	$N-1$	$\cos^2(\pi j/N)$, $1 \le j \le N$	$\mathbb{R}$	Regular $2N$-gon
3	6	2	$1/5,1$	$\mathbb{R}$	Icosahedron
7	28	2	$1/9,1$	$\mathbb{R}$	Kissing configuration for E_8
8	120	3	$0,1/4,1$	$\mathbb{R}$	Roots of E_8 lattice
23	276	2	$1/25,1$	$\mathbb{R}$	Tight simplex
23	2300	3	$0,1/9,1$	$\mathbb{R}$	Kissing configuration for Λ_{24}
24	98280	5	$0,1/16,1/4,1$	$\mathbb{R}$	Minimal vectors of Λ_{24}
d	$d+1$	1	$0,1$	$\mathbb{C}$	Cross-polytope/ONB
$d(*)$	d^2	2	$1/(d+1),1$	$\mathbb{C}$	SIC-POVM
4	40	3	$0,1/3,1$	$\mathbb{C}$	Eisenstein structure on E_8
6	126	3	$0,1/4,1$	$\mathbb{C}$	Eisenstein structure on K_{12}
d	$d+1$	1	$0,1$	$\mathbb{H}$	Cross-polytope/ONB
3	15	2	$2/7,1$	$\mathbb{H}$	Tight simplex
5	165	3	$0,1/4,1$	$\mathbb{H}$	Quaternionic reflection group
3	$d+1$	1	$0,1$	$\mathbb{O}$	Cross-polytope/ONB
3	27	2	$2/13,1$	$\mathbb{O}$	Tight simplex
3	819	5	$0,1/4,1/2,1$	$\mathbb{O}$	Generalized hexagon of order $(2,8)$

A weaker property of a design is sharpness, which will not play a role here. The paper [CK07] proves that sharp designs, and tight designs in particular, are minimizers for discrete energy minimization problems with absolutely monotone kernels.

Chapter 3

Elementary Aspects of Energy Optimization

We now provide several results which connect properties of the kernel K, the functional I_K, and the minimizers of this continuous energy. Many seem to be new, and those which are known do not appear to have been previously collected in a single text, though [BHS19, Chp. 4] provides a similar exposition for lower semi-continuous kernels on compact sets.

In Sections 3.1, 3.2, and 3.3, we present these results for general compact metric spaces. Section 3.1 discusses the equivalences and implications which hold without requiring that the potential U_K^{μ} is constant or the $\text{supp}(\mu) = \Omega$ for some probability measure μ. Bounds on the mutual energy, the convexity of I_K, and a condition for the uniqueness of the equilibrium measure are addressed in this section, as well as two results that will be particularly useful in later chapters: If μ is a local minimizer of I_K, then on $\text{supp}(\mu)$, U_K^{μ} is constant and K is positive definite modulo a constant. In Section 3.2, we assume that μ is K-invariant, i.e. that the potential U_K^{μ} is constant on all of Ω. With this assumption, we find that I_K, which is a quadratic functional, behaves linearly about μ, that the conditionally positive definiteness of K is equivalent positive definiteness modulo a constant, and that if μ is a local minimizer, then it is in fact a global minimizer. In Section 3.3 we make an additional assumption:

that μ has full support. This final assumption allows us to equate K being conditionally positive definite to μ being a global minimizer of I_K and we collect several conditions on K, I_K, or μ that are equivalent to K being conditionally positive definite, positive definite, or conditionally strictly positive definite, Theorems 3.3.1, 3.3.2, and 3.3.3, respectively.

In Sections 3.4 and 3.5 we discuss energy on two-point homogeneous spaces and, more specifically, the sphere. For these spaces, for any isometry invariant kernel F, one is often interested in determining if the surface measure η is a minimizer of I_F. Since η naturally has full support and satisfies $U_F^{\eta}(x) = I_F(\eta)$ for all $x \in \Phi$, our results from the previous sections all apply. In these sections, we discuss how these results relate to the Jacobi or Gegenbauer expansions of F, and provide the results that we will make greatest use of later in the text.

3.1 Positive Definite Functions

We start by discussing some properties and characterizations of (conditional) positive definiteness related to the behavior of the energy functionals and their minimizers.

Positive Definiteness and Inequalities for Mixed Energies

We first make the observation that the (conditional) positive definiteness of the kernel can be characterized by the inequalities for mixed energies in terms of arithmetic or geometric means. While the validity of such inequalities for positive definite kernels is well known, see e.g. Chapter 4 of [BHS19], their sufficiency doesn't seem to have appeared in the literature. We summarize these facts in the following two lemmas. The first one connects conditional positive definiteness to the arithmetic mean inequality.

Lemma 3.1.1. *Suppose K is a kernel on Ω^2. Then the following conditions are equivalent:*

1. *K is conditionally positive definite.*

2. *For every pair of Borel probability measures μ_1 and μ_2 on Ω, the mutual energy $I_K(\mu_1,\mu_2)$ satisfies*

$$I_K(\mu_1,\mu_2) \le \frac{1}{2}\big(I_K(\mu_1)+I_K(\mu_2)\big). \tag{3.1}$$

3. *Inequality* (3.1) *is satisfied for any pair of signed Borel measures of total mass one.*

If K is conditionally strictly positive definite, then equality in 3.1 holds if and only if $\mu_1 = \mu_2$ on Borel subsets of Ω.

Proof. Suppose that K is conditionally positive definite. Then for any $\mu_1,\mu_2 \in \widetilde{\mathbb{P}}(\Omega)$, $\mu_1 - \mu_2 \in \mathscr{Z}(\Omega)$, so

$$0 \le I_K(\mu_1-\mu_2) = I_K(\mu_1) - 2I_K(\mu_1,\mu_2) + I_K(\mu_2),$$

which proves (3.1). Thus, (1) implies (3), which in its turn obviously implies (2).

Now assume condition (2), i.e. that (3.1) holds for all $\mu_1,\mu_2 \in \mathbb{P}(\Omega)$. For any $\mu \in \mathscr{Z}(\Omega)$, there exists $c \ge 0$ and probability measures $\mu_1,\mu_2 \in \mathbb{P}(\Omega)$ such that $\nu = c(\mu_1-\mu_2)$. We then have that

$$I_K(\mu) = c^2\Big(I_K(\mu_1) - 2I_K(\mu_1,\mu_2) + I_K(\mu_2)\Big) \ge 0,$$

so K must be conditionally positive definite.

Let us now assume that K is conditionally strictly positive definite. Equality clearly holds in (3.1) if $\mu_1 = \mu_2$ on all Borel sets of Ω. If, however, the restriction of μ_1 to Borel subsets of Ω does not coincide with that of μ_2, the measure $\mu_1 - \mu_2$ is nonzero on some Borel subset of Ω, and the conditionally strict positive definiteness of K gives us that $I_K(\mu_1-\mu_2) > 0$, making (3.1) a strict inequality. □

The second lemma is very similar: it shows that positive definiteness is equivalent to the geometric mean inequality for the mixed energy.

Lemma 3.1.2. *Suppose K is a kernel on Ω^2. Then K is positive definite if and only if for all $\mu_1, \mu_2 \in \mathbb{P}(\Omega)$, the mutual energy $I_K(\mu_1, \mu_2)$ satisfies*

$$I_K(\mu_1, \mu_2) \leq \sqrt{I_K(\mu_1) I_K(\mu_2)}, \tag{3.2}$$

and $I_K(\mu_1) \geq 0$. If K is strictly positive definite, then equality in (3.2) *holds if and only if $\mu_1 = \mu_2$ on Borel subsets of Ω.*

Observe that, just like in Lemma 3.1.1, we could replace $\mathbb{P}(\Omega)$ with $\widetilde{\mathbb{P}}(\Omega)$.

Proof. Suppose that K is positive definite. Then for any $t \in \mathbb{R}$ and $\mu_1, \mu_2 \in \mathbb{P}(\Omega)$, $t\mu_1 - \mu_2 \in \mathscr{M}(\Omega)$ so

$$g(t) := t^2 I_K(\mu_1) - 2t I_K(\mu_1, \mu_2) + I_K(\mu_2) = I_K(t\mu_1 - \mu_2) \geq 0.$$

Thus the discriminant $4I_K(\mu_1, \mu_2)^2 - 4I_K(\mu_1)I_K(\mu_2)$ of the quadratic polynomial $g(t)$ is nonpositive, which yields (3.2).

Suppose instead that (3.2) holds for all probability measures. For any $\mu \in \mathscr{M}(\Omega)$, there exists $a, b \geq 0$ and $\mu_1, \mu_2 \in \mathbb{P}(\Omega)$ such that $\mu = a\mu_1 - b\mu_2$. We then have that

$$I_K(\mu) = a^2 I_K(\mu_1) - 2ab I_K(\mu_1, \mu_2) + b^2 I_K(\mu_2) \geq (a\sqrt{I_K(\mu_1)} - b\sqrt{I_K(\mu_2)})^2 \geq 0,$$

implying that K is positive definite.

If K is strictly positive definite and equality holds in (3.2), then $g(t)$ has a unique root t'. Since K is strictly positive definite, we have $\mu_1 = t'\mu_2$ on Borel subsets of Ω and since $\mu_1, \mu_2 \in \mathbb{P}(\Omega)$, we see that $t' = 1$ and $\mu_1 = \mu_2$. □

Finally, we use the arithmetic mean inequality of Lemma 3.1.1 to show that minimizers are unique for strictly conditionally positive definite kernels.

Theorem 3.1.3. *Suppose that K is conditionally strictly positive definite. Then I_K has a unique minimizer (either in $\mathbb{P}(\Omega)$ or in $\widetilde{\mathbb{P}}(\Omega)$).*

Proof. Suppose that $\mu_1, \mu_2 \in \mathbb{P}(\Omega)$ (the argument for $\widetilde{\mathbb{P}}(\Omega)$ is identical) are equilibrium measures of I_K, i.e. energy minimizers. Due to Lemma 3.1.1 the probability measure $\mu = \frac{1}{2}(\mu_1 + \mu_2)$ satisfies

$$I_K(\mu) = \frac{1}{4}I_K(\mu_1) + \frac{1}{2}I_K(\mu_1,\mu_2) + \frac{1}{4}I_K(\mu_2) \leq \frac{1}{2}I_K(\mu_1) + \frac{1}{2}I_K(\mu_1) = \mathscr{I}_K(\Omega). \tag{3.3}$$

Thus, μ must also be a minimizer of I_K, which means that $2I_K(\mu_1,\mu_2) = I_K(\mu_1) + I_K(\mu_2)$. By Lemma 3.1.1, $\mu_1 = \mu_2$ on Borel subset of Ω, which proves the claim. □

Positive Definiteness and Convexity of the Energy Functional

Convexity often plays an important role in optimization problems, so it is natural to suspect that the convexity of energy functionals relates to energy minimization, and it is well known that conditional positive definiteness does as well. Therefore, it is not surprising that the two notions are related. We shall demonstrate that they are, in fact, equivalent. This equivalence seems to have been overlooked in most of the literature. The proof presented below has appeared in the author and coauthors' recent paper [BFG$^+$a].

Definition 3.1.4. *Let $K : \Omega \times \Omega \to \mathbb{R}$ be a kernel. We say that I_K is **convex at** $\mu \in \mathbb{P}(\Omega)$ if for every $\nu \in \mathbb{P}(\Omega)$ there exists some $t_\nu \in (0,1]$, such that for all $t \in [0,t_\nu)$*

$$I_K((1-t)\mu + t\nu) \leq (1-t)I_K(\mu) + tI_K(\nu). \tag{3.4}$$

*We say I_K is **convex** on $\mathbb{P}(\Omega)$ if inequality (3.4) holds for every μ, $\nu \in \mathbb{P}(\Omega)$ and all $t \in [0,1]$.*

We observe that convexity of I_K on $\mathbb{P}(\Omega)$ is equivalent to the fact that I_K is convex at all $\mu \in \mathbb{P}(\Omega)$. Indeed, if (3.4) fails for some μ, $\nu \in \mathbb{P}(\Omega)$, then the polynomial $f(t) = I_K((1-t)\mu + t\nu)$ is not convex on the interval $[0,1]$, i.e. $f''(t) < 0$ on some subinterval $[a,b] \subset [0,1]$. But in this case, one can easily see that I_K fails to be convex at $\mu_a = (1-a)\mu + a\nu$.

We first show that convexity is equivalent to the arithmetic mean inequality (3.1) for mixed energies.

Lemma 3.1.5. *The energy functional I_K is convex at $\mu \in \mathbb{P}(\Omega)$ if and only if for all $\nu \in \mathbb{P}(\Omega)$,*

$$I_K(\mu,\nu) \leq \frac{1}{2}\big(I_K(\mu) + I_K(\nu)\big). \tag{3.5}$$

Consequently, I_K is convex on $\mathbb{P}(\Omega)$ if and only if inequality (3.5) *holds for all $\mu, \nu \in \mathbb{P}(\Omega)$.*

Proof. Let $\nu \in \mathbb{P}(\Omega)$ and assume that the arithmetic mean inequality (3.5) holds. Then for all $t \in [0,1]$,

$$I_K((1-t)\mu + t\nu) = (1-t)^2 I_K(\mu) + 2(1-t)t I_K(\mu,\nu) + t^2 I_K(\nu) \leq (1-t)I_K(\mu) + tI_K(\nu). \tag{3.6}$$

So I_K is indeed convex at μ.

For the converse direction, assume that I_K is convex at μ. Then for any $\nu \in \mathbb{P}(\Omega)$ and $t > 0$ sufficiently small, i.e. $t \in (0, t_\nu)$, inequality (3.6) holds, so

$$2(1-t)tI_K(\mu,\nu) \leq t(1-t)(I_K(\mu) + I_K(\nu)).$$

Dividing by $t(1-t)$, we obtain the arithmetic mean inequality (3.5). □

Lemmas 3.1.1 and 3.1.5 together clearly imply the desired equivalence.

Proposition 3.1.6. *Let $K : \Omega \times \Omega \to \mathbb{R}$ be a kernel. Then K is conditionally positive definite if and only if I_K is convex on $\mathbb{P}(\Omega)$.*

Minimizing Measures: Basic Potential Theory

It is well known that the behavior of the minimizing measures is closely connected to the behavior of the potential of the kernel with respect to the minimizing measure. For a detailed account of the topic, we refer the reader to [BHS19] book. The following simple statement is classical, see e.g. [Bjö56]. We provide its proof for completeness.

Theorem 3.1.7. *Suppose that μ is a minimizer of I_K over $\mathbb{P}(\Omega)$. Then $U_K^{\mu}(x) = I_K(\mu)$ on* $\operatorname{supp}(\mu)$ *and $U_K^{\mu}(x) \geq I_K(\mu)$ on Ω.*

Proof. Let $\nu \in \mathscr{Z}(\Omega)$ such that $\mu(A) + \varepsilon\nu(A) \geq 0$ for all Borel subsets $A \subseteq \Omega$ and $0 \leq \varepsilon \leq 1$. This clearly means that $\mu + \varepsilon\nu \in \mathbb{P}(\Omega)$, so

$$I_K(\mu) \leq I_K(\mu + \varepsilon\nu) = I_K(\mu) + 2\varepsilon I_K(\mu, \nu) + \varepsilon^2 I_K(\nu).$$

Thus, for $0 \leq \varepsilon \leq 1$,

$$0 \leq \varepsilon\left(2I_K(\mu,\nu) + \varepsilon I_K(\nu)\right).$$

This means that $I_K(\mu, \nu) \geq 0$.

Suppose, indirectly, that there exist $a, b \in \mathbb{R}$, $z \in \operatorname{supp}(\mu)$, and $y \in \Omega$ such that

$$a = U_K^{\mu}(z) > U_K^{\mu}(y) = b.$$

Let B be a ball centered at z, small enough so that $y \notin B$ and the oscillation of $U_K^{\mu}(x)$ (i.e. $\max_{x\in B} U_K^{\mu}(x) - \min_{y\in B} U_K^{\mu}(y)$) is at most $\frac{a-b}{2}$, and let $m = \mu(B)$. Let ν be defined by

$$\nu(A) = m\delta_y(A) - \mu(A \cap B). \tag{3.7}$$

Then

$$I_K(\mu, \nu) = U_K^{\mu}(y) \cdot m - \int_B U_K^{\mu}(x)d\mu(x) \leq bm - \left(a - \frac{a-b}{2}\right)m < 0,$$

which is a contradiction. Thus, if $U_K^\mu(z) = a$ for some $z \in \operatorname{supp}(\mu)$, then $U_K^\mu(x) \geq a$ for all $x \in \Omega$. Our claim then follows. □

Definition 3.1.8. *We shall say that μ is a* ***local minimizer*** *of I_K if it is a local minimizer in every direction, in other words, if for each $\nu \in \mathbb{P}(\Omega)$, there exists $\tau_\nu \in (0,1]$ such that for all $t \in [0,\tau_\nu]$ we have*

$$I_K\big((1-t)\mu + t\nu\big) \geq I_K(\mu).$$

Observe that this definition differs from the definition of local minimizers with respect to some metric, such as the Wasserstein d_∞ metric or the total variation norm (the difference is similar to that between the Gateaux and Fréchet derivatives). In particular, local minimizers with respect to total variation norm are also local minimizers in the above sense, but not vice versa. In the present work, we shall always use the words *local minimizers* in the sense of Definition 3.1.8. The following proposition provides a relation between the local and global minimizers.

Analyzing the proof of Theorem 3.1.7, we find that for ν defined in (3.7), we can write $\mu + \varepsilon\nu = (1-\varepsilon)\mu + \varepsilon\widetilde{\nu}$ with $\widetilde{\nu} = \mu + \nu \in \mathbb{P}(\Omega)$. Hence, one arrives at a contradiction even if μ is just a local minimizer.

Corollary 3.1.9. *The statement of Theorem 3.1.7 remains true if we only assume that μ is a local (not global) minimizer of I_K.*

As we shall see in Theorem 3.2.10, under some additional conditions, in particular, if K is conditionally positive definite, the statement of Theorem 3.1.7 can be reversed.

Energy Minimizers and Hilbert–Schmidt Operators

There is a close relation between energy minimizers and the properties of the associated Hilbert–Schmidt operator $T_{K,\mu}$ in $L^2(\Omega,\mu)$. We have the following statement.

Lemma 3.1.10. *Let K be a kernel on $\Omega \times \Omega$ and assume that $\mu \in \mathbb{P}(\Omega)$ is a global or local minimizer of I_K with $I_K(\mu) \geq 0$. Then the Hilbert–Schmidt operator $T_{K,\mu}$ is positive.*

Proof. We start by observing that if μ is a (global or local) minimizer of I_K, then the constant function $\mathbb{1}_\Omega$ is an eigenfunction of $T_{K,\mu}$ in $L^2(\Omega,\mu)$. Indeed, according to Theorem 3.1.7 or Corollary 3.1.9, for each $x \in \text{supp}(\mu)$,

$$T_{K,\mu}\mathbb{1}_\Omega(x) = \int_\Omega K(x,y)d\mu(y) = U_K^\mu(x) = I_K(\mu)\mathbb{1}_\Omega(x). \tag{3.8}$$

Assume, indirectly, that $T_{K,\mu}$ is not positive. By Lemma 2.3.1, $T_{K,\mu}$ is compact and self-adjoint, so there exists an eigenfunction ϕ such that $T_{K,\mu}\phi = \lambda\phi$ with $\lambda < 0$. Since ϕ is continuous, and therefore bounded, on $\text{supp}(\mu)$, we have that for sufficiently small $|t|$, the measure

$$\mu_t = (1+t\phi)\mu$$

is positive. As we noted above, $\mathbb{1}_\Omega$ is an eigenfunction of $T_{K,\mu}$ corresponding to the eigenvalue $I_K(\mu) \geq 0$. Clearly, then, $\mathbb{1}_\Omega$ and ϕ are orthogonal, so

$$\mu_t(\Omega) = \int_\Omega (1+t\phi(x))d\mu(x) = \mu(\Omega) = 1$$

and for $s > 0$

$$\begin{aligned} I_K((1-s)\mu + s\mu_t) &= I_K(\mu_{st}) \\ &= \int_\Omega\int_\Omega K(x,y)(1+st\phi(x))(1+st\phi(y)d\mu(x)d\mu(y) \\ &= I_K(\mu) + \lambda t^2 \int_\Omega |\phi(x)|^2 d\mu(x) < I_K(\mu) \end{aligned}$$

which contradicts the (local) minimality of μ over probability measures. □

Recall that according to Lemma 2.3.1, the operator $T_{K,\mu}$ is positive if and only if K is positive definite on the support of μ. If the condition $I_K(\mu) \geq 0$ in Lemma 3.1.10 is not satisfied, we can replace K by $K'(x,y) = K(x,y) - I_K(\mu)$, which does not affect energy minimizers. Then $I_{K'}(\mu) = 0$, and hence, Lemma 3.1.10 applies. Therefore $T_{K',\mu}$ is positive, i.e. K' is positive definite on $\widetilde{\Omega} = \mathrm{supp}(\mu)$. In other words, K is positive definite up to an additive constant, as a kernel on $\widetilde{\Omega} \times \widetilde{\Omega}$. We arrive at the following important fact.

Lemma 3.1.11. *Let K be a kernel on $\Omega \times \Omega$. Suppose that μ is a minimizer of I_K over $\mathbb{P}(\Omega)$. Then the kernel K must be positive definite modulo a constant on* $\mathrm{supp}(\mu)$*, i.e. as a kernel on* $\mathrm{supp}(\mu) \times \mathrm{supp}(\mu)$*. If $I_K(\mu) \geq 0$, then K is positive definite on* $\mathrm{supp}(\mu)$.

Various statements of this type are known in the literature [CFP17, FS13].

3.2 Invariant Measures

As explained in the previous section, measures with constant potentials are particularly interesting from the point of view of energy minimization. They also naturally arise in metric geometry, in connection with the so called "rendezvous numbers" [CMY86], and we draw the term "invariant" from this literature. These applications and various interesting properties warrant a separate discussion of such measures.

Definition, Examples, and Comments

We start with the following definition.

Definition 3.2.1. *Let K be a kernel on $\Omega \times \Omega$. We say that a measure $\mu \in \mathbb{P}(\Omega)$ is **K-invariant** if the potential of K with respect to this measure is constant on Ω, i.e.*

$$U_K^{\mu}(x) = I_K(\mu) \quad \text{for every} \quad x \in \Omega. \tag{3.9}$$

We shall see shortly that these measures have an array of remarkable properties. Notice that the definition does not require that μ has full support: while some of the statements in this chapter will require this additional assumption, i.e. $\mathrm{supp}(\mu) = \Omega$, the majority of them hold even in its absence.

Before proceeding to these properties we shall provide some examples, showing that K-invariant measures is a rather rich notion. Observe that most of the examples below have full support. Numerous statements that we shall prove for K-invariant measures will apply to all these natural examples.

- If μ (locally) minimizes I_K and has full support, then according to Theorem 3.1.7 and Corollary 3.1.9 , the measure μ is K-invariant.

- Let $\Omega = \mathbb{S}^{d-1}$ and assume that K is rotationally invariant, i.e. $K(x,y) = F(\langle x,y \rangle)$. Then the normalized uniform surface measure is K-invariant, since the potential $U_F^\sigma(x) = \int\limits_{\mathbb{S}^{d-1}} F(\langle x,y \rangle) d\sigma(y)$ is obviously independent of $x \in \mathbb{S}^{d-1}$.

- If, moreover, the F from the previous example is a polynomial of degree M, and μ is a spherical M-design, then μ must also be K-invariant.

- Similarly, assume that Ω is a compact two-point homogeneous space, K is invariant with respect to the group of isometries, and η is the normalized uniform measure on Ω. Then η is K-invariant. This equally applies to connected (e.g., projective spaces) and discrete (e.g., Hamming cube) two-point homogeneous spaces.

- If Ω is a compact topological group, μ is its normalized Haar measure, and K is invariant with respect to the group operation, i.e. $K(x,y) = F(x-y)$, then μ is K-invariant.

- Let $\Omega = [0,1]$ and $K(x,y) = |x-y|$. Then the measure $\mu = \frac{1}{2}(\delta_0 + \delta_1)$ is K-invariant. Notice that this example provides an invariant measure which does not have full support.

Despite an abundance of examples, the existence of a K-invariant measure is possible only under significant restrictions on the geometry of the domain Ω and the structure of the kernel K. For example, the following statement is true [CMY86].

Lemma 3.2.2. *Assume that U is a finite-dimensional vector space endowed with a strictly convex norm, i.e. $\|x+y\|_U < \|x\|_U + \|y\|_U$ unless x and y are linearly dependent. Let $\Omega \subset U$ be compact and set $K(x,y) = \|x-y\|_U$. If there exists a K-invariant measure on Ω, then either Ω is a line segment or no three points of Ω are colinear.*

For the case when $K(x,y) = \|x-y\|$ is the Euclidean distance, this lemma shows, for example, that an invariant measure doesn't exist for the unit ball, while, as we know, it does exist for the sphere.

Finally, we make the remark that if a measure μ is K-invariant, it implies that a constant function is an eigenfunction of the Hilbert–Schmidt operator $T_{K,\mu}$ in $L^2(\Omega,\mu)$ with eigenvalue $\lambda = I_K(\mu)$, which is implied by (3.8).

A Crucial Identity

The following simple relation provides a direct link between energy minimization and (conditional) positive definiteness and will play a decisive role in many results of this section. It is also an important first step in the proof of the Generalized Stolarsky principle (Theorem 5.3.1). In a nutshell, this lemma states that, while I_K is a quadratic functional, it behaves linearly around a K-invariant measure.

Lemma 3.2.3. *Let K be a kernel on $\Omega \times \Omega$ and let μ be a K-invariant measure, i.e. $U_K^{\mu}(x) = I_K(\mu)$ for all $x \in \Omega$. Then for any $\nu \in \widetilde{\mathbb{P}}(\Omega)$,*

$$I_K(\nu - \mu) = I_K(\nu) - I_K(\mu). \tag{3.10}$$

More generally, if $\mu \in \mathbb{P}(\Omega)$ such that $U_K^{\mu}(x) \geq I_K(\mu)$, with equality on $\operatorname{supp}(\mu)$, then for any $\nu \in \mathbb{P}(\Omega)$

$$I_K(\nu - \mu) \leq I_K(\nu) - I_K(\mu), \tag{3.11}$$

and equality (3.10) holds for any measure $\nu \in \widetilde{\mathbb{P}}(\Omega)$ with $\operatorname{supp}(\nu) \subseteq \operatorname{supp}(\mu)$.

Proof. If μ is K-invariant, then for any $\nu \in \widetilde{\mathbb{P}}(\Omega)$,

$$I_K(\mu,\nu) = \int_\Omega U_K^\mu(x)d\nu(x) = \int_\Omega I_K(\mu)d\nu(x) = I_K(\mu). \tag{3.12}$$

Therefore

$$I_K(\nu-\mu) = I_K(\nu) - 2I_K(\mu,\nu) + I_K(\mu).$$

For the second part of our claim, observe that for any $\nu \in \mathbb{P}(\Omega)$, instead of equality (3.12), one has the inequality $I_K(\mu,\nu) \geq I_K(\mu)$, and thus,

$$I_K(\nu-\mu) = I_K(\nu) - 2I_K(\mu,\nu) + I_K(\mu) \leq I_K(\nu) - I_K(\mu).$$

Finally, the last statement follows from the first by replacing Ω with $\mathrm{supp}(\mu)$. □

Theorem 3.1.7 and Corollary 3.1.9 show that if μ is a global (or at least local) minimizer of I_K, it satisfies the the conditions of the second statement in Lemma 3.2.3, and if in addition μ has full support, it also satisfies the first condition, i.e. μ is K-invariant. Thus Lemma 3.2.3 applies to (local) energy minimizers, which results in the following corollary:

Corollary 3.2.4. *Let K be a kernel on $\Omega \times \Omega$ and μ be a (local) minimizer of I_K. Then for any $\nu \in \mathbb{P}(\Omega)$*

$$I_K(\nu-\mu) \leq I_K(\nu) - I_K(\mu). \tag{3.13}$$

For any $\nu \in \widetilde{\mathbb{P}}(\Omega)$ such that $\mathrm{supp}(\nu) \subseteq \mathrm{supp}(\mu)$*, then*

$$I_K(\nu-\mu) = I_K(\nu) - I_K(\mu). \tag{3.14}$$

Conditional Positive Definiteness and Energy Minimization

Identity (3.10) of Lemma 3.2.3 provides a clear link between energy minimization and conditional positive definiteness. We would like to emphasize that relation (3.10) holds not just for probability measures ν, but for arbitrary signed measures of total mass one, i.e. $\nu \in \widetilde{\mathbb{P}}(\Omega)$. Therefore, one can immediately deduce the following equivalence.

Theorem 3.2.5. *Let K be a kernel on $\Omega \times \Omega$ and assume that μ is K-invariant. Then μ minimizes I_K over the set $\widetilde{\mathbb{P}}(\Omega)$ of normalized signed Borel measures if and only if K is conditionally positive definite.*

Moreover, μ uniquely minimizes I_K over $\widetilde{\mathbb{P}}(\Omega)$ if and only if K is conditionally strictly positive definite.

Proof. Suppose that K is conditionally positive definite. Then for any $\nu \in \widetilde{\mathbb{P}}(\Omega)$, equality (3.10) holds and, since $(\nu - \mu)(\Omega) = 0$, we have

$$I_K(\nu) - I_K(\mu) = I_K(\nu - \mu) \geq 0,$$

which shows that μ minimizes I_K over $\widetilde{\mathbb{P}}(\Omega)$. If K is conditionally strictly positive definite, then $I_K(\nu) = I_K(\mu)$ only if $\nu - \mu = 0$ on all Borel sets of Ω, i.e. μ is the unique minimizer.

Assume conversely that $I_K(\mu) \leq I_K(\nu)$ for each $\nu \in \widetilde{\mathbb{P}}(\Omega)$. Consider an arbitrary signed measure $\gamma \in \mathscr{Z}(\Omega)$. Define $\nu = \mu + \gamma$, then $\nu(\Omega) = 1$, i.e. $\nu \in \widetilde{\mathbb{P}}(\Omega)$. Thus, applying (3.10) once again, we find that

$$I_K(\gamma) = I_K(\nu - \mu) = I_K(\nu) - I_K(\mu) \geq 0,$$

hence K is conditionally positive definite. If μ is the unique minimizer, then the expression above equals zero only for $\gamma = 0$, i.e. K is conditionally strictly positive definite. □

Obviously, one of the implications holds for minimizers over probability measures $\mathbb{P}(\Omega)$.

Corollary 3.2.6. *Let K be a kernel on $\Omega \times \Omega$ and assume that μ is K-invariant. If K is conditionally (strictly) positive definite, then μ (uniquely) minimizes I_K over the set $\mathbb{P}(\Omega)$ of Borel measures probability measures.*

Some remarks are in order. We would like to remind the reader that in some specific cases, such as the sphere with the uniform surface measure (or more generally, two-point homogeneous spaces with the corresponding uniform measures), the relation between energy minimization and some form of positive definiteness of the kernel is well known [Sch42, BDM18]. However, it is usually demonstrated using the representation theory of the underlying space and the associated orthogonal polynomial (Gegenbauer, Jacobi, Krawtchouk) expansions. Theorem 3.2.5 above is a blanket statement that covers all of these examples and beyond. Moreover, it relies only on the completely elementary identity (3.10), thus simplifying the known proofs in all of the specific cases. In the spherical case, a similar approach has been recently employed in [BDM18].

Conditional Positive Definiteness vs. Positive Definiteness up to an Additive Constant

As we have observed in the previous discussions, two properties, which are somewhat weaker than positive definiteness, play an important role in energy minimization: namely, conditional positive definiteness and positive definiteness up to an additive constant. We have already demonstrated in Lemma 2.2.4 that the latter always implies the former, and the converse implication is not true in general. We shall now show that the converse implication also holds, i.e. conditional positive definiteness implies positive definiteness up to an additive constant, if we additionally assume the existence of a K-invariant measure. Moreover, the statement also holds for the "strict" version of these properties.

Lemma 3.2.7. *Let K be a kernel on $\Omega \times \Omega$ and assume that K is conditionally (strictly) positive definite. Suppose also that there exists a K-invariant measure $\mu \in \mathbb{P}(\Omega)$. Then K*

is (strictly) positive definite up to an additive constant.

Proof. Let K be conditionally positive definite. Set $C = -I_K(\mu)+1$. Then $K+C$ is still conditionally (strictly) positive definite, μ is $(K+C)$-invariant, and $I_{K+C}(\mu) = (\mu(\Omega))^2 = 1$. For any signed measure ν with $\nu(\Omega) = 1$, identity (3.10) implies that

$$I_{K+C}(\nu) - I_{K+C}(\mu) = I_{K+C}(\nu-\mu) = I_K(\nu-\mu) \geq 0.$$

Therefore, $I_K(\nu) \geq 1 > 0$.

Now consider an arbitrary measure $\gamma \in \mathscr{M}(\Omega)$. If $\gamma(\Omega) = 0$, then $I_{K+C}(\gamma) \geq 0$ by conditional positive definiteness (and $I_{K+C}(\gamma) > 0$ for $\gamma \neq 0$ for the "strict" version if $\gamma \neq 0$).

If $\gamma(\Omega) = c \neq 0$, we can write $\gamma = c\nu$ for some $\nu \in \widetilde{\mathbb{P}}(\Omega)$. Therefore, $I_{K+C}(\gamma) = c^2 I_{K+C}(\nu) \geq c^2 > 0$. Hence $K+C$ is (strictly) positive definite. □

Lemmas 2.2.4 and 3.2.7 together show that in the presence of a K-invariant measure, conditional positive definiteness and positive definiteness modulo an additive constant are equivalent notions. This is the case, for example, for rotationally invariant kernels K on the sphere, since the uniform surface measure σ is K-invariant for all such kernels.

Local and Global Minimizers

Under some additional assumptions local minimizers of I_K are necessarily global minimizers. Some facts of this type have been observed in the papers of the author with various coauthors [BFG$^+$a, BGM$^+$a]. Here we prove a variety of more general statements with the same flavor.

Proposition 3.2.8. *Suppose that μ is a local minimizer of I_K and any of the following two conditions holds:*

1. *the measure μ is K-invariant, i.e. $U_K^{\mu}(x) = I_K(\mu)$ for all $x \in \Omega$;*

2. *K is conditionally positive definite.*

Then μ is a global minimizer of I_K.

Observe that, according to Corollary 3.1.9, condition (1) is automatically satisfied if μ has full support.

Proof. Assume that (1) holds. Then for any $\nu \in \mathbb{P}(\Omega)$, we have $I_K(\mu,\nu) = I_K(\mu)$ and therefore, since μ is a local minimizer, for small $t > 0$, we have

$$\begin{aligned} I_K(\mu) &\le I_K((1-t)\mu + t\nu) = (1-t)^2 I_K(\mu) + 2t(1-t)I_K(\mu,\nu) + t^2 I_K(\nu) \\ &= (1-t)^2 I_K(\mu) + 2t(1-t)I_K(\mu) + t^2 I_K(\nu) = (1-t^2)I_K(\mu) + t^2 I_K(\nu). \end{aligned}$$

Thus $I_K(\mu) \le I_K(\nu)$, i.e. μ is a global minimizer of I_K in $\mathbb{P}(\Omega)$.

Now assume that K is conditionally positive definite. Then for each $\nu \in \mathbb{P}(\Omega)$, the measure $\nu - \mu$ has total mass zero. Therefore, according to conditional positive definiteness of K and inequality (3.13) of Corollary 3.2.4,

$$I_K(\nu) - I_K(\mu) \ge I_K(\nu - \mu) \ge 0. \tag{3.15}$$

Therefore, in this case, μ also minimizes I_K. □

If both conditions (1) and (2) hold simultaneously, an even stronger conclusion can be drawn.

Proposition 3.2.9. *Let μ be a local minimizer of I_K. Assume in addition that μ is K-invariant and K is conditionally positive definite. Then μ is a global minimizer of I_K over $\widetilde{\mathbb{P}}(\Omega)$, the set of all signed Borel measures with total mass one.*

Proof. Let $\nu \in \widetilde{\mathbb{P}}(\Omega)$. Since μ is a K-invariant local minimizer, we can apply conditional positive definiteness of K in conjunction with equality (3.10) of Lemma 3.2.3 to obtain

$$I_K(\nu) - I_K(\mu) = I_K(\nu - \mu) \ge 0,$$

giving us our claim. $\square$

Finally, another version of the local-to-global minimization principle may be proved under the assumption that I_K is convex at μ, which according to Lemma 3.1.5, is equivalent to the fact that the arithmetic mean inequality (3.5) holds for any measure $\nu \in \mathbb{P}(\Omega)$. We have the following statement.

Theorem 3.2.10. *Suppose that K is a kernel on $\Omega \times \Omega$ and that for some $\mu \in \mathbb{P}(\Omega)$ there exists a constant $M \in \mathbb{R}$ such that $U_K^\mu(x) \geq M$, with equality on* $\mathrm{supp}(\mu)$. *If I_K is convex at μ, then μ is a global minimizer of I_K over $\mathbb{P}(\Omega)$.*

Before proving this statement we observe that its first assumption is satisfied in any of the following two cases: (a) if μ is K-invariant; (b) if μ is a local minimizer, according to Corollary 3.1.9. In addition, if convexity at μ were replaced with convexity of I_K on $\mathbb{P}(\Omega)$, then in view of Proposition 3.1.6, this would be equivalent to the conditional positive definiteness of K. Thus, this theorem recovers and strengthens part (2) of Proposition 3.2.8. Moreover, we have the following immediate corollary, which will be used later.

Corollary 3.2.11. *Let K be a kernel on $\Omega \times \Omega$ and let $\mu \in \mathbb{P}(\Omega)$ be a K-invariant measure. If I_K is convex at μ, then μ is a global minimizer of I_K over $\mathbb{P}(\Omega)$.*

Proof of Theorem 3.2.10. Observe first that the constant M is necessarily equal to $I_K(\mu)$:

$$I_K(\mu) = \int_\Omega U_K^\mu(x)d\mu(x) = \int_{\mathrm{supp}(\mu)} M d\mu(x) = M.$$

For any $\nu \in \mathbb{P}(\Omega)$, we have that

$$I_K(\mu,\nu) = \int_\Omega U_K^\mu(x)d\nu(x) \geq I_K(\mu).$$

Convexity of I_K at μ, according to Lemma 3.1.5, is equivalent to the arithmetic mean inequality (3.5). Thus,

$$I_K(\mu) \le I_K(\mu,\nu) \le \frac{1}{2}I_K(\mu) + \frac{1}{2}I_K(\nu),$$

so $I_K(\nu) \ge M = I_K(\mu)$. □

3.3 Invariant Measures and Minimizers with Full Support

It is now time to summarize the results of the previous sections. It may not be yet obvious, but we have proven (sometimes quite surprising) equivalences between many different notions. We shall restrict our attention to the case when the measure μ is K-invariant (i.e. has constant potential) and has full support. As we have discussed before, these conditions are satisfied by many natural candidates (the uniform measure on the sphere or other two-point homogeneous spaces, the Haar measure on a compact topological group, etc). Though a majority of the implications are valid even just for K-invariant measures without the full support assumption, assuming that μ has full support truly ties the picture together. We shall carefully trace which of the conclusions require this condition.

We start with the following long list of equivalences.

Theorem 3.3.1. *Let K be a kernel on $\Omega \times \Omega$. Assume that there exists a measure $\mu \in \mathbb{P}(\Omega)$, which is K-invariant and has full support, i.e. $U_K^{\mu}(x) = I_K(\mu)$ for all $x \in \Omega$ and* $\operatorname{supp}(\mu) = \Omega$.

Then the following conditions are equivalent:

1. *K positive definite modulo a constant.*

2. *K is conditionally positive definite.*

3. *μ is a local minimizer of I_K.*

4. *μ is a global minimizer of I_K over $\mathbb{P}(\Omega)$.*

5. *μ is a global minimizer of I_K over $\widetilde{\mathbb{P}}(\Omega)$.*

6. *I_K is convex.*

7. *I_K is convex at μ.*

8. *The arithmetic mean inequality* (3.1) *holds for all $\mu_1, \mu_2 \in \mathbb{P}(\Omega)$ (or, equivalently for all $\mu_1, \mu_2 \in \widetilde{\mathbb{P}}(\Omega)$).*

9. *The arithmetic mean inequality* (3.1) *holds when $\mu_1 = \mu$.*

10. *The kernel K can be represented as*

$$K(x,y) = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \lambda_j \phi_j(x) \phi_j(y)$$

where the series converges uniformly and absolutely, the function ϕ_1 is constant, and $\lambda_j \geq 0$ for $j \geq 2$.

Proof. For the reader's convenience the implications proving this theorem are summarized in Figure 3.1.

We open with the list the implications that do not require any assumptions on μ. It is obvious that (5) implies (4), which in turn implies (3). Also, (6) implies (7), and similarly, (8) implies (9).

The equivalence between (2), (6), and (8) is proved in Lemmas 3.1.1 and 3.1.5 together with Proposition 3.1.6. Lemma 3.1.5 also establishes the equivalence between (7) and (9). Lemma 2.2.4 shows that (1) implies (2).

The following implications rely on the fact that μ is K-invariant, but do not require μ to have full support. Lemma 3.2.7 demonstrates that (2) implies (1). Theorem 3.2.5 yields the equivalence of (2) and (5). Corollary 3.2.11 to Theorem 3.2.10 shows that (4) follows

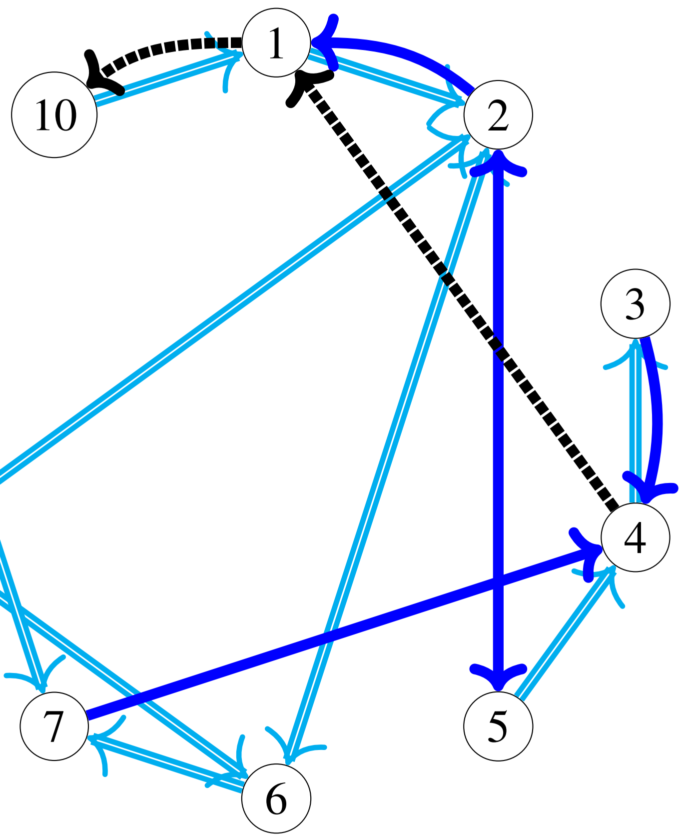

Figure 3.1: Equivalences in Theorem 3.3.1: double line (cyan) arrows are implications that hold without additional assumptions; single line (blue) ones require K-invariance, but not full support; the dashed (black) arrows represent the implications which do require the assumption of full support.

from (7). Finally, part (1) of Proposition 3.2.8 guarantees that (3) implies (4).

The equivalence between (1) and (10) is discussed in Lemma 2.2.2 and Mercer's Theorem (see Theorem 2.3.3), or more specifically Corollary 2.3.4. The fact that (1) implies (10) relies on the fact that for a K-invariant measure μ, the constant function $\mathbb{1}_\Omega$ is an eigenfunction of the Hilbert–Schmidt operator $T_{K,\mu}$ in $L^2(\Omega,\mu)$, and the condition $\text{supp}(\mu) = \Omega$ implies that the expansion in Mercer's Theorem is valid on all of Ω. The implication (10) $\Rightarrow$ (1) holds without any additional assumptions, according to Lemma 2.2.2.

In conclusion, we observe that Lemma 3.1.11 demonstrates that (4) implies (1), which closes the loop of implications – and, except for the standalone equivalence between (1) and (10), this is the only implication in our proof where the fact that $\text{supp}(\mu) = \Omega$ is used. Indeed, Lemma 3.1.11 only guarantees that the kernel K is positive definite (up to constant) on the support of the minimizer. Observe also that due to Theorem 3.1.7, if (4) holds and μ has full support. □

To reiterate, this theorem reveals several interesting novel effects that happen to a K-invariant measure (with full support):

- Equivalence between minimization over the set $\mathbb{P}(\Omega)$ of probability measures and the set $\widetilde{\mathbb{P}}(\Omega)$ of all signed measures of mass one. This effect has been observed for rotationally invariant kernels on the sphere and the surface measure σ by the author and collaborators [BDM18]. This is not necessarily the case in other settings. In particular, for the integral over the unit ball $\mathbb{B}^d$

$$\int_{\mathbb{B}^d}\int_{\mathbb{B}^d} \|x-y\| d\mu(x)d\mu(y),$$

according to [Bjö56], the unique maximizer over both $\mathbb{P}(\mathbb{B}^d)$ and $\mathbb{P}(\mathbb{S}^{d-1})$ is σ. According to the aforementioned equivalence, σ is also a maximizer over $\widetilde{\mathbb{P}}(\mathbb{S}^{d-1})$, while in the case of signed measures on the ball, the maximizer does not exist [HNW11].

- Equivalence between being a local and global energy minimizer. This effect, in a slightly less general form, has been observed by the author and collaborators in [BFG$^+$a, BGM$^+$a].

- Equivalence between other local and global properties: e.g., the energy functional I_K is convex on the whole set of probability measures if and only if it is convex just at the special measure μ.

- Equivalence between conditional positive definiteness of the kernel and positive definiteness up to constant, which is not true in general.

We now formulate similar theorems for kernels which have the "strict" version of the properties and for positive definite kernels. We start with the latter.

