Semidefinite Programming Bounds for Energy Minimization on the Sphere

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Abstract

In this thesis, we present new results regarding the continuous energy minimization problem for two types of potentials on the sphere S^{n-1}, which generalize the case of Riesz s-energy. The first kind arises from the mixed Riesz s-potential involving both Euclidean and geodesic distances; the second is the three-point potential $A_s(x, y, z)$ defined by the areas of the triangle spanned by the three vertices x, y, z on the sphere. Specifically, for any dimension $n \geq 3$, we show that the energy $\mathcal{I}(n, A_s)$ is maximized by a discrete measure that is uniformly distributed over the vertices of a regular tetrahedron for $s = 4$ and over an equilateral triangle for $s \geq 6$. These problems are investigated and solved using linear and semidefinite programming bounds, building on the existing literature on packing and kissing number problems for spherical codes.

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Chapter 1

Introduction

1.1 Discrete Energy Minimization

In 1904, J.J. Thomson proposed the atomic model, asking how to distribute a finite number of electrons on the unit sphere S^2 to minimize the electrostatic potential energy. Although the physics model was replaced by quantum physics in the early 20th century, its mathematical interest was only beginning to develop the deep theory of extreme problems on spherical codes.

Without the restriction of the dimension and the specified Coulomb potential, the generalized Thomson problem is to determine all N-point configurations on the $(n-1)$-sphere in $\mathbb{R}^n$ such that the energy

$$\mathcal{E}(n, f, N) = \inf\left\{ \sum_{1\le i\ne j\le N} f(x_i, x_j) : \{x_i\}_{i=1}^{N} \subset S^{n-1} \right\}$$

corresponding to the Riesz s-potential

$$f(x, y) = \|x - y\|^s$$

is minimized as $s < 0$ or maximized as $s > 0$.

The energy minimization problem is closely related to other extreme problems in spherical codes, such as the optimal packing and kissing number problem. The optimal packing problem, or Tammes' problem, is to determine the N-point configuration $\{x_i\}_{i=1}^N \subset S^{n-1}$ such that the minimal value of $\min_{i \neq j} \|x_i - x_j\|$ is maximized, which is equivalent to the placing N congruent spherical caps on S^{n-1} so that the radius $\delta_{n,N}$ is maximized. One way to approach this problem is to minimize Riesz s-energy for each s through the convergence of the sequence

$$\lim_{s \to -\infty} \mathcal{E}(n, s, N)^{1/s} = \delta_{n,N}, \tag{1.1}$$

though it's not useful for most cases.

A more systematic and efficient approach to problems related to spherical codes was developed by Delsarte in his thesis [11] and his collaboration with Goethals and Seidel in 1977 [12]. This method utilizes a linear programming framework, including constraints based on Delsarte's inequality for any given point set on the sphere:

$$\sum_{(x,y) \in X^2} Q_k^n(\langle x, y \rangle) \geqslant 0 \quad \text{for any} \quad X \subset S^{n-1}.$$

Here, $Q_k^n : [-1, 1] \to \mathbb{R}$ represents the Gegenbauer polynomials of degree k, which form a rotationally invariant positive definite kernel on the sphere. One of its famous uses is to solve the kissing number problem in dimensions 8 and 24 [16]. For a given dimension n, the kissing number is the largest number of points that can be arranged on S^{n-1} so that the angle between each pair of points is greater than $60°$. Currently, the problem has only been solved in the dimensions $n = 1, 2, 3, 4, 8$ and 24, where the case of $n = 4$ was first proved by Musin [15] and can be efficiently solved by utilizing a semidefinite program.

The semidefinite programming bound, or the SDP bound, was first developed by Bachoc and Vallentin [1] in 2008 for the kissing number problem. Since then, several spherical codes have been proved optimal, which cannot be shown by the linear programming bound. For example, the 10-point spherical embedding of the complement of the Petersen graph on S^3 is optimal with the maximal inner product 1/6 [2], and the rhombic dodecahedron code is universally optimal in the projective space $\mathbb{RP}^2$ [9].

1.2 Continuous Energy Minimization

In virtue of measure theory, the discrete energy minimization can be regarded as the Lebesgue integral of the signed measure with mass distributed on a finite number of points on S^{n-1}. In this way, we can generalize the discrete energy problem to its continuous setting by defining the continuous energy of a Borel probability measure $\mu \in \mathcal{P}(S^{n-1})$ supported on the unit sphere S^{n-1} to be

$$I_{n,f}(\mu) = \int_{S^{n-1}} \int_{S^{n-1}} f(x,y) d\mu(x) d\mu(y),$$

and consider the minimization of the continuous energy

$$\mathcal{I}(n,f) = \inf\{I_{n,f}(\mu) : \mu \in \mathcal{P}(S^{n-1})\}$$

Denoting the discrete measure δ_x to be the measure of mass one at point $x \in S^{n-1}$, for any finite subset $X \subset S^{n-1}$, we can write

$$\frac{1}{|X|^2} \sum_{(x,y)\in X^2} f(x,y) = \int_{S^{n-1}} \int_{S^{n-1}} f(x,y) d\mu(x) d\mu(y)$$

where $\mu = \frac{1}{|X|}\sum_{x\in X}\delta_x$. Therefore, the discrete energy is included as a part of the continuous setting. It would be interesting to explore when the energy minimizer is discrete and when it is minimized by the uniform measure for the current potential.