Theorem 3.3.2. *Suppose that K is a kernel on $\Omega \times \Omega$ and that there exists a measure $\mu \in \mathbb{P}(\Omega)$, which is K-invariant and has full support, i.e. $U_K^{\mu}(x) = I_K(\mu)$ for all $x \in \Omega$ and* $\operatorname{supp}(\mu) = \Omega$. *Then the following conditions are equivalent:*

1. *The kernel K is positive definite.*

2. *The geometric mean inequality* (3.2) *and $I_K(\mu_1) \geq 0$ hold for all $\mu_1, \mu_2 \in \mathbb{P}(\Omega)$.*

3. *The measure μ is a global minimizer of I_K and satisfies $I_K(\mu) \geq 0$.*

4. *The kernel K can be represented as*

$$K(x,y) = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \lambda_j \phi_j(x) \phi_j(y)$$

where the series converges uniformly and absolutely, and $\lambda_j \geq 0$ for $j \geq 1$.

5. *There exists some symmetric $k \in L^2(\Omega \times \Omega, \mu \times \mu)$ such that for all $x, y \in \Omega$,*

$$K(x,y) = \int_\Omega k(x,z)k(z,y)d\mu(z).$$

Proof. Lemma 3.1.2, Corollary 2.3.4, and Proposition 2.3.6 show the equivalence of (1), (2), (4), and (5). Positive definiteness, i.e. condition (1), guarantees that $I_K(\mu) \geq 0$, and that μ is a minimizer, due to Theorem 3.3.1. Conversely, Lemma 3.1.11 shows that (3) implies (1), finishing our proof. Observe also that according to Theorem 3.3.1 it does not matter whether we mean global minimization over $\mathbb{P}(\Omega)$ or $\widetilde{\mathbb{P}}(\Omega)$ in condition (3). □

Theorem 3.3.3. *Suppose that K is a kernel on Ω^2 and that that there exists a measure $\mu \in \mathbb{P}(\Omega)$ which is K-invariant, i.e. $U_K^\mu(x) = I_K(\mu)$ for all $x \in \Omega$. Then the following conditions are equivalent:*

1. *K is conditionally strictly positive definite.*
2. *K is strictly positive definite modulo a constant.*
3. *μ is the unique minimizer of I_K over $\widetilde{\mathbb{P}}(\Omega)$.*

If in addition $\mathrm{supp}(\mu) = \Omega$*, i.e. μ has full support, then each of the conditions* (1)–(3) *implies the following*

4. *The kernel K can be represented as*

$$K(x,y) = \sum_{j=1}^{\dim(L^2(\Omega,\mu))} \lambda_j \phi_j(x)\phi_j(y)$$

where $\{\phi_j\}$ is the orthonormal basis consisting of eigenfunctions of the Hilbert–Schmidt operator $T_{K,\mu}$ in $L^2(\Omega,\mu)$, the function ϕ_1 is a constant, the series converges uniformly and absolutely, and $\lambda_j > 0$ for $j \geq 2$.

Moreover, if the span of $\{\phi_j\}$ is dense in $C(\Omega)$, then (4) *also implies conditions* (1)–(3).

Proof. Lemma 2.2.4 shows that (2) implies (1), while Lemma 3.2.7 provides the converse implication. The equivalence of (3) and (1) is proved in Theorem 3.2.5.

Before we turn to dealing with condition (4), recall that K-invariance of μ implies that a constant is an eigenfunction of the operator $T_{K,\mu}$, so we shall assume that $\phi_1 = \mathbb{1}_\Omega$.

Now we show that (3) implies (4). Since μ minimizes I_K and has full support, by Theorem 3.3.1, K is positive definite up to a constant, and since $\phi_1 = 1$, by Mercer's Theorem, the expansion in part (4) holds with some $\lambda_j \in \mathbb{R}$ and with the series converging uniformly and absolutely. Suppose, indirectly, that μ is the unique minimizer of I_K over $\widetilde{\mathbb{P}}(\Omega)$, but there exists some $l \geq 2$ such that $\lambda_l \leq 0$. Let $d\nu(x) = (1+\phi_l(x))d\mu(x)$. Orthogonality implies that $\int\limits_\Omega \phi_l(x)d\mu(x) = 0$, therefore $\nu \in \widetilde{\mathbb{P}}(\Omega)$. Then we obtain

$$\begin{aligned}
I_K(\nu) &= \int\limits_\Omega \int\limits_\Omega K(x,y)(1+\phi_l(x))(1+\phi_l(y))d\mu(x)d\mu(y) \\
&= I_K(\mu) + 2\langle T_{K,\mu}\phi_l, \mathbb{1}_\Omega\rangle_{L^2(\Omega,\mu)} + \langle T_{K,\mu}\phi_l, \phi_l\rangle_{L^2(\Omega,\mu)} \\
&= I_K(\mu) + 2\lambda_l\langle \phi_l, \mathbb{1}_\Omega\rangle_{L^2(\Omega,\mu)} + \lambda_l\|\phi_l\|^2_{L^2(\Omega,\mu)} \\
&= I_K(\mu) + \lambda_l \leq I_K(\mu),
\end{aligned}$$

which contradicts the fact that μ is the unique minimizer over $\widetilde{\mathbb{P}}(\Omega)$.

Finally, we show that (4) implies (2) under the aforementioned additional assumption. Let $K'(x,y) = K(x,y) - \lambda_1 + 1$ and $\nu \in \mathscr{M}(\Omega)$. Then

$$\begin{aligned}
I_{K'}(\nu) &= \int\limits_\Omega \int\limits_\Omega K'(x,y)d\nu(x)d\nu(y) \\
&= (\nu(\Omega))^2 + \sum_{j=2}^{\dim(L^2(\Omega,\mu))} \int\limits_\Omega \int\limits_\Omega \lambda_j\phi_j(x)\phi_j(y)d\nu(x)d\nu(y) \\
&= (\nu(\Omega))^2 + \sum_{j=2}^{\dim(L^2(\Omega,\mu))} \lambda_j\Big(\int\limits_\Omega \phi_j(x)d\nu(x)\Big)^2 \geq 0.
\end{aligned}$$

Clearly, the only way that $I_{K'}(\nu) = 0$ is if $\int\limits_{\Omega} \phi_j(x) d\nu(x) = 0$ for all $j \geq 1$. By the density of $\text{span}(\{\phi_j\}_{j=1}^{\dim(L^2(\Omega,\mu))})$ in $C(\Omega)$, we can conclude that this implies $d\nu = 0$, so K' must be strictly positive definite, which completes the proof. $\square$

We conclude with the remark that the additional condition imposed for the sufficiency of condition (4) is not very restrictive in practice. For example in the case of rotationally invariant kernels on the sphere and $\mu = \sigma$, the eigenfunction ϕ_j are simply spherical harmonics, which span all polynomials on the sphere and thus their span is dense in the space continuous functions.

3.4 Energies on Two-point Homogeneous Spaces

On a compact, connected, two-point homogeneous set Φ, it is natural to ask, for an isometry invariant kernel F, whether the uniform surface measure η is a minimizer of the energy I_F. Since F is isometry invariant, we have that for every isometry θ on Φ,

$$U_F^{\eta}(\theta x) = \int\limits_{\Phi} F(\tau(\theta x, y)) d\eta(y) = \int\limits_{\Phi} F(\tau(x, \theta^{-1} y)) d\eta(\theta^{-1} y)$$
$$= \int\limits_{\Phi} F(\tau(x,y)) d\eta(y) = U_F^{\eta}(x),$$

so the potential U_F^{η} is constant on Φ. This means that η is an F-invariant measure and hence Theorems 3.3.1, 3.3.2, and 3.3.3 hold. In particular, η minimizes I_F if and only if F is positive definite modulo a constant. Due to (2.35), this means that if F is a positive definite (modulo a constant) polynomial of degree M, then any weighted M-design on Φ is a minimizer of I_F.

We now show that having nonnegative coefficients in the Jacobi expansion of F is equivalent to the fact that η is a minimizer of I_F over $\mathbb{P}(\Phi)$, which has been shown in a number of papers, see for instance [DG03, BD19, BGM$^+$a]. It immediately follows from the equivalence of η being a minimizer of I_F and positive definiteness (modulo a constant) of F, from Theorem 3.3.1, and Proposition 2.4.2, however, we will provide a direct proof. Let, as before $C_n = C_n^{(\alpha,\beta)}$ denote the normalized Jacobi polynomials associated to Φ.

Proposition 3.4.1. *Let $F \in C([-1,1])$, $F(t) = \sum_{n=0}^{\infty} \widehat{F}_n C_n(t)$, and $\mu \in \mathbb{P}(\Phi)$. Then, the following are equivalent:*

1. *$\widehat{F}_n \geq 0$ for all $n \geq 1$,*

2. *the surface measure η is a minimizer of I_F.*

Moreover, η is the unique minimizer of I_F if and only if $\widehat{F}_n > 0$ for all $n \geq 1$.

Proof. We first show that η is a minimizer of I_F. Assume that $\widehat{F}_n \geq 0$ for all $n \geq 1$. Then by Lemma 2.4.1, the Fubini theorem, and the addition formula (2.19), we have, for any $\mu \in \mathbb{P}(\Phi)$,

$$\begin{aligned}
I_F(\mu) &= \sum_{n=0}^{\infty} \widehat{F}_n \int_{\Phi} \int_{\Phi} C_n(\tau(x,y)) d\mu(x) d\mu(y) \\
&= \sum_{n=0}^{\infty} \frac{\widehat{F}_n}{\dim V_n} \sum_{n=1}^{\dim V_n} \int_{\Omega} \int_{\Omega} Y_{n,k}(x) \overline{Y_{n,k}(y)} d\mu(x) d\mu(y) \\
&= \widehat{F}_0 + \sum_{n=1}^{\infty} \frac{\widehat{F}_n}{\dim V_n} \cdot \sum_{k=1}^{\dim V_n} \left| \int_{\Omega} Y_{n,k}(x) d\mu(x) \right|^2, \\
&\geq \widehat{F}_0 = I_F(\eta).
\end{aligned}$$

If $\widehat{F}_n > 0$ for all $n \geq 1$, then equality can be achieved above only if μ is orthogonal to all spaces V_n, which directly implies that $\mu = \eta$.

If $\widehat{F}_n < 0$ for some $n \geq 1$, then set, for some $p \in \Phi$, $Y_n(x) = C_n(\tau(x,p)) \in V_n$ and $d\mu(x) = (1 + \varepsilon Y_n(x)) d\eta(x)$, where $\varepsilon > 0$ is sufficiently small so that $(1 + \varepsilon Y_n(x)) \geq 0$ on Ω. Orthogonality and the fact that $\dim(V_n) C_n(\tau(x,y))$ is the reproducing kernel of V_n show us that

$$I_F(\mu) = \int_\Phi \int_\Phi F(\tau(x,y))(1+\varepsilon Y_n(x))(1+\varepsilon Y_n(y))d\eta(x)d\eta(y)$$
$$= I_F(\eta) + \varepsilon^2 \widehat{F}_n \int_\Phi Y_n(x)^2 d\eta(x) < I_F(\eta),$$

implying that η is not a minimizer for I_F. If $\widehat{F}_n = 0$ for some $n \geq 1$, the same argument shows that $I_F(\mu) = I_F(\eta)$, i.e. η is not the unique minimizer. □

Observe that by combining the equivalence of positive definiteness (modulo a constant) on Φ and η being a minimizer with Lemma 3.1.11, we immediately achieve the following:

Corollary 3.4.2. *Let $F \in C([-1,1])$. Then either η is a minimizer of I_F, or every minimizer of I_F is supported on a proper subset of Φ.*

3.5 Energy on the Sphere

Clearly, everything that was said about the invariant measures in general and the case of compact connected two-point homogeneous spaces applies to the case of the sphere $\mathbb{S}^{d-1}$ and the uniform surface measure σ. In particular, Proposition 3.4.1 holds on $\mathbb{S}^{d-1}$ if we replace the normalized Jacobi expansion with a Gegenbauer expansion. We now collect some of our results for the sphere, for convenience.

Proposition 3.5.1. *For a function $F \in C([-1,1])$ and $\lambda = \frac{d-2}{2}$, the following conditions are equivalent:*

1. *F is positive definite on $\mathbb{S}^{d-1}$.*

2. *All Gegenbauer coefficients of F are non-negative, i.e.*

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

3. *There exists a function* $f \in L^2([-1,1], w_\lambda)$ *such that*

$$F(\langle x,y\rangle) = \int_{\mathbb{S}^{d-1}} f(\langle x,z\rangle) f(z\cdot y)\, d\sigma(z), \;\; x,y \in \mathbb{S}^{d-1}, \tag{3.16}$$

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

4. *The normalized Lebesgue measure* σ *is a minimizer of* I_F *over* $\mathbb{P}(\mathbb{S}^{d-1})$ *and* $I_F(\sigma) \geq 0$.

While this theorem clearly follows from Corollary 2.5.2, Theorem 3.3.2 and Proposition 3.4.1, we also note that the equivalence of (1) and (2) is a celebrated theorem of Schoenberg [Sch42].

In some situations, Gegenbauer coefficients can give some information about the minimizers, even when σ does not minimize the energy. In particular, the facts that Gegenbauer polynomials C_n^λ achieve their maximum at $t = 1$, are even if n is even, and are odd if n is odd, provide certain conditions, other than being a positive definite polynomial, under which *there exist* discrete minimizers or *all* minimizers are discrete. These results can be found in [BD19].

Proposition 3.5.2. *Let* $F \in C([-1,1])$. *Then the following hold:*

1. *If* $\widehat{F}(n,\lambda) \leq 0$ *for all* $n \geq 1$, *then a Dirac delta mass* $\mu = \delta_z$, *for any* $z \in \mathbb{S}^{d-1}$, *is a minimizer of* I_F. *If* F *has a strict absolute minimum at* $t = 1$ *(in particular, if* $\widehat{F}(n,\lambda) < 0$ *for all* $n \geq 1$*), then every minimizer is a Dirac mass. Observe that this case resonates with Theorem 4.1.3.*

2. *If* $(-1)^{n+1}\widehat{F}(n,\lambda) \geq 0$ *for all* $n \geq 1$, *and the Gegenbauer expansion of* F *converges uniformly to* F, *then a measure of the form* $\mu = \frac{1}{2}\big(\delta_z + \delta_{-z}\big)$, *for any* $z \in \mathbb{S}^{d-1}$, *is a minimizer of* I_F. *Moreover, all minimizers are of this form if the strict inequality* $(-1)^{n+1}\widehat{F}(n,\lambda) > 0$ *holds.*

3. *If* $\widehat{F}(2n,\lambda)=0$ *and* $\widehat{F}(2n-1,\lambda)\geq 0$ *for all* $n\geq 1$, *then every centrally symmetric measure minimizes* I_F. *In particular, there exist discrete minimizers. Moreover, if* $\widehat{F}(2n,\lambda)=0$ *and* $\widehat{F}(2n-1,\lambda)>0$ *for all* $n\geq 1$, *then all minimizers of* I_F *are centrally symmetric.*

Finally, we would like to remind the reader that Jacobi and Gegenbauer expansions are closely connected to Mercer's theorem (Theorem 2.3.3), and one could also take this approach in developing Schoenberg's theory. Indeed, the Funk–Hecke formula (2.29) shows that spherical harmonics of order n are eigenfunctions of the Hilbert–Schmidt operator $T_{K,\sigma}$ with the kernel $K(x,y)=F(\langle x,y\rangle)$, corresponding to the eigenvalue $\widehat{F}(n,\lambda)$. Thus for positive definite kernels F, all Gegenbauer coefficients are non-negative, which recovers Schoenberg's theorem [Sch42]. Moreover, using Mercer's theorem and the addition formula, we find that

$$F(\langle x,y\rangle)=K(x,y)=\sum_{n=0}^{\infty}\widehat{F}_n\sum_{k=1}^{N(n,d)}Y_{n,k}(x)Y_{n,k}(y)=\sum_{n=0}^{\infty}\widehat{F}(n,\lambda)\frac{n+\lambda}{\lambda}C_n^{\lambda}(\langle x,y\rangle),$$

and hence the Gegenbauer expansion of a function $F\in C[-1,1]$, which is positive definite on $\mathbb{S}^{d-1}$ converges absolutely and uniformly.

Chapter 4

Support of Minimizers

Lemma 3.1.11 implies that for kernels K which are not positive definite (modulo a constant), the support of any minimizing probability measure $\mu \in \mathbb{P}(\Omega)$ cannot be the entire set Ω. Moreover, parts 1 and 2 of Proposition 3.5.2 show us that for kernels of a certain type on the sphere, not only are the minimizers of the energy necessarily discrete, but we can in fact determine their cardinality. Furthermore, we can exactly characterize what those minimizers are. This led us to several interesting questions. In particular, under certain conditions on K (and Ω), are all minimizers of I_K necessarily discrete, or otherwise concentrated? Such a phenomenon has been repeatedly observed for repulsive-attractive potentials (i.e. potentials that depend only on distance and under which particles repel each other at close range, but attract each other at distant ranges) in the Euclidean space $\mathbb{R}^d$.

Definition 4.0.1. *Let (Ω, ρ) be a (not necessarily compact) metric space and suppose that $W : [0, diam(\Omega)) \to \mathbb{R}$ is continuous (with W also being defined and continuous at $diam(\Omega)$ if Ω is compact). We call a potential $K(x,y) = W(\rho(x,y))$ on Ω* ***repulsive-attractive*** *if there exist some $R_0 \in (0, diam(\Omega))$ such that W is strictly decreasing (repelling) on $(0, R_0)$ and strictly increasing (attracting) on $(R_0, diam(\Omega))$.*

As mentioned in Section 2.1, energy optimization in non-compact spaces is possible, so long as some constraint on the problem forces the support of minimizers to be bounded.

Repulsive-attractive potentials provide such a restriction, as shown by Carillo, Figalli, and Patacchini in the Euclidean setting.

Lemma 4.0.2. [CFP17, Lemma 2.6] *Let* $W : [0,\infty) \to \mathbb{R}$ *be continuous and repulsive-attractive. Suppose that there exist some* $R' > 0$ *such that for* $r > R'$, $W(r) > W(0)$. *Then the minimizers of the energy*

$$I_W(\mu) := \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W(||x-y||) d\mu(x) d\mu(y) \tag{4.1}$$

over $\mathbb{P}(\mathbb{R}^d)$ *have compact support.*

In many energy minimization problems in the compact setting, one deals with purely repulsive potentials, such as the Riesz potentials. However, there are many phenomena that can be modeled by repulsive-attractive potentials. For instance, interactions between neutral molecules, which involve repulsion due to overlapping electron orbitals and attraction due to London dispersion forces, are often simulated by the Lennard-Jones potential [ZD83] The minimization of repulsive-attractive energies has been observed to result in a clustering phenomenon in various models in computational chemistry, mathematical biology, social sciences, and physics [BLT06, BC14, CMV03, FS13, HP06, MEK99, VBUKB12, WS15]. Carrillo, Figalli, and Patacchini provided the first theoretical explanation for this discreteness of minimizers for *mildly repulsive* repulsive-attractive energies in Euclidean space.

Theorem 4.0.3 ([CFP17])**.** *Let* W *satisfy the conditions of Lemma 4.0.2. Suppose that* $W(0) = 0$ *and for some* $\gamma > 2$ *and* $C > 0$,

$$\lim_{r \to 0^+} W(r) r^{-\gamma} \to -C,$$

i.e. W *is mildly repulsive. Then any minimizer* $\mu \in \mathbb{P}(\mathbb{R}^d)$ *of* I_W *has finite support.*

An analogue of this result for certain compact sets has recently been discovered by Vlasiuk [Vla].

Though little seems to be known about the minimizers of such energies when $\gamma = 2$, this value acts as a "breaking point": for $\gamma < 2$, i.e. when W is "strongly repulsive", minimizers are no longer discrete.

Theorem 4.0.4 ([BCLR13]). *Let W be a repulsive-attractive potential such that $W(0) = 0$ and for some $\min\{0, 2-d\} < \gamma < 2$ and $C > 0$,*

$$\lim_{r \to 0^+} W(r) r^{-\gamma} \to -C.$$

Then the support of any minimizer $\mu \in \mathbb{P}(\mathbb{R}^d)$ of I_W has Hausdorff dimension greater than or equal to $2-\gamma$.

As we will soon discuss, this result is specific to the Euclidean setting, and does not hold in the compact setting.

We note that Theorem 4.0.3 is not quantitative, and except for the one dimensional case $\mathbb{R}$ [CFP17], there are few estimates on the cardinality of the support of these discrete minimizers. The recent paper of Lim and McCann [LMa] addresses this question for certain repulsive-attractive potentials with $\gamma \geq 2$, showing that the corresponding energies are uniquely minimized by discrete measures on regular simplices, and Kang, Kim, Lim, and Seo have classified certain repulsive-attractive potentials for which two-point measures appear as minimizers in [KKLS21]. However, the problem of generally determining cardinalities of minimizers in the Euclidean setting remains largely unsolved. The problem of understanding minimizers when $\gamma = 2$ is open as well, though some known energies in both the Euclidean case [LMa] and the compact case (see, e.g., Chapter 6) have only discrete minimizers.

We now turn our attention to the compact setting, where we do not require our potentials to be eventually attractive for global minimizers to be well-defined. Comparing

Theorems 4.0.3 and 4.0.4 to Theorem 2.1.2 results in a few important observations. First, weak-repulsiveness might be a sufficient condition in the compact setting to guarantee only discrete minimizers. Second, the geometry of a compact domain Ω affects the support of the minimizers to the point where even strongly-repulsive energies may have discrete minimizers, unlike the Euclidean case. Moreover, as we will show in Chapter 5, there exist strongly-repulsive kernels on the sphere (of the same strength of repulsion, in fact) for which minimizers can be discrete and for which only σ, the normalized Lebesgue measure on the sphere, is a minimizer. This clearly means that the geometry of Ω and the strength of repulsion, γ, may not be sufficient to determine discreteness or dimension of minimizers, as they are in the Euclidean case. Finally, much like the Euclidean case, there appears to be a breaking point at $\gamma = 2$ that may change the behavior of minimizers, and little is known for what generally happens in this instance. As many of the kernels we are most interested in, e.g. (6.1), (5.15), and (7.1), are not weakly-repulsive (or not weakly-attractive for the latter two), in this chapter we develop methods to determine properties of minimizers that ignore our potentials' strength of repulsion (attraction).

In Section 4.1, we prove a fairly general condition on a kernel F on the sphere guaranteeing the existence of a discrete minimizer and obtain bounds on the cardinality of the support of such minimizers. The proof relies on the analysis of the structure of extreme points of the set of moment-constrained measures.

In Section 4.2, we show that for any kernel F on the sphere that is real-analytic but not positive definite (modulo a constant), the support of any minimizer of I_F must have empty interior. Moreover, on the circle $\mathbb{S}^1$, they are discrete. This generates a certain dichotomy: for an analytic function F, either the energy I_F is minimized by the normalized Lebesgue measure σ, or *all minimizers* have support with empty interior.

In Section 4.3, we expand our focus to all connected, compact, two-point homogeneous spaces Φ, and show that for a certain class of functions, not only can we determine the existence of discrete minimizers and bounds on the cardinality of their support, we can in fact provide an explicit minimizer. Using arguments based on the linear programming method which goes back to Delsarte and Yudin [Del73, Yud92] and which are reminiscent of those appearing in [CK07], we demonstrate that tight M-designs minimize the energy I_F for all absolutely monotonic functions of degree M with $F^{(M+1)} \leq 0$. Moreover, if F is strictly absolutely monotonic of degree M, tight M-designs characterize the minimizers.

4.1 Extreme Points for Sets of Moment-constrained Measures

In the present section, we exhibit a large class of kernels K for which there exist discrete minimizers of the energies I_K. The methods that we employ are closely related to *moment problems*.

Let Ω be a compact metric space and let $\mathscr{B}(\Omega)$ denote the set of positive Borel measures on Ω. Given continuous functions $\phi_0, ..., \phi_n$ on Ω and non-negative constants c_i, we consider the set

$$H = \left\{ \mu \in \mathscr{B}(\Omega) : \int_{\Omega} \phi_i(x) d\mu(x) = c_i,\, i = 0, 1, \dots, n \right\}, \tag{4.2}$$

which consists of Borel measures whose moments with respect to $\phi_i \in C(\Omega)$ are fixed. We always set $\phi_0 \equiv 1$ and $c_0 = 1$, so that $\mu \in H$ guarantees that μ is a probability measure.

It is easy to see that H is convex, bounded, and weak* closed, and therefore is weak* compact. By the Krein–Milman Theorem, H is the weak* closure of $\text{ext}(H)$ — the set of extreme points of H (i.e. the measures $\mu \in H$ such that μ cannot be written as a convex combination of other measures in H). The results presented below describe the structure of $\text{ext}(H)$ – in particular, the discreteness of its elements.

We start with a theorem that gives a necessary condition for μ to be an extreme point of H.

Theorem 4.1.1 ([Dou64]). *Assume that* $\mu \in \text{ext}(H)$. *Then*

$$L^1(\mu) = \text{span}\{\phi_0 = 1, \phi_1, \dots, \phi_n\}. \tag{4.3}$$

Proof. Assume that $g \in L^\infty(\mu)$ satisfies

$$\int_\Omega \phi_i g d\mu = 0, \qquad i = 0, 1, \dots, n.$$

Multiplying g by a constant, we may assume that $\|g\|_{L^\infty(\mu)} < 1$. Then the measures $\mu_\pm$, defined by $d\mu_\pm = (1 \pm g)d\mu$, belong to H, since $\mu_\pm \in \mathscr{B}(\Omega)$ and

$$\int_\Omega \phi_i d\mu_\pm = \int_\Omega \phi_i (1 \pm g) d\mu = \int_\Omega \phi_i d\mu = c_i.$$

At the same time, $\mu = \frac{1}{2}(\mu_- + \mu_+)$. Since $\mu \in \text{ext}(H)$, this implies that $\mu_\pm = \mu$ and hence $g = 0$ μ-a.e. Therefore, the functions ϕ_i span $L^1(\mu)$. □

Remark: An infinite version of this statement also holds. In this case, for $\mu \in \text{ext}(H)$ the span of $\{\phi_i\}_{i=0}^\infty$ is dense in the space $L^1(d\mu)$.

We now state and prove a result, which demonstrates the discreteness of the elements of $\text{ext}(H)$. This result has a number of precursors and extensions; see [Ric57, Rog58, Rog62, Ros51, Win98, Zuh62].

Theorem 4.1.2 ([Kar83]). *Let* $\mu \in H$. *Then the following statements are equivalent:*

1. $\mu \in \text{ext}(H)$.

2. *The cardinality of* $\text{supp}(\mu)$ *is at most* $n+1$. *Moreover, if we denote* $\text{supp}(\mu) = \{x_1, \dots, x_k\}$, *then the vectors* $v_j = \big(1, \phi_1(x_j), \dots, \phi_n(x_j)\big)$, $j = 1, 2, \dots, k$, *are linearly independent.*

Proof. (1)⇒(2). Assume that there exist points $\{x_1, \dots, x_{n+2}\} \subseteq \text{supp}(\mu)$. Then one can find a vector $y \in \mathbb{R}^{n+2}$, which is not in the span of the vectors $\big(\phi_i(x_1), \phi_i(x_2), \dots, \phi_i(x_{n+2})\big)$,

$i=0,1,\dots,n$, since the latter subspace is at most $n+1$ dimensional. Appealing to Urysohn's Lemma, one can construct a function $g \in C(\Omega) \subseteq L^1(\mu)$ such that $g(x_i) = \langle y, e_i \rangle$ (where $\{e_1,...,e_{n+2}\}$ is an orthonormal basis of $\mathbb{R}^{n+2}$) for $i=1,2,\dots,n+2$. But then $g \notin \operatorname{span}\{\phi_i\}$, which contradicts Theorem 4.1.1, so $\left|\operatorname{supp}(\mu)\right| \leq n+1$.

Now that it is known that $\mu = \sum_{i=1}^{k} t_i \delta_{x_i}$ with $k \leq n+1$, $t_i > 0$, $\sum t_i = 1$, consider the linear system

$$\begin{pmatrix} 1 & \dots & 1 \\ f_1(x_1) & \dots & f_1(x_k) \\ \vdots & \ddots & \vdots \\ f_n(x_1) & \dots & f_n(x_k) \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_k \end{pmatrix} = \begin{pmatrix} 1 \\ c_1 \\ \vdots \\ c_n \end{pmatrix}. \tag{4.4}$$

This system has a unique solution $a_i = t_i$, since if the solution is not unique, then there is a whole affine subspace of solutions and one could perturb the values of t_i in opposite directions. In other words, on could find two solutions of the form $\{t_i \pm \tau_i\}$ and construct two measures $\mu_\pm = \sum_{i=1}^{k} (t_i \pm \tau_i)\delta_{x_i}$ so that $\mu_\pm \geq 0$ and $\int \phi_i d\mu_\pm = \int \phi_i d\mu$. This would mean $\mu_\pm \in K$, and since $\mu = \frac{1}{2}(\mu_+ + \mu_-)$, this would contradict the fact that $\mu \in \operatorname{ext}(H)$. This proves the linear independence of the columns of the matrix above.

(2)⇒(1). Assume that (2) holds. Then the system (4.4) has a unique solution, i.e. μ is uniquely determined by the condition $\operatorname{supp}(\mu) \subseteq \{x_1,\dots,x_k\}$. If $\mu = t\mu_1 + (1-t)\mu_2$ for some $t \in (0,1)$, then $\operatorname{supp}(\mu) \subseteq \operatorname{supp}(\mu_1) \cup \operatorname{supp}(\mu_2)$, and thus $\operatorname{supp}(\mu_j) \subseteq \{x_1,\dots,x_k\}$ for $j=1,2$. Therefore $\mu_1 = \mu_2 = \mu$, i.e. $\mu \in \operatorname{ext}(H)$. □

We remark that convex geometry plays heavily into similar characterizations of solutions to infinite dimensional optimization problems in the recent papers [BCDC+19, CRPW12, UFW17].

Applications of Karr's Theorem: Existence of Discrete Minimizers

We now apply the results on moment-constrained measures to show that for kernels K with certain expansions, there exist discrete minimizers of I_K. We specifically prove it for rotationally invariant kernels F on the sphere, but the generalization to other spaces is clear.

Let $\widehat{F}(n,\lambda)$ denote the coefficients in the Gegenbauer expansion (2.25) of the function $F \in C([-1,1])$. Consider the sets $N_+(F) = \{n \geq 0 : \widehat{F}(n,\lambda) > 0\}$ and $N_-(F) = \{n \geq 0 : \widehat{F}(n,\lambda) < 0\}$. We shall assume that

$$\big|N_+(F)\big| < \infty, \tag{4.5}$$

i.e. there are only finitely many terms of (2.25) with $\widehat{F}(n,\lambda) > 0$. In this case, Lemma 2.4.1 implies that the Gegenbauer expansion of F converges uniformly and absolutely.

Recall that $\mathscr{H}_n^d$ denotes the space of spherical harmonics of degree n on $\mathbb{S}^{d-1}$. We are now ready to state the main theorem of the section.

Theorem 4.1.3. *Assume that the Gegenbauer expansion* (2.25) *of the function* $F \in C([-1,1])$ *satisfies*

$$\big|N_+(F)\big| = \big|\{n \geq 0 : \widehat{F}(n,\lambda) > 0\}\big| < \infty,$$

i.e. the Gegenbauer expansion has only finitely many positive terms. Then there exists a discrete measure $\mu^* \in \mathbb{P}(\mathbb{S}^{d-1})$ *such that*

$$\big|\operatorname{supp}(\mu^*)\big| \leq \sum_{n \in N_+(F) \cup \{0\}} \dim(\mathscr{H}_n^d), \tag{4.6}$$

and μ^* *minimizes the energy* I_F *over* $\mathbb{P}(\mathbb{S}^{d-1})$*, i.e.*

$$I_F(\mu^*) = \mathscr{I}_F(\mathbb{S}^{d-1}). \tag{4.7}$$

Proof. Let $\nu \in \mathbb{P}(\mathbb{S}^{d-1})$ be any minimizer of I_F. We shall use the addition formula for spherical harmonics (2.28), as well as the absolute convergence of (2.25), to re-write $I_F(\mu)$, for any measure $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$, as

$$
\begin{aligned}
I_F(\mu) &= \sum_{n=0}^{\infty} \widehat{F}(n,\lambda) \int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} \frac{n+\lambda}{\lambda} C_n^{\lambda}(\langle x,y\rangle) d\mu(x) d\mu(y) \\
&= \sum_{n=0}^{\infty} \widehat{F}(n,\lambda) \left[\sum_{j=1}^{\dim(\mathscr{H}_n^d)} \left(\int\limits_{\mathbb{S}^{d-1}} Y_{n,j}(x) d\mu(x) \right)^2 \right] \\
&= \sum_{n \in N_+(F)} \widehat{F}(n,\lambda) \left[\sum_{j=1}^{\dim(\mathscr{H}_n^d)} \left(\int\limits_{\mathbb{S}^{d-1}} Y_{n,j}(x) d\mu(x) \right)^2 \right] \\
&\quad - \sum_{n \in N_-(f)} \big(-\widehat{F}(n,\lambda) \big) \left[\sum_{j=1}^{\dim(\mathscr{H}_n^d)} \left(\int\limits_{\mathbb{S}^{d-1}} Y_{n,j}(x) d\mu(x) \right)^2 \right],
\end{aligned}
$$

the last of which we define as the difference of functionals $\mathscr{F}(\mu) - \mathscr{G}(\mu)$. It is easy to see that $\mathscr{G}$ is convex with respect to μ since it is a positive linear combination of squares of linear functionals of μ. Let us set

$$
\begin{aligned}
H_F = \Bigg\{ & \mu \in \mathscr{B}(\mathbb{S}^{d-1}) : \\
& \int\limits_{\mathbb{S}^{d-1}} Y_{n,j}(x) d\mu(x) = \int\limits_{\mathbb{S}^{d-1}} Y_{n,j}(x) d\nu(x),\, n \in N_+(F),\, j = 1, \ldots, \dim(\mathscr{H}_n^d) \Bigg\},
\end{aligned}
$$

so that $\nu \in H_F$ and $\mathscr{F}(\mu) = \mathscr{F}(\nu)$ for $\mu \in H_F$. Without loss of generality, we shall assume that $0 \in N_+(F)$. This guarantees that $\mu \in H_F$ is a probability measure (similarly to setting $c_0 = 1$ and $\phi_0 \equiv 1$ earlier). Since $|N_+(F)| < \infty$, the set H_F has finitely many moment constraints and Theorem 4.1.2 is applicable. In fact, the number of constraints is exactly the right-hand side of (4.6).

Given that $\mathscr{G}$ is convex in μ and H_F is a convex weak* compact subset of $\mathscr{B}(\mathbb{S}^{d-1})$, we conclude that $\mathscr{G}(\mu)$ achieves its maximum on H_F at a point of $\mathrm{ext}(H_F)$. Hence there exists a measure $\mu^* \in \mathrm{ext}(H_F)$ such that $\mathscr{G}(\mu^*) = \sup_{\mu \in H_F} \mathscr{G}(\mu)$. We then find that

$$\begin{aligned}\mathscr{I}_F(\mathbb{S}^{d-1}) &= \inf_{\mu \in \mathbb{P}(\mathbb{S}^{d-1})} I_F(\mu) = I_F(\nu) = \mathscr{F}(\nu) - \mathscr{G}(\nu) = \mathscr{F}(\mu^*) - \mathscr{G}(\nu) \\ &\geq \mathscr{F}(\mu^*) - \mathscr{G}(\mu^*) = I_F(\mu^*) \geq \mathscr{I}_F(\mathbb{S}^{d-1}),\end{aligned}$$

i.e. $I_F(\mu^*) = M$ and μ^* is also a minimizer of I_F.

Since $\mu^* \in \mathrm{ext}(H_F)$, we can apply Karr's theorem (Theorem 4.1.2) to finish our proof.

□

4.2 Minimizers of Energies with Analytic Kernels

It follows from Lemma 3.1.11 that if K is not positive definite (modulo a constant) on Ω, then the support of a minimizer μ of I_K must be a proper subset of Ω. When Ω is a real-analytic manifold and K is real-analytic, we can make a stronger claim: the support of any minimizer must have empty interior. For simplicity, we will prove this for rotationally invariant kernels F on the sphere $\mathbb{S}^{d-1}$, though the generalization is clear.

Theorem 4.2.1. *Assume that F is a real-analytic function on $[-1,1]$, such that σ is not a minimizer of I_F, i.e. F is not (up to an additive constant) positive definite on $\mathbb{S}^{d-1}$. Let μ be a minimizer of I_F, then $(\mathrm{supp}(\mu))^\circ = \emptyset$. Moreover, if $d = 2$, then $\mathrm{supp}(\mu)$ must be discrete.*

In order to prove this theorem, we need the following lemma (see, e.g. [KP02, MT]):

Lemma 4.2.2 (Principle of Analytic Continuation)**.** *Let M be a real-analytic manifold, and $f : M \to \mathbb{R}$ be real-analytic. If f is constant on an open set of M, then f is constant on all of M. Moreover, if the manifold is one-dimensional, then it suffices that f is constant on some $U \subseteq M$ that has an accumulation point in M.*

Proof of Theorem 4.2.1. Suppose, indirectly, that $(\mathrm{supp}(\mu))^\circ \neq \emptyset$. By Theorem 3.1.7, we know that the potential

$$U_F^{\mu}(x) = \int\limits_{\mathbb{S}^{d-1}} F(\langle x,y\rangle)d\mu(y)$$

is constant on $\mathrm{supp}(\mu)$. Since $F(\langle x,y\rangle)$ is real-analytic on $\mathbb{S}^{d-1}\times\mathbb{S}^{d-1}$, $U_F^{\mu}(x)$ is real-analytic on $\mathbb{S}^{d-1}$. Since U_F^{μ} is real-analytic and constant on an open set in $\mathbb{S}^{d-1}$, it is constant on all of $\mathbb{S}^{d-1}$, by Lemma 4.2.2. In addition, $U_F^{\sigma}(x) = I_F(\sigma)$ is constant on $\mathbb{S}^{d-1}$ due to rotational invariance. We then obtain

$$\begin{aligned}
I_F(\mu) &= \int\limits_{\mathbb{S}^{d-1}}\int\limits_{\mathbb{S}^{d-1}} F(\langle x,y\rangle)d\mu(y)d\mu(x) = \int\limits_{\mathbb{S}^{d-1}} U_F^{\mu}(x)d\mu(x) = \int\limits_{\mathbb{S}^{d-1}} U_F^{\mu}(x)d\sigma(x)\\
&= \int\limits_{\mathbb{S}^{d-1}}\int\limits_{\mathbb{S}^{d-1}} F(\langle x,y\rangle)d\mu(y)d\sigma(x) = \int\limits_{\mathbb{S}^{d-1}}\int\limits_{\mathbb{S}^{d-1}} F(\langle x,y\rangle)d\sigma(x)d\mu(y)\\
&= \int\limits_{\mathbb{S}^{d-1}} U_F^{\sigma}(x)d\mu(y) = I_F(\sigma).
\end{aligned}$$

This is clearly a contradiction, as by the assumption, I_F is not minimized by σ. Our first claim then follows.

For $\mathbb{S}^1$, Lemma 4.2.2 tells us that if U_F^{μ} is constant on a set $\{z_1, z_2, \ldots\} \subset \mathbb{S}^1$ with an accumulation point, U_F^{μ} is constant on $\mathbb{S}^1$. The proof of our second claim then follows as above. □

If $\mathbb{S}^{d-1}$ is replaced with one of the projective spaces $\mathbb{FP}^{d-1}$, we can derive a similar result.

In the spirit of Theorem 4.2.1, as well as Corollary 3.4.2, it may be tempting to conjecture that if F (not necessarily analytic) is not positive definite on $\mathbb{S}^{d-1}$ (up to constant), i.e $I_F(\mu)$ is *not* minimized by σ, then the support of any minimizer of I_F must have empty interior. However, this is not true, as the following simple example shows.

Example 4.2.3. *Assume that* $F \in C([-1,1])$ *is constant near* $t = 1$ *and strictly decreasing* *otherwise, i.e. it satisfies for some fixed* $\gamma \in (0,1)$*,*

$$F(1) = F(t') = \min_{t \in [-1,1]} F(t) \text{ for any } t' \in [1-\gamma, 1],$$

and $F(t') > F(1)$ *for all* $t' \in [-1, 1-\gamma)$*. It is then evident that for any* $z \in \mathbb{S}^{d-1}$

$$\min_{\mu \in \mathbb{P}(\mathbb{S}^{d-1})} I_F(\mu) = I_F\left(\delta_z\right) = F(1),$$

and $I_F(\sigma) > I_F(\delta_z)$*, i.e.* σ *is not a minimizer of* I_F*. Let* $C(z,h) = \{x \in \mathbb{S}^{d-1} : \langle x, z\rangle > h\}$ *denote the* spherical cap *of "height"* h *centered at* $z \in S^{d-1}$*. Let* ν *be the normalized uniform measure on* $C(z,h)$*, i.e.*

$$d\nu(x) = \frac{\mathbb{1}_{C(z,h)}(x)}{\sigma\big(C(z,h)\big)} d\sigma(x),$$

with $h = 1 - \frac{\gamma}{4}$*. Then for each* $x, y \in C(z,h)$*, we have* $\langle x, y\rangle > 1-\gamma$*, and hence*

$$I_F(\nu) = I_F\left(\delta_z\right) = F(1),$$

i.e. ν *is also a minimizer of* I_F*, but its support has non-empty interior.*

Applications to Polynomial Energies

We observe that the results of Sections 4.1 and 4.2 apply if F is a polynomial. Indeed, Theorem 4.2.1 is applicable since polynomials are analytic, while the conditions of Theorem 4.1.3 hold because the Gegenbauer expansion has only finitely many terms. We summarize these statements in the following corollary. As in the preceding sections, this can be generalized to the other two-point homogeneous spaces.

Corollary 4.2.4. *Assume that F is a polynomial whose Gegenbauer expansion is*

$$F(t) = \sum_{n=0}^{m} a_n C_n^{\lambda}(t).$$

1. *There exists a discrete minimizer $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ with*

$$\big|\operatorname{supp}(\mu)\big| \leq 1 + \sum_{\{n:\ a_n>0,\ 1\leq n\leq m\}} \dim(\mathscr{H}_n^d).$$

2. *If, moreover, σ is not a minimizer of I_F over $\mathbb{P}(\mathbb{S}^{d-1})$, i.e. there exists $n \geq 1$ such that $a_n < 0$, then the support of any minimizer of I_F has empty interior. For $\mathbb{S}^1$, the support is finite.*

We observe that when $a_n \geq 0$ for $n = 1, \ldots, m$, i.e. F is a polynomial that is positive definite on $\mathbb{S}^{d-1}$ (up to constant), the statement of Theorem 4.1.3 (and hence also part (1) of the above corollary) is known. In this case, the discrete minimizers $\mu = \sum w_{z_i}\delta_{z_i}$ are exactly *weighted spherical m-designs*, see Section 2.6.

Existence of weighted m-designs of cardinality $\sum_{n=0}^{m} \dim(\mathscr{H}_n^d)$ has been shown in [Tch57, Rog62]. A certain well-known generalization of this fact can also be easily deduced from part (1) of Corollary 4.2.4. Let $\mathscr{N} \subset \mathbb{N}_0$ with $0 \in \mathscr{N}$. Call a set $\{z_i\}_{i=1}^N \subset \mathbb{S}^{d-1}$ with positive weights ω_{z_i} a *weighted $\mathscr{N}$-design* if for every $m \in \mathscr{N}$ and every spherical harmonic $Y \in \mathscr{H}_m^d$ one has

$$\sum_{i=1}^{N} \omega_{z_i} Y(z_i) = \int_{\mathbb{S}^{d-1}} Y(x)\,d\sigma(x).$$

When $\mathscr{N} = \{0,1,\ldots,m\}$, this definition coincides with the definition of a weighted m-design. Such objects arise naturally for some configurations. For example, the 600-cell, one of the six 4-dimensional convex regular polytopes with vertices which form a 120-point subset of $\mathbb{S}^3$, yields an exact cubature formula for spherical harmonics of degrees up to 19, *excluding* degree 12 (see, e.g., [CK07, Section 7]). In other words, it is an $\mathscr{N}$-design for $\mathscr{N} = \{0,1,\ldots,11\} \cup \{13,\ldots,19\}$. By taking $a_n > 0$ only for $n \in \mathscr{N}$ and applying part (1) of Corollary 4.2.4, one easily concludes existence of weighted $\mathcal{N}$-designs on the sphere $\mathbb{S}^{d-1}$ of cardinality at most $\sum_{n\in\mathcal{N}} \dim(\mathcal{H}_n^d)$. This statement is encompassed by more general results [Tch57, Rog62].

Theorem 4.1.3 and part (1) of Corollary 4.2.4 vastly generalize these well-known statements, essentially showing that the addition of any number of negative definite terms does not destroy the statement: discrete minimizers with the same cardinality still exist.

4.3 Linear Programming and Optimality of Tight Designs

Though results such as Theorem 4.0.3 are useful in showing that minimizers of some energy must be discrete, and results along the lines of Theorem 4.1.3 tell us that discrete minimizers of a certain cardinality must exist, it would be ideal to determine what those minimizers are. The main goal of this section is to show that for those dimensions d and values of M for which tight designs exist, these measures minimize the energy I_F for a large class of potentials F. We will use linear programming bounds, discussed below, to this end.

The main result of this section is the following:

Theorem 4.3.1. *Let F be absolutely monotonic of degree M, with $F^{(M+1)}(t) \leq 0$ for $t \in (-1,1)$. Then for a tight M-design $\mathscr{C}$, the measure*

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

is a minimizer of

$$I_F(\mu) = \int_\Phi \int_\Phi F(\tau(x,y))\, d\mu(x) d\mu(y)$$

over $\mathbb{P}(\Phi)$.

Linear Programming

In the 1970s, Delsarte developed a method to bound codes on finite fields that yielded an upper bound on the kissing numbers and upper bounds for the size of spherical codes given minimal distance as solutions to linear programs [Del73]. This linear programming method provides bounds for optima in various optimization problems, and its use is often aided by computational tools, where a problem is approximated by a finite-dimensional or discretized counterpart, then solved with a computer. Despite being a relatively simple method, it often provides optimal bounds, such as those in Theorem 2.6.6. In particular, the linear programming method has been used to find the kissing number in dimensions 8 and 24 by Odlyzko and Sloane [OS79], and independently by Levenshtein [Lev79], as well as in dimension 4 by Musin [Mus08]. This technique applies to all the compact two-point homogeneous spaces Φ described in Section 2.4. Our application of the method can be summed up in the following lemma, which is a measure-theoretic counterpart of the linear programming bound of Yudin [Yud92]. In what follows, we will use the notion from Section 2.4, i.e. C_n is the appropriate normalized Jacobi polynomial of degree n, and $\widehat{h}_n$ is the corresponding coefficient in the Jacobi expansion of h.

Lemma 4.3.2. *Let $h \in C([-1,1])$ be positive-definite modulo a constant, i.e.*

$$h(t) = \sum_{n=0}^{\infty} \widehat{h}_n C_n(t)$$

with $\widehat{h}_n \geq 0$ for all $n \geq 1$.

1. *Assume that $h(t) \leq F(t)$ for all $t \in [-1,1]$. Then for any $\mu \in \mathbb{P}(\Phi)$,*

$$I_F(\mu) \geq \widehat{h}_0 = I_h(\eta).$$

2. *Assume further that h is a polynomial of degree k and that there exists a k-design*

$\mathscr{C} \subset \Phi$ such that $h(t) = F(t)$ for each $t \in \mathscr{A}(\mathscr{C})$. Then for any $\mu \in \mathbb{P}(\Phi)$,

$$I_F(\mu) \geq I_F\Big(\frac{1}{|\mathscr{C}|}\sum_{x\in\mathscr{C}}\delta_x\Big),$$

i.e. I_F is minimized by the uniform distribution on $\mathscr{C}$.

Proof. For the first part observe that

$$I_F(\mu) \geq I_h(\mu) \geq I_h(\eta) = \widehat{h}_0,$$

where the first inequality follows from the fact that $F \geq h$, while the second one is due to Proposition 3.4.1, since h is positive definite modulo a constant.

For the second part, one can continue as follows

$$I_h(\eta) = I_h\Big(\frac{1}{|\mathscr{C}|}\sum_{x\in\mathscr{C}}\delta_x\Big) = I_F\Big(\frac{1}{|\mathscr{C}|}\sum_{x\in\mathscr{C}}\delta_x\Big).$$

The first equality follows from the fact that $\mathscr{C}$ is a k-design, and the second from the fact that F and h coincide on the set $\mathscr{A}(\mathscr{C})$. Together with part (1) this proves the statement in part (2). □

This lemma provides insights in two different ways for how the linear programming method can be applied. If a candidate $\mathscr{C}$ is available, one can apply part (2) of Lemma 4.3.2 by constructing a polynomial $h \leq F$ as a Hermite interpolant of the function F at the points of $\mathscr{A}(\mathscr{C})$. This reasoning, which lies behind the proof of Theorems 4.3.1 and 6.2.3, explains the appearance of tight designs: indeed, the number of elements in the set of interpolation points (i.e. distinct distances between the points of $\mathscr{C}$) determines the degree of the interpolant h – hence one wants a design of high strength, but low degree.

The same reasoning as above applies to the emergence of sharp designs as universally optimal sets in [CK07], and it also explains why this slightly weaker notion does not suffice for our purposes: since we are working with general measures rather than point sets with fixed cardinality, we cannot avoid interpolating at the point $t = 1$, which requires a design of higher strength. The main technical difficulty in this setting is proving positive definiteness of the Hermite interpolating polynomial h. We take this approach to Theorem 4.3.1 and carry out the technicalities in the following subsections.

If a suitable candidate is not available, one can still rely on part (1) of Lemma 4.3.2 and attempt to optimize the value of the energy $I_h(\eta)$ over auxiliary polynomials h (i.e. polynomials h satisfying the conditions of Lemma 4.3.2), obtaining a lower bound for the energy over all probability measures. If the degree of an auxiliary function h is bounded by D, we have $D+1$ non-negative variables $\widehat{h}_i$, $0 \leq i \leq D$, and infinitely many linear constraints $h(t) \leq F(t)$ for all $t \in [-1,1]$. In order to get the best possible lower bound, we need to maximize $\widehat{h}_0$ given these linear conditions. This particular method will be used in Sections 7.2.

This problem is, generally, intractable as a linear optimization problem. However, when F is a polynomial, the condition $F(t) - h(t) \geq 0$ for all $t \in [-1,1]$ may be represented as a finite-size positive semi-definite constraint on the coefficients $\widehat{h}_i$. In particular, the polynomial inequality may be rewritten as a sum-of-squares optimization problem (see, for instance, [Nes00]) and thus solved as a semi-definite program.

Properties of Orthogonal Polynomials

Recall that, for fixed Φ, we write simply $C_n(t) = C_n^{(\alpha,\beta)}(t)$ and have $C_n(1) = 1$. In some of the arguments below we will use instead the monic Jacobi polynomials, which we will denote as $Q_n(t) = Q_n^{(\alpha,\beta)}(t)$.

We now collect several results about orthogonal polynomials relevant to the proof of Theorem 4.3.1 and which are presented and covered in greater detail in [CK07]. Fix a space Φ, and let α and β be the corresponding parameters of the associated Jacobi polynomials. According to Proposition 3.4.1, positive definiteness on Φ is equivalent to the positivity of coefficients in the monic Jacobi expansion, i.e. the expansion with respect to $Q_n^{(\alpha,\beta)}$.

It will be useful to consider *adjacent* Jacobi polynomials, defined as one of the three sequences $Q_n^{k,l} = Q_n^{(\alpha+k,\beta+l)}$ with $k,l \in \{0,1\}$, $k+l > 0$. Specifically, we will need the following corollary which comes out of representing $Q_n^{1,0}$ through $Q_n^{0,0}$ [Lev92, equation (3.4)]:

Proposition 4.3.3. *Adjacent Jacobi polynomials $Q_n^{1,0}$ are positive definite on Φ.*

On the other hand, adjacent polynomials $Q_n^{1,1}$, defined as orthogonal with respect to the measure $(1-t^2)\,d\nu^{(\alpha,\beta)}$, are not positive definite on Φ. The following property, a special case of the strengthened Krein condition [Lev98, Lemma 3.22], can serve as a substitute.

Lemma 4.3.4. *$(t+1)Q_n^{1,1}(t)$ are positive definite on Φ for $n \geq 0$.*

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

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

for some constant b. Since all the roots of $Q_n^{1,0}$ lie in $(-1,1)$, $\operatorname{sgn} Q_n^{1,0}(-1) = (-1)^n$. Substituting $t=-1$ in the last equation gives $Q_{n+1}^{1,0}(-1) + bQ_n^{1,0}(-1) = 0$, and so $b \geq 0$. By Proposition 4.3.3, each $Q_n^{1,0}(t)$ is positive definite, and thus $(t+1)Q_n^{1,1}(t)$ is also positive definite. □

Lastly, we will need the strict positive-definiteness of polynomials annihilated by subsets of roots of $Q_n + \gamma Q_{n-1}$, which is provided by the following result.

Proposition 4.3.5 ([CK07, Theorem 3.1])**.** *Let $\mu \in \mathscr{B}(\mathbb{R})$ such that all polynomials are integrable with respect to μ and for all polynomials p, $\int_{\mathbb{R}} (p(t))^2 d\mu(t) > 0$ if p is not identically zero. Set $p_0(t), p_1(t), \ldots$ to be a sequence of monic orthogonal polynomials for μ such that* $\deg(p_k) = k$ *for all $k \in \mathbb{N}$. If $t_1 < \ldots < t_n$ are the zeros of $p_n + \gamma p_{n-1}$ for some* *fixed γ, then the polynomials*

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

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

Hermite Interpolation

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

$$\max\{k_1, \ldots, k_m\} \le B+1.$$

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

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

Such a p is called the *Hermite interpolating polynomial* that agrees with F to order k_i at each t_i (we will simply call it the Hermite interpolating polynomial for short); it always exists and is unique because the linear map that takes a polynomial p of degree less than D to

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

is bijective.

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

$$g(t) = \prod_{i=1}^{m}(t-t_i)^{k_i} \tag{4.8}$$

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

We can now state an important remainder formula for Hermite interpolation [Dav63, Theorem 3.5.1].

Lemma 4.3.6. *Suppose that $F \in C^B[a,b] \cap C^D(a,b)$ and g is as in* (4.8). *Then for each $t \in [a,b]$, there exists $\xi \in (a,b)$ such that* $\min(t,t_1,...,t_m) < \xi < \max(t,t_1,...,t_m)$ *and*

$$F(t) - H[F,g](t) = \frac{F^{(D)}(\xi)}{D!} g(t). \tag{4.9}$$

Similarly, we let

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

be the *divided difference* associated with the polynomial g. Since, for $1 \leq i \leq m$,

$$F(t) - H[F,g](t) = O((t-t_i)^{k_i})$$

as $t \to t_i$, it follows that $Q[F,g]$ extends to a continuous function at the roots of g. If we assume that $F \in C^D(a,b)$, then the continuity of $F^{(D)}$ and Lemma 4.3.6 implies that for all $t \in [a,b]$, there there exists some $\xi \in (a,b)$ such that $\min(t,t_1,...,t_m) < \xi < \max(t,t_1,...,t_m)$ and

$$Q[F,g](t) = \frac{F^{(D)}(\xi)}{D!}. \tag{4.10}$$

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

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

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

By the Newton's formula [DL93, Chapter 4.6–7], the Hermite interpolating polynomial $H[F,g]$ can be represented as

$$H[F,g](t) = F(s_1) + \sum_{j=1}^{D-1} g_j^*(t)\, Q[F,g_j^*](s_{j+1}). \tag{4.11}$$

It will be convenient to introduce notation for this number of nonnegative derivatives of a function.

Definition 4.3.7. *Let $F \in C^D(a,b)$. We say that F is* ***absolutely monotonic of degree*** *D if $F^{(k)}(t) \geq 0$ for $0 \leq k \leq D$ and $t \in (a,b)$. If these derivatives are positive, we say that F is* ***strictly absolutely monotonic of degree*** *D.*

The benefit of these nonnegative derivatives lies in the fact that the Hermite interpolant of an absolutely monotonic function, F, of degree D with negative $(D+1)$st derivative will stay below F, as shown in the following observation.

Lemma 4.3.8. *Let $F : [-1,1] \to \mathbb{R}$ be absolutely monotonic of degree D, and $F^{(D+1)}(t) \leq 0$ for all $t \in (-1,1)$. If the roots of a polynomial g of the form* (4.8) *(and thus of degree D) are contained in $[-1,1]$, and, in addition, $g(t) \leq 0$ for $t \in [-1,1]$, then,*

$$F(t) \geq H[F,g](t), \qquad t \in [-1,1].$$

Proof. According to Lemma 4.3.6, for all $t \in [-1,1]$ there exists $\xi \in (-1,1)$ such that $\min(t,t_1) < \xi < \max(t,t_m)$, where the roots of g are $t_1 < \ldots < t_m$, and

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

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

Optimality of Tight Designs

As above, Φ is a compact, connected two-point homogeneous space and $Q_0, Q_1, Q_2, \ldots$ are the corresponding monic orthogonal polynomials. Recall that Q_n are orthogonal with respect to the measure $d\nu^{(\alpha,\beta)} = \frac{1}{\gamma_{\alpha,\beta}}(1-t)^{\alpha}(1+t)^{\beta}dt$, where the parameters α, β are chosen as in Section 2.4.

In what follows, we give a proof of the Theorem 4.3.1, splitting it into two separate cases, depending on whether the code $\mathscr{C}$ contains two points separated by the diameter of Φ, or, equivalently, depending on the parity of the strength M of $\mathscr{C}$.

Proposition 4.3.9. *Theorem 4.3.1 holds when $M = 2m$, $m \geq 1$.*

Proof. Let $-1 \leq t_1 < \ldots < t_m < t_{m+1} = 1$ be the values within $\mathscr{A}(\mathscr{C})$ and define

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

and

$$g(t) := g_m(t)\, g_{m+1}(t) = (t-1)g_m^2(t) \tag{4.12}$$

To prove the statement of the proposition, we verify the following chain of inequalities, satisfied for arbitrary $\mu \in \mathbb{P}(\Phi)$, similar to the proof of Lemma 4.3.2,

$$I_F(\mu) \geq I_{H[F,g]}(\mu) \geq I_{H[F,g]}(\eta) = I_{H[F,g]}(\mu_{\mathscr{C}}) = I_F(\mu_{\mathscr{C}}). \tag{4.13}$$

The equality $I_{H[F,g]}(\eta) = I_{H[F,g]}(\mu_{\mathscr{C}})$ follows since $\mathscr{C}$ is a design of strength $2m \geq \deg H[F,g]$. The last equality holds since $H[F,g]$ agrees with F at the cosines of distances occurring in $\mathscr{C}$. Since $g(t) \leq 0$ for $t \in [-1,1]$, Lemma 4.3.8 implies that $F(t) \geq H[F,g](t)$ for $t \in [-1,1]$, which gives the first inequality. It remains to show the second inequality: it will follow from the positive definiteness of $H[F,g]$, which we will now demonstrate.

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

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

since, by construction, g_{m+1} is annihilated on all the t_i. The constants c_i are given by

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

Since both g_{m+1} and Q_{m+1} are monic and g_{m+1} is orthogonal to each Q_n for $n < m$, we conclude that

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

for some $\gamma \in \mathbb{R}$. By Proposition 4.3.5, subproducts of factors of g_{m+1}, which we denote by g_k, $1 \le k \le m$, can be expressed as linear combinations of Q_n with positive coefficients, and therefore are positive definite.

According to Newton's formula (4.11), the Hermite interpolant of F can be expressed as the sum of partial products of factors of g multiplied by the appropriate divided difference. We will use this formula to show that $H[F,g]$ is positive definite. Indeed, (4.11) gives

$$
H\left[F,g\right](t) = F(t_1) + \sum_{k=1}^{m}\left(g_k(t)g_{k-1}(t)\,Q\left[F,g_kg_{k-1}\right](t_k) + g_k^2(t)\,Q\left[F,g_k^2\right](t_{k+1})\right), \quad (4.14)
$$

where, as usual, $g_0 = 1$. Observe that the divided differences in the last equation are non-negative due to (4.10), as the function F is absolutely monotonic of degree $2m$. Since we have shown that each g_k is positive definite, Schur's theorem implies that so are g_k^2 and g_kg_{k+1}, and it follows that $H[F,g]$ is positive definite as well. □

Before turning to the proof of Theorem 4.3.1 for tight designs of odd strength, recall the definition of the adjacent polynomials $Q_n^{1,1} = Q_n^{(\alpha+1,\beta+1)}$ for $n \geq 0$. They are monic and orthogonal with respect to the measure

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

Proposition 4.3.10. *Theorem 4.3.1 holds when $M = 2m-1$, $m \geq 1$.*

Proof. Suppose that $\mathscr{C} \subset \Phi$ is a tight $(2m-1)$-design. As discussed in Section 2.6 tight designs of odd strength necessarily contain antipodal points, i.e. there exist $x, y \in \mathscr{C}$ such that $\vartheta(x,y) = \pi$ and thus $-1 \in \mathscr{A}(\mathscr{C})$. Let $-1 = t_1 < \ldots < t_m < t_{m+1} = 1$ be the values of $\mathscr{A}(\mathscr{C})$, and set

$$w(t) = \prod_{j=2}^{m}(t-t_j)$$

and

$$g(t) = w^2(t)(t^2-1). \tag{4.15}$$

As in the proof of Proposition 4.3.9, we need to verify the inequalities (4.13). Applying Lemma 4.3.8 to $H[F,g]$ gives the first inequality; it remains to show positive-definiteness of $H[F,g]$.

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

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

as $(1-t^2)w(t)$ is annihilated on the cosines of distances from $\mathscr{C}$. Because $w(t)$ is a degree

$(m-1)$ monic polynomial, the above implies $w(t) = Q^{1,1}_{m-1}(t)$. By Proposition 4.3.5, this also means that for $2 \leq k \leq m-1$, polynomials $\prod_{j=2}^{k}(t-t_j)$ are linear combinations of $Q^{1,1}_n$ with positive coefficients. Since the cone of functions with nonnegative Jacobi coefficients with respect to $Q^{1,1}_n$ is closed under multiplication, for $2 \leq k \leq m$, polynomials $\prod_{j=2}^{k}(t-t_j)^2$ and $(t-t_k)\prod_{j=2}^{k-1}(t-t_j)^2$ also have nonnegative Jacobi coefficients in $Q^{1,1}_n$. Due to Lemma 4.3.4, since $t - t_1 = t+1$, we obtain that

$$a_k(t) := (t-t_1)(t-t_k)\prod_{j=2}^{k-1}(t-t_j)^2 \quad \text{and} \quad b_k(t) := (t-t_1)\prod_{j=2}^{k}(t-t_j)^2, \tag{4.16}$$

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

We conclude by the same observations as in the proof of Proposition 4.3.9; in particular, the positive definiteness of the Hermite interpolant $H[F,g]$ follows from the representation

$$\begin{aligned} H\left[F,g\right](t) &= F(t_1) + b_1(t)Q[F,b_1](t_2) \\ &\quad + \sum_{k=2}^{m}\Big(a_k(t)\,Q\left[F,a_k\right](t_k) + b_k(t)\,Q\left[F,b_k\right](t_{k+1})\Big), \end{aligned} \tag{4.17}$$

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

Example 4.3.11. *As an example of another application of Theorem 4.3.1, consider the case that $F(t) = a + bt + ct^2 + dt^3$ is given as the potential function. In this case, some elementary considerations show that if*

(i) $d \leq 0$,

(ii) $c \geq -3d$,

(iii) $c^2 - 3bd \geq 0$,

(iv) $-c - \sqrt{c^2 - 3bd} \leq 3d$, *and,*

(v) $-c+\sqrt{c^2-3bd} \geq 3d$,

then F is absolutely monotonic of degree 2 up to a constant. Hence, the energy of any potential function of the above form on a two-point homogeneous space Φ is minimized by a tight 2-design. Note that the constant term can be ignored, so it suffices to only consider the sign of derivatives. In particular, if $b > 0$ and d becomes sufficiently small in magnitude, the above inequalities will hold.

As discussed earlier this chapter, we would like to determine conditions for which all minimizers of an energy are discrete, as well as characterize the minimizers whenever possible. This is possible when F is strictly absolutely monotonic of degree M and tight M-designs exist, as then the tight designs are exactly the minimizers of I_F.

Theorem 4.3.12. *Suppose that a tight M-design $\mathscr{C}$ minimizes the F-energy integral, for F strictly absolutely monotonic of degree M and such that $F^{(M+1)}(t) < 0$ for $t \in (-1,1)$. Then any minimizer of I_F must be a tight M-design.*

Proof. The argument developed to prove Theorem 4.3.1 may be described concisely through the following string of inequalities

$$I_F(\mu) \geq I_{H[F,g]}(\mu) \geq I_{H[F,g]}(\eta) = I_{H[F,g]}(\mu_{\mathscr{C}}) = I_F(\mu_{\mathscr{C}}),$$

where g is of the form (4.12) or (4.15), as is appropriate. In order for $I_F(\mu) = I_F(\mu_{\mathscr{C}})$ to hold, the inequalities must be equalities. The first inequality can only be sharp in the case that $\mathscr{A}(\text{supp}(\mu)) \subseteq \mathscr{A}(\mathscr{C})$. This follows from the fact that $H[F,g](t) < F(t)$ for all $t \notin \mathscr{A}(\mathscr{C})$ by the remainder formula from Lemma 4.3.8. In particular, this shows that $|\text{supp}(\mu)|$ is finite.

We now wish to show that the second inequality is sharp only when μ is a weighted design of at least the strength of the minimizing tight design. We first note that since F is strictly absolutely monotonic, the divided differences appearing in (4.14) or (4.17) are all positive due to (4.10). Thus, $H[F,g]$ (possibly modulo a constant) is a linear combination, with positive coefficients, of positive definite polynomials of degrees $0,1,\ldots,M$, so $H[F,g] = a_0 + \sum_{j=1}^{M} a_j C_j$, where $a_j > 0$ for $j > 0$. We see that μ must indeed be a weighted M-design, and due to Theorem 2.6.6 and the fact that $\mathscr{C}$ is a tight M-design, $|\operatorname{supp}(\mu)| \geq |\mathscr{C}|$. Lemmas 2.6.3 and 2.6.5 then tell us that this is only possible if

$$|\mathscr{A}(\operatorname{supp}(\mu))| \geq |\mathscr{A}(\mathscr{C})|.$$

Thus, the distance sets must be the same, and therefore so are the cardinalities of the sets, making $\operatorname{supp}(\mu)$ a tight M-design. Since μ is a weighted M-design, it must be a tight M-design. □

Causal Variational Principle

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

$$F(t) = F_\tau(t) := \max\{0, 2\tau^2\big(1+t\big)\big(2-\tau^2(1-t)\big)\}. \tag{4.18}$$

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

$$I_F(\mu) = \int_{\mathbb{S}^2}\int_{\mathbb{S}^2} F(\langle x,y\rangle)d\mu(x)d\mu(y) \tag{4.19}$$

is known as the *causal variational principle* on the sphere and is connected to relativistic quantum field theory. It is conjectured in [FS13] that there exist discrete minimizers for $\tau \geq 1$ and, moreover, that all the minimizers of (4.19) are discrete whenever $\tau > \sqrt{2}$. The background on this problem can be found in [FS13, BFSvdM19].

Here we confirm this conjecture for two values of $\tau > 0$, for which we can show that the cross-polytope (or orthoplex) and the icosahedron indeed minimize the energy, which was suggested by numerical experiments in [FS13]. The proofs are another application of the linear programming framework. In this instance, Hermite interpolation is unavailable to us as F is not differentiable on $(-1,1)$. However, as we are dealing with a single kernel, instead of a class of them as in the previous section, we need only construct the correct auxiliary function.

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

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

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

$$\nu = \frac{1}{6}\sum_{i=1}^{3}\left(\delta_{e_i} + \delta_{-e_i}\right),$$

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

Proposition 4.3.13. *The measure ν is a minimizer for the energy $I_{F_{\sqrt{2}}}$ over $\mathbb{P}(\mathbb{S}^2)$.*

Proof. The function

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

is positive definite on $\mathbb{S}^2$ and clearly satisfies

$$h(t) \leq F_{\sqrt{2}}(t) \qquad \text{for all } t \in [-1,1],$$

and

$$h(-1) = F_{\sqrt{2}}(-1) = 0, \quad h(0) = F_{\sqrt{2}}(0) = 0, \quad h(1) = F_{\sqrt{2}}(1) = 16,$$

so that h coincides with $F_{\sqrt{2}}$ on the set $\mathscr{A}(\mathrm{supp}(\nu))$.

We obtain that for any measure $\mu \in \mathbb{P}(\mathbb{S}^2)$,

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

where we have used the fact that $h(t) \leq F_{\sqrt{2}}(t)$ for $t \in [-1,1]$, so $I_{F_{\sqrt{2}}}(\mu) \geq I_h(\mu)$. Since h is positive definite, according to Proposition 3.4.1, we have that σ minimizes I_h, i.e. $I_h(\mu) \geq I_h(\sigma)$. We have also used that the cross-polytope is a 3-design and h is a quadratic polynomial, hence $I_h(\sigma) = I_h(\nu)$. Finally, $h(t) = F_{\sqrt{2}}(t)$ for $t \in \mathscr{A}(\mathrm{supp}(\nu)) = \{0, \pm 1\}$, hence $I_h(\nu) = I_{F_{\sqrt{2}}}(\nu)$. □

We now focus on the case of the icosahedron. Here we set $\tau = \sqrt{\frac{2\sqrt{5}}{\sqrt{5}-1}}$ so that $F_\tau(\frac{1}{\sqrt{5}}) = 0$. Let $\mathscr{C} \subset \mathbb{S}^2$ be the vertices of a regular icosahedron and let

$$\nu = \frac{1}{12} \sum_{x \in \mathscr{C}} \delta_x$$

be the uniform measure on the vertices of the icosahedron.

Proposition 4.3.14. *The measure ν is a minimizer for the energy, I_{F_τ}, over $\mathbb{P}(\mathbb{S}^2)$ for $\tau = \sqrt{\frac{2\sqrt{5}}{\sqrt{5}-1}}$.*

Proof. We shall need two facts about the icosahedron: namely that the set of inner products between elements of $\mathscr{C}$ is $\mathscr{A}(\mathscr{C}) = \left\{\pm 1, \pm 1/\sqrt{5}\right\}$, and $\mathscr{C}$ is a 5-design. For simplicity let us consider the function $F(t) = \frac{F_\tau(t)}{F_\tau(1)}$ so that $F(1) = 1$ (which does not effect the minimizers).

We construct the following polynomial:

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

where C_k are the standard Legendre polynomials (i.e. the Gegenbauer polynomials $C_k^{\frac{1}{2}}$). We observe then that h is positive definite, and that $h(t) \leq F(t)$ for $-1 \leq t \leq 1$, which follows from the factored form

$$h(t) = \frac{5}{32}(5-\sqrt{5})(t+1)(t - \frac{1}{\sqrt{5}})(t + \frac{1}{\sqrt{5}}).$$

A glance at this formula gives $h \leq F$ for $t \in [-1, \frac{1}{\sqrt{5}}]$, and the fact that $F - h$ is a polynomial with roots

$$t = -1, \frac{1}{\sqrt{5}}, \frac{-1 \pm 4\sqrt{10+4\sqrt{5}}}{\sqrt{5}},$$

gives $h \leq F$ for $t \in [\frac{1}{\sqrt{5}}, 1]$ which is a subset of the interval $[\frac{1}{\sqrt{5}}, \frac{-1+4\sqrt{10+4\sqrt{5}}}{\sqrt{5}}]$.

By construction, the function h (which was obtained by solving the linear equations $h(t) = F(t)$ for $t = \pm 1, \pm 1/\sqrt{5}$, as well as $h'(-1/\sqrt{5}) = 0$) has a local maximum at $-\frac{1}{\sqrt{5}}$ and coincides with F on the set $\mathscr{A}(\mathscr{C}) = \left\{\pm 1, \pm 1\sqrt{5}\right\}$. The same argument as in the proof of Proposition 4.3.13 finally shows

$$I_F(\nu) = \inf_{\mu \in \mathbb{P}(\mathbb{S}^2)} I_F(\mu),$$

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

Chapter 5

Stolarsky-type Principles

In numerous areas of mathematics and other sciences, one is faced with the problem of distributing large finite sets of points in a set Ω as uniformly as possible. There exist various quantitative measures of uniformity of point distributions. It should be evident from our discussion of Riesz energies in Section 2.1 that energy is one. Another popular candidate is discrepancy. We will focus on the sphere in this chapter, but a more complete exposition on general Discrepancy Theory can be found in [DT97, Mat99].

Let $\omega_N = \{z_1, \ldots, z_N\} \subset \mathbb{S}^{d-1}$. For a given subset of the sphere, $A \subset \mathbb{S}^{d-1}$, the discrepancy of ω_N with respect to A is defined as

$$D(\omega_N, A) = \frac{1}{N} \sum_{k=1}^{N} \mathbb{1}_A(z_k) - \sigma(A), \tag{5.1}$$

in other words, $D(\omega_N, A)$ indicates how well the Lebesgue measure of A is approximated by the counting measure $\frac{1}{N}\sum_{k=1}^{N} \delta_{z_k}$. To obtain good finite distributions ω_N, one usually evaluates and strives to minimize the supremum (extremal discrepancy) or average (e.g., L^2 discrepancy) of $|D(\omega_N, A)|$ over some rich and well-structured collection of sets A. Typical examples of such collections include spherical caps, slices, convex sets, etc. – the specific choice depends on the problem at hand.

It is known that in some cases these two ways of quantifying equidistribution are closely connected. One of the first instances of such a connection was obtained in 1973 by Stolarsky [Sto73], who proved that minimizing the L^2 discrepancy with respect to spherical caps is equivalent to maximizing the pairwise sum of Euclidean distances, i.e. $E_{\mathscr{D}}(\omega_N)$. More precisely, he established the identity

$$c_d [D_{L^2,\text{cap}}(\omega_N)]^2 = \int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} ||x-y||\, d\sigma(x)\, d\sigma(y) \;-\; \frac{1}{N^2} \sum_{i,j=1}^{N} ||z_i - z_j||,$$

which came to be known as the *Stolarsky Invariance Principle* (see section 5.1 for more details).

Recently, there has been a spike in interest in applications, analogues, and generalizations of the Stolarsky Invariance Principle in different settings: Brauchart and Dick studied it from the point of view of numerical integration on the sphere [BD13], Bilyk and Lacey connected it to tessellations of the sphere in [BL17], Basu, He, Owen, and Zhao used it in applications to genomics [HBZO19], Skriganov explored Stolarsky principles in general compact metrics space, proving an analogue of the result in projective spaces in [Skr17, Skr20], and Barg and Skriganov further explore this on the Hamming Cube in [Bar20, BS21]. In [BD19, BDM18, BMV], Bilyk, Dai, Vlasiuk, and the author explore a generalization of the Stolarsky Invariance Principle from the context of energy optimization. The results of these papers make up the bulk of this chapter.

We note that the basic strategy behind most versions of Stolarsky principle, at a very low level, is straightforward. Computing the L^2 discrepancy, one squares out the expression in (5.1), thus pairwise interactions between points of ω_N arise from cross terms of the form $\mathbb{1}_A(z_i) \cdot \mathbb{1}_A(z_j)$. When integrated over the test sets A in a given class, this yields the interaction potential $K(z_i, z_j)$, which is often represented as the volume of intersection of test sets "centered" at z_i and z_j, see e.g. (5.8), however, the details in some settings get rather technical. This approach is employed in Sections 5.1 and 5.2. A similar idea has been used by Torquato [Tor10] for "number variance", a quantity very similar to L^2

discrepancy. In Section 5.3 we go in the opposite direction and show that for any positive definite interaction potential one can construct an appropriate notion of discrepancy, so that a version of the Stolarsky principle holds.

In Section 5.1, we revisit the classical Stolarsky Invariance Principle. In Section 5.2, we observe that by replacing *all* spherical caps with *hemispheres* one obtains a variant of the Stolarsky Invariance Principle involving the *Geodesic Riesz* (-1)*-energy*. This allows one to easily characterize the finite point sets on $\mathbb{S}^{d-1}$ which maximize the sum of geodesic distances in all dimensions $d \geq 2$. We then take this idea a step further and show that our analogue of the Stolarsky Invariance Principle holds for general probability measures, which points to a drastic difference between the geodesic and Euclidean Riesz (-1)-energies. We finish the section with a discussion of the Geodesic Riesz s-energies for $s < 0$.

In Section 5.3, we explore the connections between energy optimization and discrepancy on a more general level, showing that for any positive definite function F, one can define a natural notion of discrepancy so that an analogue of the Stolarsky Invariance Principle holds for general probability measures. In Section 5.4, we take this a step further, showing that a similar result holds on all compact metric spaces.

5.1 Stolarsky Invariance Principle

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

$$C(x,h) = \{z \in \mathbb{S}^{d-1} : \langle z,x \rangle > h\}.$$

We define the L^2 discrepancy of $\omega_N = \{z_1, ..., z_N\}$ with respect to spherical caps by

$$[D_{L^2,\mathrm{cap}}(\omega_N)]^2 = \int_{-1}^{1} \int_{\mathbb{S}^{d-1}} \left| \frac{1}{N} \sum_{j=1}^{N} \mathbb{1}_{C(x,h)}(z_j) - \sigma\big(C(x,h)\big) \right|^2 d\sigma(x)\, dh. \tag{5.2}$$

The following result was proved by Stolarsky in 1973 [Sto73]:

Theorem 5.1.1 (Stolarsky Invariance Principle)**.** *Let $\omega_N = \{z_1, z_2, \dots, z_N\} \subset \mathbb{S}^{d-1}$. Then the following relation holds:*

$$[D_{L^2,\mathrm{cap}}(\omega_N)]^2 = C_{d-1}\left(\int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \|x-y\|\, d\sigma(x)\, d\sigma(y) \;-\; \frac{1}{N^2}\sum_{i,j=1}^{N} \|z_i - z_j\| \right). \tag{5.3}$$

The constant C_{d-1} satisfies

$$\begin{aligned} C_{d-1} &= \frac{1}{2}\int_{\mathbb{S}^{d-1}} |\langle p, z\rangle|\, d\sigma(z) = \frac{1}{d-1}\frac{A_{d-2}}{A_{d-1}} = \frac{Vol_{d-1}}{A_{d-1}} \\ &= \frac{1}{d-1}\frac{\Gamma\big(d/2\big)}{\sqrt{\pi}\,\Gamma((d-1)/2)} \sim \frac{1}{\sqrt{2\pi(d-1)}} \quad \text{as } d \to \infty, \end{aligned} \tag{5.4}$$

where A_{d-1} is the surface area of $\mathbb{S}^{d-1}$, Vol_d is the volume of the unit ball in $\mathbb{R}^d$, and p is an arbitrary point on the sphere $\mathbb{S}^{d-1}$.

This theorem states that

- minimizing the L^2 spherical cap discrepancy of ω_N is equivalent to maximizing the sum of Euclidean distances between the points of ω_N.
- the L^2 spherical cap discrepancy can be realized as the difference between the continuous and discrete energies $I_F(\sigma) - E_F(\omega_N)$, with $F(\langle x,y\rangle) = ||x-y|| = \sqrt{2-2\langle x,y\rangle}$, or, equivalently, the error of numerical integration of the distance integral

  $$I_{\mathscr{D}_1}(\sigma) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \|x-y\|\, d\sigma(x)\, d\sigma(y)$$

  by the cubature formula with knots at the points of ω_N.

It is well known [Bec84a, Bec84b] that the optimal order of the L^2 spherical cap discrepancy is $N^{-\frac{1}{2}-\frac{1}{2(d-1)}}$, i.e.

$$c_{d-1} N^{-\frac{1}{2}-\frac{1}{2(d-1)}} \le \inf_{\omega_N \subset \mathbb{S}^{d-1}} D_{L^2,\mathrm{cap}}(\omega_N) \le c'_{d-1} N^{-\frac{1}{2}-\frac{1}{2(d-1)}}, \tag{5.5}$$

which in turn bounds the difference of continuous and discrete energies in (5.3).

In addition to the original proof in [Sto73], an alternative proof has been given in [BD13]. Here we present a new short and simple proof of the Stolarsky invariance principle (5.3) [BDM18]. It strongly resonates with the proof in [BD13], but is completely elementary in nature. A similar proof in a probabilistic interpretation has been independently given in [HBZO19] (compare Lemmas 5.1.2 and 5.1.3 below to Proposition 1 of [HBZO19]), and analogous ideas are used in [Skr17] on compact, connected, two-point homogeneous spaces and [Bar20] for the Hamming Cube.

The proof of (5.3) follows the aforementioned strategy: one squares out the integrand, and the discrete part (pairwise interactions) arises naturally from the cross terms. The important ingredient is the following relation between intersections of spherical caps and the Euclidean distance between their centers:

Lemma 5.1.2. *For arbitrary $x, y \in \mathbb{S}^{d-1}$ we have*

$$\int_{-1}^{1} \int_{S^{d-1}} \mathbb{1}_{C(x,h)}(z) \cdot \mathbb{1}_{C(y,h)}(z) d\sigma(z)\, dh = \int_{-1}^{1} \sigma\big(C(x,h) \cap C(y,h)\big)\, dh = 1 - C_{d-1} \|x - y\|, \tag{5.6}$$

where the constant C_{d-1} is given by (5.4).

Proof. We have

$$\begin{aligned}
\int_{-1}^{1} \sigma\big(C(x,h) \cap C(y,h)\big)\, dh &= \int_{-1}^{1} \int_{\mathbb{S}^{d-1}} \mathbb{1}_{C(x,h)}(z) \cdot \mathbb{1}_{C(y,h)}(z) d\sigma(z)\, dh \\
&= \int_{\mathbb{S}^{d-1}} \int_{-1}^{1} \mathbb{1}_{C(z,h)}(x) \cdot \mathbb{1}_{C(z,h)}(y)\, dh\, d\sigma(z) \\
&= \int_{\mathbb{S}^{d-1}} \int_{-1}^{\min\{\langle x,z\rangle, \langle y,z\rangle\}} dh\, d\sigma(z) \\
&= \int_{\mathbb{S}^{d-1}} \big(\min\{\langle x,z\rangle, \langle y,z\rangle\} + 1\big)\, d\sigma(z).
\end{aligned}$$

We now write $\min\{\langle x,z\rangle,\langle y,z\rangle\} = \frac{1}{2}\big(\langle x,z\rangle + \langle y,z\rangle - \big|\langle (x-y),z\rangle\big|\big)$. Clearly, $\int_{\mathbb{S}^{d-1}} \langle x,z\rangle\, d\sigma(z) = \int_{\mathbb{S}^{d-1}} \langle y,z\rangle\, d\sigma(z) = 0$ and by rotational invariance, we observe that

$$\int_{\mathbb{S}^{d-1}} \big|\langle (x-y),z\rangle\big|\, d\sigma(z) = \|x-y\| \cdot \int_{\mathbb{S}^{d-1}} \left|\left\langle \frac{x-y}{\|x-y\|}, z\right\rangle\right| d\sigma(z) = 2C_{d-1}\|x-y\|,$$

and this finishes the proof. □

Here we essentially repeated the proof from [BD13], but the proof of the next lemma, which gives the quadratic mean value of the size of the spherical caps, is simpler (does not use reproducing kernels).

Lemma 5.1.3. *For any $p \in \mathbb{S}^{d-1}$ we have*

$$\int_{-1}^{1} \big(\sigma\big(C(p,h)\big)\big)^2\, dh = 1 - C_d \int_{\mathbb{S}^{d-1}} \|x-p\|\, d\sigma(x), \tag{5.7}$$

Proof. It is clear that

$$\int_{\mathbb{S}^{d-1}} \|x-p\|\, d\sigma(x) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \|x-y\|\, d\sigma(x)\, d\sigma(y).$$

We use the result of the previous lemma, i.e. relation (5.6), to compute

$$\begin{aligned} 1 - C_{d-1} \int_{\mathbb{S}^{d-1}} \|x-p\|\, d\sigma(x) &= \int_{\mathbb{S}^{d-1}} \big(1 - C_{d-1}\|x-p\|\big)\, d\sigma(x) \\ &= \int_{\mathbb{S}^{d-1}} \int_{-1}^{1} \int_{\mathbb{S}^{d-1}} \mathbb{1}_{C(x,h)}(z) \cdot \mathbb{1}_{C(p,h)}(z) d\sigma(z)\, dh\, d\sigma(x) \\ &= \int_{-1}^{1} \int_{\mathbb{S}^{d-1}} \mathbb{1}_{C(p,h)}(z) \left(\int_{\mathbb{S}^{d-1}} \mathbb{1}_{C(z,h)}(x)\, d\sigma(x) \right) d\sigma(z)\, dh \\ &= \int_{-1}^{1} \big(\sigma\big(C(p,h)\big)\big)^2\, dh. \end{aligned}$$

□

This is one of numerous examples of a situation in which averaging over scales simplifies computations. For the L^2 discrepancy for spherical caps of fixed height h:

$$D^{(h)}_{L^2,\mathrm{cap}}(\omega_N) := \left(\int\limits_{\mathbb{S}^{d-1}} \left| \frac{1}{N} \sum_{j=1}^{N} \mathbb{1}_{C(x,h)}(z_j) - \sigma\big(C(x,h)\big) \right|^2 d\sigma(x) \right)^{1/2}, \tag{5.8}$$

one would have to deal with $\sigma\big(C(x,h) \cap C(y,h)\big)$, which has complicated structure, and no short relation akin to (5.6) is available, see e.g. [HBZO19]. Hence in this case, there is no formula as succinct and explicit as the Stolarsky principle, however one can still write down a generic relation where the interactions between z_j's would involve $\sigma\big(C(z_i,h) \cap C(z_j,h)\big)$.

Proposition 5.1.4. *For any $\omega_N = \{z_1, z_2, \dots, z_N\} \subset \mathbb{S}^{d-1}$ and a fixed $h \in [-1,1]$, the following relation holds*

$$\left[D^{(h)}_{L^2,\mathrm{cap}}(\omega_N)\right]^2 = \frac{1}{N^2} \sum_{i,j=1}^{N} \sigma\big(C(z_i,h) \cap C(z_j,h)\big) - \big(\sigma\big(C(p,h)\big)\big)^2, \tag{5.9}$$

where $p \in \mathbb{S}^{d-1}$ is arbitrary.

Proof. We note that $\sigma\big(C(x,h)\big)$ is independent of $x \in \mathbb{S}^{d-1}$, hence

$$\begin{aligned}
\left[D^{(h)}_{L^2}(\omega_N)\right]^2 &= \int\limits_{\mathbb{S}^{d-1}} \left| \frac{1}{N} \sum_{j=1}^{N} \mathbb{1}_{C(x,h)}(z_j) - \sigma\big(C(x,h)\big) \right|^2 d\sigma(x) \qquad (5.10) \\
&= \frac{1}{N^2} \sum_{i,j=1}^{N} \int\limits_{\mathbb{S}^{d-1}} \mathbb{1}_{C(x,h)}(z_i) \cdot \mathbb{1}_{C(x,h)}(z_j) d\sigma(x) \\
&\quad - \frac{2}{N} \int\limits_{\mathbb{S}^{d-1}} \sum_{j=1}^{N} \mathbb{1}_{C(z_j,h)}(x) \cdot \sigma\big(C(x,h)\big)\, d\sigma(x) + \big(\sigma\big(C(p,h)\big)\big)^2 \\
&= \frac{1}{N^2} \sum_{i,j=1}^{N} \sigma\big(C(z_i,h) \cap C(z_j,h)\big) - \big(\sigma\big(C(p,h)\big)\big)^2.
\end{aligned}$$

□

Integrating identity (5.9) with respect to h, as

$$[D_{L^2,\mathrm{cap}}(\omega_N)]^2 = \int_{-1}^{1} [D^{(h)}_{L^2,\mathrm{cap}}(\omega_N)]^2 dh,$$

and applying relations (5.6) and (5.7) we finish the proof of the Stolarsky principle (5.3).

5.2 Hemispheric Stolarsky Principle and Geodesic Riesz s-Energy

In this section, we see that by restricting to only hemispheres, we produce a new invariance principle that involves the discrete geodesic Riesz (-1)-energy in place of the standard Riesz (-1)-energy. This allows one to characterize the finite point sets on $\mathbb{S}^{d-1}$ which maximize the sum of geodesic distances (see Theorem 5.2.10). This can be taken one step further to show that this analogue of the Stolarsky Invariance Principle holds for general probability measures, providing a way to characterize the maximizers of the continuous geodesic Riesz (-1)-energy $I_{\vartheta^*_{-1}}$. This brings up a surprising difference between the geodesic and standard Riesz (-1)-energies. Writing the negative geodesic Riesz (-1)-kernel as a function of the Euclidean distance

$$-\vartheta^*_{-1}(x,y) = -\frac{2}{\pi}\arccos(\langle x,y\rangle) = -\frac{2}{\pi}\arccos\left(1-\frac{||x-y||^2}{2}\right)$$

we see it has the same order of repulsion as $-\mathscr{D}_{-1}$, i.e.

$$\lim_{r\to 0^+}\frac{-\frac{2}{\pi}\arccos\left(1-\frac{r^2}{2}\right)}{r} = \frac{4}{\pi}. \tag{5.11}$$

Thus, both $-\mathscr{D}_{-1}$ and $-\vartheta^*_{-1}$ are *strongly repulsive*, with $\gamma = 1$ in the notation of Theorem 4.0.4. This might lead one to think that the maximizers of $I_{\vartheta^*_{-1}}$ and $I_{\mathscr{D}_{-1}}$ would exhibit similar behavior. However, any symmetric measure is optimal in the former case, which includes both discrete and absolutely continuous measures, while only the uniform measure σ maximizes the latter energy.

Hemispheric Stolarsky Principle

An (open) hemisphere in the direction of $x \in \mathbb{S}^{d-1}$ is simply a spherical cap of height $h = 0$:

$$H(x) = \{z \in \mathbb{S}^{d-1} : \langle z, x\rangle > 0\} = C(x, 0). \tag{5.12}$$

Since $\sigma\big(H(x)\big) = \frac{1}{2}$, the natural L^2 discrepancy for this set system is

$$D_{L^2,\mathrm{hem}}(\omega_N) := \left(\int\limits_{\mathbb{S}^{d-1}} \left| \frac{1}{N} \sum_{j=1}^{N} \mathbb{1}_{H(x)}(z_j) - \frac{1}{2} \right|^2 d\sigma(x) \right)^{1/2} = D^{(0)}_{L^2,\mathrm{cap}}(\omega_N). \tag{5.13}$$

While, as mentioned above, generally the quantity $\sigma\big(C(x,h) \cap C(y,h)\big)$ is complicated, in the case $h = 0$ (hemispheres) it has a very simple representation: for $x, y \in \mathbb{S}^{d-1}$

$$\sigma\big(H(x) \cap H(y)\big) = \sigma\big(C(x,0) \cap C(y,0)\big) = \frac{1}{2} \cdot \Big(1 - \vartheta^*(x,y)\Big), \tag{5.14}$$

where

$$\vartheta^*(x,y) := \frac{\vartheta(x,y)}{\pi} \tag{5.15}$$

is the normalized geodesic distance on the sphere between x and y. This can be very easily seen from Figure 5.1.

Combining (5.14), Proposition 5.1.4 and the fact that $\int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} \vartheta^*(x,y)\, d\sigma(x)\, d\sigma(y) = \frac{1}{2}$, one arrives at the following result:

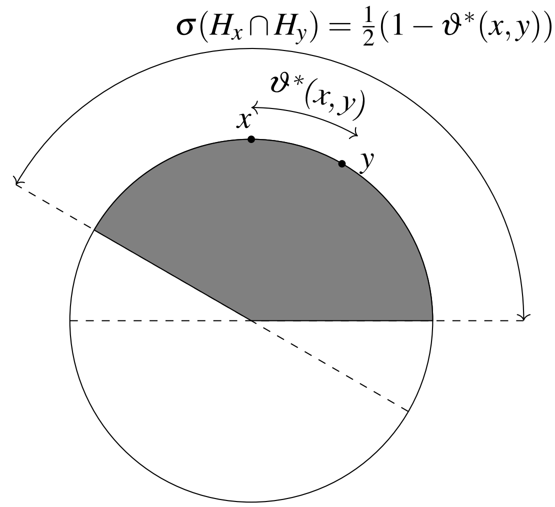

Figure 5.1: The size $\sigma(H_x \cap H_y)$ of the intersection of two hemispheres depends linearly on the geodesic distance $\vartheta^*(x,y)$.