In some cases, the continuous energy minimization can be solved by understanding the finite-point case. For instance, as the potential $f(x, y)$ is well-defined at $x = y$, the sequence of minimal discrete energy $\{\frac{\mathcal{E}(n,f,N)}{N(N-1)}\}_{N=2}^{\infty}$ is increasing in N. Moreover, if f is lower semi-continuous, the sequence converges to the minimal continuous energy $\mathcal{I}(n, f)$ (see Theorem 4.2.2 in [8]).

On the other hand, the linear programming bound for discrete minimal energy can be extended to the continuous setting without difficulty. For the two-point potential, an old theorem of Schoenberg [18] shows that a potential function on the sphere S^{n-1} is positive definite if and only if the Gegenbauer coefficients a_k in its Gegenbauer expansion

$$f(x, y) = \sum_{k=0}^{\infty} a_k Q_k^n(\langle x, y\rangle)$$

are all non-negative, which is equivalent to the situation when the energy $\mathcal{I}(n, f)$ is minimized by the uniform measure on the sphere.

For the Riesz s-potential, the function $f_s(x, y) = -\|x-y\|^s$ is strictly positive definite in the interval $0 < s < 2$, and hence the uniform measure minimizes the continuous energy $\mathcal{I}(n, f_s)$ regardless of the dimension n. As $s > 0$, the case is solved for any infinite compact set in $\mathbb{R}^n$ by Bjorck [7], where the pair of points giving the maximum distance among the set maximizes the Riesz s-energy for $s > 2$. In this case, there is only one simple jump in the optimal configuration at the power $s = 2$, which we call the *phase transition* of the energy problem. If the Euclidean distance in the Riesz s-energy is replaced by the geodesic distance $\arccos\langle x, y\rangle$, the phase transition comes to $s = 1$ with the same energy minimizer on both sides [3].

For multivariate potentials involving more than two points on the sphere, it remains unclear under what conditions the uniform measure minimizes the energy. In the study conducted by Bilyk et al. [6], the authors investigate geometric k-point potentials $V(x_1, \ldots, x_k)$ and $A(x_1, \ldots, x_k)$ on the sphere S^{n-1} as $n \geq k+1$. Here, $V(x_1, \ldots, x_k)$ is defined as the k-dimensional volume of the k-simplex spanned by the points $x_1, \ldots, x_k$ and the origin, while $A(x_1, \ldots, x_k)$ represents the $(k-1)$-dimensional volume of the $(k-1)$-simplex whose vertices are $x_1, \ldots, x_k$. In particular, the three-point potential $V(x, y, z)^s$ is maximized by a discrete measure uniformly distributed over the vertices of an orthonormal basis when $s > 2$, while it is maximized by the uniform measure when $s = 2$. In contrast, the potential $A(x, y, z)^s$ is only known to be maximized by the uniform measure when $s = 2$.

1.3 Main Results

In the present work, we consider the continuous energy maximization and estimate the existence of phase transitions as the power s varies for the following two potentials on the sphere S^{n-1}:

- the two-point potential mixing the Euclidean and geodesic distance

$$F_{\gamma,s}(x, y) = (\gamma\|x - y\| + (1 - \gamma) \arccos \langle x, y\rangle)^s$$

  with parameter $\gamma \in [0, 1]$ and the power $s > 0$.

- the three-point potential $A_s(x, y, z) = \text{area}(x, y, z)^s$, where $\text{area}(x, y, z)$ is the area of the triangle spanned by the three vertices x, y, z on the sphere.

In Chapter 2, we review the theory of the linear programming bound on two-point potentials and present numerical results for our mixed potential $F_{\gamma,s}(x, y)$. In Chapter

3, we review the semidefinite programming method and implement it for the three-point potential, showing that the continuous energy of $A_s(x, y, z)$ is maximized by a discrete measure that is uniformly distributed over the vertices of a regular tetrahedron for $s = 4$ and over an equilateral triangle for $s \geq 6$.

Chapter 2

Linear Programming Bound

The linear programming bound developed by Delsarte [11] in 1973 is based on the linear constraints of spherical codes, expressed as follows:

$$\sum_{(x,y)\in X^2} Q_k^n(\langle x,y\rangle) \geq 0$$

Here, Q_k^n represents the Gegenbauer polynomials of degree k on S^{n-1}. These polynomials serve as positive definite functions on the sphere and play a crucial role in extreme problems in discrete geometry.

In this chapter, we will first review the mechanics of linear programming bounds, particularly focusing on the rotationally invariant positive definite functions on the sphere. Next, we will apply this tool to two examples of Riesz s-energy, denoted as $F_s = \rho(x,y)^s$, where ρ is either the Euclidean or geodesic distances. Finally, we will examine the mixed potential:

$$F_{\gamma,s}(x,y) = \left(\gamma\sqrt{2-2\langle x,y\rangle} + (1-\gamma)\arccos\langle x,y\rangle\right)^s$$

which involves both types of distances. We will present numerical results on its phase transition using the linear programming bound and conjugate gradient descent.