Theorem 5.2.1 (Stolarsky Principle for Hemispheres)**.** *For any $\omega_N \in \mathbb{S}^{d-1}$, the following relation holds:*

$$[D_{L^2,\mathrm{hem}}(\omega_N)]^2 = \frac{1}{2}\left(\int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} \vartheta^*(x,y)\, d\sigma(x)\, d\sigma(y) - \frac{1}{N^2} \sum_{i,j=1}^{N} \vartheta^*(z_i,z_j) \right). \tag{5.16}$$

The statement looks strikingly similar to the original Stolarsky principle (5.3). One can say that the Euclidean distance corresponds to the *mean* over $t \in [-1,1]$, while the geodesic distance corresponds to the *median* ($h = 0$) of the heights of the spherical caps. Despite the fact that the original Stolarsky principle was proved in 1973, the Hemispheric version has only been discovered very recently, and independently, in [Skr17] and [BDM18]. Relation (5.16) has several interesting features and consequences.

Sum of Geodesic Distances

First of all, the principle of *irregularities of distribution*, discussed in great detail in [BC87], does not hold in this situation, that is, the hemisphere discrepancy can be very small, even zero, for large N. Indeed, for any symmetric distribution ω_N, it is easy to see that the L^2

hemisphere discrepancy is equal to zero. Moreover, (5.16) allows us to characterize finite point distributions in $\mathbb{S}^{d-1}$, which maximize the sum of geodesic distances.

Theorem 5.2.2. *Let $d \geq 2$. Then the following holds:*

1. *For any point distribution $\omega_N = \{z_1, \dots, z_N\} \subset \mathbb{S}^{d-1}$,*

$$\frac{1}{N^2} \sum_{i,j=1}^{N} \vartheta^*(z_i, z_j) \leq \frac{1}{2}. \tag{5.17}$$

2. *For a given $N \in \mathbb{N}$ the sum above is maximized if and only if the following condition holds: for any $x \in \mathbb{S}^{d-1}$, such that the hyperplane $x^\perp$ contains no points of ω_N, the numbers of points of ω_N on either side of $x^\perp$ differ by at most one, i.e.*

$$\Big| |\omega_N \cap H(x)| - |\omega_N \cap H(-x)| \Big| \leq 1. \tag{5.18}$$

3. *If N is even,*

$$\max_{\omega_N \subset \mathbb{S}^{d-1}} \frac{1}{N^2} \sum_{i,j=1}^{N} \vartheta^*(z_i, z_j) = \frac{1}{2}, \tag{5.19}$$

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

4. *If N is odd,*

$$\max_{\omega_N \subseteq \mathbb{S}^{d-1}} \frac{1}{N^2} \sum_{i,j=1}^{N} \vartheta^*(z_i, z_j) = \frac{1}{2} - \frac{1}{2N^2}, \tag{5.20}$$

and this maximum is achieved if and only if ω_N can be represented as a union $\omega_N = Z_1 \cup Z_2$, where Z_1 is symmetric, while Z_2 lies on a two-dimensional hyperplane (i.e. on a great circle) and satisfies

$$\frac{1}{M^2} \sum_{z_i, z_j \in Z_2} \vartheta^*(z_i, z_j) = \frac{1}{2} - \frac{1}{2M^2},$$

where $M = |Z_2|$. In other words, Z_2 is a maximizer of the sum of geodesic distances on $\mathbb{S}^1$.

Before we turn to the proof of the theorem, we briefly discuss the history of these questions. The problem of maximizing the sum of geodesic distances on the sphere was first introduced by Fejes Tóth in [FT59]. In his work, Fejes Tóth proved parts (3) and (4) on $\mathbb{S}^1$ and conjectured that they held on $\mathbb{S}^2$ (which he showed for $N \leq 6$). This conjecture was proven for N even (i.e. part (3)) soon after by Sperling [Spe60], and later for odd N (i.e. part (4)) by Nielsen [Nie65]. An earlier proof of part (4) for $d = 3$ was provided by Larcher in [Lar62], however, there is a mistake in his proof (statement (ii) at the bottom of page 48). Kelly then proved the bounds (5.19) and (5.20) for all N and in all dimensions in [Kel70], though no characterization of maximizers was found. Though parts (1) and (2) can be inferred from parts (3) and (4), they were recently proven directly for $d = 2$ in [Jia08] in relation to musical rhythms.

Our Stolarsky principle (5.16) allows us to directly prove parts (1) and (2), and makes the proofs of (5.19) and (5.20) simple in all dimensions $d \geq 2$. Moreover, we can now provide a characterization of maximizers, something that was previously known only for $d \leq 3$. In the case of odd N, we exploit a spherical version of the Sylvester–Gallai theorem (an interesting result from combinatorial geometry), much as Nielsen did in their paper [Nie65], though the main methods are different. We now turn to the proof of Theorem 5.2.2.

Proof. Part (1) of the theorem is now obvious since the left-hand side of (5.16) is non-negative and $\int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} \vartheta^*(x,y)\, d\sigma(x)\, d\sigma(y) = \frac{1}{2}$.

Part (2) also follows easily from (5.16). Indeed, for every $x \in \mathbb{S}^{d-1}$ such that $x^\perp$ does not contain any points of ω_N, the minimal value of the integrand in the left-hand side of (5.16), i.e. the integrand in (5.13), equals 0 for even N (if exactly half the points lie on either side of $x^\perp$), and is $\frac{1}{4N^2}$ for odd N (if the numbers of points on both sides of $x^\perp$ differ exactly by 1). Obviously, configurations ω_N for which this is achieved for each such $x \in \mathbb{S}^{d-1}$ are possible: e.g., $\lfloor N/2 \rfloor$ and $\lceil N/2 \rceil$ points in antipodal poles. Moreover, if for some $x \in \mathbb{S}^{d-1}$ with $x^\perp \cap \omega_N = \emptyset$ this condition is not satisfied, then it also fails on a small set of positive measure around x, hence $D_{L^2,\text{hem}}(\omega_N)$ is not minimal, and therefore $\frac{1}{N^2}\sum \vartheta^*(z_i, z_j)$ is not maximized.

To prove part (3), first observe that symmetric sets ω_N trivially satisfy the condition of part (2). Now assume that for some $x \in \mathbb{S}^{d-1}$ the number of points of ω_N located at x and $-x$ is not the same. Consider a hyperplane passing through x, which contains no other points of ω_N. Perturbing the hyperplane in opposite directions, we find that the difference of number of points on either side changes by at least 2, i.e. cannot stay equal to zero. Thus non-symmetric sets ω_N with an even number of points do not satisfy the condition of part (2), and so cannot maximize the sum of geodesic distances.

We now turn to part (4). We shall rely on the Sylvester–Gallai theorem. In the Euclidean case it states the following: *if a finite set ω_N in $\mathbb{R}^d$ has the property that for every two points of ω_N, the straight line passing through them contains at least one other point of ω_N, then all points of ω_N lie on the same straight line.* A spherical version of this theorem also holds.

Theorem 5.2.3 (Spherical Sylvester–Gallai Theorem)**.** *Assume that a set ω_N of N points on the sphere $\mathbb{S}^{d-1}$ contains no antipodal points and satisfies the following condition: for every two points of ω_N, the great circle passing through them contains at least one more point of ω_N. Then all points of ω_N lie on the same great circle.*

For the history and several proofs of these theorems we refer the reader to the book [AZ14, pages 73 and 88]. Normally, these theorems are stated in dimension $d = 3$, but higher dimensional extensions are simple. Indeed, for $\omega_N \subset \mathbb{S}^{d-1}$, consider a copy of $\mathbb{S}^2$ which contains z_1, z_2, $z_3 \in \omega_N$. The lower-dimensional version of Theorem 5.2.3 applies, and hence z_1, z_2, z_3 lie on the same great circle. In the same manner, considering a copy of $\mathbb{S}^2$ containing this great circle and any other point $z_i \in \omega_N$, we find that z_i has to lie on the same great circle.

We are now ready to prove part (4). Assume that N is odd. It follows from (5.16) and the proof of part (2) that the maximal value of $\frac{1}{N^2}\sum \vartheta^*(z_i, z_j)$ is $\frac{1}{2} - \frac{1}{2N^2}$. Observe that adding a pair of antipodal points to ω_N does not change maximality of ω_N, i.e. ω_N is a maximizer if and only if $\omega_N \cup \{p, -p\}$ is a maximizer (with N replaced by $N+2$). Indeed, since $\vartheta^*(x, p) + \vartheta^*(x, -p) = 1$, it is easy to check that

$$\sum_{x,y \in \omega_N \cup \{-p,p\}} \vartheta^*(x,y) = \sum_{x,y \in \omega_N} \vartheta^*(x,y) + 2(N+1),$$

thus the second sum equals $\frac{N^2}{2} - \frac{1}{2}$ if and only if the first sum is $\frac{(N+2)^2}{2} - \frac{1}{2}$. This immediately proves sufficiency of the condition in (4). Moreover, it shows that, in order to prove necessity, it is enough to consider maximizers without antipodal points and to prove that they have to be contained in some great circle.

Assume that ω_N maximizes $\frac{1}{N^2} \sum \vartheta^*(z_i, z_j)$ and contains no pair of antipodal points. Consider two arbitrary points z_1, $z_2 \in \omega_N$, and assume that no other point of ω_N lies on the great circle defined by z_1 and z_2. Since ω_N is finite, there exists a hyperplane containing z_1 and z_2, which does not contain any other points of ω_N. Since z_1 and z_2 are not antipodal, one can perturb the hyperplane in such a way that it does not touch other points of ω_N and both points z_1 and z_2 end up on the same side of the hyperplane. Perturbing in the opposite direction, we observe that the difference between the numbers of points on opposite sides of the hyperplane changes by 4, and therefore cannot stay equal to ± 1, so by part (2), ω_N cannot be a maximizer.

We thus conclude that, for any two points of ω_N, at least one other point of ω_N has to lie on the same great circle, i.e. the spherical Sylvester–Gallai theorem, Theorem 5.2.3, applies. Hence ω_N is contained in a great circle. □

Remark: Observe that the one-dimensional maximizers of odd cardinality N, which arise in part (4) of Theorem 5.2.2, 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 $d = 2$ and $N = 3$.

Theorem 5.2.2 demonstrates that the situation is drastically different from the spherical cap discrepancy and the sum of Euclidean distances. 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 ω_N [Bec84a, Bec84b, Mat99]. In particular, for $d = 2$ the sum is maximized by the vertices of a regular N-gon [FT56], and in higher dimensions maximizing distributions have to be well-separated [Sto75]. The sum of *geodesic* distances, however, may be maximized by very non-uniform sets, e.g. $N/2$ points in two antipodal poles.

Geodesic Distance Energy Integral

We now turn our sights to the problem of finding equilibrium distributions of the geodesic distance energy integral. As in the discrete case, we are interested in the maximum value of the energy I_{ϑ^*}, as well as the maximizers of this expression. The former follows from Theorem 5.2.2 and the weak* density of discrete measures in $\mathbb{P}(\mathbb{S}^{d-1})$:

$$\max_{\mu \in \mathbb{P}(\mathbb{S}^{d-1})} I_{\vartheta^*}(\mu) = \lim_{n\to\infty} \sup_{\omega_N \subset \mathbb{S}^{d-1}} E_{\vartheta^*}(\omega_N) = \frac{1}{2}. \tag{5.21}$$

One possible way to determine maximizing measures would be to show that the Gegenbauer expansion of $F(\langle x,y\rangle) = \frac{1}{2} - \vartheta^*(x,y)$ satisfies the conditions of part (3) of 3.5.2, so symmetric measures are uniquely optimal. However, we shall instead provide a proof making use of our Hemisphere Stolarsky principle (i.e. Theorem 5.2.1), which may be extended to more general measures than the counting measure $\mu = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i}$.

Theorem 5.2.4 (Hemisphere Stolarsky principle for general measures)**.** *Let* $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$. *Then the following relation holds*

$$\int_{\mathbb{S}^{d-1}} \left(\mu\big(H(x)\big) - \frac{1}{2}\right)^2 d\sigma(x) = \frac{1}{2} \cdot \left(\frac{1}{2} - I_{\vartheta^*}(\mu)\right). \tag{5.22}$$

Proof. Notice that

$$\int_{\mathbb{S}^{d-1}}\int_{H(x)} d\mu(y)d\sigma(x) = \int_{\mathbb{S}^{d-1}}\int_{H(y)} d\sigma(x)d\mu(y) = \frac{1}{2}\cdot\int_{\mathbb{S}^{d-1}} d\mu(y) = \frac{1}{2}$$

and, according to (5.14),

$$\begin{aligned}\int_{\mathbb{S}^{d-1}}\int_{H(x)}\int_{H(x)} d\mu(y)d\mu(z)d\sigma(x) &= \int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \sigma\big(H(y)\cap H(z)\big)\,d\mu(y)d\mu(z)\\ &= \int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \frac{1}{2}\cdot\big(1-\vartheta^*(y,z)\big)\,d\mu(y)d\mu(z) = \frac{1}{2}-\frac{1}{2}I_{\vartheta^*}(\mu).\end{aligned}$$

Using the two relations above we obtain

$$\begin{aligned}\int_{\mathbb{S}^{d-1}}\left(\mu\big(H(x)\big)-\frac{1}{2}\right)^2 d\sigma(x) &= \int_{\mathbb{S}^{d-1}}\left(\int_{H(x)}\int_{H(x)} d\mu(y)d\mu(z) - \int_{H(x)} d\mu(y)+\frac{1}{4}\right)d\sigma(x)\\ &= \frac{1}{2}-\frac{1}{2}I_{\vartheta^*}(\mu)-\frac{1}{2}+\frac{1}{4} = \frac{1}{2}\cdot\left(\frac{1}{2}-I_{\vartheta^*}(\mu)\right),\end{aligned}$$

which proves (5.22). □

Since the left-hand side of identity (5.22) is non-negative, Theorem 5.2.4 provides another way of showing that $I_{\vartheta^*}(\mu)\le\frac{1}{2}$ for all probability measures, and an immediate necessary condition to achieve that bound:

Corollary 5.2.5. *Measures $\mu\in\mathbb{P}(\mathbb{S}^{d-1})$ for which $I_{\vartheta^*}(\mu)=\frac{1}{2}$, are exactly the measures which satisfy the following condition:*

$$\mu\big(H(x)\big)=\frac{1}{2}\ \text{ for }\sigma\text{-a.e. } x\in\mathbb{S}^{d-1}. \tag{5.23}$$

It is easy to see that if the measure μ is symmetric, it is a maximizer of the energy I_{ϑ^*}. Consider the reflection of a measure μ, which we will call μ^*, i.e. $\mu^*(E)=\mu(-E)$. It is easy to see that

$$I_{\vartheta^*}(\mu,\mu^*) = \int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \vartheta^*(x,y)d\mu(x)d\mu^*(y) = \int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \vartheta^*(x,-y)d\mu(x)d\mu(y)$$
$$= \int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \big(1-\vartheta^*(x,y)\big)d\mu(x)d\mu(y) = 1 - I_{\vartheta^*}(\mu).$$

If, moreover, μ is symmetric, i.e. $\mu^* = \mu$, then $I_{\vartheta^*}(\mu) = \frac{1}{2}$, as

$$I_{\vartheta^*}(\mu) = I_{\vartheta^*}(\mu,\mu^*) = 1 - I_{\vartheta^*}(\mu). \tag{5.24}$$

Therefore, in particular, every symmetric measure $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ satisfies (5.23). The converse of this fact is less obvious.

Proposition 5.2.6. *Assume that the measure $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ satisfies the condition*

$$\mu\big(H(x)\big) = \frac{1}{2} \text{ for } \sigma\text{-a.e. } x \in \mathbb{S}^{d-1}. \tag{5.25}$$

Then the measure μ is symmetric, i.e. $\mu(E) = \mu(-E)$ for every Borel set $E \subseteq \mathbb{S}^{d-1}$.

The proof for this Proposition is based on spherical harmonics and Gegenbauer polynomials and requires the following auxiliary lemma, which will also be used in Section 5.3.

Lemma 5.2.7. *Let γ be a finite signed Borel measure on $\mathbb{S}^{d-1}$ and $F \in L^2([-1,1],w_\lambda)$ with $\lambda = \frac{d-3}{2}$. Assume that*

$$\int_{\mathbb{S}^{d-1}} F(\langle x,y\rangle)\,d\gamma(y) = 0 \text{ for } \sigma\text{-almost every } x \in \mathbb{S}^{d-1}. \tag{5.26}$$

Assume also that $\widehat{F}(n,\lambda) \neq 0$ *for some* $n \geq 1$. *Then for every spherical harmonic* $Y_n \in \mathscr{H}_n^d$,

$$\int_{\mathbb{S}^{d-1}} Y_n(y) d\gamma(y) = 0. \tag{5.27}$$

Proof. Applying the Funk-Hecke formula (2.29), we find that

$$\begin{aligned}\int_{\mathbb{S}^{d-1}} Y_n(y) d\gamma(y) &= \frac{1}{\widehat{F}(n,\lambda)} \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} F(\langle x,y\rangle) Y_n(x) d\sigma(x) d\gamma(y) \\ &= \frac{1}{\widehat{F}(n,\lambda)} \int_{\mathbb{S}^{d-1}} \left(\int_{\mathbb{S}^{d-1}} F(\langle x,y\rangle) d\gamma(y) \right) Y_n(x) d\sigma(x) = 0.\end{aligned}$$

□

Proof of Proposition 5.2.6. Let μ^* be the reflection of μ, defined by $\mu^*(E) = \mu(-E)$, and set $\gamma = \mu - \mu^*$. Condition (5.25) then implies that

$$\gamma\big(H(x)\big) = \int_{\mathbb{S}^{d-1}} \mathbb{1}_{(0,1]}(\langle x,y\rangle)\, d\gamma(y) = 0 \quad \text{for } \sigma\text{-a.e. } x \in \mathbb{S}^{d-1}.$$

The Gegenbauer coefficients $\widehat{F}(n,\lambda)$ of the function $F(t) = \mathbb{1}_{(0,1]}(t)$ are non-zero for odd n (Lemma 3.4.6 in [Gro96]). Therefore, according to Lemma 5.2.7, relation (5.27) holds for all odd n. For even values of n, the relation also holds, since $Y_n \in \mathscr{H}_n^d$ is an even function in this case, and γ is antisymmetric. Therefore, $\int_{\mathbb{S}^{d-1}} Y(y) d\gamma(y) = 0$ for every polynomial Y, and hence for each $Y \in C(\mathbb{S}^{d-1})$, which implies that $\gamma = 0$. Hence $\mu = \mu^*$, i.e. μ is symmetric. □

From the above discussion we obtain the following characterization of the maximizers of $I_{\vartheta^*}(\mu)$:

Theorem 5.2.8. *For a measure* $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$,

$$I_{\vartheta^*}(\mu) = \sup_{\gamma \in \mathbb{P}(\mathbb{S}^{d-1})} I_{\vartheta^*}(\gamma) = \frac{1}{2}$$

if and only if μ is centrally symmetric.

This behavior of $I_{\vartheta^*}(\mu)$ goes in sharp contrast with the behavior of the seemingly similar energy integral $\int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \|x-y\|\, d\mu(x)d\mu(y)$. It is known [Bjö56] that the unique maximizer of this energy integral is $\mu=\sigma$, the uniform distribution on $\mathbb{S}^{d-1}$. In this sense the behavior of $I_{\vartheta^*}(\mu)$ is more similar (albeit still different) to that of $\int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \|x-y\|^2\, d\mu(x)d\mu(y)$ which is maximized by any measure with center of mass at the origin, which may be easily seen from the relation

$$\int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \|x-y\|^2\, d\mu(x)d\mu(y) = 2-2\cdot\left\|\int_{\mathbb{S}^{d-1}} x d\mu(x)\right\|^2. \tag{5.28}$$

It is thus natural to analyze the *Geodesic Riesz s-energy* for general powers $s<0$, and contrast it with the standard Riesz s-energies, discussed in Section 2.1.

Geodesic Riesz s-Energy

We would like to understand which measures $\mu\in\mathbb{P}(\mathbb{S}^{d-1})$ maximize the Geodesic Riesz s-energy

$$I_{\vartheta_s^*}(\mu) = \int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \left(\vartheta^*(x,y)\right)^{-s} d\mu(x)d\mu(y), \tag{5.29}$$

for $s<0$, and how maximizers depend on s. The case of $0<s<d-1$ was studied by Bilyk and Dai in [BD19], where they found that σ was the unique minimizer of $I_{\vartheta_s^*}$.

While the study of the geodesic Riesz s-energies is quite recent, the Riesz s-energies for Euclidean distance are well investigated, as discussed in Section 2.1. In addition to the properties of maximizers given in Theorem 2.1.2 for general compact spaces, Björck was able to further refine his results in the case $\Omega=\mathbb{S}^{d-1}$.

Theorem 5.2.9 ([Bjö56]). *For $s<0$, the maximizers of the Euclidean Riesz s-energy*

$$I_{\mathscr{D}_s}(\mu) = \int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} \|x-y\|^{-s} d\mu(x)d\mu(y)$$

over $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ *can be characterized as follows:*

1. $0 > s > -2$*: the unique maximizer of* $I_{\mathscr{D}_s}(\mu)$ *is* $\mu = \sigma$.

2. $s = -2$*:* $I_{\mathscr{D}_s}(\mu)$ *is maximized if and only if the center of mass of* μ *is at the origin.*

3. $s < -2$*:* $I_{\mathscr{D}_s}(\mu)$ *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.*

The proof of part (1) uses potential analysis, in particular, the semigroup property of the Riesz potentials; part (2) is explained in (5.28); and part (3) follows from part (2) and simple linear programming bounds.

We observe that there is a "breaking point" $s = -2$ in the behavior of maximizers of the Euclidean Riesz s-energy. Surprisingly, for the seemingly similar geodesic Riesz s-energy, this critical value is different: $s = -1$. We have the following theorem:

Theorem 5.2.10. *For* $s < 0$*, the maximizers of the geodesic Riesz s-energy*

$$I_{\vartheta_s^*}(\mu) = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \big(\vartheta^*(x,y)\big)^{-s} d\mu(x) d\mu(y)$$

over $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ *can be characterized as follows:*

1. $0 > s > -1$*: the unique maximizer of* $I_{\vartheta_s^*}(\mu)$ *is* $\mu = \sigma$.

2. $s = -1$*:* $I_{\vartheta_s^*}(\mu)$ *is maximized if and only if* μ *is centrally symmetric .*

3. $s < -1$*:* $I_{\vartheta_s^*}(\mu)$ *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.*

Part (1) is proved in [BD19] through extensive analysis of spherical harmonic expansions. Part (2) is the result of Theorem 5.2.8 above, which is a consequence of the hemisphere Stolarsky principle (5.22). The proof of part (3) is quite simple, following from

Lemma 4.3.2: since $\vartheta^*(x,y) \le 1$, we have for $s < -1$

$$I_{\vartheta_s^*}(\mu) \le \int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} \vartheta^*(x,y)\, d\mu(x) d\mu(y) \le \frac{1}{2}.$$

The first inequality turns into an equality when $(\mu \times \mu)\big\{(x,y) :\ \vartheta^*(x,y) = 0 \text{ or } 1\big\} = 1$, while the second bound becomes exact when μ is symmetric, according to part (2). This readily implies that $\mu = \frac{1}{2}(\delta_p + \delta_{-p})$.

This peculiar effect (that geodesic distance energy behaves differently from its Euclidean counterpart) was previously noticed in dimension $d = 2$, i.e. on the circle, in [BHS12], where the one-dimensional case of parts (1) and (3) of the above theorem have been proved.

5.3 The Generalized Stolarsky Principle for the Sphere

In this section we turn to a generalization of the Stolarsky Invariance Principle for positive definite functions. Assume that $F \in C([-1,1])$ is positive definite, $\lambda = \frac{d-2}{2}$, and the function $f \in L^2([-1,1], w_\lambda)$ is as in Corollary 2.5.2, i.e.

$$F(\langle x,y \rangle) = \int\limits_{\mathbb{S}^{d-1}} f(\langle x,z \rangle) f(\langle z,y \rangle) d\sigma(z).$$

For a Borel probability measure $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ we define the L^2 discrepancy of μ with respect to f as

$$D_{L^2,f}(\mu) = \left(\int\limits_{\mathbb{S}^{d-1}} \Big| \int\limits_{\mathbb{S}^{d-1}} f(\langle x,y \rangle)\, d\mu(y) - \int\limits_{\mathbb{S}^{d-1}} f(\langle x,y \rangle)\, d\sigma(y) \Big|^2 d\sigma(x) \right)^{\frac{1}{2}}. \qquad (5.30)$$

The L^2 discrepancy of a finite point-set $\omega_N \subset \mathbb{S}^{d-1}$ is simply

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

Notice that various choices of f recover different geometric notions of discrepancy (e.g., $\mathbb{1}_{(h,1]}$ for spherical caps of a fixed height, see (5.9)), although this object is more general. We now prove a general version of the Stolarsky principle, which connects the energies with respect to F with the L^2 discrepancy built upon f.

Theorem 5.3.1 (Generalized Stolarsky principle)**.** *Let $\mu \in \mathbb{P}^*(\mathbb{S}^{d-1})$, i.e. a signed Borel probability measure, and let F be positive definite with f as in* (3.16). *Then*

$$I_F(\mu) - I_F(\sigma) = D^2_{L^2,f}(\mu). \tag{5.31}$$

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

$$\frac{1}{N^2}\sum_{i,j=1}^{N} F(\langle z_i, z_j\rangle) - \int\limits_{\mathbb{S}^{d-1}}\int\limits_{\mathbb{S}^{d-1}} F(\langle x,y\rangle) d\sigma(x) d\sigma(y) = D^2_{L^2,f}(\omega_N). \tag{5.32}$$

Proof. According to the definition of $D_{L^2,f}(\mu)$, (3.16), and Lemma 3.2.3, we have

$$\begin{aligned} D^2_{L^2,f}(\mu) &= \int\limits_{\mathbb{S}^{d-1}} \Big(\int\limits_{\mathbb{S}^{d-1}} f(\langle x,y\rangle)\, d(\mu-\sigma)(y)\Big)^2 d\sigma(x) \\ &= \int\limits_{\mathbb{S}^{d-1}}\int\limits_{\mathbb{S}^{d-1}}\int\limits_{\mathbb{S}^{d-1}} f(\langle x,y\rangle) f(\langle x,z\rangle) d(\mu-\sigma)(y) d(\mu-\sigma)(z) d\sigma(x) \\ &= \int\limits_{\mathbb{S}^{d-1}}\int\limits_{\mathbb{S}^{d-1}} F(\langle y,z\rangle) d(\mu-\sigma)(y) d(\mu-\sigma)(z) = I_F(\mu-\sigma) = I_F(\mu) - I_F(\sigma). \end{aligned}$$

□

This approach brings up several novel points. First of all, in most contexts the Stolarsky identity arises from the notion of the L^2 discrepancy, which in turn dictates the specific form of the interaction potential F. Theorem 5.3.1, on the other hand, allows one to go in the opposite direction: starting with the 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 obtain estimates for $D_{L^2,f}(\mu)$, as shown by Bilyk and Dai in [BD19] (Theorem 4.2, part (ii)).

Proposition 5.3.2. *Suppose that F is positive definite and $f \in L^2_{w_\lambda}([-1,1])$ is as in Corollary 2.5.2. Then there exist $c_{d-1}, c'_{d-1} > 0$ such that for all $N \in \mathbb{N}$,*

$$c'_{d-1} \min_{1 \le k \le c_{d-1} N^{\frac{1}{d-1}}} \widehat{F}(k,\lambda) \le \inf_{\omega_N \subset \mathbb{S}^{d-1}} D^2_{L^2,f}(\omega_N) \le N^{-1} \max_{0 \le \theta \le c_{d-1} N^{-\frac{1}{d-1}}} F(1) - F(\cos\theta) \tag{5.33}$$

Hence, e.g., lower bounds can be proved using information about either F or f. In [BD19], the authors use these estimates to give an alternative proof of the spherical cap discrepancy bounds (5.5), and employ (5.32) to obtain sharp asymptotic behavior of the difference between discrete and continuous energies, $E_F(\omega_N) - I_F(\sigma)$, as the number of points $N \to \infty$, both in the case of Euclidean Riesz energies, $F(\langle x,y\rangle) = \mathscr{D}_s(x,y)$ (recovering results of [Wag92, KS98, Bra06]), and the geodesic Riesz energies, $F(\langle x,y\rangle) = \vartheta_s^*(x,y)$, introduced in [BD19, BDM18].

Since $D^2_{L^2,f}(\mu) \ge 0$, the generalized Stolarsky identity (5.31) gives yet another proof that for F positive definite, the uniform measure σ is a minimizer of I_F over $\mathbb{P}(\mathbb{S}^{d-1})$ (in fact, over $\widetilde{\mathbb{P}}(\mathbb{S}^{d-1})$). Furthermore, the identity also provides an alternative way of showing that F having all positive Gegenbauer coefficients implies that σ is the unique minimizer of I_F. Indeed, without loss of generality, we may assume that $\widehat{F}(0,\lambda) > 0$. Assume also that for each $n \ge 1$, we have $\widehat{f}(n,\lambda) = (\widehat{F}(n,\lambda))^{1/2} \neq 0$. Let μ be a minimizer of $I_F(\mu)$, i.e. $I_F(\mu) = I_F(\sigma)$. Therefore, the Stolarsky principle (5.31) implies that $D^2_{L^2,f}(\mu) = 0$, i.e.

$$\int_{\mathbb{S}^{d-1}} f(\langle x,y\rangle)\, d(\sigma-\mu)(y) = 0$$

for σ-almost every x. Then by Lemma 5.2.7, relation (5.27), with $\gamma = \sigma - \mu$, holds for every polynomial, and thus for every $Y \in C(\mathbb{S}^{d-1})$. Hence σ is the unique minimizer of $I_F(\mu)$.

5.4 The Generalized Stolarsky Principle on Compact Metric Spaces

The generalized Stolarsky principle on the sphere, Theorem 5.3.1, extends to arbitrary compact domains without significant difficulty.

Let (Ω,ρ) be a compact metric space and let us fix a measure $\mu \in \mathbb{P}(\Omega)$ – this will usually be an energy minimizing (equilibrium) measure or an invariant measure (its role is similar to that of σ in the spherical case). We now define the *L^2 discrepancy of an arbitrary probability measure $\nu \in \mathbb{P}(\Omega)$ (or even a signed measure $\nu \in \widetilde{\mathbb{P}}(\Omega)$) relative to the equilibrium measure μ with respect to the function* $k : \Omega\times\Omega \to \mathbb{R}$ by the identity

$$\begin{aligned} D^2_{L^2,k,\mu}(\nu) &= \int_\Omega \left| \int_\Omega k(x,y)d\nu(y) - \int_\Omega k(x,y)d\mu(y) \right|^2 d\mu(x) \\ &= \int_\Omega \left| \int_\Omega k(x,y)d\big(\nu-\mu\big)(y) \right|^2 d\mu(x). \end{aligned} \tag{5.34}$$

When ν is the equal-weight discrete measure associated to the N-point set $\omega_N = \{z_1,...,z_N\} \subset \Omega$, i.e. $\nu = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i}$, this becomes the discrepancy of the set ω_N with respect to k:

$$D^2_{L^2,k,\mu}(\omega_N) = D^2_{L^2,k,\mu}\Big(\frac{1}{N}\sum_{i=1}^{N}\delta_{z_i}\Big) = \int_\Omega \left| \frac{1}{N}\sum_{i=1}^{N} k(x,z_i) - \int_\Omega k(x,y)d\mu(y) \right|^2 d\mu(x) \tag{5.35}$$

Observe that changing the function k by an additive constant does not change the value of the discrepancy.

We can now obtain the following general version of the Stolarsky Invariance Principle:

Theorem 5.4.1. *Let K be a positive definite (modulo and additive constant C) kernel on $\Omega \times \Omega$. Let us assume that $\mu \in \mathbb{P}(\Omega)$ is a K-invariant measure with full support (* $\operatorname{supp}(\mu) = \Omega$*). Then for every measure $\nu \in \widetilde{\mathbb{P}}(\Omega)$, we have the following identity.*

$$I_K(\nu) - I_K(\mu) = D^2_{L^2,k,\mu}(\nu), \tag{5.36}$$

where the function $k \in L^2(\Omega \times \Omega, \mu \times \mu)$ is as in part (5) of Theorem 3.3.2 applied to the positive definite kernel $K + C$.

In particular, for a discrete set $\omega_N = \{z_1, ..., z_N\} \subset \Omega$,

$$E_K(\omega_N) - I_K(\mu) = D^2_{L^2,k,\mu}(\omega_N). \tag{5.37}$$

This theorem has the following immediate corollary:

Corollary 5.4.2. *Let K be a kernel on $\Omega \times \Omega$. Assume that $\mu \in \mathbb{P}(\Omega)$ is a global minimizer of the energy functional I_K over $\mathbb{P}(\Omega)$ with $\operatorname{supp}(\mu) = \widetilde{\Omega} \subseteq \Omega$. Then identity (5.36) holds for any signed measure ν with total mass one, whose support is contained in the support of μ, i.e. $\nu \in \widetilde{\mathbb{P}}(\widetilde{\Omega})$. Similarly, relation (5.37) holds for any point set $\omega_N = \{z_1, ..., z_N\} \subset \widetilde{\Omega}$.*

Proof. If μ is a global minimizer of I_K, by Theorem 3.1.7, the potential U_K^{μ} is constant on $\widetilde{\Omega}$, i.e. μ is K-invariant and has full support if viewed as an element of $\mathbb{P}(\widetilde{\Omega})$. Moreover, according to Lemma 3.1.11, the kernel K is positive definite (modulo a constant) on $\widetilde{\Omega}$. Therefore, the statement follows directly from Theorem 5.4.1 applied to $\widetilde{\Omega}$ in place of Ω. □

We now turn to the proof of the generalized Stolarsky principle:

Proof of Theorem 5.4.1. Without loss of generality, we can assume that K is positive definite, since adding a constant to K does affects neither the invariance of μ nor the difference $I_K(\nu) - I_K(\mu)$. We can now use the crucial identity (3.10) of Lemma 3.2.3, as well as part (5) of Theorem 3.3.2, to obtain

$$\begin{aligned} I_K(\nu) - I_K(\mu) = I_K(\nu-\mu) &= \int_\Omega \int_\Omega K(x,y) d\big(\nu-\mu\big)(x) d\big(\nu-\mu\big)(y) \\ &= \int_\Omega \int_\Omega \int_\Omega k(x,z)k(z,y)\, d\mu(z) d\big(\nu-\mu\big)(x) d\big(\nu-\mu\big)(y) \\ &= \int_\Omega \left| \int_\Omega k(x,z) d\big(\nu-\mu\big)(x)\right|^2 d\mu(z) = D^2_{L^2,k,\mu}(\nu). \end{aligned} \tag{5.38}$$

□

Remark: Observe that, for $k \in L^2(\Omega\times\Omega, \mu\times\mu)$, it is not technically obvious that the definition of $D^2_{L^2,k,\mu}(\nu)$ in (5.34) is properly justified: we do not know a priori that k is integrable with respect to ν, only with respect to μ. (This problem does not occur in the discrete case since we know that $k(\cdot, z_i) \in L^2(\Omega,\mu)$ for each $i = 1, ..., N$.) However, the proof of Stolarsky principle (5.36) demonstrates that the L^2 discrepancy $D^2_{L^2,k,\mu}$ is well-defined for any Borel measure ν. Indeed, the inner integral with respect to $d\mu(z)$ in (5.38) is defined according to part (5) of Theorem 3.3.2, and, moreover, produces the function $K(x,y)$, which is continuous and therefore integrable with respect to the finite Borel measure $(\nu-\mu)\times(\nu-\mu)$ on $\Omega\times\Omega$. Hence Fubini's theorem applies and

$$\int_\Omega \int_\Omega k(x,z)k(y,z) d\big(\nu-\mu\big)(x) d\big(\nu-\mu\big)(y) = \left| \int_\Omega k(x,z) d\big(\nu-\mu\big)(x)\right|^2$$

is finite for μ-a.e. z and is integrable with respect to $d\mu(z)$, i.e. $D^2_{L^2,k,\mu}(\nu)$ is well-defined.

Chapter 6

P-frame Energy

We now turn our attention to a specific family of energies: the p-frame energies, given by kernels of the form

$$F_p(\langle x,y\rangle) := |\langle x,y\rangle|^p \qquad p>0 \tag{6.1}$$

on $\mathbb{S}_{\mathbb{F}}^{d-1}$, for $\mathbb{F}=\mathbb{R},\mathbb{C},\mathbb{H}$. Of course, since this energy does not depend on unitary transformations, the analysis of such energies naturally lends itself to the projective spaces $\mathbb{FP}^{d-1}$, where the p-frame energies correspond to taking kernels of the form (using the notation from Section 2.4, e.g. $\tau(x,y)=\cos(\vartheta(x,y))$)

$$F_p^*(\tau(x,y)) = \Big(\frac{1+\tau(x,y)}{2}\Big)^{\frac{p}{2}}, \tag{6.2}$$

as, for any $w,z\in\mathbb{S}_{\mathbb{F}}^{d-1}$, we have

$$F_p^*(\tau(w\mathbb{F},z\mathbb{F})) = F_p^*(2|\langle w,z\rangle|^2-1) = |\langle w,z\rangle|^p.$$

For $\mathbb{F}=\mathbb{R}$ or $\mathbb{C}$, the p-frame energies have a rich history. The case of $p=2$ and $\mathbb{F}=\mathbb{R}$ was studied in [Sid74] and later again in [BF03], In the latter paper, it was proved that the minimizers of the discrete energy are precisely the finite unit norm tight frames (FUNTFs), resulting in a recent increase in interest of this energy. We will discuss this in greater detail in Section 6.1.

In the case $p = 4$, the p-frame energy is closely connected to the maximal equiangular tight frames, which in the complex case are tight projective 2-designs, which are best known by their alternative name *symmetric informationally complete positive operator-valued measures* (SIC-POVMs). These are unit norm tight frames $\{z_j\}_{j=1}^N$ with the property that $|\langle z_i, z_j\rangle|^2 = \frac{1}{d+2}$ or $\frac{1}{d+1}$ for $i \neq j$, in the real and complex case respectively. In $\mathbb{C}^d$, Zauner's conjecture [Zau11] states that SIC-POVMs exist in all dimensions $d \geq 2$, which is supported by extensive numerical evidence [SG10, RBKSC04]. In the real case, the existence of analogous objects (i.e. tight projective 2-designs) is also mysterious: they may exist only in dimensions $d = (2m-1)^2 - 2$ [BD79, BD80, DGS77, LS73], but do not exist for infinitely many values of m [BMV04, Mak02]. When these objects do exist, they minimize the 4-frame energy.

More generally, for even integers p, these energies were considered in [Sid74, Wel74, Ven01], and it is known that for $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$ projective k-designs minimize the $p = 2k$ energy. In this terminology, FUNTFs are equivalent to projective 1-designs, while spherical 2-designs are exactly the FUNTFs with center of mass at the origin. Spherical 2-designs were constructively shown to exist for $d \geq 2$ precisely when the number of points N satisfies $N \geq d+1$ and $N \neq d+2$ when d is odd [Mim90], whereas FUNTFs of cardinality N exist for all $N \geq d$ [BF03]. Surface measure is also known to be a minimizer for $p \in 2\mathbb{N}$: this can be seen either from the definition of k-designs, or from the fact that the function F_p^* is positive definite in this case, and was originally proved in the real case in [Sid74].

Conversely, when $p \notin 2\mathbb{N}$, the situation is much less studied. The problem of minimizing general p-frame energies on $\mathbb{S}_{\mathbb{R}}^{d-1}$ was first posed by Ehler and Okoudjou in [EO12], where they also provided some initial results on both the discrete and continuous energies, in particular showing that distributing mass equally on the vertices of the cross-polytope yields the unique symmetric minimizer of the continuous p-frame energy for $p \in (0,2)$, up to orthogonal transformations. There have since been developments in determining minimizers of the discrete energy [CGG$^+$20, GP20, XX21] and continuous energy [BGM$^+$a, BGM$^+$b], the latter of which will be the main focus of this chapter.

In addition to the connections and applications in other areas of mathematics, the p-frame energy is an interesting subject to study from a Potential Theoretical point of view. In the introduction of Chapter 4, we discussed how, in the Euclidean setting, the discreteness of minimizers follows from the potential W being mildly repulsive, i.e. that the potential, as a function of $r = ||x-y||$, behaves as $W(0) - Cr^\gamma$ for small r, with $\gamma > 2$ and C some positive constant. Since, on the sphere $\mathbb{S}^{d-1}$,

$$|\langle x,y\rangle||^p = \left(1 - \frac{||x-y||^2}{2}\right)^p = \sum_{m=0}^{\infty} \binom{p}{m} \frac{(-r^2)^m}{2^m} \approx 1 - \frac{pr^2}{2},$$

the p-frame potential corresponds to the to the endpoint case $\gamma = 2$ and thus is quite delicate. Indeed, we know for some values of p, there exist non-discrete minimizers, while for others all minimizers are discrete, as we will show in Section 6.2. On the sphere, for $p \notin 2\mathbb{N}$, the p-frame potentials also have Gegenbauer expansions with infinitely many positive and negative coefficients (see 6.7), so they fall outside the scope of Theorem 4.1.3. This means that there is no guarantee that discrete minimizers exist, though we conjecture that all minimizers are discrete in these cases (see Conjecture 6.2.5). Thus, characterizing the behavior of minimizers of the p-frame energy may provide some insights on minimizing energies with similar behaviors, something that the current theory is not equipped to handle.

We discuss the 2-frame energy, or simply “frame energy”, in Section 6.1 and the more general p-frame energy in Section 6.2, in particular applying the results of Section 4.3 to show that in certain circumstances, tight designs are minimizers of the p-frame energy, and conjecture that for $p \notin 2\mathbb{N}$, all minimizers of $I_{F_p^*}$ are discrete. In Section 6.3, we show that the 600-cell is minimizer of certain p-frame energies as well, though it is not a tight design. While the discreteness of minimizers claimed in Conjecture 6.2.5 remains out of reach, we establish that the support of measures minimizing the p-frame energy I_{F_p}, with

$p \notin 2\mathbb{N}$, on the real sphere must have empty interior in Section 6.4. Section 6.5 extends some of our results to the non-compact setting. In Section 6.6, we show a connection to Convex Geometry, applying our results to the problem of minimizing mixed volumes of convex bodies.

6.1 Frame Energy

For $\mathbb{F} = \mathbb{R}$, the 2-frame energy, or simply *frame energy*, with the potential $F_2(t) = t^2$, was studied in [Sid74] and later again in [BF03]. In the latter paper, which coined the name for this energy, Benedetto and Fickus studied the discrete frame energy E_{F_2} in order to characterize all finite unit norm tight frames.

Given a finite dimensional Hilbert space H, a sequence $\{z_j\}_{j=1}^N$ in H is called a *frame* for H if there exist constants $0 < A \leq B < \infty$ such that for all $y \in H$

$$A||y||_H^2 \leq \sum_{j=1}^{N} |\langle y, z_j \rangle|^2 \leq B||y||_H^2. \qquad (6.3)$$

A frame is *tight* if $A = B$ in (6.3), and a tight frame is called a *unit norm tight frame* if $||z_j||_H = 1$ for $1 \leq j \leq N$. While it is possible to define frames for infinite-dimensional Hilbert spaces as well, in which case the frames may be infinite sequences, if one focuses on finite dimensional spaces, then it makes sense to only consider frames that are finite sequences, thus the term finite unit norm tight frames (FUNTFs).

Frames play an important role in signal processing and other branches of applied mathematics, as they act as overcomplete (or redundant) spanning sets of vectors that provide stable signal representations and allow modeling for noisy environments [BL98, BT93]. They were introduced in 1952 by Duffin and Schaeffer [DS52] as part of an on-going development of non-harmonic Fourier series, and have since been the subject of much research (see, e.g., [BCHL03, DGM86, SH03]). FUNTFs are of particular interest, as their characterization means that they provide an analogue of Parseval's Identity: If $\{z_j\}_{j=1}^N$ is a

FUNTF, then there exists some $A > 0$ such that

$$y = \frac{1}{A} \sum_{j=1}^{N} \langle y, z_j \rangle z_j \qquad \forall y \in H. \tag{6.4}$$

This property has led to various applications (see, e.g.,[CK03, Tyl87]), and connects FUNTFs to problems such as the Kadison-Singer conjecture [CFTW06]. For a more complete exposition on Frame Theory, see [Chr03].

In [BF03], Benedetto and Fickus provided a means of characterizing FUNTFs that connected them to energy minimization:

Theorem 6.1.1. *Let $N \in \mathbb{N}$ and $\omega_N = \{z_1, ..., z_N\} \subset \mathbb{S}^{d-1}$. Then*

1. *Treating $E_{F_2}(\omega_N)$ as a function of $z_1, ..., z_N$, every local minimizer of the frame energy is a global minimizer.*

2. *If $N \leq d$, then*
$$\mathscr{E}_{F_2}(\mathbb{S}^{d-1}, N) = \frac{1}{N}$$
and the minimizers are exactly the orthonormal sequences in $\mathbb{R}^d$.

3. *If $N \geq d$, then*
$$\mathscr{E}_{F_2}(\mathbb{S}^{d-1}, N) = \frac{1}{d} \tag{6.5}$$
and the minimizers are exactly the N-element FUNFT's.

We now provide a few remarks about this theorem. The first is that it shows that for all $N \geq d$, a FUNTF, or a spherical $\{2\}$-design as defined in Section 4.2, of N points exists. Though less wide in scope than Theorem 2.6.1, this result has the advantage of giving an explicit value after which such objects exist, rather than just the order. In addition, part (1) is an interesting and unusual result. As discussed in Section 3.3 we know that whenever F is conditionally positive definite on $\mathbb{S}^{d-1}$, all local minimizers of I_F are in fact global minimizers. Such a result rarely holds in the discrete setting, where the definition of local minimizer is necessarily quite different, and is one aspect that makes discrete energy optimization so difficult.

Since the minimum in (6.5) is independent of N, the weak*-density of discrete probability measures shows that the result of Benedetto and Fickus also implies (6.6), below. Moreover, inequality (6.6) for arbitrary measures $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ was stated in [Sid74,EO12], and Ehler and Okoudjou also characterized all minimizers of the continuous frame energy, I_{F_2}, as probabilistic tight frames. The author and coauthor provided a new proof of these results in [BM19], as well as an alternate characterization the minimizers of I_{F_2} (Lemma 6.1.3), which uses the following definition.

Definition 6.1.2. *A probability measure $\mu \in \mathbb{P}(\mathbb{S}^{d-1}$ is called **isotropic** if its second moment matrix is a multiple of the identity, i.e. $\left[\int\limits_{\mathbb{S}^{d-1}} x_i x_j \, d\mu(x)\right]_{i,j=1}^{d} = c\,\mathbb{I}_d$, with $x_i = \langle x, e_j \rangle$ for $1 \leq j \leq d$ and $\{e_1, ..., e_d\}$ and orthonormal basis of $\mathbb{R}^d$.*

Lemma 6.1.3. *For any $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$, we have*

$$I_{F_2}(\mu) \geq \frac{1}{d}. \tag{6.6}$$

Equality is achieved precisely for isotropic measures.

Proof. We expand the square, throw away off-diagonal terms, and apply the Cauchy–Schwartz inequality:

$$\begin{aligned} I_{F_2}(\mu) &= \int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} (\langle x, y \rangle)^2 \, d\mu(x) d\mu(y) = \sum_{i,j=1}^{d} \left(\int\limits_{\mathbb{S}^{d-1}} x_i x_j \, d\mu(x) \right)^2 \\ &\geq \sum_{i=1}^{d} \left(\int\limits_{\mathbb{S}^{d-1}} x_i^2 \, d\mu(x) \right)^2 \geq \frac{1}{d} \left(\sum_{i=1}^{d} \int\limits_{\mathbb{S}^{d-1}} x_i^2 \, d\mu(x) \right)^2 = \frac{1}{d}. \end{aligned}$$

From this, the characterization of the minimizers follows immediately. □

6.2 P-frame Energy

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

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

Since $\alpha + 1 = \frac{d-1}{2} \cdot \dim_{\mathbb{R}}(\mathbb{F}) > 0$ and $\beta + 1 = \frac{1}{2} \cdot \dim_{\mathbb{R}}(\mathbb{F}) > 0$, we see that the function $1+t$ is positive definite on Ω. It easily follows from repeated application of Schur's Theorem that $F^*_{2k}(t) = 2^{-k} \cdot (1+t)^k$ is positive definite on Φ, and therefore $I_{F^*_{2k}}$ is minimized by the surface measure η. This also means that on the sphere $\mathbb{S}^{d-1}_{\mathbb{F}}$, F_{2k} is positive definite and minimized by the normalized uniform surface measure on $\mathbb{S}^{d-1}_{\mathbb{F}}$, which we denote $\sigma_{\mathbb{F}}$.

The minimal values of the $p = 2k$ energy, in either the spherical or projective setting, may be expressed in elementary functions for each $\mathbb{F}$. The values for the real case were given by Sidel'nikov in [Sid74] and all values were determined by Shatalov in [Sha01].

Proposition 6.2.1. *Let $k \in \mathbb{N}$. Then*

$$\begin{aligned}
\mathscr{I}_{F_{2k}}(\mathbb{S}^{d-1}_{\mathbb{R}}) = \mathscr{I}_{F^*_{2k}}(\mathbb{RP}^{d-1}) &= \frac{1 \cdot 3 \cdot 5 \ldots (2k-1)}{d \cdot (d+2) \ldots (d+2(k-1))}, \\
\mathscr{I}_{F_{2k}}(\mathbb{S}^{d-1}_{\mathbb{C}}) = \mathscr{I}_{F^*_{2k}}(\mathbb{CP}^{d-1}) &= 1 \Big/ \binom{d+k-1}{k}, \\
\mathscr{I}_{F_{2k}}(\mathbb{S}^{d-1}_{\mathbb{H}}) = \mathscr{I}_{F^*_{2k}}(\mathbb{HP}^{d-1}) &= (k+1) \Big/ \binom{2d+k-1}{k}.
\end{aligned}$$

When p is not an even integer, the p-frame energies are not positive definite. While this could be checked by showing that the Jacobi expansion of F^*_p has negative coefficients in each setting, we may show this without these computations. The kernel F^*_p is clearly positive definite on $\mathbb{FP}^{d-1}$ if and only if F_p is positive definite on $\mathbb{S}_{\mathbb{F}}^{d-1}$. Since $\mathbb{S}_{\mathbb{H}}^{d-1}$ and $\mathbb{S}_{\mathbb{C}}^{d-1}$ each contain a copy of $\mathbb{S}_{\mathbb{R}}^{d-1}$, it is enough to show that F_p is not positive definite on the real sphere, which follows from its Gegenbauer expansion. Since it is an even function, all of F_p's odd coefficients are zero, so we need only calculate the even ones.

Lemma 6.2.2. *Let $k \in \mathbb{N}$, $p \in (0,\infty)$ and $\lambda = \frac{d-2}{2}$. Then*

$$\widehat{F}_p(2k,\lambda) = \frac{\Gamma(\lambda+1)\Gamma(\frac{p+1}{2})}{\sqrt{\pi}\,\Gamma(k+\frac{p}{2}+\lambda+1)} \prod_{l=0}^{k-1}\left(\frac{p}{2}-j\right). \tag{6.7}$$

In particular, the signs of the even coefficients alternate in sign for k sufficiently large.

Proof. Let us define, for all $n \in \mathbb{N}_0$, $p > 0$ and $\lambda > \frac{-1}{2}$

$$G(n,\lambda,p) = \int_0^1 t^p C_n^\lambda(t)(1-t^2)^{\lambda-\frac{1}{2}}dt. \tag{6.8}$$

From (2.26) and the fact that F_p is even, we see that

$$\widehat{F}_p(2k,\lambda) = \frac{\Gamma(\lambda+1)G(2k,\lambda,p)}{\sqrt{\pi}\Gamma(\lambda+\frac{1}{2})C_{2k}^\lambda(1)}. \tag{6.9}$$

We claim that for all $k \in \mathbb{N}_0$,

$$G(2k,\lambda,p) = \frac{2^{k-1}\Gamma(\lambda+k+\frac{1}{2})\Gamma(\frac{p+1}{2})}{(2k)!\Gamma(k+\frac{p}{2}+\lambda+1)}\left(\prod_{l=0}^{k-1}(\lambda+l)\right)\left(\prod_{j=0}^{k-1}(p-2j)\right) \tag{6.10}$$

and

$$G(2k+1,\lambda,p) = \frac{2^k\Gamma(\lambda+k+\frac{1}{2})\Gamma(\frac{p}{2}+1)}{(2k+1)!\Gamma(k+\frac{p}{2}+\lambda+\frac{3}{2})}\left(\prod_{l=0}^{k}(\lambda+l)\right)\left(\prod_{j=0}^{k-1}(p-2j-1)\right). \tag{6.11}$$

A quick computation shows that these hold for $k = 0$.

Now assume that (6.10) and (6.11) hold for some $k \geq 0$. Using the recurrence relation

$$C_n^\lambda(t) = \frac{2(n+\lambda-1)}{n} t C_{n-1}^\lambda(t) - \frac{n+2\lambda-2}{n} C_{n-2}^\lambda(t) \tag{6.12}$$

for $n \geq 2$, we find that

$$\begin{aligned}
G(2k+2,\lambda,p) &= \frac{2(2k+\lambda+1)}{2k+2} G(2k+1,\lambda,p+1) - \frac{2k+2\lambda}{2k+2} G(2k,\lambda,p) \\
&= \frac{1}{2k+2}\left[\frac{2^{k-1}\Gamma(\lambda+k+\frac{1}{2})\Gamma(\frac{p+1}{2})}{(2k+1)!\Gamma(k+\frac{p}{2}+\lambda+2)}\Big(\prod_{l=0}^{k-1}(\lambda+l)\Big)\Big(\prod_{j=0}^{k-1}(p-2j)\Big)\right] \\
&\quad \times \left[4(2k+\lambda+1)(\frac{p+1}{2})(\lambda+k) - (2k+1)(2k+2\lambda)(k+\frac{p}{2}+\lambda+1)\right] \\
&= \left[\frac{2^{k-1}\Gamma(\lambda+k+\frac{1}{2})\Gamma(\frac{p+1}{2})}{(2k+2)!\Gamma(k+\frac{p}{2}+\lambda+2)}\Big(\prod_{l=0}^{k-1}(\lambda+l)\Big)\Big(\prod_{j=0}^{k-1}(p-2j)\Big)\right] \\
&\quad \times \left[2(\lambda+k+\frac{1}{2})(\lambda+k)(p-2k)\right] \\
&= \frac{2^{k}\Gamma(\lambda+k+\frac{3}{2})\Gamma(\frac{p+1}{2})}{(2k+2)!\Gamma(k+\frac{p}{2}+\lambda+2)}\left(\prod_{l=0}^{k}(\lambda+l)\right)\left(\prod_{j=0}^{k}(p-2j)\right)
\end{aligned}$$

and so

$$\begin{aligned}
G(2k+3,\lambda,p) &= \frac{2(2k+\lambda+2)}{2k+3} G(2k+2,\lambda,p+1) - \frac{2k+2\lambda+1}{2k+3} G(2k+1,\lambda,p) \\
&= \frac{1}{2k+3}\left[\frac{2^{k}\Gamma(\lambda+k+\frac{1}{2})\Gamma(\frac{p}{2}+1)}{(2k+2)!\Gamma(k+\frac{p}{2}+\lambda+\frac{5}{2})}\Big(\prod_{l=0}^{k}(\lambda+l)\Big)\Big(\prod_{j=0}^{k-1}(p-2j-1)\Big)\right] \\
&\quad \times (2k+2\lambda+1)\left[(2k+\lambda+2)(p+1) - (2k+2)(k+\frac{p}{2}+\lambda+\frac{3}{2})\right] \\
&= \left[\frac{2^{k}\Gamma(\lambda+k+\frac{1}{2})\Gamma(\frac{p}{2}+1)}{(2k+3)!\Gamma(k+\frac{p}{2}+\lambda+\frac{5}{2})}\Big(\prod_{l=0}^{k}(\lambda+l)\Big)\Big(\prod_{j=0}^{k-1}(p-2j-1)\Big)\right] \\
&\quad \times 2(k+\lambda+\frac{1}{2})(k+\lambda+1)(p-2k-1) \\
&= \frac{2^{k+1}\Gamma(\lambda+k+\frac{3}{2})\Gamma(\frac{p}{2}+1)}{(2k+3)!\Gamma(k+\frac{p}{2}+\lambda+\frac{5}{2})}\left(\prod_{l=0}^{k+1}(\lambda+l)\right)\left(\prod_{j=0}^{k}(p-2j-1)\right).
\end{aligned}$$

Thus, inductively, we have that (6.10) and (6.11) hold for all $k \in \mathbb{N}_0$. From (6.9) and (6.10), we can now compute $\widehat{F}_p(2k,\lambda)$, giving us our claim. □

Thus, the p-frame energy is not positive definite when p is not even, so the uniform measure is not a minimizer. Moreover, by applying our linear programming results, we find that in certain instances, only discrete minimizers exist.

Theorem 6.2.3. *With $F_p(t) = |t|^p$ for $t \in [-1,1]$, we have the following.*

1. *Suppose there exists a tight spherical $(2t+1)$-design $\mathscr{C} \subset \mathbb{S}^{d-1}$, then the measure*

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

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

2. *Let $\mathbb{F} = \mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$. Assume that there exists a tight projective t-design $\widetilde{\mathscr{C}} \subset \mathbb{FP}^{d-1}$, and let the code $\mathscr{C} \subset \mathbb{S}_{\mathbb{F}}^{d-1}$ consist of the representers of $\widetilde{\mathscr{C}}$ in $\mathbb{S}_{\mathbb{F}}^{d-1}$ according to* (2.16)*. Then the measure*

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

is a minimizer of the p-frame energy I_{F_p} with $2t-2 \leq p \leq 2t$ over $\mu \in \mathbb{P}(\mathbb{S}_{\mathbb{F}}^{d-1})$. Furthermore, if the inequalities are strict, then $\mu \in \mathbb{P}(\mathbb{S}_{\mathbb{F}}^{d-1})$ is a minimizer of I_{F_p} only if the push-forward of μ, $(p_{\mathbb{F}})_*\mu$ is a tight projective t-design.

3. *If $p \notin 2\mathbb{N}$, then the minimizers of I_{F_p} on the circle $\mathbb{S}^1$ are discrete.*

Proof. We observe that part (3) is a special case of part (1), as on the circle $\mathbb{S}^1$, there exists a tight $(2t+1)$-design for all $t \in \mathbb{N}_0$: the vertices of a regular $(2t+2)$-gon. In addition, part (1) is itself essentially contained in part (2) with $\mathbb{F} = \mathbb{R}$: indeed, odd-strength tight spherical designs are necessarily symmetric, and by taking one point in each antipodal pair one obtains a tight projective design, as discussed in Section 2.6. Since tight projective t-designs on $\mathbb{RP}^1$ exist for all $t \in \mathbb{N}$ (i.e. $t+1$ equally spaced points on $\mathbb{RP}^1$), part 2 fully characterizes the minimizers of the p-frame energy. Thus, it is enough to prove part 2, which follows from Theorem 4.3.1 and the fact that $F_p^*(t) = (\frac{1+t}{2})^{\frac{p}{2}}$ is strictly absolutely monotonic of degree $\lceil p/2 \rceil$ and has as its first nonpositive derivative $(F_p^*)^{(\lceil p/2 \rceil+1)}(t)$, $-1 < t < 1$. If p is not an even integer then this derivative is in fact negative, so Theorem 4.3.12 applies, finishing the proof. □

Minimizing the continuous energy over all probability measures and obtaining discrete minimizers allows us to make new conclusions about the minimizing configurations of the discrete p-frame energies for certain values of the cardinality N. One directly obtains the following corollary:

Corollary 6.2.4. *Let $\mathbb{F}$, d, p, and $\mathscr{C} = \{x_1, ..., x_N\}$ be as in any of the parts of Theorem 6.2.3. Let $k \in \mathbb{N}$ and $\omega_{kN} = \{z_1, ..., z_{kN}\} \subset \mathbb{S}_{\mathbb{F}}^{d-1}$ such that for $0 \leq j \leq k-1$ and $1 \leq m \leq N$, $z_{kN+m} = x_m$. Then N-point discrete p-frame energy is minimized by ω_{kN}, i.e. the configuration $\mathscr{C}$ repeated k times. In other words*

$$E_{F_p}(\omega_{kN}) = \mathscr{E}_{F_p}(\mathbb{S}_{\mathbb{F}}^{d-1}, N). \tag{6.13}$$

Thus, for example, if N is a multiple of 6, then repeated copies of a "half" of the icosahedron minimize the N-point p-frame energy on $\mathbb{S}^2$ for $p \in [2,4]$.

Extensive numerical experiments, the results of which were compiled and discussed in [BGM$^+$b], together with Theorem 6.2.3, the fact that the p-frame energy is almost mildly repulsive, and the lack of positive definiteness leads us to the following conjecture:

Conjecture 6.2.5 ([BGM$^+$b])**.** *For all $d \geq 2$ and $p > 0$ such that $p \notin 2\mathbb{N}$, the minimizing measures of $I_{F_p^*}$ on $\mathbb{FP}^{d-1}$ are discrete.*

While we have yet to prove this conjecture, in Section 6.4, we show that on $\mathbb{S}^{d-1}$, whenever p is not even, the support of any minimizer of the p-frame energy I_{F_p} necessarily has empty interior.

6.3 Optimality of the 600-cell

In addition to tight designs, the vertices of the 600-cell also provide a minimizer for certain p-frame energies, specifically those on $\mathbb{S}^3$ for $8 < p < 10$. The 600-cell is one of the six 4-dimensional convex regular polytopes; it has 600 tetrahedral faces, which explains the origin of its name. When its 120 vertices are identified with unit quaternions, they give a representation of the elements of a group known as the binary icosahedral group [Sti01].

As discussed above, optimization of p-frame energy I_{F_p} on the sphere $\mathbb{S}^3$ is equivalent to optimization of the expression

$$I_{F_p^*}(\mu) = \int\limits_{\mathbb{RP}^3} \int\limits_{\mathbb{RP}^3} F_p^*(\tau(x,y))\, d\mu(x) d\mu(u)$$

over probability measures μ on $\mathbb{RP}^3$, where the kernel F_p^* is given by

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

We therefore assume for the rest of this section the underlying space to be $\mathbb{RP}^3$, and use the corresponding normalized Jacobi polynomials $C_n^{(-1/2,1/2)}(t)$. Following the approach in Section 4.3, we will establish a sequence of inequalities similar to (4.13).

The 600-cell is only a projective 5-design and therefore not tight. The authors in [CK07], motivated by an approach found in the paper [And99], found means to prove universal optimality of the 600-cell by using a higher degree interpolating polynomial. The 600-cell has the notable property that the averages of the 7th, 8th, and 9th degree Jacobi polynomials vanish over it, although this is not the case for 6th degree Jacobi polynomial. This allows for constructing a degree 8 polynomial h which is less than or equal to F_p^*, positive definite, and agrees with F_p^* at the distances appearing in the 600-cell, and which finally has the property that its 6th Jacobi coefficient vanishes.

For a polynomial h of the form,

$$h = \sum_{\substack{n=0 \\ n \neq 6}}^{8} \widehat{h}_n C_n^{(1/2,-1/2)}(t), \tag{6.14}$$

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

$$\begin{aligned} h(t_i) &= f(t_i), \qquad 1 \leq i \leq 5 \\ h'(t_i) &= f'(t_i), \qquad 2 \leq i \leq 4, \end{aligned}$$

where $-1 = t_1 < t_2 < \ldots < t_5 = 1$ are the elements of $\mathscr{A}(\mathscr{C})$, for $\mathscr{C}$ the projective 600-cell. It turns out that for all $p \in [8,10]$, the coefficients $\widehat{h}_n(p)$ are nonnegative when $0 \leq n \leq 8$, $n \neq 6$. This was shown through a computer-assisted approach carried out by Glazyrin, Park, and Vlasiuk; specifically, using interval arithmetic, we compute values of $\widehat{h}_n(p)$ on a grid fine enough to guarantee that $\widehat{h}_n(p) \geq 0$. The details of these computations are available in the auxiliary files of the arXiv submission [BGM$^+$b].

Lemma 6.3.1. *If $p \in [8,10]$ and the polynomial h is constructed as above, the coefficients $\widehat{h}_n$ in the Jacobi expansion* (6.14) *satisfy $\widehat{h}_n(p) \geq 0$.*

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

Theorem 6.3.2. *For $p \in [8,10]$, the* 600*-cell minimizes the p-frame energy $I_{F_p^*}$ over Borel probability measures on $\mathbb{RP}^3$.*

Note that this also means that the 600-cell is a minimizer of I_{F_p} on the sphere $\mathbb{S}^3$.

Proof. Let $F_p^*(t) = \left(\frac{t+1}{2}\right)^{p/2}$ for some $8 < p < 10$, $t_1 = -1$, $t_2 = \frac{-\sqrt{5}-1}{4}$, $t_3 = -\frac{1}{2}$, $t_4 = \frac{\sqrt{5}-1}{4}$, and $t_5 = 1$. Let $h(t)$ be the 8th degree polynomial given by (6.14), such that $h(t_i) = p(t_i)$ for $1 \leq i \leq 5$, and $h'(t_i) = p'(t_i)$ for $2 \leq i \leq 4$. By Lemma 6.3.1, the coefficients $\widehat{h}_n$ are non-negative for $p \in [8,10]$.

Let $g(t) = (t^2-1)\prod_{i=2}^{4}(t-t_i)^2$ and $\tilde{h}(t) = H[F_p^*(t), g](t)$. Then we also have $\tilde{h}(t) = H[h,g](t)$. By Lemma 4.3.6, this gives that for all $t \in [-1,1]$ there exist some $\xi, s \in (\min(t,t_1), \max(t,t_5))$ such that

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

and

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

We thus have $F_p^*(t)(t) - h(t) = F_p^*(t)(t) - \tilde{h}(t) + \tilde{h}(t) - h(t) \geq 0$. Since $h(t)$ is positive definite and $\widehat{h}_6 = 0$, for the 600-cell $\mathscr{C}$, we have the following sequence of inequalities

$$I_{F_p^*(t)}(\mu) \geq I_h(\mu) \geq I_h(\sigma) = I_h(\mu_{\mathscr{C}}) = I_F(\mu_{\mathscr{C}}),$$

implying that equally weighted vertices of $\mathscr{C}$ minimize p-frame energy. □

6.4 Empty Interior of p-frame Energy Minimizers

Outside of some specific cases covered by Theorem 6.2.3, Conjecture 6.2.5, which states that the minimizers of the p-frame energy with $p \notin 2\mathbb{N}$ on the real sphere (and on projective spaces) are necessarily discrete, remains open. In the present section, we prove a weaker statement for the real sphere: namely that the support of every minimizer of such energies has empty interior.

Theorem 6.4.1. *Let $F_p(t) = |t|^p$, for $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$. Let μ be a minimizer of the p-frame energy I_{F_p}. Then* $\mathrm{supp}(\mu)$ *has empty interior.*

While we proved a similar result in Theorem 4.2.1, it is clear that when $p \notin 2\mathbb{N}$, the p-frame potential (given on the sphere or on a projective space) is not analytic, meaning that result does not apply. A similar result to Theorem 6.4.1 was proven in [FS13] for the Causal

Variational Principle, given by the kernel (4.19), on $\mathbb{S}^2$. While our approach is inspired by theirs and the main line of reasoning follows an analogous path, specific constructions and arguments in the proofs of Propositions 6.4.2 and 6.4.3 below are much more peculiar and significantly more involved in the case of the p-frame energy.

The proof of Theorem 6.4.1 is based on two properties of interior points of $\mathrm{supp}(\mu)$. The following statements hold:

Proposition 6.4.2. *Let $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$, $F_p(t) = |t|^p$, and μ be a minimizer of I_{F_p}. Then for $z \in \big(\mathrm{supp}(\mu)\big)^\circ$,*

$$\mathrm{supp}(\mu) \cap z^\perp = \emptyset.$$

Proposition 6.4.3. *Let the same conditions as in Proposition 6.4.2 hold. Then for $z \in \big(\mathrm{supp}(\mu)\big)^\circ$,*

$$\mathrm{supp}(\mu) \cap z^\perp \neq \emptyset.$$

Since these two statements are clearly mutually exclusive whenever $\big(\mathrm{supp}(\mu)\big)^\circ$ is non-empty, their validity proves Theorem 6.4.1, 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 these propositions.

We now sketch the argument for the first proposition. In short, the idea of the proof is the following: Let $z \in \big(\mathrm{supp}(\mu)\big)^\circ$ and assume that there exists a point $y \in \mathrm{supp}(\mu)$ such that $\langle y, z\rangle = 0$. We shall construct a finite set of points $X = \{x_i\}_{i=1}^N \subset \mathrm{supp}(\mu)$, such that the matrix $\big[F(\langle x_i, x_j\rangle)\big]_{i,j}$ is not positive semidefinite, thus violating Lemma 3.1.11. The set X 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.

Proof of Proposition 6.4.2. Fix z in the interior of $\mathrm{supp}(\mu)$ and let $y \in \mathbb{S}^{d-1}$ 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 3.1.11, we consider the matrix $A = \left[F_p(\langle x_i, x_j \rangle)\right]_{i,j=0}^{2k+1}$.

We will 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 $m \in \{0, 1, ..., 2k-1\}$,

$$\sum_{j=0}^{2k} j^m v_j = 0, \tag{6.15}$$

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

$$v_j = \prod_{\substack{i=0 \\ i \neq j}}^{2k} \frac{1}{j-i} = \frac{(-1)^j}{(2k-j)!\,j!}. \tag{6.16}$$

Such a vector can be seen to be in the kernel of the matrix above by use of the formula for the inverse of the square Vandermonde matrix (see Ex. 40 on page 38 of [Knu97]).

Consider a vector $u = [av_0, av_1, ..., av_{2k}, b]^T \in \mathbb{R}^{2k+2}$, where $a, b \in \mathbb{R}$. Then we have

$$\langle Au, u \rangle = a^2 \left(\sum_{i,j=0}^{2k} v_i v_j F_p(\langle x_i, x_j \rangle) \right) + 2ab \left(\sum_{j=0}^{2k} v_j F_p(\langle x_{2k+1}, x_j \rangle) \right) + b^2. \tag{6.17}$$

We shall show that the real numbers a and b 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

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

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 (6.17) as follows

$$\begin{aligned}
\sum_{i,j=0}^{2k} v_i v_j F_p(\langle x_i, x_j\rangle) &= \sum_{i,j=0}^{2k} v_i v_j \cos^p\big((i-j)\varepsilon\big) \\
&= \sum_{i,j=0}^{2k} v_i v_j \left(1 + \sum_{m=1}^{2k-1} c_m \varepsilon^{2m} (i-j)^{2m} + O(\varepsilon^{4k})\right) \\
&= \left(\sum_{j=0}^{2k} v_j\right)\left(\sum_{i=0}^{2k} v_i\right) + \sum_{m=1}^{2k-1} c_m \varepsilon^{2m} \left(\sum_{i,j=0}^{2k} v_i v_j (i-j)^{2m}\right) + O(\varepsilon^{4k}) \\
&= \sum_{m=1}^{2k-1} c_m \varepsilon^{2m} \sum_{i,j=0}^{2k} v_i v_j \sum_{l=0}^{2m} \binom{2m}{l} i^l j^{2m-l} + O(\varepsilon^{4k}) \\
&= \sum_{m=1}^{2k-1} c_m \varepsilon^{2m} \sum_{l=0}^{2m} \binom{2m}{l} \left(\sum_{i=0}^{2k} v_i i^l\right)\left(\sum_{j=0}^{2k} v_j j^{2m-l}\right) + O(\varepsilon^{4k}) \\
&= O(\varepsilon^{4k}),
\end{aligned} \tag{6.18}$$

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

We now turn to the second term of (6.17). Observe that for $j = 0,\dots,2k$ we have

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

We then find that

$$\begin{aligned}\sum_{j=0}^{2k} v_j F_p(\langle y, x_j\rangle) &= \sum_{j=0}^{2k} v_j \sin^p(|k-j|\varepsilon) = \sum_{j=0}^{2k} v_j \left(|k-j|\varepsilon + O(\varepsilon^3)\right)^p \\ &= \sum_{j=0}^{2k} v_j (|k-j|\varepsilon)^p \left(1+O(\varepsilon^2)\right)^p = \varepsilon^p \sum_{j=0}^{2k} v_j |k-j|^p + O(\varepsilon^{p+2}).\end{aligned} \tag{6.19}$$

We now analyze the coefficient of ε^p in the above expression using (6.16)

$$\sum_{j=0}^{2k} v_j |k-j|^p = \sum_{j=0}^{2k} (-1)^j \frac{|k-j|^p}{(2k-j)!j!} = 2\sum_{j=0}^{k-1} (-1)^j \frac{(k-j)^p}{(2k-j)!j!}. \tag{6.20}$$

Since the right-hand side of (6.20) 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. Ex. 75 from [PS76, pg. 46]. We will show that these zeros are exhausted by the even integer values $p = 2, 4, \dots, 2k-2$. 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 (6.17), (6.18), and (6.19) we have

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

Since $p < 2k$, for ε sufficiently small, the discriminant of this quadratic form is positive, hence we can choose a and b so that $\langle Au, u\rangle < 0$. However, since $F_p(t) = |t|^p$ is a positive definite function on $\mathbb{S}^{d-1}$ for any even integer 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

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

and by the previous argument, for ε sufficiently small, we could choose a and b so that $\langle Au,u\rangle < 0$, i.e. A is not positive definite. Thus, according to Lemma 3.1.11, $\{x_0,...,x_{2k},y\}$ is not a subset of $\mathrm{supp}(\mu)$. Since, by assumption, for small $\varepsilon > 0$ the points $x_0,x_1,\dots,x_{2k}$ all lie in a neighborhood of z and hence in $\mathrm{supp}(\mu)$, this implies that $y \notin \mathrm{supp}(\mu)$ and so $\mathrm{supp}(\mu) \cap z^{\perp} = \emptyset$. □

We would like to make the following remark. Observe that for $p \notin 2\mathbb{N}$, the number of points used to disprove positive definiteness of $F_p(t) = |t|^p$ in the argument above is of the order p. A restriction of this type is actually necessary. Indeed, according to the result of Fitzgerald and Horn [FH77], for any positive definite matrix $C = \left[c_{ij}\right]_{i,j=1}^{N}$ with non-negative entries $c_{ij} \geq 0$, its Hadamard powers $C^{(a)} = \left[c_{ij}^{a}\right]_{i,j=1}^{N}$ are also positive definite when $a \geq N-2$. Let $G = \left[\langle x_i,x_j\rangle\right]_{i,j=1}^{N}$ be the Gram matrix of the set $X = \{x_1,\dots,x_N\} \subset \mathbb{S}^{d-1}$. Since the matrix $G^{(2)} = \left[|\langle x_i,x_j\rangle|^2\right]_{i,j=1}^{N}$ is positive definite and has non-negative entries, we have that the matrix

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

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.

We now prove Proposition 6.4.3, completing the proof of Theorem 6.4.1.

The proof of Proposition 6.4.3. Suppose a neighborhood of a point $z \in \mathbb{S}^{d-1}$ is contained in the support of μ. We shall demonstrate that $\mathrm{supp}(\mu)$ must intersect the hyperplane $z^{\perp}$.

Let us assume the contrary, i.e. $\mathrm{supp}(\mu) \cap z^{\perp} = \emptyset$. We may move all the mass of μ to the hemisphere centered at z by defining a new measure $\mu_z \in \mathbb{P}(\mathbb{S}^{d-1})$:

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

As our discussion in Section 2.4 about kernels that depend on $|\langle x, y\rangle|$ shows,

$$I_{F_p}(\mu) = I_{F_p}(\mu_{U(\mathbb{R})}) = I_{F_p}((\mu_z)_{U(\mathbb{R})}) = I_{F_p}(\mu_z),$$

so that μ_z is also a minimizer.

Since $\mathrm{supp}(\mu) \cap z^{\perp} = \emptyset$, we also have that $\mathrm{supp}(\mu_z) \cap z^{\perp} = \emptyset$, i.e. $\mathrm{supp}(\mu_z) \subset \{x \in \mathbb{S}^{d-1} : \langle z, x\rangle > 0\}$. 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 $y \in \mathrm{supp}(\mu_z)$. Let us choose an open neighborhood U_z of z, small enough so that $U_z \subseteq \mathrm{supp}(\mu_z)$ and so that for each $x \in U_z$ and each $y \in \mathrm{supp}(\mu_z)$, $\langle y, x\rangle > \delta > 0$.

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

$$U_{F_p}^{\mu_z}(x) = \int\limits_{\mathbb{S}^{d-1}} |\langle x, y\rangle|^p \, d\mu_z(y) = \int\limits_{\mathrm{supp}(\mu_z)} \langle x, y\rangle^p \, d\mu_z(y). \tag{6.21}$$

The discussion above implies that the last expression is well-defined for all $p > 0$. According to Theorem 3.1.7, the potential $U_{F_p}^{\mu_z}(x)$ is constant on $U_z \subseteq \mathrm{supp}(\mu_z)$.

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

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

is well-defined for each $x \in \mathbb{S}^{d-1}$ and yields an analytic function on the sphere (actually, a polynomial). Hence, being constant on an open set implies that it is constant on all of

$\mathbb{S}^{d-1}$, by Lemma 4.2.2, which is not possible since, obviously, $g(-z) = -g(z) = -U_{F_p}^{\mu_z}(z) = -I_{F_p}(\mu_z) \neq 0$. Compare this argument to Theorem 4.2.1.

We now will 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:

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

2. $D_x(\langle x,y\rangle^p) < 0$ 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 $x \in U_z$

$$0 = D_x U_{F_p}^{\mu_z}(x) = \int_{\operatorname{supp}(\mu_z)} D_x(\langle x,y\rangle^p)\, d\mu_z(y) < 0, \tag{6.22}$$

which is a contradiction. Note that that switching to $D_x(\langle x,y\rangle^p) > 0$ in condition (2) does not affect the proof.

We now construct such an operator D. Let Δ denote the Laplace–Beltrami operator on $\mathbb{S}^{d-1}$. Writing it in the standard spherical coordinates $\theta_1, \dots, \theta_d$ one obtains (see, e.g., equation (2.2.4) in [KMR01])

$$\Delta = \sum_{j=1}^{d-1} \frac{1}{q_j (\sin\theta_j)^{d-1-j}} \frac{\partial}{\partial \theta_j} \left((\sin\theta_j)^{d-1-j} \frac{\partial}{\partial \theta_j} \right), \tag{6.23}$$

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

For a fixed $y \in \mathbb{S}^{d-1}$, 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

$$\Delta_x(\langle x,y\rangle^p) = p(p-1)\langle x,y\rangle^{p-2} - p(p+d-1)\langle x,y\rangle^p. \tag{6.24}$$

Observe that if $p \in (0,1]$, then the operator Δ_x satisfies conditions (1) and (2), 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

$$\begin{aligned} D_x\left(\langle x,y\rangle^p\right) &= p(p-1)\Delta_x\left(\langle x,y\rangle^{p-2}\right) \\ &= p(p-1)(p-2)\langle x,y\rangle^{p-4}\cdot\big((p-3)-(p+d-3)\langle x,y\rangle^2\big). \end{aligned} \tag{6.25}$$

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

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 (2) holds with the inequality reversed, 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 $2k+2$

$$\begin{aligned} D^{(k)} = \Delta\left(\Delta + (p+d-2k+1)\prod_{j=0}^{2k-2}(p-j)\right)\left(\Delta + (p+d-2k-1)\prod_{j=0}^{2k-4}(p-j)\right) \\ \cdots\left(\Delta + p(p-1)(p-2)(p+d-3)\right)\big(\Delta + p(p+d-1)\big). \end{aligned}$$

Let $p \in \mathbb{R}_+ \setminus 2\mathbb{N}$ and choose $k \in \mathbb{N}_0$ so that $2k-1 < p \leq 2k+1$. An iterative computation similar to (6.25) gives us

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

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

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 Proposition 6.4.3 for p in the range $(2k-1,2k)\cup(2k,2k+1]$. □

6.5 p-frame Energies in Non-compact Spaces

As discussed in Section 2.1, energy optimization on non-compact spaces is possible so long as there is some constraint that forces minimizing measures to have bounded support. This can be done by placing certain constraints on the kernel, as was discussed in the introduction of Chapter 4. Another possibility is to place constraints on the set of probability measures. Just as above, we consider $\mathbb{F}=\mathbb{R},\mathbb{C},\mathbb{H}$. In this setting, we consider the set of probability measures $\mu\in\mathbb{P}(\mathbb{F}^d)$ with the additional restriction

$$\int_{\mathbb{F}^d}||x||^2 d\mu(x)=1, \tag{6.26}$$

and denote this set by $\mathbb{P}^*(\mathbb{F}^d)$. Note that $\mu(\{0\})=0$ for all $\mu\in\mathbb{P}^*(\mathbb{F}^d)$.

We have previously used linear programming to bound energies and determine minimizers on compact, connected, two-point homogeneous spaces. This approach can be extended to p-frame energies in non-compact spaces as well. The normalization from (6.26) allows us to obtain a direct extension of above results for the spherical case, and by scaling, solutions to more general problems can be obtained from these results. A similar problem of finding minimizers for p-frame energies for $p\leq 2$, subject to the condition that measures be isotropic, was investigated in [Gla].

In what follows, we shall assume $F_p:\mathbb{F}\to[0,\infty)$ is the p-frame potential $F(\langle x,y\rangle)=|\langle x,y\rangle|^p$ on $\mathbb{F}^d$, $F_p^*(t)=\left(\frac{t+1}{2}\right)^p$ is the projective p-frame kernel on $\mathbb{FP}^{d-1}\times\mathbb{FP}^{d-1}$

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

We shall also define $q_{\mathbb{F}} : \mathbb{F}^d \setminus \{0\} \to \mathbb{FP}^{d-1}$ to be the projection from $\mathbb{F}^d$ to $\mathbb{FP}^{d-1}$. From the discussion in Section 2.4 about the relationships between energies on the spheres and projective spaces, we can see that for all $x, y \in \mathbb{F}^d \setminus \{0\}$,

$$\begin{aligned} F_p(\langle x,y\rangle) &= ||x||^p||y||^p\Big|\Big\langle \frac{x}{||x||}, \frac{y}{||y||}\Big\rangle\Big|^p \\ &= ||x||^p||y||^p F_p^*\Big(\tau\Big(p_{\mathbb{F}}\Big(\frac{x}{||x||}\Big), p_{\mathbb{F}}\Big(\frac{y}{||y||}\Big)\Big)\Big) \\ &= ||x||^p||y||^p F_p^*\Big(\tau(q_{\mathbb{F}}(x), q_{\mathbb{F}}(x))\Big). \end{aligned}$$

As above, the normalized Jacobi polynomials for the projective spaces $\mathbb{FP}^{d-1}$ are denoted C_m.

Lemma 6.5.1. *Let $p \geq 2$, and assume $F_p^*(t) \geq h(t) = \sum\limits_{m=0}^{\infty} \widehat{h}_m C_m(t)$ for all $t \in [-1,1]$, where $\widehat{h}_m \geq 0$ for all $m \geq 0$. Then $I_{F_p}(\mu) \geq \widehat{h}_0$ for all $\mu \in \mathbb{P}^*(\mathbb{F}^d)$.*

Proof. Since discrete measures are weak* dense in $\mathbb{P}(\mathbb{F}^d)$, it is sufficient to prove the inequality for them only. Let μ take the form $\mu = \frac{1}{N}\sum\limits_{i=1}^{N}\delta_{x_i}$, $x_i \in \mathbb{F}^d$. Then,

$$\begin{aligned} I_{F_p}(\mu) &= \frac{1}{N^2}\sum_{i,j=1}^{N} ||x_i||^p||x_j||^p F_p^*(\tau(q_{\mathbb{F}}(x_i), q_{\mathbb{F}}(x_j))) \\ &\geq \frac{1}{N^2}\sum_{i,j=1}^{N} ||x_i||^p||x_j||^p h(\tau(q_{\mathbb{F}}(x_i), q_{\mathbb{F}}(x_j))) \\ &= \frac{1}{N^2}\sum_{m=0}^{\infty}\widehat{h}_m \sum_{i,j=1}^{N} ||x_i||^p||x_j||^p C_m(\tau(q_{\mathbb{F}}(x_i), q_{\mathbb{F}}(x_j))). \end{aligned}$$

For any $m \geq 1$, C_m is positive definite on $\mathbb{FP}^{d-1}$ so that each sum

$$\sum_{i,j=1}^{N} ||x_i||^p||x_j||^p C_m(\tau(q_{\mathbb{F}}(x_i), q_{\mathbb{F}}(x_j)))$$

is non-negative. Thus,

$$I_{F_p}(\mu) \geq \widehat{h}_0 \frac{1}{N^2} \sum_{i,j=1}^{N} ||x_i||^p ||x_j||^p C_0(\tau(q_{\mathbb{F}}(x_i), q_{\mathbb{F}}(x_j))) = \widehat{h}_0 \left(\frac{1}{N} \sum_{i=1}^{N} ||x_i||^p \right)^2.$$

Since $p \geq 2$,

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

holds by Jensen's inequality. The constraint (6.26) is equivalent to $\frac{1}{N} \sum\limits_{i=1}^{N} ||x_i||^2 = 1$, and so combining all inequalities, we complete the proof of the lemma. □

Lemma 6.5.1 gives that any linear programming bounds for p-frame energies for the spherical/projective case will work in the non-compact setting as well. As a consequence of this approach we obtain the following result.

Theorem 6.5.2. *Let $\mathscr{C}$ be a set of arbitrary unit representatives of a tight projective M-design, $M \geq 2$, in $\mathbb{FP}^{d-1}$ and $p \in [2M-2, 2M]$. Alternatively, let $\mathscr{C}$ be a set of arbitrary unit representatives of the projective* 600*-cell in $\mathbb{RP}^3$ and $p \in [8, 10]$. Then*

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

is a minimizer of

$$I_{F_p}(\mu) = \int\limits_{\mathbb{F}^d} \int\limits_{\mathbb{F}^d} F_p(\langle x, y \rangle) d\mu(x) d\mu(y)$$

over $\mathbb{P}^*(\mathbb{F}^d)$.

Proof. Set h to be the interpolating polynomial $H[F_p^*, g]$ used in the proof of Theorem 4.3.1 or the polynomial h from Theorem 6.3.2, depending on $\mathscr{C}$. Let us define

$$h_p(x, y) := ||x||^p ||y||^p h(\tau(q_{\mathbb{F}}(x), q_{\mathbb{F}}(y))), \tag{6.27}$$

for $x, y \in \mathbb{F}^d \setminus \{0\}$.

By construction, we see that for all $\mu \in \mathbb{P}^*(\mathbb{F}^d)$,

$$I_{F_p}(\mu) \geq I_{h_p}(\mu)$$

with equality if $\mu = \mu_{\mathscr{C}}$. From the proof of Lemma 6.5.1, it is also clear that

$$I_{h_p}(\mu) \geq \widehat{h}_0$$

with equality if $\mu(\mathbb{S}_F^{d-1}) = 1$ and $I_h((q_{\mathbb{F}})_*\mu) = \widehat{h}_0$. Once again, this condition is satisfied if $\mu = \mu_{\mathscr{C}}$, since h is a positive definite polynomial and $(q_{\mathbb{F}})_*\mu_{\mathscr{C}}$ is a projective design of the appropriate strength. □

6.6 Mixed Volume Inequalities

In this section we demonstrate an intriguing connection between the p-frame energy and convex geometry. We begin by briefly recalling some of the basic notions from convex geometry. See [Kol05, Ch. 2] for a more thorough development.

Let $K \subset \mathbb{R}^d$ be a convex body and σ_K be the surface measure of K, that is, a measure supported on the unit sphere $\mathbb{S}^{d-1}$, satisfying

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

for all Borel sets $B \subseteq \mathbb{S}^{d-1}$, where $|\cdot|_{d-1}$ denotes the $(d-1)$-dimensional Hausdorff measure. For example, if K is a polytope with faces $\{K_i\}_{i=1}^m$ and normals $\{n_i\}_{i=1}^m$, σ_K is atomic with mass $|K_i|_{d-1}$ at each n_i,

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

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

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

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

and uniquely determines K.

Given two convex bodies K and L, and $p \geq 1$, define the L_p-mixed volume

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

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

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

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

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

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

Now, let us call a probability measure $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ *admissible*, if it is symmetric and not concentrated on a proper subspace. A classical result, which follows from Minkowski's theorem, says that any admissible measure can be realized as the surface area measure of a symmetric convex body; see more in [Sch93, Ch. 7].

The *L_p-projection body* $\Pi_p K$ of a convex body K is defined to be the origin-symmetric body whose support function is given by

$$h_{\Pi_p K}(u) = \Big(c_{d,p} \int\limits_{\mathbb{S}^{d-1}} |\langle u, v \rangle|^p d\sigma_K^p(u) \Big)^{\frac{1}{p}}, \tag{6.28}$$

where $c_{d,p}$ is the normalization chosen so that for the unit ball $\mathbb{B}^d$, $\Pi_p\mathbb{B}^d = \mathbb{B}^d$ (see [LYZ00, LZ97]). Thus, the identities

$$I_{F_p}(\sigma_K^p) = \int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} |\langle u,v\rangle|\, d\sigma_K^p(u) d\sigma_K^p(v) = \int\limits_{\mathbb{S}^{d-1}} h_{\Pi_p K}(u)^p \, d\sigma_K^p(u) = dV_p(K,\Pi K)$$

finally establish the connection between L_p-mixed volumes and p-frame energies.

Theorems 6.2.3 and 6.3.2 show that minimizers of $I_{F_p}(\mu)$ over probability measures are admissible when a corresponding tight design (or the 600-cell) exists, as this measure is symmetric and the support spans $\mathbb{R}^d$. Therefore, minimizing the p-frame energy in these cases is equivalent to minimizing the L_p mixed volume of a convex body K with its L_p-projection body $\Pi_p K$ over all convex bodies satisfying $\sigma_K^p(\mathbb{S}^{d-1}) = 1$. In the case that the design is supported on the vertices of a polyhedron C, the minimizing K will be the dual of C, scaled so that σ_K^p is a probability measure. In particular, due to the fact that $\sigma_K^1 = \sigma_K$ we obtain the following:

Proposition 6.6.1. *The minimum of the quantity*

$$\frac{V_1(K,\Pi_1 K)}{|\partial K|^2}$$

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

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

In accordance with Conjecture 6.2.5, we also anticipate that whenever p is not an even integer, the L_p-mixed volume $V_p(K,\Pi_p K)$ is always minimized by a convex body which is polyhedral (with discrete surface measure).

Chapter 7

Acute Angle Energy

The famous Hungarian geometer László Fejes Tóth formulated a variety of problems and conjectures about point distributions on the sphere, two of which, pertaining to the maximizers of the discrete Euclidean and geodesic Riesz energies, were discussed in Section 5.2. In this chapter, we discuss another conjecture of his that is currently open. In 1959, Fejes Tóth posed the following question [FT59]: what is the maximal value of the sum of pairwise acute angles defined by N vectors in the sphere $\mathbb{S}^2$? More precisely, setting the kernel

$$\varphi(\langle x,y\rangle) := \arccos(|\langle x,y\rangle|) = \min\left\{\arccos(\langle z_i,z_j\rangle), \pi - \arccos(\langle z_i,z_j\rangle)\right\}, \tag{7.1}$$

determine which N-element point sets $\omega_N = \{z_1,\ldots,z_N\} \subset \mathbb{S}^2$ maximize the discrete energy E_φ.

He conjectured that this sum is maximized by the periodically repeated copies of the standard orthonormal basis. Though he only stated this for $d \leq 3$, the generalization is clear, and has been independently stated in [Pet14] for all $d \geq 2$.

Conjecture 7.0.1 (Fejes Tóth, 1959 [FT59]). *Let $d \geq 2$ and $N = md + k$ with $m \in \mathbb{N}_0$ and $0 \leq k \leq d-1$. Then the discrete energy E_φ on $\mathbb{S}^{d-1}$ is maximized by the point set $\omega_N = \{z_1,\ldots,z_N\} \subset \mathbb{S}^{d-1}$ with $z_{pd+i} = e_i$, where $\{e_i\}_{i=1}^d$ is the standard orthonormal basis* *of $\mathbb{R}^d$, i.e. ω_N consists of $m+1$ copies of k elements of the orthonormal basis of $\mathbb{R}^d$ and m copies of the remaining $d-k$ basis elements. In this case,*

$$E_\varphi(\omega_N) = \frac{\pi}{2N^2}\left(k(k-1)(m+1)^2 + 2km(d-k)(m+1) + (d-k-1)(d-k)m^2\right). \quad (7.2)$$

In particular, if $N = md$, the sum is maximized by m copies of the orthonormal basis:

$$\max_{\omega_N \subset \mathbb{S}^{d-1}} E_\varphi(\omega_N) = \frac{\pi}{2} \cdot \frac{d-1}{d}. \quad (7.3)$$

Due to Lemma 2.1.1 and because (7.3) is independent of N, we may also formulate a continuous version of the conjecture: that the continuous energy I_φ is maximized by a measure whose mass is equally distributed between elements of the standard orthonormal basis, i.e.

$$\mu_{ONB} := \frac{1}{d}\sum_{i=1}^{d} \delta_{e_i}. \quad (7.4)$$

Conjecture 7.0.2. *The energy integral I_φ is maximized by μ_{ONB}:*

$$\max_{\mu \in \mathbb{P}(\mathbb{S}^{d-1})} I_\varphi(\mu) = I\big(\mu_{ONB}\big) = \frac{\pi}{2} \cdot \frac{d-1}{d}. \quad (7.5)$$

Since the maximal value in (7.3) is independent of N, Lemma 2.1.1 shows that the case $N = md$ of Conjecture 7.0.1 implies Conjecture 7.0.2, and the converse implication is obvious.

The case $d = 2$ of Conjecture 7.0.1 has been settled in [FVZ16, Pet14]. We shall return to this case in Section 7.2 and shall give several alternative proofs.

In dimension $d = 3$, Fejes Tóth confirmed Conjecture 7.0.1 for $N \leq 6$ and established an asymptotic upper bound $E_\varphi(\omega_N) \leq \frac{2\pi}{5}$ for large N. In [FVZ16] Fodor, Vígh, and Zarnócz proved that for any point distribution $\omega_N \subset \mathbb{S}^2$

$$E_\varphi(\omega_N) \leq \frac{3\pi}{8} \text{ when } N \text{ is even,} \tag{7.6}$$

with a small correction for N odd.

In their recent papers [LM21, LMb], Lim and McCann considered a different approach to this problem, studying the kernel $\varphi_s^*(x,y) := \left(\frac{2}{\pi}\arccos(|\langle x,y\rangle|)\right)^{-s}$ for $s<0$ (the Riesz s-energy for the normalized acute angle potential φ^*). Among other results, they showed that there exists some $s_d \leq -1$ such that for all $s < s_d$, the set

$$\begin{aligned} \mathbb{P}_{ONB}(\mathbb{S}^{d-1}) :&= \{\mu \in \mathbb{P}(\mathbb{S}^{d-1}) : \mu(\{e_i, -e_i\}) = \frac{1}{d}, \\ & i \in \{1,...,d\}, \{e_i\}_{i=1}^d \text{ an orthonormal basis of } \mathbb{R}^d\} \end{aligned} \tag{7.7}$$

characterizes the maximizers of $I_{\varphi_s^*}$ up to rotation. The also found that at this endpoint s_d, there must exist a maximizer which is not in $\mathbb{P}_{ONB}(\mathbb{S}^{d-1})$. In response to an earlier draft of Lim and McCann's work, the author and coauthors Bilyk, Glazyrin, Park, and Vlasiuk provided a proof that $s_d > -2$, improving a previously discovered bound. This result now appears in the appendix of [LMb], but we provide it here as well.

Proposition 7.0.3. *If $s \leq -2$, then the the maximizers of*

$$I_{\varphi_s^*}(\mu) := \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \left(\frac{2}{\pi}\arccos(|\langle x,y\rangle|)\right)^{-s} d\mu(x) d\mu(y) \tag{7.8}$$

are precisely the elements of $\mathbb{P}_{ONB}(\mathbb{S}^{d-1})$.

Proof. For $t \in [-1,1]$ and $s<0$, let $F_s(t) = \left(\frac{2}{\pi}\arccos(|t|)\right)^{-s}$ and $g(t) = 1-t^2$. We first show that $s \leq -2$ if and only if $g(t) \geq F_s(t)$ on $[-1,1]$ and $g(t) = F_s(t)$ exactly when $t \in \{-1,0,1\}$.

Setting $h_s(t) := g(t)^{\frac{1}{-s}} - F_s(t)^{\frac{1}{-s}}$, the computation $h''_{-2}(t) = (2t\pi^{-1} - 1)(1-t^2)^{-3/2}$ shows $h_{-2}(t)$ to be strictly concave on the interval $[0,1]$ and to vanish at both endpoints.

This establishes the above equivalence for $s=-2$. For $s<-2$, the same conclusion then follows from $\frac{dh_s}{ds}(t)\leq 0$. For $s>-2$ we have that

$$\lim_{t\to 1} F_s'(t) = -\infty < g'(t)$$

and $F_s(1)=0=g(1)$, so domination of F_s by g fails. Thus we indeed have that $s\leq -2$ if and only if $g(t)\geq F_s(t)$ on $[-1,1]$ and $g(t)=F_s(t)$ exactly when $t\in\{-1,0,1\}$.

We now use linear programming to complete the proof. Using the fact that g bounds F_s from above, with equality on $\{-1,0,1\}$, and our knowledge of frame energy (see Lemma 6.1.3), we find that for all $s\leq -2$ and $\mu\in\mathbb{P}(\mathbb{S}^{d-1})$

$$I_{F_s}(\mu)\leq I_g(\mu)\leq I_g(\mu_{ONB}) = I_{F_s}(\mu_{ONB}). \tag{7.9}$$

The first inequality becomes an equality precisely when $\mathscr{A}(\text{supp}(\mu))\subseteq\{-1,0,1\}$ and the second when μ is an isotropic measure. The two properties characterize $\mathbb{P}_{ONB}(\mathbb{S}^{d-1})$, and our claim now follows. □

Though Proposition 7.0.3 clearly does not prove Conjecture 7.0.2, it may be seen as some further evidence to suggest the conjecture is correct: in [LM21], the Lim and McCann showed that Conjecture 7.0.2 is true if and only if $s_d=-1$.

The kernel

$$\tilde{\varphi}(t) := \frac{\pi}{2} - \varphi(t) = \arcsin(|t|)$$

(for which minimization of $I_{\tilde{\varphi}}$ is naturally equivalent to the maximization of I_{φ}) has quite a bit in common with the p-frame potentials discussed in Chapter 6. It is clearly even and repulsive-attractive, with a minimum at $t=0$, and for $d\geq 3$, $\tilde{\varphi}$ is not positive definite on the sphere $\mathbb{S}^{d-1}$. This can be seen by the fact that on $\mathbb{S}^2$, σ is not a minimizer of the energy:

$$I_{\tilde{\varphi}}(\sigma) = \frac{\pi}{2} - 1 > \frac{\pi}{6} = I_{\tilde{\varphi}}(\mu_{ONB}).$$

Since spheres of higher dimensions contain a copy of $\mathbb{S}^2$ within them, $\tilde{\varphi}$ cannot be positive definite on them either. However, $\tilde{\varphi}$ defers from the p-frame potentials in two interesting ways. Unlike the p-frame potentials, $\tilde{\varphi}$ is positive definite on the circle $\mathbb{S}^1$, as will be shown in Section 7.2. As we will discuss in that section, this suggests that there exists one-dimensional (in the sense of Hausdorff dimension) minimizers of $I_{\tilde{\varphi}}$, rather than exclusively discrete ones, as we suspect for the p-frame energy. The second is that $\lim_{t\to\pm 1} \tilde{\varphi}'(t) = \infty$, which prevents us from creating a Hermite interpolant as we did in Section 4.3.

In Section 7.1, we prove a new upper bound for I_φ in all dimensions, and show that the validity of Conjecture 7.0.2 in some dimension $d \geq 3$ implies its validity in all lower dimensions. In Section 7.2, we provide several proofs of Conjectures 7.0.1 and 7.0.2 on $\mathbb{S}^1$: two based on orthogonal expansions, and one based on a variant of the Stolarsky Invariance Principle.

7.1 New Results in all Dimensions

New Bound

As discussed in Section 4.3, when a suitable candidate for an interpolant does not present itself, we may find bounds on the energy I_φ by determining an auxiliary polynomial h that bounds φ from above and for which we know the maximizers. In the present section, we prove a new upper bound for I_φ in all dimensions $d \geq 3$ through the use of a quadratic auxiliary function. In addition to being the first result which determines a bound for all dimension, this result also provides a stronger bound than (7.6) when restricted to $\mathbb{S}^2$.

Theorem 7.1.1. *In all dimensions $d \geq 3$*

$$\max_{\mu \in \mathbb{P}(\mathbb{S}^{d-1})} I_\varphi(\mu) \leq \frac{\pi}{2} - \frac{69}{50d}. \tag{7.10}$$

In particular, for $d = 3$*,*

$$\max_{\mu \in \mathbb{P}(\mathbb{S}^2)} I_\varphi(\mu) \le \frac{\pi}{2} - \frac{69}{150} = 1.110796... < \frac{3\pi}{8} = 1.178097..., \tag{7.11}$$

thus improving upon (7.6)*.*

We recall that, according to (7.3) and (7.5), the conjectured maximal value in dimension $d = 3$ is $\frac{\pi}{3} = 1.047198\ldots$.

Proof. It suffices to demonstrate that the inequality

$$\arccos|t| \le \frac{\pi}{2} - \frac{69}{50}t^2 \tag{7.12}$$

holds for all $t \in [-1, 1]$, as then Lemma 6.1.3 would imply that, for all $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$,

$$I_\varphi(\mu) \le \frac{\pi}{2} - \frac{69}{50d}. \tag{7.13}$$

For $b \ge 1$, $\frac{\pi}{2} - bt^2 - \arccos(|t|)$ is an even function, increasing on $\left[0, \sqrt{\frac{b-\sqrt{b^2-1}}{2b}}\right)$ and $\left(\sqrt{\frac{b+\sqrt{b^2-1}}{2b}}, 1\right)$, and decreasing on $\left(\sqrt{\frac{b-\sqrt{b^2-1}}{2b}}, \sqrt{\frac{b+\sqrt{b^2-1}}{2b}}\right)$. Thus, $\arccos|t| \le \frac{\pi}{2} - bt^2$ for all $t \in [-1, 1]$ if and only if

$$\frac{\pi}{2} - \frac{b+\sqrt{b^2-1}}{2} - \arccos\left(\sqrt{\frac{b+\sqrt{b^2-1}}{2b}}\right) \ge 0,$$

which holds for $b \le \frac{69}{50}$, completing our proof. Figure 7.1 illustrates inequality (7.12). $\square$

Figure 7.1 indicates that there is very little room for improvement via this method (one can check that $\frac{\pi}{2} - bt^2 + \arccos(|t|)$ takes negative values if $b \ge \frac{7}{5}$), and therefore it cannot yield Conjecture 7.0.2.

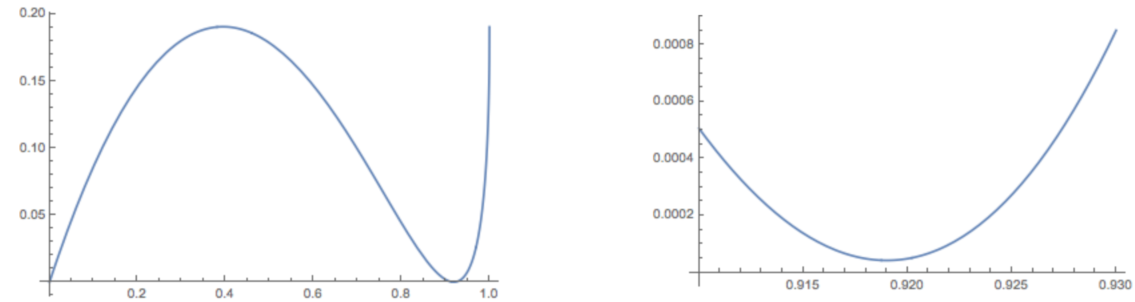

Figure 7.1: An illustration of inequality (7.12): the graph of the function $F(t) = \frac{\pi}{2} - \frac{69}{50}t^2 - \arccos(|t|)$ for $0 \le t \le 1$.

Dimension Reduction Argument

Here we show generally that if a measure's components are orthogonal and that measure is a maximizer of the energy integral of some function, then the components are maximizers of this energy in lower dimensions. Naturally, the simplest case of this occurs when the measure is an orthonormal basis.

Let $F : [-1,1] \to \mathbb{R}$ be a bounded, measurable function that achieves its maximum at 0. Let $\nu \in \mathbb{P}(\mathbb{S}^k)$ and $\lambda \in \mathbb{P}(\mathbb{S}^l)$, with $k+l = d-2$. Construct a measure $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ as follows:

$$\mu = a\widetilde{\nu} + b\widetilde{\lambda}, \tag{7.14}$$

where $0 \le a, b \le 1$, $a+b = 1$, and $\widetilde{\nu}$ and $\widetilde{\lambda}$ are copies of ν and λ, supported on mutually orthogonal subspheres of $\mathbb{S}^{d-1}$ of dimensions k and l, respectively. It is easy to see that

$$I_F(\mu) = a^2 I_F(\nu) + b^2 I_F(\lambda) + 2abF(0), \tag{7.15}$$

which implies that if μ is a maximizer of I_F over $\mathbb{P}(\mathbb{S}^{d-1})$, then ν and λ maximize I_F respectively over $\mathbb{P}(\mathbb{S}^k)$ and $\mathbb{P}(\mathbb{S}^l)$.

The orthonormal basis measure μ_{ONB} is precisely of the form (7.14), with ν and λ as orthonormal basis measures in lower dimensions. Therefore, in particular, we have just proved that the validity of Conjecture 7.0.2 on $\mathbb{S}^{d-1}$ for some dimension $d \ge 3$ implies its validity on $\mathbb{S}^k$ for $k < d-1$, i.e. in all lower dimensions.

Moreover, in our case, for $\varphi(t) = \arccos(|t|)$, we have $\varphi(0) = \frac{\pi}{2}$. Let $l = 0$ and $k = d-2$. Then $I_\varphi(\lambda) = \varphi(1) = 0$, and thus (7.15) becomes

$$I_\varphi(\mu) = a^2 I_\varphi(\nu) + \pi a(1-a).$$

Optimizing this quadratic polynomial in a we find that for $a = \dfrac{\pi}{2\big(\pi - I_\varphi(\nu)\big)}$,

$$I_\varphi(\nu) = \pi - \frac{\pi^2}{4 I_\varphi(\mu)}.$$

This discussion leads to the following conclusion.

Proposition 7.1.2 (Dimension reduction). *Denote* $M_{d-1} = \max\{I_\varphi(\mu) : \mu \in \mathbb{P}(\mathbb{S}^{d-1})\}$. *We have the following:*

1. *For* $d \geq 3$,
$$M_{d-2} \leq \pi - \frac{\pi^2}{4M_{d-1}}.$$
2. *Assume that Conjecture 7.0.2 holds on* $\mathbb{S}^{d-1}$, *i.e.* $M_{d-1} = \frac{\pi(d-1)}{2d}$. *Then it also holds on* $\mathbb{S}^{d-2}$, *and consequently in all lower dimensions.*

Observe, that part (2) follows both from part (1), and, in a more general setting, from the discussion in the beginning of this section. We also see that Proposition 7.1.2 implies that, in order to prove Conjecture 7.0.2 in all dimensions $d \geq 3$, it is enough to establish its validity for infinitely many values of d.

7.2 The Case of $\mathbb{S}^1$ Revisited

We now revisit the case $d = 2$, in which Conjecture 7.0.2 (and hence also Conjecture 7.0.1) has been settled in [FVZ16, Jia08] through a geometric proof. We shall provide three analytic approaches to this case (one based on a Chebyshev expansion, one based on a Fourier expansion, and one based on connections to discrepancy theory), which first appeared in [BM19].

Before we proceed, we observe that on $\mathbb{S}^1$

$$I_\varphi(\mu_{ONB}) = I_\varphi(\sigma) = I_\varphi(\sigma_{4N}) = \frac{\pi}{4}, \tag{7.16}$$

where σ_N is the measure with mass equally concentrated at N equally spaced points, i.e. with $x_{N,k} = \begin{pmatrix} \cos(2\pi k/N) \\ \sin(2\pi k/N) \end{pmatrix}$,

$$\sigma_N = \frac{1}{N}\sum_{k=1}^{N} \delta_{x_{N,k}}.$$

Hence, to prove Conjecture 7.0.2 it suffices to prove that any of these measures is a maximizer.

It is worth noting the implications of the uniform measure σ being a minimizer for $I_{\tilde{\varphi}}$ (maximizer for I_φ) on $\mathbb{S}^1$. If the Conjecture 7.0.2 is true, then $\mu = \frac{1}{4}\sum_{j=1}^{4}\delta_{e_j}$ is a minimizer of $I_{\tilde{\varphi}}$ on $\mathbb{S}^3$. Following the dimension-reduction discussion above, the normalized uniform 1-dimensional Hausdorff measure on two orthogonal copies of $\mathbb{S}^1$, i.e. on the set

$$\{(x_1,x_2,0,0) : x_1^2 + x_2^2 = 1\} \cup \{(0,0,x_3,x_4) : x_3^2 + x_4^2 = 1\},$$

would also yield a minimizer. This naturally generalizes to higher dimensions. Thus, assuming the validity of the conjecture, this energy has non-discrete minimizers.

Chebyshev Polynomial Expansion

From Proposition 3.5.2, we know that σ is a maximizer of the energy integral I_F on $\mathbb{S}^1$ if and only if F is a negative definite function on $\mathbb{S}^1$ (up to the constant term), which is equivalent to the fact that in the orthogonal expansion of F into Chebyshev polynomials,

$F(t) \sim \sum_{n=0}^{\infty} \widehat{F}(n,0) T_n(t)$, the coefficients of all non-constant terms are non-positive, i.e.

$$\widehat{F}(n,0) \leq 0 \quad \text{for} \quad n \geq 1.$$

Since the Chebyshev coefficients of $\varphi(t) = \arccos|t|$,

$$\widehat{\varphi}(n,0) = \frac{1}{\pi} \int_{-1}^{1} F(t) T_n(t) (1-t^2)^{-\frac{1}{2}} dt = \begin{cases} \frac{\pi}{4}, & \text{if } n = 0, \\ \frac{-4}{\pi n^2}, & \text{if } n \equiv 2 \bmod 4, \\ 0, & \text{otherwise} \end{cases} \tag{7.17}$$

σ clearly maximizes I_φ on $\mathbb{S}^1$, which together with (7.16) implies Conjecture 7.0.2.

Fourier Series

Our second orthogonal expansion is a Fourier series. Every point in $\mathbb{S}^1$ can be defined by its angle, so setting $\mathbb{T} = \mathbb{R}/(2\pi\mathbb{Z})$ and defining, for every $\mu \in \mathscr{M}(\mathbb{S}^1)$, a corresponding measure $\tilde{\mu} \in \mathscr{M}(\mathbb{T})$ by

$$\tilde{\mu}(B) = \mu\Big(\Big\{ \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} : \theta \in B \Big\} \Big)$$

for all Borel sets $B \subseteq \mathbb{T}$, we see that for any $F \in C([-1,1])$ and $\mu \in \mathscr{M}(\mathbb{S}^1)$,

$$I_F(\mu) = \int_{\mathbb{T}} \int_{\mathbb{T}} F(\cos(\theta - \phi)) d\tilde{\mu}(\theta) \tilde{\mu}(\phi) = \int_{\mathbb{T}} \int_{\mathbb{T}} G(\theta - \phi) d\tilde{\mu}(\theta) d\tilde{\mu}(\phi).$$

Let $G(\theta) = F(\cos(\theta))$ be an even function. Then for $\nu, \mu \in \mathbb{P}(\mathbb{S}^{d-1})$ such that $d\tilde{\nu}(\theta) = \frac{d\tilde{\mu}(\theta) + d\tilde{\mu}(-\theta)}{2}$ for all $\theta \in \mathbb{T}$, we have $I_F(\mu) = I_F(\nu)$. Thus, for the rest of this subsection, we may assume that $\mu \in \mathbb{P}(\mathbb{S}^1)$ such that $\tilde{\mu}$ is an even measure. We note that since G is an even function, its Fourier series is a cosine series, i.e. $G(\theta) \sim \sum_{n=0}^{\infty} \widehat{G}(n)\cos(n\theta)$. As long as this series converges absolutely, we can use it to compute the energy:

$$\begin{aligned} I_F(\mu) &= \sum_{n=0}^{\infty} \widehat{G}(n) \int_{\mathbb{T}} \int_{\mathbb{T}} \cos(n(\theta-\phi))\, d\tilde{\mu}(\theta) d\tilde{\mu}(\phi) \\ &= \sum_{n=0}^{\infty} \widehat{G}(n) \int_{\mathbb{T}} \int_{\mathbb{T}} \Big(\cos(n\theta)\cos(n\phi) + \sin(n\theta)\sin(n\phi) \Big)\, d\tilde{\mu}(\theta) d\tilde{\mu}(\phi). \end{aligned} \tag{7.18}$$

Since $\tilde{\mu}$ is an even measure, the sines do not contribute to the integral, and we have

$$I_F(\mu) = \sum_{n=0}^{\infty} \widehat{G}(n) \left(\int_{\mathbb{T}} \cos(n\theta) d\tilde{\mu}(\theta) \right)^2 \le \widehat{G}(0) + \sum_{n\ge 1:\, \widehat{G}(n)\ge 0} \widehat{G}(n). \tag{7.19}$$

The equality above is achieved if and only if $\int_{\mathbb{T}} \cos(n\theta) d\tilde{\mu}(\theta) = 0$ for each value of $n \ge 1$ for which $\widehat{G}(n) < 0$ and $\int_{\mathbb{T}} \cos(n\theta) d\tilde{\mu}(\theta) = 1$ for each value of $n \ge 1$ such that $\widehat{G}(n) > 0$.

Lemma 7.2.1. *Let G be even and have an absolutely convergent Fourier (cosine) series and let $\tilde{\sigma}_N$ be the probability measure generated by point masses at N equally spaced points, i.e.*

$$\tilde{\sigma}_N := \frac{1}{N} \sum_{k=0}^{N-1} \delta_{2\pi k/N}.$$

Assume that for all $n \ge 1$ we have $\widehat{G}(n) \ge 0$ if n is a multiple of N, and $\widehat{G}(n) \le 0$ otherwise. Then the measure σ_N maximizes I_F over $\mathbb{T}$.

The proof easily follows from the discussion above and the fact that

$$\int_{\mathbb{T}} \cos(n\theta) d\tilde{\sigma}_N(\theta) = \frac{1}{N} \sum_{k=0}^{N-1} \cos \frac{2\pi nk}{N} = \begin{cases} 1, & \text{if } n \text{ is a multiple of } N, \\ 0, & \text{otherwise.} \end{cases}$$

Remark: The conditions on $\widehat{G}(n)$ in Lemma 7.2.1 also become necessary if we assume that σ_N maximizes I_F over all signed probability measures, $\widetilde{\mathbb{P}}(\mathbb{S}^1)$. This can be proved by considering signed measures of the form $d\tilde{\mu} = d\tilde{\sigma} - \cos n\theta \, d\tilde{\sigma}$.

Returning to our specific case, $G(\theta) = \varphi(\cos(\theta)) = \min\{|\theta|, \pi - |\theta|\}$, we observe that according to definition (2.27) and relation (7.17), we have $\widehat{G}(n) = \widehat{\varphi}(n,0) = -\frac{4}{\pi n^2}$ whenever $n \equiv 2 \bmod 4$, and $\widehat{G}(n) = 0$ for all other values of $n \geq 1$. Therefore, Lemma 7.2.1 with $N = 4$ applies and σ_4 maximizes I_φ. Since φ is an even function, symmetry implies that μ_{ONB} is also a maximizer, i.e. Conjecture 7.0.2 holds on $\mathbb{S}^1$.

Notice that alternatively, since $\widehat{G}(n) \leq 0$ for all $n \geq 1$, one could deduce from (7.19) that $I_\varphi(\mu) \leq \widehat{G}(0) = I_\varphi(\sigma)$. Therefore σ is a maximizer of the energy integral I_φ, and, due to (7.16), so is μ_{ONB}, leading to another proof of Conjecture 7.0.2 (almost identical to our proof involving the Chebyshev expansion). However, Lemma 7.2.1 could be applied to determine a maximizer for an energy with both positive and negative Fourier coefficients, allowing one to address a wider range of energy optimization problems, so we wanted to include it here.

Stolarsky Principle

Finally, our last approach is yet another analogue of the Stolarsky Invariance Principle (Theorem 5.1.1).

For $x \in \mathbb{S}^1$, define the *antipodal quadrants* in the direction of x as $Q(x) = \{y : |\langle x, y\rangle| > \frac{\sqrt{2}}{2}\}$, i.e. $Q(x)$ is a union of two symmetric quarter-circle arcs with midpoints at x and $-x$. The size of the intersection of two such sets is given by

$$\sigma\big(Q(y) \cap Q(z)\big) = \frac{1}{2} - \frac{1}{\pi} \arccos|y \cdot z| \tag{7.20}$$

as the left-hand side is $\frac{1}{2}$ if $z = y$ and 0 if z and y are orthogonal, and clearly changes linearly with respect to the acute angle between the points.

We define the L^2 discrepancy of a point set $\omega_N = \{z_1, \ldots, z_N\} \subset \mathbb{S}^1$ with respect to these antipodal quadrants as the quadratic average of the difference between the empirical measure $\frac{|Q(x)\cap\omega_N|}{N}$ and the uniform measure $\sigma\big(Q(x)\big)=\frac{1}{2}$.

$$D^2_{L^2,\text{quad}}(\omega_N)=\int\limits_{\mathbb{S}^1}\left|\frac{1}{N}\sum_{i=1}^{N}\mathbb{1}_{Q(x)}(z_i)-\sigma\big(Q(x)\big)\right|^2 d\sigma(x). \tag{7.21}$$

More generally, for a measure $\mu\in\mathbb{P}(\mathbb{S}^1)$ we can define its discrepancy as

$$D^2_{L^2,\text{quad}}(\mu)=\int\limits_{\mathbb{S}^1}\left|\mu\big(Q(x)\big)-\sigma\big(Q(x)\big)\right|^2 d\sigma(x), \tag{7.22}$$

i.e. $D^2_{L^2,\text{quad}}(\omega_N)=D^2_{L^2,\text{quad}}\big(\frac{1}{N}\sum_{z\in\omega_N}\delta_z\big)$.

The following version of the Stolarsky principle holds:

Proposition 7.2.2 (Stolarsky principle for quadrants)**.** *For any measure $\mu\in\mathbb{P}(\mathbb{S}^1)$ we have*

$$D^2_{L^2,\text{quad}}(\mu)=\frac{1}{\pi}\big(I_\varphi(\sigma)-I_\varphi(\mu)\big)=\frac{1}{4}-\frac{1}{\pi}I_\varphi(\mu). \tag{7.23}$$

In particular, for a discrete point set $\omega_N=\{z_1,\dots,z_N\}\subset\mathbb{S}^1$

$$D^2_{L^2,\text{quad}}(\omega_N)=\frac{1}{4}-\frac{1}{\pi}E_\varphi(\omega_N). \tag{7.24}$$

Proof. We use relations (7.22) and (7.20) to obtain

$$\begin{aligned}D^2_{L^2,\text{quad}}(\mu)&=\int\limits_{\mathbb{S}^1}\int\limits_{\mathbb{S}^1}\int\limits_{\mathbb{S}^1}\mathbb{1}_{Q(x)}(y)\cdot\mathbb{1}_{Q(x)}(z)\,d\sigma(x)\,d\mu(y)\,d\mu(z)\\&\quad-\int\limits_{\mathbb{S}^1}\int\limits_{\mathbb{S}^1}\mathbb{1}_{Q(x)}(y)d\sigma(x)\,d\mu(y)+\frac{1}{4}\\&=\int\limits_{\mathbb{S}^1}\int\limits_{\mathbb{S}^1}\sigma\big(Q(y)\cap Q(z)\big)-\frac{1}{4}=\frac{1}{4}-\frac{1}{\pi}\int\limits_{\mathbb{S}^1}\int\limits_{\mathbb{S}^1}\arccos(|\langle y,z\rangle|)\,d\mu(y)\,d\mu(z),\end{aligned}$$

which proves (7.23). □

Remarks: Discrepancy with respect to similar sets, but with arbitrary apertures, (“wedges”) on $\mathbb{S}^{d-1}$ arose in [BL17] in connection to sphere tessellations and one-bit sensing, which led to a Stolarsky principle involving energies with the potential $F(t) = \arcsin(t)^2$. Observe also that Proposition 7.2.2 follows from our Generalized Stolarsky Principle (Theorem 5.3.1), with $f(t) = \mathbb{1}_{[-1,\frac{-\sqrt{2}}{2})\cup(\frac{\sqrt{2}}{2},1]}(t)$ and $F(t) = \frac{1}{2} - \frac{1}{\pi}\arccos(|t|)$. However, we have provided a proof here that does not assume any positive definiteness.

Our Stolarsky principle (7.23) proves that $I_\varphi(\mu) \leq \frac{\pi}{4}$ and σ maximizes this energy, and by (7.16) so does ν_{ONB} proving Conjecture 7.0.2. In the discrete case, (7.24) shows that $E_\varphi(\omega_N) \leq \frac{\pi}{4}$ for even N and $E_\varphi(\omega_N) \leq \frac{\pi}{4} \cdot \frac{N^2-1}{N^2}$ for odd N. It also allows one to characterize the maximizers of $E_\varphi(\omega_N)$ and prove Conjecture 7.0.1: (7.24) implies that maximizing $E_\varphi(\omega_N)$ is equivalent to minimizing the discrepancy $D^2_{L^2,\text{quad}}(\omega_N)$. It is easy to see from (7.21) that this happens exactly when the following holds: for σ-almost every $x \in \mathbb{S}^1$ the difference between the number of points of ω_N in $Q(x)$ and in its complement $\big(Q(x)\big)^c$ is zero (when N is even) or ± 1 (when N is odd). Equivalently, this should hold for any x such that the boundary of $Q(x)$ doesn't intersect ω_N, which recovers the characterization in [FVZ16]. The extremizing configurations in Conjecture 7.0.1 obviously satisfy this condition.

This method unfortunately does not hold for dimensions $d \geq 3$, as $\frac{1}{2} - \frac{1}{\pi}\arccos(|t|)$ is not positive definite on these spheres, so we cannot create an appropriate Stolarsky-type invariance principle.

Chapter 8

Energy with Multivariate Potentials

In this final chapter, we discuss optimization problems for more complicated energies, defined by interactions of triples, quadruples, or even higher numbers of particles, i.e. energies of the type

$$E_K(\omega_N) = \frac{1}{N^n} \sum_{x_1,\dots,x_n \in \omega_N} K(x_1,...,x_n), \tag{8.1}$$

$$I_K(\mu) = \int_\Omega \cdots \int_\Omega K(x_1,\dots,x_n)\, d\mu(x_1) \dots d\mu(x_n), \tag{8.2}$$

with $n \geq 3$. Energies of this type arise naturally in various fields:

1. In different branches of *physics* (nuclear, quantum, chemical, condensed matter, material science, etc.), it has been suggested that, if the behavior of the system cannot be accurately modeled by two-body interactions, more precise information may be obtained from three-body or many-body interactions. Such forces are observed among nucleons in atomic nuclei (three-nucleon force) [Zel09], in carbon nanostructures [MS14], crystallization of atomistic configurations [FT15], cold polar molecules in optical lattices [BMZ07], interactions of solid and liquid forms of silicon [SW85], interactions between atoms [AT43], in "perfect glass" potentials [ZST16], and many other areas.

2. Energy integrals with multivariate kernels defined in (8.2) play the role of polynomials on the space $\mathbb{P}(\Omega)$ of probability measures on Ω – e.g., their linear span over all $n \in \mathbb{N}$ is dense in the space of continuous functions on $\mathbb{P}(\Omega)$, according to the Stone–Weierstrass theorem. Such functionals on the space of measures appear in optimal transport [San15] and mean field games [Lio08].

3. A classical example of a three-input energy, coming from geometric measure theory, is given by the total Menger curvature of a measure μ

$$c^2(\mu) = \int_\Omega \int_\Omega \int_\Omega c^2(x,y,z)\, d\mu(x)\, d\mu(y)\, d\mu(z), \tag{8.3}$$

where $c(x,y,z) = \frac{1}{R(x,y,z)}$ and $R(x,y,z)$ is the circumradius of the triangle xyz. This object plays an important role in the study of the L^2-boundedness of the Cauchy integral, analytic capacity, and uniform rectifiability [Dav99, MMV96].

4. Some questions in *probabilistic geometry* admit natural reformulations in terms of multi-input energies (8.1) or (8.2). For example, assume that three points are chosen in a domain Ω, e.g. $\Omega = \mathbb{S}^2$, independently at random, according to the probability distribution μ. Which probability distribution maximizes the expected area of the triangle generated by these random points or the volume of the parallelepiped spanned by the random vectors? These quantities can be written as energy integrals (8.1) with $n = 3$, and higher dimensional versions of such questions call for energies with more inputs, which may be viewed as natural extensions of the classical Riesz energy. Questions of this type are discussed in Section 8.8 and are explored in more detail in [BFG$^+$b].

5. Energies with more than two inputs akin to (8.1) appear in three-point bounds [CW12] and, more generally, k-point bounds [dLMdOFV, Mus14] in semidefinite programming [BV08] – a very fruitful method, which led to numerous breakthroughs in dis-

crete geometry. We shall briefly revisit this method in Section 8.7 and show some applications to the aforementioned geometric problems in Section 8.8. A more complete discussion of this method in the context of the multivariate energy optimization and, in particular, applications to the geometric problems described in Section 8.8 can be found in [BFG⁺b].

6. Relations between the L^2-discrepancy and the two-input energies, in particular, the Stolarsky principle [Sto73], are well known [BDM18, Skr20]. In a similar spirit, other L^n-norms of the discrepancy or "number variance" with integer values of n lead to n-particle interaction energies (8.1). Some similar ideas have been put forward in [Tor10].

Despite the abundance of applications, there seems to have been no systematic development of a general theory of multi-input energies preceding [BFG⁺a, BFG⁺b], unlike the case of classical two-input energies, which has been deeply and extensively explored. This chapter covers the results of [BFG⁺a] (as well as some from [BFG⁺b]) which made the first attempt to remedy this shortcoming. In these works, the author and coauthors study the general properties of point configurations and measures, minimization of the multi-input energies (8.1) and (8.2), and the relations between the structure of the multivariate kernel K and the energy minimizers. This theory presents many intrinsic obstacles and is far from a straightforward generalization of the two-input case. For instance, in the spherical case $\Omega = \mathbb{S}^{d-1}$ with rotationally invariant two-input kernel $F(\langle x,y \rangle)$, we know that the uniform surface measure σ minimizes I_F if and only if the F is conditionally positive definite 3.3.1. However, in the multi-input case, such a characterization is still elusive: while we obtain various natural sufficient conditions for the surface measure σ to minimize the energy (8.1) in Section 8.4, counterexamples presented in Section 8.5 show that none of them are necessary.

In Section 8.1 we introduce the notation and some of the main definitions, including the notion of n-positive definiteness. In Section 8.2 we explore some basic properties of multivariate energies. In particular, we analyze the connections between (conditional) positive definiteness of the kernel K, convexity of the energy functional $I_K(\mu)$, and arithmetic and geometric mean inequalities for the mixed energies.

Section 8.3 deals with analogues of various results from Section 3.3, which provide certain necessary (Theorem 8.3.2) and sufficient (Theorem 8.3.3) conditions for a measure μ to be a minimizer of the n-input energy integral in terms of the $(n-1)$-fold potential of the kernel K with respect to μ. Even though some of these results by themselves are clear-cut generalizations of standard statements for two-input energies, they yield several interesting consequences in the n-input case. In particular, Theorem 8.3.7 states that, under some additional assumptions (e.g., if K is n-positive definite), for any $1 \leq k \leq n-2$, if the measure μ minimizes the $(n-k)$-input energy $I_{U_K^{\mu^k}}$, where $U_K^{\mu^k}$ is the k-fold integral of K with respect to μ, then μ also minimizes the n-input energy I_K. This statement allows one to simplify proving that a given measure is a minimizer of a multi-input energy by considering energies with a lower number of inputs. A partial converse to Theorem 8.3.7, for $k = n-2$, is given in Theorem 8.3.8. In addition, in Lemma 8.3.5, we show that, for n-positive definite kernels, every local minimizer of I_K is necessarily a global minimizer.

In Section 8.4 we adapt the methods of Section 8.3 to energies with rotationally invariant kernels on the sphere $\mathbb{S}^{d-1}$, where symmetries allow for a more delicate analysis, and one has a natural candidate for a minimizer: the uniform surface measure σ. Theorem 8.4.1 states that energies with conditionally n-positive definite rotationally invariant kernels on the sphere are minimized by the surface measure σ (without any additional assumptions). As mentioned above, it turns out that, in contrast to the classical case $n = 2$, conditional n-positive definiteness is not necessary for σ to minimize the n-input energy, which is shown by examples presented in Propositions 8.6.3 and 8.6.4. Nevertheless, Theorem 8.4.1 allows one to prove that σ minimizes a variety of interesting energies, which did not seem to be accessible by different methods, see e.g. Corollary 8.4.2. In Theorem 8.4.3 we obtain very close necessary and sufficient conditions for σ to be a *local* minimizer of the n-input energy

I_K in terms of the minimization properties of the two-input energy with the kernel given by the $(n-2)$-fold integral of K (or the conditional positive definiteness of this kernel). We also conjecture these are the correct conditions for σ to be a *global* minimizer of I_K.

Section 8.5 is dedicated to constructing various classes of n-positive definite kernels, proving that certain kernels of interest are (conditionally) n-positive definite, whereas Section 8.6 exhibits some naturally arising 3-input kernels on the sphere which are not conditionally 3-positive definite, yet the corresponding energies are minimized by the surface measure σ. These examples are presented in Propositions 8.6.1, 8.6.2, 8.6.3, and 8.6.4. The first two are closely related to the semidefinite programming method, while the last two are geometric.

In Section 8.7 we adapt the powerful method of semidefinite programming bounds [BV08, CW12, Mus14] to our setting. While multi-input energies arise naturally in this method, its applications were mainly focused on discrete configurations and energies, rather than on minimizing measures and energy integrals. By adapting the results of [BV08] to our setting, the formulation of Theorem 8.7.1 provides a way to determine that σ minimizes the three-input energy for a wide class of functions.

Section 8.8 addresses some problems from probabilistic discrete geometry, which deal with objects that can be viewed as multi-input analogues of the classical Riesz energies. We show that if three random vectors are chosen in the sphere $\mathbb{S}^{d-1}$ independently according to the probability distribution μ, then the expected volume squared of the tetrahedron generated by these vectors (Theorem 8.8.1) as well as the square of the area of the triangle defined by these points (Theorem 8.8.4) are maximized if the distribution is uniform, $\mu = \sigma$. Both statements can be proved either by semidefinite programming or directly, using ideas from linear algebra. While for the volume and area (without the square) these questions remain open, we use our results to show that, for $N = d+1$ points, the corresponding discrete energy (the average area of the triangle or the average volume of the tetrahedron) is maximized when the point configuration consists of the vertices of a regular simplex in $\mathbb{S}^{d-1}$, see Corollary 8.8.6.

8.1 Background and Definitions

In what follows, we always assume that (Ω,ρ) is a compact metric space, $n \in \mathbb{N} \setminus \{1\}$, and the kernel $K : \Omega^n \to \mathbb{R}$ is continuous and symmetric, i.e. for any permutation $\pi \in S_n$ and $x_1,...,x_n \in \Omega$, $K(x_1,...,x_n) = K(x_{\pi(1)},...,x_{\pi(n)})$. Let $\omega_N = \{z_1,z_2,...,z_N\}$ be an N-point configuration (multiset) in Ω for $N \geq n$. We define the discrete K-energy of ω_N to be

$$E_K(\omega_N) := \frac{1}{N^n} \sum_{j_1=1}^{N} \cdots \sum_{j_n=1}^{N} K(z_{j_1},...,z_{j_n}), \tag{8.4}$$

and the minimal discrete N-point K-energy of Ω as

$$\mathscr{E}_K(\Omega,N) := \inf_{\omega_N \subseteq \Omega} E_K(\omega_N). \tag{8.5}$$

Let $\mu_1,...,\mu_n \in \mathscr{M}(\Omega)$, then we define their mutual energy as

$$I_K(\mu_1,...,\mu_n) = \int_\Omega \cdots \int_\Omega K(x_1,...,x_n) d\mu_1(x_1) \cdots d\mu_n(x_n), \tag{8.6}$$

and, for $j < n$, the j-th potential function as

$$U_K^{\mu_1,...,\mu_j}(x_{j+1},...,x_n) = \int_\Omega \cdots \int_\Omega K(x_1,...,x_n) d\mu_1(x_1) \cdots d\mu_j(x_j). \tag{8.7}$$

Note that since we are working with continuous K, the energy is well-defined for all finite signed Borel measures. We will abuse notation by writing μ^k if k of the measures are the same and define the *K-energy* of a measure $\mu \in \mathscr{M}(\Omega)$ by

$$I_K(\mu) = I_K(\mu^n) = I_K(\mu,...,\mu), \tag{8.8}$$

and the minimal K-energy over all probability measures by

$$\mathscr{I}_K(\Omega) = \inf_{\mu \in \mathbb{P}(\Omega)} I_K(\mu). \tag{8.9}$$

The definitions of discrete (8.4) and continuous (8.8) energies are compatible in the sense that

$$E_K(\omega_N) = I_K(\mu_{\omega_N}), \quad \text{where } \mu_{\omega_N} = \frac{1}{N}\sum_{j=1}^{N} \delta_{z_j} \tag{8.10}$$

and due to the weak* density of the linear span of Dirac masses in $\mathbb{P}(\Omega)$

$$\lim_{N\to\infty} \mathscr{E}_K(\Omega, N) = \mathscr{I}_K(\mu). \tag{8.11}$$

We can extend the classical notion of positive definiteness for two-input kernels to n-input kernels by demanding that, if one fixes arbitrary values of all but two variables, the resulting two-input kernel is positive definite in the classical sense. For every $m < n$ and $z_1, z_2, \ldots, z_m \in \Omega$, we define

$$K_{z_1,z_2,\ldots,z_m}(x_1,\ldots,x_{n-m}) := K(z_1,\ldots,z_m,x_1,\ldots,x_{n-m}). \tag{8.12}$$

Definition 8.1.1. *We shall say that a continuous symmetric kernel $K : \Omega^n \to \mathbb{R}$ is **(conditionally) n-positive definite** if, for all $z_1, z_2, \ldots, z_{n-2} \in \Omega$, the two-input kernel $K_{z_1,\ldots,z_{n-2}}$ is (conditionally) positive definite in the sense of Definition 2.2.1.*

We would like to emphasize that this definition relies more on the pointwise two-variable structure, rather than the full set of variables. In particular, it does not have any connection to positive definite tensors [Qi05]. Thus, it may appear that the name *n-positive definite* might be somewhat misleading. However, from the point of view of energy optimization, which is the main theme of this work, this nomenclature seems absolutely justified. Indeed, in various statements about minimal energy (e.g., Theorem 8.3.3, Corollary 8.3.4, Theorem 8.4.1), this condition naturally replaces positive definiteness of classical two-input kernels. In addition, non-symmetric multivariate kernels of similar flavor have been considered in the context of k-point bounds in semidefinite programming [dLMdOFV, Mus14]. The class of n-positive definite kernels is rather rich: throughout this chapter, particularly in Section 8.5, we present numerous examples of functions with this property.

We immediately observe that this property is inherited by kernels with a lower number of inputs, which are obtained as potentials of K with respect to arbitrary probability measures.

Lemma 8.1.2. *Let $n > 2$ and assume that K is (conditionally) n-positive definite. Then for every $\mu \in \mathbb{P}(\Omega)$, the potential $U_K^{\mu}(x_1, \dots, x_{n-1})$ is (conditionally) $(n-1)$-positive definite.*

Proof. Let ν be a finite signed Borel measure on Ω (with $\nu(\Omega) = 0$ if K is conditionally n-positive definite). Then by Fubini–Tonelli

$$
\begin{aligned}
I_{\left(U_K^{\mu}\right)_{z_2,\dots,z_{n-2}}}(\nu) &= \int_{\Omega}\int_{\Omega}\int_{\Omega} K(z_1, z_2, \dots, z_{n-3}, z_{n-2}, x, y) d\mu(z_1)\, d\nu(x) d\nu(y) \\
&= \int_{\Omega}\int_{\Omega}\int_{\Omega} K_{z_1,\dots,z_{n-2}}(x,y) d\nu(x) d\nu(y)\, d\mu(z_1) \geq 0,
\end{aligned}
$$

since $K_{z_1,\dots,z_{n-2}}$ is (conditionally) positive definite for all $z_1, \dots, z_{n-2} \in \Omega$. ☐

As a corollary of Lemma 8.1.2, we observe that if $K : \Omega^n \to \mathbb{R}$ is (conditionally) n-positive definite, then for all $\mu_1, \dots, \mu_k \in \mathbb{P}(\Omega)$, with $k \leq n-2$, $U_K^{\mu_1,\dots,\mu_k}(x_{k+1}, \dots, x_n)$ is (conditionally) $(n-k)$-positive definite.

Naturally, (conditionally) n-positive definite kernels enjoy the same basic properties as their classical two-variable counterparts. The following result generalizes Lemma 2.2.3 to n-input kernels and immediately follows this lemma as well.

Lemma 8.1.3. *If K and L are n-positive definite, then so are $K + L$ and KL. If $K_1, K_2, \dots$ are n-positive definite and $\lim_{n\to\infty} K_n = K$ uniformly, then K is n-positive definite. The* *statements about the sum and the limit (but not about the product) continue to hold if we replace n-positive definite with conditionally n-positive definite.*

8.2 First Principles

In this section we explore some basic properties related to (conditional) n-positive definiteness, such as inequalities for mixed energies and convexity of the energy functionals, as well as connections between these notions, much as we did in the two input case in Section 3.3. All the kernels in this section are assumed to be continuous and symmetric.

Bounds on Mutual Energies

The arithmetic and geometric mean inequalities (3.1) and (3.2) can be extended to n-input energies with (conditionally) n-positive definite kernels.

Lemma 8.2.1. *Suppose K is a conditionally n-positive definite kernel on Ω^n. Then for every n-tuple of Borel probability measures $\mu_1, \ldots, \mu_n$ on Ω, the mutual energy $I_K(\mu_1, \ldots, \mu_n)$ satisfies*

$$I_K(\mu_1, \ldots, \mu_n) \leq \frac{1}{n} \sum_{j=1}^{n} I_K(\mu_j). \tag{8.13}$$

If, moreover, K is n-positive definite,

$$I_K(\mu_1, \ldots, \mu_n) \leq \prod_{j=1}^{n} \sqrt[n]{I_K(\mu_j)}. \tag{8.14}$$

Proof. We only prove (8.14), as one could repeat the proof below verbatim, with the multiplicative notation replaced by the additive, to arrive at (8.13) (when K is n-positive definite, it would also follow from the arithmetic–geometric mean inequality).

By Lemma 3.1.2, our claim holds for $n = 2$. Now, suppose our claim holds for some $k \geq 2$, and let $\mu_1, ..., \mu_{k+1} \in \mathbb{P}(\Omega)$. Lemma 8.1.2 tells us that for $1 \leq j \leq k+1$, $U_K^{\mu_j}$ is

k-positive definite, so by our inductive hypothesis

$$I_K(\mu_1,...,\mu_{k+1}) = I_{U_K^{\mu_1}}(\mu_2,...,\mu_{k+1}) \le \prod_{j=1}^{k} \sqrt[k]{I_K(\mu_1,\mu_{j+1}^k)}. \tag{8.15}$$

Again using the inductive hypothesis, and the fact that K is symmetric, we have that for $1 \le j \le k$,

$$\begin{aligned} I_K(\mu_1,\mu_{j+1}^k) &= I_K(\mu_{j+1},\mu_1,\mu_{j+1}^{k-1}) \\ &\le \sqrt[k]{I_K(\mu_{j+1},\mu_1^k)}\sqrt[k]{I_K(\mu_{j+1})^{k-1}} \\ &= \sqrt[k]{I_K(\mu_1,\mu_{j+1},\mu_1^{k-1})}\sqrt[k]{I_K(\mu_{j+1})^{k-1}} \\ &\le \sqrt[k^2]{I_K(\mu_1)^{k-1}}\sqrt[k^2]{I_K(\mu_1,\mu_{j+1}^k)}\sqrt[k]{I_K(\mu_{j+1})^{k-1}}, \end{aligned}$$

where in the second and last lines we have used (8.15). Rearranging the terms, we have

$$\left(I_K(\mu_1,\mu_{j+1}^k)\right)^{\frac{k^2-1}{k^2}} \le I_K(\mu_1)^{\frac{k-1}{k^2}} I_K(\mu_{j+1})^{\frac{k-1}{k}},$$

so that

$$\sqrt[k]{I_K(\mu_1,\mu_{j+1}^k)} \le I_K(\mu_1)^{\frac{1}{k(k+1)}} I_K(\mu_{j+1})^{\frac{1}{k+1}}.$$

Plugging this back into (8.15), we have

$$I_K(\mu_1,...,\mu_{k+1}) \le \prod_{j=1}^{k} \sqrt[k]{I_K(\mu_1,\mu_{j+1}^k)} \le \prod_{j=1}^{k+1} \sqrt[k+1]{I_K(\mu_j)}. \tag{8.16}$$

Our claim then follows via induction. □

The upper bound (8.13) allows us to prove a corresponding lower bound for the mixed energy:

Corollary 8.2.2. *If K is n-positive definite on Ω^n, then for all $\mu_1,...,\mu_n \in \mathbb{P}(\Omega)$,*

$$-\frac{1}{n}\sum_{j=1}^{n} I_K(\mu_j) \leq I_K(\mu_1,...,\mu_n). \tag{8.17}$$

Proof. Suppose $n = 2$, and let $\mu_1, \mu_2 \in \mathbb{P}(\Omega)$. Setting $\mu = \frac{1}{2}(\mu_1 + \mu_2)$, we have

$$0 \leq 4I_K(\mu) = I_K(\mu_1) + I_K(\mu_2) + 2I_K(\mu_1, \mu_2),$$

since K is positive definite, and (8.17) follows.

Now suppose our claim holds for some $k \geq 2$, and let $\mu_1,...,\mu_{k+1} \in \mathbb{P}(\Omega)$. Since by Lemma 8.1.2 the potential $U_K^{\mu_1}$ is k-positive definite, the inductive hypothesis implies that

$$-\frac{1}{k}\sum_{j=1}^{k} I_{U_K^{\mu_1}}(\mu_{j+1}) \leq I_{U_K^{\mu_1}}(\mu_2,...,\mu_{k+1}) = I_K(\mu_1,...,\mu_{k+1}).$$

For $1 \leq j \leq k$, Lemma 8.2.1 gives us that

$$I_{U_K^{\mu_1}}(\mu_{j+1}) = I_K(\mu_1, \mu_{j+1}^k) \leq \frac{1}{k+1}\Big(I_K(\mu_1) + kI_K(\mu_{j+1})\Big),$$

leading to

$$-\frac{1}{k+1}\sum_{j=1}^{k+1} I_K(\mu_j) \leq I_K(\mu_1,...,\mu_{k+1}),$$

which finishes the proof of the claim. □

Lemma 8.2.1 and Corollary 8.2.2 imply that if K is n-positive definite on Ω^n and $\mu_1,...,\mu_n \in \mathbb{P}(\Omega)$, then

$$\big|I_K(\mu_1,...,\mu_n)\big| \leq \frac{1}{n}\sum_{j=1}^{n} I_K(\mu_j). \tag{8.18}$$

Of course, since we can choose the probability measures μ_k to be Dirac masses, inequality (8.18) yields pointwise bounds on K. For instance, if K is n-positive definite, then for all

$z_1, \ldots, z_n \in \Omega$,

$$\left|K(z_1, \ldots, z_n)\right| \leq \frac{1}{n} \sum_{j=1}^{n} K(z_j, \ldots, z_j),$$

and for conditionally n-positive definite kernels K, this inequality holds without the absolute value. Clearly then, K must achieve its maximum value on its diagonal, something that is already known for the two-input case.

Corollary 8.2.3. *Suppose K is a conditionally n-positive definite kernel. Then*

$$K(z_1, \ldots, z_n) \leq \max_{z \in \Omega} \{K(z, \ldots, z)\}. \tag{8.19}$$

Convexity

As in the two-input case, convexity of the underlying energy functionals naturally plays an important role in energy minimization.

Definition 8.2.4. *Suppose $K : \Omega^n \to \mathbb{R}$. We say that I_K is **convex at** $\mu \in \mathbb{P}(\Omega)$ if for every $\nu \in \mathbb{P}(\Omega)$ there exists some $t_\nu \in (0,1]$, such that for all $t \in [0, t_\nu)$,*

$$I_K((1-t)\mu + t\nu) \leq (1-t) I_K(\mu) + t I_K(\nu). \tag{8.20}$$

*We say I_K is **convex** on $\mathbb{P}(\Omega)$ if inequality (8.20) holds for every μ, $\nu \in \mathbb{P}(\Omega)$ and all $t \in [0,1]$.*

As in the two-input case, we observe that convexity of I_K on $\mathbb{P}(\Omega)$ is equivalent to the fact that I_K is convex at all $\mu \in \mathbb{P}(\Omega)$. Indeed, if (8.20) fails for some μ, $\nu \in \mathbb{P}(\Omega)$, then the polynomial $f(t) = I_K((1-t)\mu + t\nu)$ is not convex on the interval $[0,1]$, i.e. $f''(t) < 0$ on some subinterval $[a,b] \subset [0,1]$. But in this case, one can easily see that I_K fails to be convex at $\mu_a = (1-a)\mu + a\nu$.

We know that conditional positive definiteness of the kernel K is equivalent to convexity of the corresponding energy functional I_K in the case $n = 2$ (Proposition 3.1.6). As the next proposition shows, a one-sided implication holds for $n \geq 3$: convexity of I_K can be deduced from relaxed arithmetic or geometric mean inequalities akin to (8.13) and (8.14). This implies, due to Lemma 8.2.1, that conditionally n-positive definite kernels K give rise to convex energies.

Proposition 8.2.5. *Let $K : \Omega^n \to \mathbb{R}$ be continuous and symmetric and fix $\mu \in \mathbb{P}(\Omega)$. Suppose that for all $\nu \in \mathbb{P}(\Omega)$ and $0 \leq k \leq n$,*

$$I_K(\mu^k, \nu^{n-k}) \leq \frac{k}{n} I_K(\mu) + \frac{n-k}{n} I_K(\nu). \tag{8.21}$$

Alternatively, assume that for all $\nu \in \mathbb{P}(\Omega)$ we have $I_K(\nu) \geq 0$ and for all $0 \leq k \leq n$

$$I_K(\mu^k, \nu^{n-k}) \leq \big(I_K(\mu)\big)^{\frac{k}{n}} \cdot \big(I_K(\nu)\big)^{\frac{n-k}{n}}. \tag{8.22}$$

Then I_K is convex at μ. If (8.21) or (8.22) holds for all $\mu \in \mathbb{P}(\Omega)$, then I_K is convex on $\mathbb{P}(\Omega)$.

Proof. Assume that (8.21) holds. For all $t \in [0,1]$, we have

$$\begin{aligned}
I_K((1-t)\mu + t\nu) &= \sum_{k=0}^{n} (1-t)^k t^{n-k} \binom{n}{k} I_K(\mu^k, \nu^{n-k}) \\
&\leq \sum_{k=0}^{n} (1-t)^k t^{n-k} \binom{n}{k} \left(\frac{k}{n} I_K(\mu) + \frac{n-k}{n} I_K(\nu) \right) \\
&= \sum_{k=1}^{n} (1-t)^k t^{n-k} \binom{n-1}{k-1} I_K(\mu) + \sum_{k=0}^{n-1} (1-t)^k t^{n-k} \binom{n-1}{k} I_K(\nu) \\
&= (1-t) I_K(\mu) + t I_K(\nu),
\end{aligned}$$

which proves convexity of the energy functional. The multiplicative inequality (8.22) implies (8.21) by the arithmetic-geometric mean inequality, leading to convexity of K in this case. □

Observe that Proposition 8.2.5 admits a partial converse:

Lemma 8.2.6. *Suppose $\mu \in \mathbb{P}(\Omega)$ is such that I_K is convex at μ. Then for all $\nu \in \mathbb{P}(\Omega)$,*

$$I_K(\mu^{n-1}, \nu) \leq \frac{n-1}{n} I_K(\mu) + \frac{1}{n} I_K(\nu). \tag{8.23}$$

Proof. Let $\nu \in \mathbb{P}(\Omega)$. Assume $t \in (0,1)$ such that (8.20) holds. Then

$$\begin{aligned} tI_K(\nu) + (1-t)I_K(\mu) &\geq I_K(t\nu + (1-t)\mu) \\ &= \sum_{j=0}^{n} (1-t)^j t^{n-j} \binom{n}{j} I_K(\mu^j, \nu^{n-j}). \end{aligned}$$

Clearly then

$$\Big(t - t^n\Big) I_K(\nu) + \Big((1-t) - (1-t)^n\Big) I_K(\mu) \geq \sum_{j=1}^{n-1} (1-t)^j t^{n-j} \binom{n}{j} I_K(\mu^j, \nu^{n-j}),$$

and dividing by $t(1-t)$, we obtain

$$\Big(\sum_{k=0}^{n-2} t^k\Big) I_K(\nu) + \Big(\sum_{l=0}^{n-2} (1-t)^l\Big) I_K(\mu) \geq \sum_{j=1}^{n-1} (1-t)^{j-1} t^{n-j-1} \binom{n}{j} I_K(\mu^j, \nu^{n-j}).$$

If I_K is convex at μ, then we may take the limit as t goes to 0, which gives us

$$I_K(\nu) + (n-1)I_K(\mu) \geq nI_K(\mu^{n-1}, \nu).$$

□

We note that if I_K is convex (in particular, convex at ν), then by switching the roles of μ and ν we obtain

$$(n-1)I_K(\nu) + I_K(\mu) \geq nI_K(\mu, \nu^{n-1}).$$

Therefore, in the case $n = 2, 3$, Lemma 8.2.6 provides the converse of Proposition 8.2.5, in other words, I_K is convex if and only if it satisfies the arithmetic mean inequalities (8.21).

Lemma 8.2.1 with $\mu_1 = \cdots = \mu_k = \mu$ and $\mu_{k+1} = \cdots = \mu_n = \nu$ shows that inequality

(8.21) holds if K is conditionally n-positive definite. This leads to the following corollary.

Corollary 8.2.7. *If K is conditionally n-positive definite, then I_K is convex on $\mathbb{P}(\Omega)$.*

It is not completely clear whether the equivalence from Proposition 3.1.6 holds for $n \geq 3$ in the equivalence holds for $n \geq 3$, but evidence suggests that it does not. Indeed, Proposition 8.6.1 provides an example of a rotationally invariant three-input kernel with $\Omega = \mathbb{S}^{d-1}$, which is not conditionally 3-positive definite, but at the same time the energy functional is convex at σ (although we do not know if it is convex at *all* measures in $\mathbb{P}(\mathbb{S}^{d-1})$) and is minimized by σ, which we know would be impossible in the two-input case.

In this regard, we would also like to point out that a number of our results about energy minimizers do not require the full power of convexity of I_K on $\mathbb{P}(\Omega)$, but rather just the convexity at the presumptive minimizer μ. In particular, condition (8.26), which appears in Theorems 8.3.3 and 8.3.7, is implied by inequality (8.23) of Lemma 8.2.6, and hence it holds if I_K is convex at μ.

Using convexity of the energy functional, one can draw a connection between minimizing the n-input energy I_K and the $(n-1)$-input energy $I_{U_K^\mu}$, thus obtaining our first result about minimizers of multi-input energies.

Proposition 8.2.8. *Let $n \geq 3$. Assume that $K : \Omega^n \to \mathbb{R}$ is continuous and symmetric, I_K is convex, and that $\mu \in \mathbb{P}(\Omega)$ is a minimizer of $I_{U_K^\mu}$. Then μ is a minimizer of I_K.*

Proof. We first prove that if the energy I_K is convex and μ, $\nu \in \mathbb{P}(\Omega)$, then

$$I_K(\nu) - I_K(\mu) \geq \frac{n}{n-1}\Big(I_{U_K^\mu}(\nu) - I_{U_K^\mu}(\mu)\Big). \tag{8.24}$$

Indeed, we have $I_{U_K^\mu}(\mu) = I_K(\mu)$ and, by Lemma 8.2.6, $I_{U_K^\mu}(\nu) = I_K(\mu, \nu^{n-1}) \leq \frac{1}{n} I_K(\mu) +$

$\frac{n-1}{n} I_K(\nu)$. Thus,

$$I_K(\nu) - I_K(\mu) - n\Big(I_{U_K^\mu}(\nu) - I_{U_K^\mu}(\mu)\Big) = I_K(\nu) - nI_K(\mu, \nu^{n-1}) + (n-1)I_K(\mu)$$
$$\geq (n-2)\Big(I_K(\mu) - I_K(\nu)\Big),$$

which implies inequality (8.24).

Inequality (8.24), together with the fact that μ is a minimizer of $I_{U_K^\mu}$, implies that for all $\nu \in \mathbb{P}(\Omega)$, we have

$$I_K(\nu) - I_K(\mu) \geq \frac{n}{n-1}\Big(I_{U_K^\mu}(\nu) - I_{U_K^\mu}(\mu)\Big) \geq 0,$$

hence μ minimizes I_K. □

Proposition 8.2.8 can be viewed as a precursor of some of our more advanced results from Section 8.3 which show that there is a strong relation between μ minimizing the n-input energy I_K and the energy functional $I_{U_K^{\mu^k}}$ with a lower number of inputs. In fact, Theorem 8.3.7 contains Proposition 8.2.8 as a special case. We have nevertheless decided to include this proposition, as it admits a very transparent and elementary proof, which also provides a quantitative relation between the minimization of I_K and $I_{U_K^\mu}$.

8.3 Minimizers of the Energy Functional

We finally turn to some of the general results about minimizers of energies with multivariate kernels. It is clear from various results in Chapter 3 that in the classical two-input case, properties of minimizing measures are closely related to their potentials. Direct analogues of these statements can be obtained for multi-input energies. We start with the necessary condition, which is a generalization of Theorem 3.1.7 and Corollary 3.1.9, stating that the potential of a local minimizer is constant on its support. As before, in all of the statements of this section we assume that $K : \Omega^n \to \mathbb{R}$ is continuous and symmetric, even if not explicitly stated.

We define a local minimizer the same way we did for the two-input case:

Definition 8.3.1. *We shall say that μ is a **local minimizer** of I_K if it is a local minimizer in every direction, in other words, if for each $\nu \in \mathbb{P}(\Omega)$, there exists $t_\nu \in (0,1]$ such that for all $t \in [0,t_\nu]$ we have*

$$I_K\big((1-t)\mu + t\nu\big) \geq I_K(\mu).$$

Observe that this definition differs from the definition of local minimizers with respect to some metric, such as the Wasserstein d_∞ metric or the total variation norm (the difference is similar to that between the Gateaux and Fréchet derivatives).

Theorem 8.3.2. *Let $K : \Omega^n \to R$ be continuous and symmetric. Suppose that μ is a local minimizer of I_K over $\mathbb{P}(\Omega)$. Then $U_K^{\mu^{n-1}}(x) = I_K(\mu)$ on* $\operatorname{supp}(\mu)$ *and $U_K^{\mu^{n-1}}(x) \geq I_K(\mu)$ on Ω.*

Proof. The proof is a simple extension of the proof of Theorem 3.1.7 and we include it for the sake of completeness. Let $\nu \in \mathbb{P}(\Omega)$, t_ν be as in Definition 8.3.1, and $\tilde{\nu} = \nu - \mu \in \mathscr{Z}(\Omega)$. Then for all $0 \leq t \leq 1$ and $\mu + t\tilde{\nu} = (1-t)\mu + t\nu \in \mathbb{P}(\Omega)$, and satisfies

$$I_K(\mu) \leq I_K(\mu + t\tilde{\nu}) = \sum_{k=0}^{n} \binom{n}{k} t^k I_K(\mu^{n-k}, \tilde{\nu}^k).$$

Thus, for $0 \leq t \leq t_\nu$,

$$0 \leq t \left(\sum_{k=1}^{n} \binom{n}{k} t^{k-1} I_K(\mu^{n-k}, \tilde{\nu}^k) \right).$$

This means that $I_K(\mu^{n-1}, \tilde{\nu}) \geq 0$.

Suppose, indirectly, that there exist $a, b \in \mathbb{R}$, $z \in \operatorname{supp}(\mu)$ and $y \in \Omega$ such that

$$a = U_K^{\mu^{n-1}}(z) > U_K^{\mu^{n-1}}(y) = b.$$

Let B be a ball centered at z, small enough so that $y \notin B$ and oscillation of $U_K^{\mu^{n-1}}(x)$ is at most $\frac{a-b}{2}$, and let $m=\mu(B)$. Let ν be defined by

$$\nu(A)=\mu(A)+m\delta_y(A)-\mu(A\cap B). \tag{8.25}$$

Then

$$I_K(\mu^{n-1},\tilde{\nu})=U_K^{\mu^{n-1}}(y)\cdot m-\int_B U_K^{\mu^{n-1}}(x)d\mu(x)\leq bm-\left(a-\frac{a-b}{2}\right)m<0,$$

which is a contradiction. Thus, if $U_K^{\mu^{n-1}}(z)=a$ for some $z\in\operatorname{supp}(\mu)$, then $U_K^{\mu^{n-1}}(x)\geq a$ for all $x\in\Omega$. Our claim then follows. □

In general, the converse to Theorem 8.3.2 is not true. However, with some additional convexity assumptions, the necessary condition for μ to be a global minimizer also becomes sufficient.

Theorem 8.3.3. *Let $K:\Omega^n\to\mathbb{R}$ be symmetric and continuous. Suppose that for some $\mu\in\mathbb{P}(\Omega)$, there exists a finite constant M such that $U_K^{\mu^{n-1}}(x)\geq M$ on Ω and $U_K^{\mu^{n-1}}(x)=M$ on* $\operatorname{supp}(\mu)$. *Suppose further that for all $\nu\in\mathbb{P}(\Omega)$, there exists some $a\in(0,1)$, possibly depending on ν, such that*

$$I_K(\mu^{n-1},\nu)\leq aI_K(\nu)+(1-a)I_K(\mu). \tag{8.26}$$

Then μ is a minimizer of I_K.

Proof. For any $\nu\in\mathbb{P}(\Omega)$, for some $a\in(0,1)$, we have

$$I_K(\mu)=\int_\Omega U_K^{\mu^{n-1}}(x)d\mu(x)\leq\int_\Omega U_K^{\mu^{n-1}}(x)d\nu(x)=I_K(\mu^{n-1},\nu)\leq aI_K(\nu)+(1-a)I_K(\mu),$$

hence $I_K(\mu)\leq I_K(\nu)$. □

Some remarks concerning the assumptions of Theorem 8.3.3, i.e. condition (8.26), are in order. Due to Lemma 8.2.6, convexity of the energy functional I_K at μ implies condition (8.26) with $a = \frac{1}{n}$. In turn, if K is conditionally n-positive definite, Corollary 8.2.7 states that I_K is convex, and hence again condition (8.26) is satisfied (alternatively, Lemma 8.2.1 shows directly that conditional n-positive definiteness of K implies the convexity condition (8.26) of Theorem 8.3.3 with $a = \frac{1}{n}$). The hierarchy of these conditions can be summarized in the following diagram:

$$\begin{aligned} &K \text{ is } n\text{-positive definite} \implies K \text{ is conditionally } n\text{-positive definite} \implies \\ &\implies I_K \text{ is convex} \implies I_K \text{ is convex at } \mu \implies \text{condition (8.26) holds.} \end{aligned} \tag{8.27}$$

Therefore, Theorem 8.3.3 (as well as other statements relying on (8.26), e.g. Lemma 8.3.5 or Theorem 8.3.7) may be applied under the assumptions that K is (conditionally) n-positive definite or that I_K is convex at μ.

We also make the following remark: in the case when μ has full support, i.e. $\operatorname{supp}(\mu) = \Omega$, if the first condition of Theorem 8.3.3 holds, i.e. $U_K^{\mu^{n-1}}(x) = M$ for all $x \in \Omega$, then $I_K(\mu^{n-1}, \nu) = I_K(\mu)$, and the assumption (8.26) is obviously the same as the conclusion of Theorem 8.3.3. This does not, however, render this case of the theorem useless – on the contrary, if one replaces (8.26) with one of the stronger conditions in (8.27), one obtains an interesting and meaningful statement. (This shows that most of the content is hidden in the implications presented in (8.27).) We summarize this case in a separate corollary, as it will be of use later.

Corollary 8.3.4. *Let $K : \Omega^n \to \mathbb{R}$ be symmetric and continuous. Suppose that $\mu \in \mathbb{P}(\Omega)$ has full support (*$\operatorname{supp}(\mu) = \Omega$*) and that there exists a constant M such that $U_K^{\mu^{n-1}}(x) = M$ on Ω. Assume also that any of the conditions in* (8.27) *holds (e.g., K is n-positive definite or I_K is convex). Then μ is a minimizer of I_K.*

We also observe that Theorems 8.3.2 and 8.3.3 imply the following local-to-global principle for minimizers of I_K under convexity assumptions.

Lemma 8.3.5. *Let $n \geq 2$ and let μ be a local minimizer of the energy functional I_K. Assume also that condition* (8.26) *is satisfied. Then μ is a global minimizer of I_K over $\mathbb{P}(\Omega)$.*

Proof. Theorem 8.3.2 shows that the first condition of Theorem 8.3.3 holds. Together with condition (8.26), this implies that μ is a global minimizer of I_K. □

Naturally, the set of minimizers of a convex functional is convex. By Corollary 8.2.7, for conditionally n-positive definite kernels, the energy I_K is convex, i.e. minimizers of I_K form a convex set in this case.

Proposition 8.3.6. *Let K be a conditionally n-positive definite kernel. Then the set of minimizers of the energy I_K is convex.*

Proof. For two minimizers μ, ν of I_K, and all $t \in [0,1]$, by convexity of energy,

$$I_K(\nu) \leq I_K\big((1-t)\mu + t\nu\big) \leq (1-t)I_K(\mu) + tI_K(\nu) = I_K(\nu).$$

Hence, $I_K\big((1-t)\mu + t\nu\big) = I_K(\nu)$ and $(1-t)\mu + t\nu$ minimizes I_K. □

While Theorems 8.3.2 and 8.3.3 are straightforward generalizations of the corresponding facts for the classical two-input energies, they lead to some interesting consequences for energies with multivariate kernels. In particular, we start by showing that under condition (8.26), if μ minimizes the lower input energy with the kernel $U_K^{\mu^k}$, then it also minimizes the original n-input energy I_K.

Theorem 8.3.7. *Let $K : \Omega^n \to \mathbb{R}$, $n \geq 3$, be symmetric and continuous. Assume that for some $1 \leq k \leq n-2$, the measure $\mu \in \mathbb{P}(\Omega)$ (locally) minimizes the $(n-k)$-input energy $I_{U_K^{\mu^k}}$. Assume also that μ satisfies condition* (8.26) *of Theorem 8.3.3. Then μ minimizes the n-input energy I_K.*

Proof. Theorem 8.3.2 applied to the kernel $U_K^{\mu^k}$ implies that for all $x \in \Omega$

$$U_K^{\mu^{n-1}}(x) = U_{U_K^{\mu^k}}^{\mu^{n-k-1}}(x) \geq I_{U_K^{\mu^k}}(\mu) = I_K(\mu)$$

with equality for $x \in \mathrm{supp}(\mu)$. Condition (8.26) then allows one to invoke Theorem 8.3.3, which shows that μ minimizes I_K. □

The converse to Theorem 8.3.7 holds for $k = n-2$ even without any convexity assumptions: in this case, if μ locally minimizes I_K, it also locally minimizes the two-input energy $I_{U_K^{\mu^{n-2}}}$. Moreover, under the additional condition that μ has full support, one can deduce that the measure μ is a *global* minimizer of $I_{U_K^{\mu^{n-2}}}$, which follows from Theorem 3.3.1, though we prove it directly here. Furthermore, this implication may be reversed, if one additionally assumes that μ *uniquely* minimizes $I_{U_K^{\mu^{n-2}}}$. Observe that, unlike Theorem 8.3.7, part (3) of Theorem 8.3.8 does not require any of the conditions of (8.27) and, unlike part (2), it does not require the condition $\mathrm{supp}(\mu) = \Omega$.

Theorem 8.3.8. *Let $K : \Omega^n \to \mathbb{R}$, $n \geq 3$, be symmetric and continuous and let $\mu \in \mathbb{P}(\Omega)$.*

1. *Let μ be a local minimizer of I_K. Then μ is a local minimizer of the two-input energy $I_{U_K^{\mu^{n-2}}}$.*
2. *Let μ be a local minimizer of I_K and assume, in addition, that μ has full support, i.e. $\mathrm{supp}(\mu) = \Omega$. Then μ minimizes the two-input energy $I_{U_K^{\mu^{n-2}}}$ over $\mathbb{P}(\Omega)$.*
3. *If μ is the unique minimizer of $I_{U_K^{\mu^{n-2}}}$ in $\mathbb{P}(\Omega)$, then μ is a local minimizer of I_K.*

Proof. Fix an arbitrary measure $\nu \in \mathbb{P}(\Omega)$. For $t \in [0,1]$, let us define two functions $g_\nu(t) = I_K\big((1-t)\mu + t\nu\big)$ and $h_\nu(t) = I_{U_K^{\mu^{n-2}}}\big((1-t)\mu + t\nu\big) = I_K\big(\mu^{n-2}, \big((1-t)\mu + t\nu\big)^2\big)$. We have

$$g_\nu(t) = (1-t)^n I_K(\mu) + nt(1-t)^{n-1} I_K(\mu^{n-1}, \nu) + \binom{n}{2} t^2 (1-t)^{n-2} I_K(\mu^{n-2}, \nu^2) + R_\nu(t),$$

where each term in $R_\nu(t)$ contains a factor of the form t^k with $k \geq 3$ and, therefore, $R'_\nu(0) = R''_\nu(0) = 0$,

$$h_\nu(t) = (1-t)^2 I_K(\mu) + 2t(1-t) I_K(\mu^{n-1}, \nu) + t^2 I_K(\mu^{n-2}, \nu^2).$$

A direct (elementary, but lengthy) computation, which we omit, shows that

$$h_\nu'(0) = \frac{2}{n} g_\nu'(0) = 2\big(I_K(\mu^{n-1}, \nu) - I_K(\mu)\big), \tag{8.28}$$

$$h_\nu''(0) = \frac{2}{n(n-1)} g_\nu''(0) = 2\big(I_K(\mu) - 2I_K(\mu^{n-1}, \nu) + I_K(\mu^{n-2}, \nu^2)\big). \tag{8.29}$$

We now start by proving (1). Let μ be a local minimizer of I_K. According to Corollary 3.1.9, we have that $U_K^{\mu^{n-1}}(x) \geq I_K(\mu)$ on Ω and therefore, $I_K(\mu^{n-1}, \nu) \geq I_K(\mu)$ for any $\nu \in \mathbb{P}(\Omega)$. Since g_ν has a local minimum at $t = 0$, either $g_\nu'(0) > 0$, or $g_\nu'(0) = 0$ and $g_\nu''(0) \geq 0$. In the first case, we also have $h_\nu'(0) > 0$. In the second case, $h_\nu'(0) = 0$ and $h_\nu''(0) \geq 0$, and since h_ν is quadratic, this implies that $h_\nu(t) = at^2 + b$ with $a \geq 0$. Thus, h_ν has a local minimum at $t = 0$ for each $\nu \in \mathbb{P}(\Omega)$, i.e. μ is a local minimizer of $I_{U_K^{\mu^{n-2}}}$.

If in addition μ has full support, then Corollary 3.1.9 implies that for any $\nu \in \mathbb{P}(\Omega)$, we have $I_K(\mu^{n-1}, \nu) = I_K(\mu)$. Therefore, relations (8.28)-(8.29), together with the fact that g_ν has a local minimum at $t = 0$, show that $g_\nu'(0) = 0$, hence $g_\nu''(0) \geq 0$, and at the same time

$$g_\nu''(0) = n(n-1)\big(I_K(\mu^{n-2}, \nu^2) - I_K(\mu)\big) = n(n-1)\Big(I_{U_K^{\mu^{n-2}}}(\nu) - I_{U_K^{\mu^{n-2}}}(\mu)\Big). \tag{8.30}$$

Hence, μ is a global minimizer of $I_{U_K^{\mu^{n-2}}}$, which proves part (2).

To prove (3), assume that μ is the unique global minimizer of $I_{U_K^{\mu^{n-2}}}$. Observe that, since the potential of $U_K^{\mu^{n-2}}$ with respect to μ is $U_K^{\mu^{n-1}}$, Theorem 8.3.2 applied to $U_K^{\mu^{n-2}}$ implies that, just like in part (1), we have $I_K(\mu^{n-1}, \nu) \geq I_K(\mu)$. Thus, $g_\nu'(0) \geq 0$ by (8.28). If $g_\nu'(0) > 0$, there is a local minimum at $t = 0$. If, however, $g_\nu'(0) = 0$, then $I_K(\mu^{n-1}, \nu) = I_K(\mu)$ and relation (8.30) holds. Since μ uniquely minimizes $I_{U_K^{\mu^{n-2}}}$, this proves that $g_\nu''(0) > 0$ for $\nu \neq \mu$. Hence, in each case, g_ν has a local minimum at $t = 0$, i.e. μ is a local minimizer of I_K. □

Applying Theorem 3.3.1, we obtain the following corollary to part (2) of Theorem 8.3.8:

Corollary 8.3.9. *Assume that* $\mu \in \mathbb{P}(\Omega)$ *with* $\operatorname{supp}(\mu) = \Omega$ *is a local minimizer of* I_K. *Then the* $(n-2)$*-fold potential of* K *with respect to* μ*, i.e. the two-variable function* $U_K^{\mu^{n-2}}(x,y)$*, is conditionally positive definite on* Ω.

Observe that, if the kernel K is conditionally n-positive definite, then, according to Lemma 8.1.2, $U_K^{\mu^{n-2}}(x,y)$ is conditionally positive definite. Moreover, Theorem 8.3.7 applies for conditionally positive definite kernels K. Therefore, the statement of Corollary 8.3.9 may be viewed as a partial converse of Theorem 8.3.7 for conditionally positive definite kernels. This interplay will manifest itself in an even stronger fashion on the sphere, the situation to be explored in Section 8.4.

8.4 Multi-input Energy on the Sphere

We now restrict our attention to the unit sphere $\mathbb{S}^{d-1}$, where the symmetries and structure of the domain allow one to deduce additional information about energy minimization. One of the most natural questions is whether the normalized uniform surface measure σ minimizes the energy functional over $\mathbb{P}(\mathbb{S}^{d-1})$, or, in other words, whether energy minimization induces uniform distribution.

In this section, we shall be interested in kernels, which (in addition to being continuous and symmetric) are *rotationally invariant*, i.e. have the form

$$K(x_1,\dots,x_n) = F\Big((\langle x_i, x_j \rangle)_{i,j=1}^n \Big), \tag{8.31}$$

in other words, they depend only on the Gram matrix of $\{x_1,\dots,x_n\} \subset \mathbb{S}^{d-1}$. When $n=2$, one obtains classical pairwise interaction kernels of the form $K(x,y) = F(\langle x,y \rangle)$, which has been thoroughly discussed in previous chapters. In the case $n=3$ rotationally invariant kernels are functions of the form

$$K(x,y,z) = F(\langle x,y \rangle, \langle x,z \rangle, \langle z,y \rangle) = F(t,u,v), \tag{8.32}$$

where we set $t = \langle x,y\rangle$, $u = \langle x,z\rangle$, $v = \langle z,y\rangle$, and we shall keep this notation, which comes from [BV08], throughout the text.

Observe that, if the n-input kernel K is rotationally invariant, its potential with respect to σ is again rotationally invariant. Indeed, for any $V \in SO(d)$, we have

$$U_K^{\sigma}(Vx_1,\dots,Vx_{n-1}) = U_K^{\sigma}(x_1,\dots,x_{n-1}), \tag{8.33}$$

which easily follows from (8.31) and the facts that $\langle x_i,x_j\rangle = \langle Vx_i,Vx_j\rangle$ and $\langle Vx_i,x_n\rangle = \langle x_i,V^{-1}x_n\rangle$, $1 \le i,j \le n-1$, together with the rotational invariance of σ, i.e. $d\sigma(x_n) = d\sigma(V^{-1}x_n)$. Iterating this observation, one finds that all k-fold potentials of K with respect to σ, i.e. functions $U_K^{\sigma^k}$ with $1 \le k \le n-1$, are rotationally invariant. In particular, when $k = n-2$, the two-input kernel $U_K^{\sigma^{n-2}}$ depends only on the inner product of the inputs, and for $k = n-1$, the potential $U_K^{\sigma^{n-1}}$ is just a constant:

$$U_K^{\sigma^{n-2}}(x,y) = G(\langle x,y\rangle) = G(t) \ \text{ and } \ U_K^{\sigma^{n-1}}(x) = \text{const} = I_K(\sigma). \tag{8.34}$$

Recall that Theorem 8.3.2 would guarantee the latter condition in the case when σ is a minimizer of I_K. However, for rotationally invariant kernels, this is automatically satisfied, which facilitates the application of the results of Section 8.3 and will play an important role later, in Theorem 8.4.1.

Turning to the primary task of understanding when σ minimizes I_K, we first remind ourselves that in the classical case of a two-input energy with a rotationally invariant kernel $G(\langle x,y\rangle)$ on $\mathbb{S}^{d-1}$, the answer to this question is well understood, see, e.g. Theorem 3.3.1 and Proposition 3.5.1. In particular, the following three conditions are equivalent:

1. The uniform surface measure σ minimizes I_G over $\mathbb{P}(\mathbb{S}^{d-1})$.

2. The kernel G is conditionally positive definite on $\mathbb{S}^{d-1}$.

3. The kernel G is positive definite on $\mathbb{S}^{d-1}$ up to a constant term, i.e. there exists a

constant $c \in \mathbb{R}$ such that $G + c$ is positive definite on $\mathbb{S}^{d-1}$ (in fact, one can take $c = -I_G(\sigma)$).

Our goal is to generalize these statements (at least partially) to the case of multi-input energies. We observe that, if a symmetric rotationally invariant kernel K is conditionally n-positive definite on $\mathbb{S}^{d-1}$, then, according to Lemma 8.1.2, the potential $G(\langle x,y\rangle) = U_K^{\sigma^{n-2}}(x,y)$ is also conditionally positive definite, and hence, by the discussion above, σ is a minimizer of the two-input energy $I_{U_K^{\sigma^{n-2}}}$. Therefore, since conditionally n-positive definite kernels satisfy condition (8.26), Theorem 8.3.7 with $k = n-2$ applies and we obtain the following statement:

Theorem 8.4.1. *Suppose that $K : (\mathbb{S}^{d-1})^n \to \mathbb{R}$ is continuous, symmetric, rotationally invariant, and conditionally n-positive definite on $\mathbb{S}^{d-1}$. Then σ is a minimizer of I_K over $\mathbb{P}(\Omega)$.*

This theorem also easily follows from Theorem 8.3.3 and the remarks thereafter (or, more precisely, from Corollary 8.3.4), since, as explained above, the potential $U_K^{\sigma^{n-1}}$ is constant on $\mathbb{S}^{d-1}$. In addition, we notice that, unlike some statements of Section 8.3, such as Theorem 8.3.7, for rotationally invariant kernels in the theorem above, one does not need to assume anything about energies with a lower number of inputs – conditional n-positive definiteness alone suffices.

Theorem 8.4.1 immediately yields some interesting examples:

Corollary 8.4.2. *Let $f : [-1,1] \to \mathbb{R}$ be a real-analytic function with nonnegative Maclaurin coefficients and let $F(t,u,v) = f(tuv)$. Then, for K defined as in* (8.32)*, the uniform surface measure σ minimizes the energy I_K over $\mathbb{P}(\mathbb{S}^{d-1})$.*

Proof. Observe first that in this setup, if K_z is positive definite for one point $z \in \mathbb{S}^{d-1}$, it is also positive definite for each $z \in \mathbb{S}^{d-1}$ due to rotational invariance, i.e. Definition 8.1.1 only needs to be checked at one point. Consider first $F(t,u,v) = tuv$ and fix any $z \in \mathbb{S}^{d-1}$, e.g., $z = e_1$. Then for any $\nu \in \mathscr{M}(\mathbb{S}^{d-1})$,

$$I_{K_{e_1}}(\nu) = \int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} \langle x,y\rangle x_1 y_1 d\nu(x) d\nu(y) = \sum_{i=1}^{d} \left(\int\limits_{\mathbb{S}^{d-1}} x_1 x_i d\nu(x) \right)^2 \geq 0,$$

i.e. the kernel $K(x,y,z) = \langle x,y\rangle\langle x,z\rangle\langle z,y\rangle = tuv$ is 3-positive definite, and hence, by Lemma 8.1.3, so are all of its integer powers, positive linear combinations and their limits. The conclusion now follows from Theorem 8.4.1. □

This corollary provides a whole array of examples: for instance, three-input energies with kernels $K(x,y,z) = tuv$, or $(tuv)^n$, or e^{tuv} are all minimized by σ. We remark that, while for $K = tuv$ this statement could be proved using semidefinite programming methods, for higher powers $(tuv)^n$ this would be extremely difficult technically, and for kernels like e^{tuv} almost impossible.

For even exponents, the energies with the kernels $K = (uvt)^{2k}$ can be viewed as three-input generalizations of the well-known p-frame potentials discussed in Chapter 6. We also point out that Proposition 8.5.2 provides a more general class of n-positive definite kernels, which contains $K = tuv$ as a special case.

Unfortunately, unlike the classical two-input case, the converse to Theorem 8.4.1 is not true: Propositions 8.6.1, 8.6.2, 8.6.3, and 8.6.4 show that some kernels, naturally arising in semidefinite programming and geometry, fail to be conditionally n-positive definite, even though σ minimizes corresponding energies (see Theorems 8.7.1, 8.8.1, and 8.8.3). In other words, conditional n-positive definiteness of the kernel is not equivalent to the fact that σ minimizes the energy.

We suspect that the property that σ minimizes I_K is equivalent to $U_K^{\sigma^{n-2}}$ being conditionally positive definite, i.e. the two-input energy $I_{U_K^{\sigma^{n-2}}}$ is minimized by σ. This conjecture is supported by all examples currently known to us. Conditional positive-definiteness of $U_K^{\sigma^{n-2}}$ obviously follows from conditional n-positive definiteness of K, due to Lemma 8.1.2, but the converse implication is not true. In fact, all the kernels discussed in Section 8.6 possess this property: they are not 3-positive definite, but their potentials U_K^σ with respect to σ are (conditionally) positive definite, and the corresponding energies I_K are minimized by σ.

Theorem 8.4.3 below (which is essentially a restatement of Theorem 8.3.8 for the spherical case, along with the fact that σ has full support) shows that conditional positive definiteness of $U_K^{\sigma^{n-2}}$ is implied if σ is a *local* minimizer of I_K, and a partial converse to this statement also holds. Observe that, if the conjecture above is true, then being a local and global minimizer are equivalent for σ, a fact is indeed true for the two-input energies (Theorem 3.3.1).

Theorem 8.4.3. *Let $K : (\mathbb{S}^{d-1})^n \to \mathbb{R}$ be a continuous, symmetric, and rotationally invariant kernel.*

1. *Assume that σ is a local minimizer of I_K in $\mathbb{P}(\mathbb{S}^{d-1})$. Then the uniform measure σ is a global minimizer of the two-input energy $I_{U_K^{\sigma^{n-2}}}$, or, equivalently, $U_K^{\sigma^{n-2}}$ is conditionally positive definite on the sphere $\mathbb{S}^{d-1}$.*

2. *Assume that σ is the unique global minimizer of $I_{U_K^{\sigma^{n-2}}}$ over $\mathbb{P}(\mathbb{S}^{d-1})$. Then σ is a local minimizer of the n-input energy I_K.*

Theorem 8.4.3 above shows that if σ is a global minimizer of I_K, then the potential $U_K^{\sigma^{n-2}}$ is conditionally positive definite. We do not know whether the converse of this statement holds. One can show, however, at least for $n = 3$ that if σ minimizes $I_{U_K^\sigma}$ (in other words, U_K^σ is conditionally positive definite), but fails to minimize I_K, then the global minimizer of I_K cannot be supported on the whole sphere.

Lemma 8.4.4. *Let $K : (\mathbb{S}^{d-1})^3 \to \mathbb{R}$ be a continuous, symmetric, and rotationally invariant three-input kernel. Assume that U_K^σ is conditionally positive definite on the sphere $\mathbb{S}^{d-1}$ (i.e. σ minimizes $I_{U_K^\sigma}$), but at the same time σ is not a minimizer of I_K. Let μ be a minimizer of I_K. Then* $\operatorname{supp}(\mu) \subsetneq \mathbb{S}^{d-1}$.

Proof. Assume, by contradiction, that $\text{supp}(\mu) = \mathbb{S}^{d-1}$. Then, by Theorem 8.3.2, $U_K^{\mu^2}(x) = I_K(\mu)$ for every $x \in \mathbb{S}^{d-1}$, and therefore,

$$I_{U_K^\sigma}(\mu) = I_K(\mu,\mu,\sigma) = \int\limits_{\mathbb{S}^{d-1}} U_K^{\mu^2}(x)\, d\sigma(x) = I_K(\mu).$$

On the other hand, obviously, $I_K(\sigma) = I_{U_K^\sigma}(\sigma)$. Since μ is a minimizer of I_K, and σ is not, we have $I_K(\mu) < I_K(\sigma)$. This implies that $I_{U_K^\sigma}(\mu) < I_{U_K^\sigma}(\sigma)$, which contradicts the conditional positive definiteness of U_K^σ. □

8.5 Positive Definite Kernels

Corollary 8.4.2 of the previous section already provided a class of 3-positive definite functions. In this section we provide several other classes of kernels that are (conditionally) n-positive definite.

General Classes of (Conditionally) n-positive Definite Kernels

We start with some very natural examples, which show how to construct (conditionally) n-positive definite kernels from kernels with fewer inputs. In particular, we show that an n-input kernel can be constructed from m-input ones, $m < n$, by considering the sum or product over all m-element subsets of inputs. We first deal with the statement about the sum.

Proposition 8.5.1. *Let $2 \le m \le n-1$, and suppose $H : \Omega^m \to \mathbb{R}$ is continuous, symmetric, and conditionally m-positive definite. Then*

$$K(z_1,\dots,z_n) := \sum_{1 \le j_1 < j_2 < \cdots < j_m \le n} H(z_{j_1}, z_{j_2}, \dots, z_{j_m})$$

is conditionally n-positive definite.

Proof. Let ν be a finite signed Borel measure on Ω such that $\nu(\Omega)=0$. Then for any fixed $z_1,\ldots,z_{n-2}\in\Omega$, since H is conditionally m-positive definite, we have

$$\begin{aligned}
\int_\Omega\int_\Omega K(z_1,\ldots,z_{n-2},x,y)d\nu(x)d\nu(y) &= \int_\Omega\int_\Omega \sum_{1\le l_1<\cdots<l_m\le n-2} H(z_{l_1},\ldots,z_{l_m})d\nu(x)d\nu(y)\\
&+\int_\Omega\int_\Omega \sum_{1\le k_1<\cdots<k_{m-1}\le n-2}\Big(H(z_{k_1},\ldots,z_{k_{m-1}},x)+H(z_{k_1},\ldots,z_{k_{m-1}},y)\Big)d\nu(x)d\nu(y)\\
&+\int_\Omega\int_\Omega \sum_{1\le j_1<\cdots<j_{m-2}\le n-2} H(z_{j_1},\ldots,z_{j_{m-2}},x,y)d\nu(x)d\nu(y)\\
&= \sum_{1\le j_1<\cdots<j_{m-2}\le n-2}\int_\Omega\int_\Omega H(z_{j_1},\ldots,z_{j_{m-2}},x,y)d\nu(x)d\nu(y)\ge 0,
\end{aligned}$$

which shows that K is conditionally n-positive definite. □

We can also prove an analogue of Proposition 8.5.1 for products of positive definite functions.

Proposition 8.5.2. *Let $2\le m\le n-1$ and assume that $H:\Omega^m\to\mathbb{R}$ is continuous, symmetric, and m-positive definite. If H is a nonnegative function or $m=n-1$, then*

$$K(z_1,\ldots,z_n)=\prod_{1\le j_1<\cdots<j_m\le n} H(z_{j_1},\ldots,z_{j_m})$$

is n-positive definite.

Proof. Fix $z_1, \dots, z_{n-2} \in \Omega$. We can write

$$K(z_1, \dots, z_{n-2}, x, y) = \prod_{1 \le j_1 < \cdots < j_m \le n-2} H(z_{j_1}, \dots, z_{j_m}) \tag{8.35}$$

$$\times \prod_{1 \le j_1 < \cdots < j_{m-1} \le n-2} H(z_{j_1}, \dots, z_{j_{m-1}}, x) \tag{8.36}$$

$$\times \prod_{1 \le j_1 < \cdots < j_{m-1} \le n-2} H(z_{j_1}, \dots, z_{j_{m-1}}, y) \tag{8.37}$$

$$\times \prod_{1 \le j_1 < \cdots < j_{m-2} \le n-2} H(z_{j_1}, \dots, z_{j_{m-2}}, x, y). \tag{8.38}$$

Observe that the product in line (8.35) is non-negative when $H \ge 0$ or if $m = n-1$ (the product is empty in the latter case). The product of lines (8.36) and (8.37) is positive definite as a function of x and y: indeed, it has the form $F(x,y) = \phi(x)\phi(y)$ and hence

$$I_F(\mu) = \left(\int_{\Omega} \phi(x) d\mu(x) \right)^2 \ge 0$$

for any $\mu \in \mathscr{M}(\Omega)$. Finally, every factor in the product in line (8.38) is positive definite as a function of x and y, because H is m-positive definite. Thus, Schur's product theorem (see Lemma 8.1.3) ensures that the whole product is positive definite as a function of x and y, therefore, K is n-positive definite. □

Propositions 8.5.1 and 8.5.2 provide us with large classes of n-positive definite kernels. However, these constructions do not exhaust all such kernels. In the following subsection, we provide examples of three-positive definite kernels on the sphere, which are not obtained from two-input kernels by the methods described above.

Three-positive Definite Kernels on the Sphere

We use the same notation as in Section 8.4: for $x, y, z \in \mathbb{S}^{d-1}$, we set $t = \langle x, y \rangle$, $u = \langle x, z \rangle$, and $v = \langle z, y \rangle$.

In Corollary 8.4.2, we showed that $K = tuv$ is 3-positive definite on the sphere. Observe that this is a specific case of Proposition 8.5.2 above, since $\langle x,y \rangle$ is a positive definite function on $\mathbb{S}^{d-1}$. More generally, Proposition 8.5.2 implies that any kernel of the form $K(x,y,z) = h(t)h(u)h(v)$ is 3-positive definite, as long as h is a positive definite function on the sphere.

The kernels considered in Lemmas 8.5.3 and 8.5.4 are closely related to the parallelepiped spanned by the vectors x, y, and $z \in \mathbb{S}^{d-1}$. Indeed, setting $a = 2$ in (8.39), one obtains negative volume squared of this parallelepiped: this kernel is not conditionally 3-positive definite according to Proposition 8.6.3, even though σ is a minimizer of the corresponding energy, as shown in Theorem 8.8.1. However, positive definiteness does hold for other values of the parameter a.

Lemma 8.5.3. *For* $a < 1$*,*

$$K(x,y,z) = t^2 + u^2 + v^2 - auvt + \frac{1}{1-a} \tag{8.39}$$

is 3*-positive definite.*

Proof. Due to rotational invariance, we need only check one value of z. Let $z = e_1$. We have that

$$\begin{aligned}
K(x,y,e_1) &= \langle x,y\rangle^2 + x_1^2 + y_1^2 - ax_1y_1\langle x,y\rangle + \frac{1}{1-a} \\
&= \left(\langle x,y\rangle^2 - ax_1y_1\langle x,y\rangle - (1-a)x_1^2y_1^2\right) + (1-a)x_1^2y_1^2 + x_1^2 + y_1^2 + \frac{1}{1-a} \\
&= \left(\langle x,y\rangle^2 - ax_1y_1\langle x,y\rangle - (1-a)x_1^2y_1^2\right) \\
&\quad + \left(x_1^2\sqrt{1-a} + \frac{1}{\sqrt{1-a}}\right)\left(y_1^2\sqrt{1-a} + \frac{1}{\sqrt{1-a}}\right) \\
&= \sum_{j=2}^{d}\sum_{k=2}^{d} x_jy_jx_ky_k + (2-a)\sum_{m=2}^{d} x_1y_1x_my_m \\
&\quad + \left(x_1^2\sqrt{1-a} + \frac{1}{\sqrt{1-a}}\right)\left(y_1^2\sqrt{1-a} + \frac{1}{\sqrt{1-a}}\right).
\end{aligned}$$

We quickly see that for any finite signed Borel measure $\nu \in \mathscr{M}(\mathbb{S}^{d-1})$,

$$\begin{aligned}
\int_{\mathbb{S}^{d-1}}\int_{\mathbb{S}^{d-1}} K(x,y,e_1)d\nu(x)d\nu(y) &= \sum_{j=2}^{d}\sum_{k=2}^{d}\Big(\int_{\mathbb{S}^{d-1}} x_jx_kd\nu(x)\Big)^2 + (2-a)\sum_{m=2}^{d}\Big(\int_{\mathbb{S}^{d-1}} x_1x_md\nu(x)\Big)^2 \\
&\quad + \Big(\int_{\mathbb{S}^{d-1}} \Big(x_1^2\sqrt{1-a} + \frac{1}{\sqrt{1-a}}\Big)d\nu(x)\Big)^2 \geq 0,
\end{aligned}$$

hence, K is 3-positive definite. □

Lemma 8.5.4. *For $a \leq 1$, $K(x,y,z) = t^2 + u^2 + v^2 - auvt$ is conditionally 3-positive definite.*

Proof. For $a < 1$, according to Lemma 8.5.3, $K + \frac{1}{1-a}$ is 3-positive definite. Thus, for any fixed $z \in \mathbb{S}^{d-1}$ and any $\nu \in \mathscr{M}(\mathbb{S}^{d-1})$ with $\nu(\mathbb{S}^{d-1}) = 0$,

$$I_{K_z}(\nu) = I_{K_z + \frac{1}{1-a}}(\nu) \geq 0,$$

i.e. K is conditionally 3-positive definite. Lemma 8.1.3 then gives the result for $a = 1$. □

8.6 Some Counterexamples

While our results provide new and less complicated means to determine minimizers for a wide range of kernels, it is clear that more general ideas are necessary to categorize all kernels on the sphere for which σ is a minimizer. In this subsection, we present naturally arising kernels on the sphere which are *not* conditionally 3-positive definite on the sphere, but yet the three-input energies generated by these kernels are minimized by the uniform measure σ.

The semidefinite programming methods of Bachoc and Vallentin [BV08], which we will discuss in Section 8.7 in the context relevant to this paper, are more computationally difficult than ours, and would likely be infeasible for non-polynomial kernels in the context relevant to this paper. At the same time, they apply to certain functions which are not covered by our methods from Section 8.4. In particular, Theorem 8.7.1 shows that the energies with kernels given by polynomials

$$S^d_{0,1,1}(x,y,z) = uv + vt + tu \tag{8.40}$$

and

$$S^d_{1,0,0}(x,y,z) = (t-uv) + (u-vt) + (v-tu) \tag{8.41}$$

are both minimized by σ. However, neither function is conditionally 3-positive definite, as we demonstrate below. This implies that the converse to Theorem 8.4.1 does not hold. In addition, the potential of both kernels with respect to σ is a positive definite two-input kernel, which provides evidence that this might indeed be the correct necessary and sufficient condition for σ to minimize the three-input energy (see the discussion before Theorem 8.4.3).

The former example (8.40) is particularly interesting, since the energy functional with this kernel is convex at the minimizer σ, which suggests that conditional n-positive definiteness and convexity of the energy functional are perhaps not equivalent for $n \geq 3$, unlike the two-input case (see Proposition 3.1.6). We summarize these properties in the following proposition:

Proposition 8.6.1. *Let* $\Omega = \mathbb{S}^{d-1}$ *and set*

$$K(x,y,z) = S^d_{0,1,1}(x,y,z) = uv + vt + tu.$$

The kernel K satisfies the following:

1. *the uniform measure* σ *minimizes the energy* I_K*,*
2. *the energy functional* I_K *is convex at* σ*,*
3. $U^\sigma_K(x,y)$ *is positive definite,*
4. *K is not conditionally* 3*-positive definite.*

Proof. As mentioned above, part (1) follows from the semidefinite programming method as stated in Theorem 8.7.1. However, there is also a simple direct proof of this fact. Observe that by symmetry, for any $\nu \in \mathbb{P}(\mathbb{S}^{d-1})$,

$$I_K(\nu) = 3 \int\limits_{\mathbb{S}^{d-1}} \left(\int\limits_{\mathbb{S}^{d-1}} \langle x,y \rangle d\nu(x) \right)^2 d\nu(y) \geq 0 = I_K(\sigma). \tag{8.42}$$

We now turn to parts (2) and (3). We first note that

$$U^\sigma_K(x,y) = \int\limits_{\mathbb{S}^{d-1}} \langle z,x \rangle \langle y,z \rangle d\sigma(z) = \frac{1}{d} \langle x,y \rangle,$$

which follows from Corollary 2.5.2. Hence, the kernel $U^\sigma_K(x,y)$ is positive definite, i.e. (3) holds. Therefore σ minimizes the two-input energy with this kernel, i.e., for any $\nu \in \mathbb{P}(\mathbb{S}^{d-1})$,

$$I_{U^\sigma_K}(\nu) = I_K(\nu,\nu,\sigma) \geq I_{U^\sigma_K}(\sigma) = I_K(\sigma) = 0.$$

Observe also that $U_K^{\sigma^2}(x) = 0$ and thus $I_K(\sigma, \sigma, \nu) = 0$.

For an arbitrary $\nu \in \mathbb{P}(\mathbb{S}^{d-1})$ and $t \in [0,1]$, define $\sigma_t = (1-t)\sigma + t\nu$. Then

$$\begin{aligned} I_K(\sigma_t) &= (1-t)^3 I_K(\sigma) + 3(1-t)^2 t I_K(\sigma,\sigma,\nu) + 3(1-t)t^2 I_K(\nu,\nu,\sigma) + t^3 I_K(\nu) \\ &= 3(1-t)t^2 I_K(\nu,\nu,\sigma) + t^3 I_K(\nu). \end{aligned}$$

If $I_K(\nu) > 0$, we can choose t_ν sufficiently small so that for all $t \in (0, t_\nu)$, we have $I_K(\nu,\nu,\sigma) \le \frac{1+t}{3t} I_K(\nu)$, since the right-hand side goes to $+\infty$ as $t \to 0$. Then

$$I_K(\sigma_t) \le (1-t^2) t I_K(\nu) + t^3 I_K(\nu) = t I_K(\nu) = t I_K(\nu) + (1-t) I_K(\sigma).$$

It remains to consider the case $I_K(\nu) = 0$. According to (8.42), in this situation, $\int\limits_{\mathbb{S}^{d-1}} \langle x, y \rangle d\nu(x) = 0$ for ν-a.e. $y \in \mathbb{S}^{d-1}$, and therefore

$$\int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} \langle x, y \rangle d\nu(x) d\nu(y) = 0.$$

But this implies that

$$I_K(\nu,\nu,\sigma) = I_{U_K^\sigma}(\nu) = \int\limits_{\mathbb{S}^{d-1}} \int\limits_{\mathbb{S}^{d-1}} \frac{1}{d} \langle x, y \rangle d\nu(x) d\nu(y) = 0.$$

Thus, when $I_K(\nu) = 0$, we have

$$I_K(\sigma_t) = 3(1-t)t^2 I_K(\nu,\nu,\sigma) + t^3 I_K(\nu) = 0 = (1-t) I_K(\sigma) + t I_K(\nu)$$

for all $t \in [0,1]$. This finishes the proof that I_K is convex at σ.

Finally, we show that I_K is not conditionally 3-positive definite, i.e. part (4). Taking

$\mu = \delta_{e_2} - \delta_{-e_1}$ and $z = e_1$, a straightforward computation shows that

$$I_{K_z}(\mu) = I_K(\delta_{e_1}, \mu, \mu) = -1 < 0,$$

which proves our claim. □

The behavior of the kernel $S^d_{1,0,0}$ is somewhat different.

Proposition 8.6.2. *Let* $\Omega = \mathbb{S}^{d-1}$ *and set*

$$K(x,y,z) = S^d_{1,0,0}(x,y,z) = (t - uv) + (u - vt) + (v - tu).$$

The kernel K satisfies the following:

1. *the uniform measure σ minimizes the energy I_K,*
2. *the energy functional I_K is not convex at σ,*
3. *K is not conditionally 3-positive definite,*
4. *$U^\sigma_K(x,y)$ is positive definite.*

Proof. As in Proposition 8.6.1, part (1) follows from Theorem 8.7.1. For part (2), we see that since

$$I_K(\delta_{e_1}, \delta_{e_1}, \sigma) = \int_{\mathbb{S}^{d-1}} (1 - z_1^2) d\sigma(z) > 0 = I_K(\sigma) = I_K(\sigma, \sigma, \delta_{e_1}) = I_K(\delta_{e_1}),$$

we have that for all $t \in (0,1)$,

$$I_K(t\delta_{e_1} + (1-t)\sigma) = 3t^2(1-t) I_K(\delta_{e_1}, \delta_{e_1}, \sigma) > t I_K(\delta_{e_1}) + (1-t) I_K(\sigma),$$

so I_K is not convex at σ, and therefore K is not conditionally 3-positive definite, according to Corollary 8.2.7. Applying Corollary 2.5.2, we find that

$$U_K^{\sigma}(x,y) = \int_{\mathbb{S}^{d-1}} \langle x,y\rangle - \langle x,z\rangle\langle z,y\rangle d\sigma(z) = \frac{d-1}{d}\langle x,y\rangle,$$

is indeed positive definite. □

This shows that convexity of I_K at σ and the fact that σ is a minimizer of I_K are not equivalent for three-input energies, unlike in the classical two-input case (see Theorem 3.3.1).

Our remaining two functions arise from geometric problems and are the focus of Section 8.8, where we shall demonstrate that the corresponding energies are nevertheless minimized by the uniform measure σ (Theorems 8.8.1 and 8.8.4). These three-input kernels are related to the volume of the parallelepiped spanned by three unit vectors and the area of the triangle defined by three points on the sphere. We start with the former.

Proposition 8.6.3. *Assume $d \geq 3$, and let $V(x,y,z)$ be the volume of the parallelepiped spanned by the vectors $x,y,z \in \mathbb{S}^{d-1}$. Define the kernel $K(x,y,z) = -V^2(x,y,z)$. Then K is not conditionally 3-positive definite.*

Proof. It is well-known that the volume squared of the parallelepiped spanned by three vectors is given by the determinant of their Gram matrix, i.e.

$$V^2(x,y,z) = \det\begin{pmatrix} 1 & u & v \\ u & 1 & t \\ v & t & 1 \end{pmatrix} = 1 - u^2 - v^2 - t^2 + 2uvt.$$

Fixing $z = e_1$, we find that $K_{e_1}(x,y) = t^2 + y_1^2 + x_1^2 - 2tx_1y_1 - 1$. It is easy to check that $K_{e_1}(e_1,e_1) = K_{e_1}(e_1,y) = K_{e_1}(x,e_1) = 0$ and hence

$$K_{e_1}(x,y) + K_{e_1}(e_1,e_1) - K_{e_1}(e_1,y) - K_{e_1}(x,e_1) = K_{e_1}(x,y). \tag{8.43}$$

Taking $\nu = \delta_{e_2} + \delta_{e_3}$, one can compute

$$I_{K_{e_1}}(\nu) = -2 < 0,$$

i.e. K_{e_1} is not positive definite. Lemma 2.2.6 and (8.43) then tell us that K_{e_1} is not conditionally positive definite and thus K is not conditionally 3-positive definite. □

We now turn to area squared of a triangle and prove an analogous statement.

Proposition 8.6.4. *Assume that $d \geq 2$. Let $A(x,y,z)$ be the area of the triangle with vertices at $x,y,z \subset \mathbb{S}^{d-1}$ and set $K(x,y,z) = -A^2(x,y,z)$. Then K is not conditionally 3-positive definite.*

Proof. Using Heron's formula or linear algebra, see (8.53), one can compute that

$$A^2(x,y,z) = \frac{3}{4} - \frac{1}{2}(u+v+t) + \frac{1}{2}(uv+vt+tu) - \frac{1}{4}(u^2+v^2+t^2).$$

Fixing $z = e_1$, we find that

$$4K_{e_1}(x,y) = t^2 + x_1^2 + y_1^2 + 2t + 2x_1 + 2y_1 - 2x_1y_1 - 2tx_1 - 2ty_1 - 3.$$

The rest of the argument almost repeats the proof of Proposition 8.6.3: we have that

$$K_{e_1}(x,y) + K_{e_1}(e_1,e_1) - K_{e_1}(e_1,y) - K_{e_1}(x,e_1) = K_{e_1}(x,y), \tag{8.44}$$

as well as

$$I_{K_{e_1}}(\delta_{e_2} + \delta_{-e_1}) = -2 < 0,$$

and an application of Lemma 2.2.6 finishes the proof. □

8.7 Semidefinite Programming

The semidefinite programming method is a powerful and delicate tool that has been successfully applied to numerous optimization problems on the sphere [BV08, CW12, dLMdOFV, Mus14]. Some intrinsic features of the method (the so-called three-point bounds or, more generally, k-point bounds [CW12, dLMdOFV]) naturally give rise to certain multi-input energies. Thus, it comes as no surprise that this method is also useful in our context.

We briefly recall some of the main notions of the method. We start with the fundamental class of polynomials constructed by Bachoc and Vallentin in [BV08]. The role of these polynomials in semidefinite programming is similar to that of the classical Gegenbauer polynomials in linear programming. The construction starts with a class of infinite matrices and associated polynomials of the form

$$(Y_k^d)_{i+1,j+1}(x,y,z) := Y_{k,i,j}^d(x,y,z) := \lambda_{i,j}^{k,d} P_i^{d+2k}(u) P_j^{d+2k}(v) Q_k^d(u,v,t), \tag{8.45}$$

where $k,i,j \in \mathbb{N}_0$, P_m^h is the Gegenbauer polynomial of degree m on $\mathbb{S}^{h-1}$, normalized so that $P_m^h(1) = 1$, i.e. $P_m^h = C_m^{(\frac{h-3}{2},\frac{h-3}{2})}$,

$$\lambda_{i,j}^{k,d} := \frac{A_{d-1}}{A_{d-2}} \frac{A_{d+2k-2}}{A_{d+2k-1}} \big(\dim(\mathscr{H}_i^{d+2k}) \dim(\mathscr{H}_j^{d+2k}) \big)^{1/2}$$

(recall that A_{h-1} is the surface area of $\mathbb{S}^{h-1}$ and $\mathscr{H}_n^h$ is the space of spherical harmonics of degree n on $\mathbb{S}^{h-1}$), and

$$Q_k^d(u,v,t) = ((1-u^2)(1-v^2))^{\frac{k}{2}} P_k^{d-1} \left(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}} \right).$$

Below we provide the upper left 3×3, 2×2, and 1×1 submatrices of infinite matrices Y_0^d, Y_1^d, and Y_2^d, respectively, which is all that will be needed for the geometric results in

Section 8.8:

$$\begin{pmatrix} 1 & \sqrt{d}v & \sqrt{\frac{(d+1)d}{2}-1}\,\frac{dv^2-1}{d-1} \\ \sqrt{d}u & duv & \sqrt{\frac{(d+1)d^2}{2}-d}\,u\frac{dv^2-1}{d-1} \\ \sqrt{\frac{(d+1)d}{2}-1}\,\frac{dv^2-1}{d-1} & \sqrt{\frac{(d+1)d^2}{2}-d}\,\frac{du^2-1}{d-1}v & \left(\frac{(d+1)d}{2}-1\right)\frac{du^2-1}{d-1}\frac{dv^2-1}{d-1} \end{pmatrix}$$

$$\begin{pmatrix} \frac{d}{d-1}(t-uv) & \frac{d\sqrt{d+2}}{d-1}u(t-uv) \\ \frac{d\sqrt{d+2}}{d-1}v(t-uv) & \frac{d(d+2)}{d-1}uv(t-uv) \end{pmatrix}, \left(\frac{d(d+2)}{(d-1)(d+1)} \frac{(d-1)(t-uv)^2-(1-u^2)(1-v^2)}{d-2} \right).$$

Note that the polynomials comprising these matrices are not symmetric. Averaging over all permutations π of the variables x, y, and z, one obtains the following symmetric matrices and associated polynomials

$$(S_k^d)_{i+1,j+1}(x,y,z) := S_{k,i,j}^d(x,y,z) := \frac{1}{6}\sum_{\pi} Y_{k,i,j}^d(\pi(x),\pi(y),\pi(z)). \tag{8.46}$$

These polynomials and matrices have a variety of nice properties, which we summarize below in the form pertinent to our discussion. In [BV08], all the results are stated for discrete energies of points set. However, the extension to energy integrals and measures, which we need, follows immediately from the weak* density of discrete measures in $\mathbb{P}(\mathbb{S}^{d-1})$. The following statements hold:

- For any $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ and $e \in \mathbb{S}^{d-1}$, the infinite matrices

$$\int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} Y_k^d(x,y,e)\,d\mu(x)\,d\mu(y)$$

and

$$S_k^d(\mu) := \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} S_k^d(x,y,z)\,d\mu(x)\,d\mu(y)\,d\mu(z)$$

are positive semidefinite (to be more precise, all finite principal minors are positive semidefinite).

- For $(k,i,j) \neq (0,0,0)$, we have $I_{S^d_{k,i,j}}(\sigma) = 0$ and $I_{Y^d_{k,i,j}}(\sigma,\sigma,\delta_e) = 0$ for all $e \in \mathbb{S}^{d-1}$.

- For $k \geq 1$ and any $e \in \mathbb{S}^{d-1}$, one has $I_{S^d_{k,i,j}}(\delta_e) = I_{Y^d_{k,i,j}}(\delta_e) = 0$.

Consider an infinite, symmetric, positive semidefinite matrix A with finitely many nonzero entries. Then for any $k \geq 1$ and $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$, one easily sees that $\mathrm{tr}(S^d_k(\mu)A) \geq 0$, with equality if $\mu = \sigma$. Likewise, when $k = 0$, if A_0 is an infinite, positive semidefinite matrix A with finitely many nonzero entries and such that all entries in the first row and first column are zeros, then $\mathrm{tr}(S^d_0(\mu)A_0) \geq 0$ for any probability measure μ, with equality if $\mu = \sigma$. (Requiring zeros in the first row and column guarantees that equality for $\mu = \sigma$; due to the fact that $S^d_{0,0,0}$ is a constant, equality might not be achieved otherwise.) This yields the following sufficient condition for σ to be a minimizer of a three-input energy integral I_K.

Theorem 8.7.1. *Let $m \in \mathbb{N}_0$. For each $k \leq m$, let A_k be an infinite, symmetric, positive semidefinite matrix with finitely many nonzero entries, with the additional requirement that A_0 has only zeros in its first row and first column. Let*

$$K(x,y,z) = C + \sum_{k=0}^{m} \mathrm{tr}(S^d_k(x,y,z), A_k), \tag{8.47}$$

where C is an arbitrary constant. Then σ minimizes I_K in $\mathbb{P}(\mathbb{S}^{d-1})$.

Under appropriate convergence assumptions, the theorem also holds with $m = \infty$. Notice that the fact that σ minimizes the energies with kernels (8.40) and (8.41) immediately follows from Theorem 8.7.1. In general, in order to apply Theorem 8.7.1, one needs to represent the kernel in the form (8.47) – a task which becomes more complex as m grows.

8.8 Results in Probabilistic Geometry

Riesz s-energies with the kernel $K(x,y) = \|x-y\|^{-s}$, discussed in Section 2.1, are one of the most important classes of two-input energies. In particular, when $s = -1$, maximizing the sum of distances between points on various spaces (as well as corresponding distance integrals) is a classical optimization problem from metric geometry [AS74, Bjö56, FT56]. One can construct interesting multi-input analogues of Riesz energies by replacing the distance with other geometric characteristics which depend on n points, such as area and volume.

For $n = 3$, some of the most natural examples include the area of the triangle generated by three points or the volume of the tetrahedron (or the parallelepiped) spanned by three vectors. This can be generalized to higher values of n by considering volumes of various simplices or polytopes generated by n points or vectors.

It is reasonable to conjecture that on the sphere, energy integrals with these three-input kernels (namely, the area of the triangle and the volume of the parallelepiped) are *maximized* by the uniform measure σ. Probabilistically, this can be reformulated in the following way: assume that three random points are chosen on the sphere $\mathbb{S}^{d-1}$ independently according to a probability distribution μ. The conjecture then states that the expected value of these geometric quantities is maximized when the distribution μ is uniform, i.e. $\mu = \sigma$. The question was posed in this form in [Rom19].

This conjecture is supported, among other reasons, by the fact that for the classical case $n = 2$, the analogous kernels $|\sin(\arccos\langle x, y\rangle)| = \sqrt{1-t^2}$ and $\|x-y\| = \sqrt{2-2t}$ (i.e. the area of the parallelogram spanned by vectors x and y and the Euclidean distance between x and y, respectively) are both negative definite kernels on the sphere (up to an additive constant), and hence the corresponding two-input energies are maximized by σ.

In this section, we verify the conjecture above for the slightly different, yet closely related kernels V^2 and A^2: the *squares* of the aforementioned volume and area. In these cases, the kernels are multivariate polynomials, which substantially simplifies the analysis. For both kernels, we provide two proofs: one based on the semidefinite programming methods as outlined in Section 8.7, the other a more direct proof based on geometry and linear algebra.

Volume of the Tetrahedron/Parallelepiped

Let $V(x,y,z)$ denote the three-dimensional volume of the parallelepiped spanned by the vectors x, y, $z \in \mathbb{S}^{d-1}$. (Observe that the volume of the tetrahedron with vertices at x, y, z, and the origin is given by $\frac{1}{6}V(x,y,z)$.) The square of the volume $V(x,y,z)$ is given by the determinant of the Gram matrix. Thus we consider the kernel

$$K(x,y,z) = V^2(x,y,z) = \det \begin{pmatrix} 1 & t & u \\ t & 1 & v \\ u & v & 1 \end{pmatrix} = 1 - t^2 - u^2 - v^2 + 2tuv, \tag{8.48}$$

where, as before, we set $t = \langle x,y \rangle$, $u = \langle x,z \rangle$, $v = \langle z,y \rangle$.

As shown by Proposition 8.6.3, the kernel $-V^2$ is not conditionally 3-positive definite. Nevertheless, we shall show that σ is a minimizer of I_{-V^2}, i.e. a maximizer of $I_K = I_{V^2}$.

One can check directly that

$$\begin{aligned} K(x,y,z) = \frac{(d-1)(d-2)}{d^2} &- \frac{2(d-2)}{d^2(d+2)} S_{0,2,2} \\ &- \frac{4(d-1)(d-2)}{d^2(d+2)} S_{1,1,1} - \frac{(3d-4)(d+1)(d-2)}{d^2(d+2)} S_{2,0,0}, \end{aligned} \tag{8.49}$$

hence, Theorem 8.7.1 implies that σ is a maximizer of I_K.

Theorem 8.8.1. *Assume that $d \geq 3$ and $\Omega = \mathbb{S}^{d-1}$. Let $K(x,y,z) = V^2(x,y,z) = 1 - t^2 - u^2 - v^2 + 2uvt$. Then σ is a maximizer of I_K over $\mathbb{P}(\mathbb{S}^{d-1})$.*

Moreover, since K in this case is a polynomial of degree two in every variable, and has no linear terms, any isotropic measure on the sphere, i.e., any measure $\mu \in \mathbb{P}(\mathbb{S}^{d-1})$ satisfying $\int\limits_{\mathbb{S}^{d-1}} xx^T d\mu(x) = \frac{1}{d} I_d$, is also a maximizer, and in fact this classifies all maximizers.

This statement can be generalized to a higher number of inputs. As discussed in Section 6.5, we may consider optimization for probability measures on $\mathbb{R}^d$ with the additional normalizing condition: $\int\limits_{\mathbb{R}^d} \|x\|^2 d\mu(x) = 1$. As before, we will denote the space of such measures by $\mathbb{P}^*(\mathbb{R}^d)$, and we say that $\mu \in \mathbb{P}(\mathbb{R}^d)$ is an isotropic measure if $\int\limits_{\mathbb{R}^d} xx^T d\mu(x) = \frac{1}{d} I_d$. One can easily see that any isotropic measure $\mu \in \mathbb{P}(\mathbb{R}^d)$ satisfies the normalizing condition as well, i.e. $\mu \in \mathbb{P}^*(\mathbb{R}^d)$.

Let $3 \leq n \leq d$ and consider the n-input kernel $K(x_1, \ldots, x_n)$ defined as the determinant of the Gram matrix of the set of vectors $\{x_1, \ldots, x_n\} \subset \mathbb{R}^d$. Observe that for $n = 3$, this coincides with the 3-input kernel (8.48). The following result contains Theorem 8.8.1 as a special case. The case $n = d$ has been proved by Rankin [Ran56] and the general case is due to Cahill and Casazza [CC].

Theorem 8.8.2. *Let $d \geq 3$ and let the n-input kernel K be as defined above. Then the set of maximizing measures of I_K in $\mathbb{P}^*(\mathbb{R}^d)$ is the set of isotropic measures on $\mathbb{R}^d$. As a corollary, any isotropic measure on $\mathbb{S}^{d-1}$, in particular, the uniform surface measure σ, maximizes I_K over $\mathbb{P}(\mathbb{S}^{d-1})$.*

The proof of the case $n = d$ is particularly concise and elegant, so we include it below.

Proof. We start with the discrete case, which was considered in [Ran56]. Let $\mu \in \mathbb{P}^*(\mathbb{R}^d)$ be an equal-weight discrete measure, i.e. $\mu = \frac{1}{N} \sum \delta_{x_i}$, with support consisting of $N \geq d$ vectors $x_1, \ldots, x_N$. Let D be a matrix formed by these vectors as columns. The normalization condition then implies that $\mathrm{tr}(DD^T) = \mathrm{tr}(D^T D) = \sum \|x_i\|^2 = N$.

We denote the set of all d-subsets of $\{1, \ldots, N\}$ by $[N]_d$ and set $[d] = \{1, \ldots, d\}$. For two sets of indices $S_1 \subset [d]$ and $S_2 \subset [N]$, let D_{S_1,S_2} stand for the minor of D defined by rows with indices in S_1 and columns with indices in S_2. Observe that for $S = \{i_1, \ldots, i_d\} \in [N]_d$, the kernel K satisfies

$$K(x_{i_1}, \ldots, x_{i_d}) = \det\big((D^T)_{[d],S} D_{S,[d]}\big) = \det^2(D_{[d],S}).$$

Therefore, the energy can be expressed as

$$I_K(\mu) = E_K\big(\{x_i\}_{i=1}^N\big) = \frac{d!}{N^d} \sum_{S \in [N]_d} \det^2(D_{[d],S}) = \frac{d!}{N^d} \sum_{S \in [N]_d} \det(D_{[d],S}) \det((D^T)_{S,[d]}).$$

By the Cauchy–Binet formula, the sum above is just $\det(DD^T)$, i.e.

$$I_K(\mu) = \frac{d!}{N^d}\det(DD^T).$$

The matrix DD^T is positive definite, hence all eigenvalues are nonnegative, and their sum equals $\mathrm{tr}(DD^T) = N$ due to the normalizing condition. Since the determinant of DD^T is the product of eigenvalues, by the geometric-arithmetic mean inequality, it satisfies

$$\det(DD^T) \le \left(\frac{\mathrm{tr}(DD^T)}{d}\right)^d = \left(\frac{N}{d}\right)^d. \tag{8.50}$$

Hence, the energy is bounded above by

$$I_K(\mu) = \frac{d!}{N^d}\det(DD^T) \le \frac{d!}{N^d}\left(\frac{N}{d}\right)^d = \frac{d!}{d^d}. \tag{8.51}$$

Equality in (8.50)–(8.51) is possible if and only if all eigenvalues of DD^T are equal to $\frac{N}{d}$, i.e. $DD^T = \frac{N}{d}I_d$, which is equivalent to the fact that μ is an isotropic measure, since for the discrete measure $\mu = \frac{1}{N}\sum \delta_{x_i} \in \mathbb{P}(\mathbb{S}^{d-1})$ we would have

$$\int\limits_{\mathbb{S}^{d-1}} xx^T d\mu(x) = \frac{1}{N}DD^T = \frac{1}{d}I_d.$$

Observe that this is equivalent to saying that the set $\{x_1,\dots,x_N\} \subset \mathbb{S}^{d-1}$ is a projective 1-design.

Since the right-hand side of (8.51) does not depend on N, one may easily pass from discrete to arbitrary measures μ, thus finishing the proof of the theorem. □

Area of the Triangle

We now turn to exploring the area $A(x,y,z)$ of the triangle with vertices x, y, and z. As in the previous section, rather than considering the spherical case directly, we shall consider probability measures μ on the whole space $\mathbb{R}^d$ which satisfy the normalizing condition $\int_{\mathbb{R}^d} \|x\|^2 d\mu(x) = 1$, i.e. measures in the class $\mathbb{P}^*(\mathbb{R}^d)$. It is a standard geometrical fact that

$$A^2(x,y,z) = \frac{1}{4}\big(\|y-x\|^2 \cdot \|z-x\|^2 - \langle y-x, z-x\rangle^2\big). \tag{8.52}$$

We shall keep the notation $t = \langle x,y\rangle$, $u = \langle x,z\rangle$, $v = \langle z,y\rangle$ despite the fact that the vectors $x,y,z \in \mathbb{R}^d$ do not necessarily lie on the sphere $\mathbb{S}^{d-1}$. A straightforward computation shows that

$$\begin{aligned} A^2(x,y,z) = &\ \frac{1}{4}(\|x\|^2\|y\|^2 + \|y\|^2\|z\|^2 + \|z\|^2\|x\|^2) \\ &+ \frac{1}{2}(uv + vt + tu) - \frac{1}{2}(t\|z\|^2 + v\|x\|^2 + u\|y\|^2) \\ &- \frac{1}{4}(u^2 + v^2 + t^2). \end{aligned} \tag{8.53}$$

We are now ready to prove that the expectation of the area of the triangle *squared* is maximized by isotropic measures with barycenter at zero – in particular, the uniform surface measure σ on the sphere $\mathbb{S}^{d-1}$ is a maximizer.

Theorem 8.8.3. *Suppose $d \geq 2$, and let $K : (\mathbb{R}^d)^3 \to \mathbb{R}$ be defined by $K(x,y,z) = A^2(x,y,z)$. Then μ is a maximizer of $I_K(\mu)$ over $\mathbb{P}^*(\mathbb{R}^d)$ if and only if μ is isotropic and has center of mass at the origin.*

Observe that for discrete measures, this condition yields exactly the weighted spherical 2-designs.

Proof. Fix an arbitrary measure $\mu \in \mathbb{P}^*(\mathbb{R}^d)$. First of all, observe that the normalizing condition implies that the first line in the representation (8.53) contributes the constant $\frac{3}{4}$ to the energy. Invoking the normalizing condition again, we observe that

$$\begin{aligned} I_{t\|z\|^2}(\mu) &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \langle x,y\rangle \|z\|^2 d\mu(x) d\mu(y) d\mu(z) \\ &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \langle x,y\rangle d\mu(x) d\mu(y) = \left\| \int_{\mathbb{R}^d} x\, \mu(x) \right\|^2. \end{aligned} \tag{8.54}$$

Furthermore, applying the Cauchy–Schwarz inequality and the normalization condition, we obtain

$$\begin{aligned} I_{tu}(\mu) &= \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \langle x,y\rangle\langle z,x\rangle d\mu(x)d\mu(y)d\mu(z) = \int\limits_{\mathbb{R}^d}\left\langle x, \int\limits_{\mathbb{R}^d} y d\mu(y)\right\rangle^2 d\mu(x) \\ &\leq \int\limits_{\mathbb{R}^d}\|x\|^2\cdot\left\|\int\limits_{\mathbb{R}^d} y d\mu(y)\right\|^2 d\mu(x) = \left\|\int\limits_{\mathbb{R}^d} y d\mu(y)\right\|^2 = I_{t\|z\|^2}(\mu). \end{aligned} \tag{8.55}$$

This inequality implies that the contribution of the two middle terms in the representation (8.53) is non-positive, i.e.

$$I_{\frac{1}{2}(uv+vt+tu)-\frac{1}{2}(t\|z\|^2+v\|x\|^2+u\|y\|^2)}(\mu) \leq 0,$$

and therefore,

$$I_K(\mu) \leq \frac{3}{4} - \frac{1}{4} I_{u^2+v^2+t^2}(\mu). \tag{8.56}$$

Finally, we have a well-known estimate for the frame energy (discussed in Section 6.1)

$$I_{t^2}(\mu) = \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \langle x,y\rangle^2 d\mu(x)d\mu(y) \geq \frac{1}{d}, \tag{8.57}$$

with the equality holding if and only if μ is isotropic. This can be inferred from Lemmas 6.1.3 and 6.5.1, but for completeness, we include a simple proof of (8.57):

$$\begin{aligned} \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \langle x,y\rangle^2 d\mu(x)d\mu(y) &= \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \sum_{i,j=1}^{d} x_i y_i x_j y_j d\mu(x)d\mu(y) \\ &= \sum_{i,j=1}^{d}\left(\int\limits_{\mathbb{R}^d} x_i x_j d\mu(x)\right)^2 \geq \sum_{i=1}^{d}\left(\int\limits_{\mathbb{R}^d} x_i^2 d\mu(x)\right)^2 \\ &\geq \frac{1}{d}\left(\sum_{i=1}^{d}\int\limits_{\mathbb{R}^d} x_i^2 d\mu(x)\right)^2 = \frac{1}{d}\left(\int\limits_{\mathbb{R}^d}\|x\|^2 d\mu(x)\right)^2 = 1, \end{aligned}$$

where we have dropped the off-diagonal terms and used the Cauchy–Schwarz inequality, which implies that equality holds if and only if $\int_{\mathbb{R}^d} xx^T d\mu(x) = \frac{1}{d} I_d$, i.e. μ is isotropic.

Putting together (8.56) and (8.57), we find that

$$I_K(\mu) \leq \frac{3}{4} - \frac{1}{4} I_{u^2+v^2+t^2}(\mu) \leq \frac{3}{4} - \frac{3}{4d} = \frac{3}{4}\frac{d-1}{d}.$$

The equality holds if and only if it holds in inequalities (8.55) and (8.57). In the latter case, it means that μ is isotropic. In the former, it means that, for μ-almost every $x \in \operatorname{supp}(\mu)$, the vector x is collinear to $\int y d\mu(y)$. However, if $\int y d\mu(y) \neq 0$ that would imply that the support of μ is contained in a one-dimensional subspace, which is impossible for an isotropic measure. Therefore, $\int y d\mu(y) = 0$, in other words, the center of mass of μ has to be at the origin. This finishes the proof of the theorem. $\square$

Theorem 8.8.3 immediately implies the characterization of the maximizers among probability measures on the sphere.

Theorem 8.8.4. *Suppose $d \geq 2$, and let $K : (\mathbb{S}^{d-1})^3 \to \mathbb{R}$ be defined by $K(x,y,z) = A^2(x,y,z)$. Then μ is a maximizer of $I_K(\mu)$ over $\mathbb{P}(\mathbb{S}^{d-1})$ if and only if μ is isotropic and has center of mass at the origin. In particular, the uniform measure σ maximizes I_K.*

We want to point out that this statement can also be proved using semidefinite programming. Representation (8.53) for x, y, $z \in \mathbb{S}^{d-1}$ yields

$$K(x,y,z) = A^2(x,y,z) = \frac{3}{4} - \frac{u+v+t}{2} + \frac{ut+uv+tv}{2} - \frac{u^2+t^2+v^2}{4}. \tag{8.58}$$

This kernel can be rewritten as

$$K = \frac{3(d-1)}{4d} - \frac{3(d+1)(d-2)}{4d(d+2)} S_{2,0,0} - \frac{3(d-1)}{2d} S_{1,0,0} - \frac{3(d-1)}{2d(d+2)} S_{1,1,1} - \frac{3}{2d(d+2)} S_{0,2,2},$$

and Theorem 8.7.1 then tells us that σ maximizes I_K. The fact that μ is isotropic and has center of mass at the origin is easily seen to be equivalent to the relation $\int_{\mathbb{S}^{d-1}} p(x)d\mu(x) = \int_{\mathbb{S}^{d-1}} p(x)d\sigma(x)$ for each polynomial p of degree two. Since K is a polynomial of degree two in each variable, the conclusion of Theorem 8.8.4 follows.

Discrete Maximizers

While the kernels given by the volume of the parallelepiped and the area of the triangle are far more complicated to deal with than their squares, the results of Theorems 8.8.1 and 8.8.4 can nevertheless be used to show that a regular simplex is optimal for discrete energies with these kernels when the number of points is $d+1$. We have the following general statement.

Theorem 8.8.5. *Let $d \geq n-1$ and let $B : (\mathbb{S}^{d-1})^n \to [0,\infty)$ be a symmetric, rotationally invariant polynomial of degree no more than two in each of its variables, with the property that if $x_i = x_j$ for some $i \neq j$, then $B(x_1, x_2, \ldots, x_n) = 0$. Assume further that σ is a maximizer of I_B over $\mathbb{P}(\mathbb{S}^{d-1})$.*

Let the function $f : [0,\infty) \to \mathbb{R}$ be concave, increasing, and right continuous at 0, and define the kernel $K(x_1, \ldots, x_n) = f(B(x_1, \ldots, x_n))$. If $N = d+1$, then the vertices of regular N-simplices inscribed in $\mathbb{S}^{d-1}$ with centers at the origin maximize the discrete energy $E_K(\omega_N)$ over all N-point configurations on the sphere.

Proof. Let $\omega_N = \{z_1, \ldots, z_N\}$ be an arbitrary point configuration on $\mathbb{S}^{d-1}$. Then we have

$$E_B(\omega_N) = \frac{1}{N^n} \sum_{m_1=1}^{N} \cdots \sum_{m_n=1}^{N} B(z_{m_1}, \ldots, z_{m_n}) \leq I_B(\sigma),$$

with equality occurring if the point configuration is a spherical 2-design. Since B is zero if two of its inputs are the same, we can restrict the sum to n-tuples with distinct entries.

Combining this with the fact that f is increasing and concave, we have

$$
\begin{aligned}
E_K(\omega_N) &:= \frac{1}{N^n} \sum_{j_1=1}^{N} \cdots \sum_{j_n=1}^{N} f(B(z_{j_1}, \dots, z_{j_n})) \\
&\le \frac{N(N-1)\cdots(N-n+1)}{N^n} f\left(\sum_{\substack{z_{j_1},\dots,z_{j_n} \in \omega_N \\ j_1,\dots,j_n \text{ distinct}}} \frac{B(z_{j_1}, \dots, z_{j_n})}{N(N-1)\cdots(N-n+1)} \right) \\
&= \frac{N(N-1)\cdots(N-n+1)}{N^n} f\left(\frac{N^n E_B(\omega_N)}{N(N-1)\cdots(N-n+1)} \right) \\
&\le \frac{N(N-1)\cdots(N-n+1)}{N^n} f\left(\frac{N^n I_B(\sigma)}{N(N-1)\cdots(N-n+1)} \right).
\end{aligned}
$$

The second inequality is achieved if ω_N is a spherical 2-design, in particular, if ω_N is a regular simplex. The first one becomes an equality if

$$
B(y_1, \dots, y_n) = \frac{N^n E_B(\omega_N)}{N(N-1)\cdots(N-n+1)}
$$

for all distinct $y_1, \dots, y_n \in \omega_N$. Since B is rotationally invariant, the simplex satisfies this condition as well. Hence, the regular simplex is a maximizer of E_K for $N = d+1$. □

Theorem 8.8.5 immediately applies to the energies considered in Theorems 8.8.1 and 8.8.4.

Corollary 8.8.6. *Let $K(x,y,z)$ denote the area of the triangle with vertices x,y,z or the volume of the parallelepiped spanned by x, y, and z. If $N = d+1$, then the regular N-simplices inscribed in $\mathbb{S}^{d-1}$ with centers at the origin maximize $E_K(\omega_N)$ over all N-point configurations on the sphere.*

Proof. From Theorems 8.8.4 and 8.8.1, we see that in both cases, $K^2(x,y,z)$ satisfies the conditions of Theorem 8.8.5. Setting $f(x) = \sqrt{x}$ in Theorem 8.8.5 finishes the proof. □

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