2.1 Positive Definite Functions on the Sphere

A function $f : S^{n-1} \times S^{n-1} \to \mathbb{R}$ is called positive definite if for any sequence of points $\{x_i\}_{i=1}^N$ on the sphere S^{n-1} and $\{c_i\}_{i=1}^N \subset \mathbb{R}$, we have

$$\sum_{1 \leqslant i,j \leqslant N} c_i c_j f(x_i, x_j) \geq 0,$$

or equivalently, the matrix $(f(x_i, x_j))_{1 \leqslant i,j \leqslant N}$ is positive semidefinite. A quick example is the inner product $f(x, y) = \langle x, y \rangle$, where $(\langle x_i, x_j \rangle)_{1 \leqslant i,j \leqslant N}$ is the Gram matrix of $\{x_i\}_{i=1}^N$. If the potential f is continuous on $S^{n-1} \times S^{n-1}$, the weak* density of discrete measures in the space of signed finite regular Borel measures $\mathcal{M}(S^{n-1})$ implies that

$$I_{n,f}(\mu) = \int_{S^{n-1}} \int_{S^{n-1}} f(x, y) d\mu(x) d\mu(y) \geq 0 \tag{2.1}$$

for any $\mu \in \mathcal{M}(S^{n-1})$, where the converse is true by taking discrete measures in (2.1).

The investigation of positive definite functions began with Schoenberg in 1941, who explored the criteria for isometrically embedding point sets from any metric space into Euclidean space. His work demonstrated that Gegenbauer polynomials Q_k^n are positive definite on the sphere. Additionally, he showed that all rotationally invariant positive definite functions can be expressed as non-negative combinations of these Gegenbauer polynomials.

Theorem 2.1.1. *Let $f : S^{n-1} \times S^{n-1} \to \mathbb{R}$ be a rotationally invariant continuous function, i.e., $f(x, y) = F(\langle x, y \rangle)$ for each $x, y \in S^{n-1}$ for some $F \in C[-1, 1]$. The following conditions are equivalent:*

(i) f is positive definite on S^{n-1},

(ii) All the coefficients in the Gegenbauer expansion

$$f(x,y)=\sum_{n=0}^{\infty} a_k Q_k^n(\langle x,y\rangle)$$

are non-negative,

(iii) The energy $\mathcal{I}(n,f)$ is minimized by the uniform measure σ on S^{n-1}.

The equivalence of (i) and (ii) was established by Schoenberg [18], whereas (iii) is well-known and stated in the papers [4], [3], [6]. To derive the Gegenbauer polynomials in the theorem, it requires the representation theory of the rotation group $\mathcal{O}(n)$.

Now, let $f: S^{n-1}\times S^{n-1}\to\mathbb{R}$ be an $\mathcal{O}(n)$-invariant function and denote $f(x,y)=F(\langle x,y\rangle)$ for some $F\in C[-1,1]$. Then, we can define the linear operator on $L^2(S^{n-1})$

$$T_f(\psi)(x)=\int_{S^{n-1}} f(x,y)\psi(y)d\sigma(y)$$

for all $\psi\in L^2(S^{n-1})$. Based on the following lemma, it's enough for us to characterize all the positive operators on $L^2(S^{n-1})$.

Lemma 2.1.1. *The following properties are equivalent:*

(i) f is positive definite.

(ii) T_f is a positive operator, i.e., $\langle T_f(\psi),\psi\rangle_{L^2}\geq 0$ for all $\psi\in L^2(S^{n-1})$.

Next, recall that the space $L^2(S^{n-1})$ as a $\mathcal{O}(n)$-module has the irreducible orthogonal decomposition

$$L^2(S^{n-1})=\overset{\bullet}{\bigoplus_{k\geq 0}}\mathcal{H}_k^n \tag{2.2}$$

where $\mathcal{H}_k^n$ is the subspace of all harmonic polynomials on the sphere S^{n-1} of degree k. Since the linear operator T_f is commutative with the rotation action defined by $g.\psi(x) = \psi(gx)$, by Schur's Lemma, T_f must be a scalar multiple of the identity operator on each irreducible component

$$T_f|_{\mathcal{H}_k} = \lambda_k \mathrm{Id}_{\mathcal{H}_k}.$$

For each k, we denote $d_k = \dim\mathcal{H}_k^n = \binom{n+k-1}{k} + \binom{n+k-2}{k-1}$ and $\{Y_{k,j}^n\}_{j=1}^{d_k}$ to be an orthonormal basis of $\mathcal{H}_k$. By Stone-Weierstrass' Theorem, the union $\bigcup_k \mathcal{H}_k^n$ is dense in $\mathcal{C}(S^{n-1})$, and hense dense in $L^2(S^{n-1})$. Therefore, the set $\{Y_{k,j}^n : k = 0, 1, 2, ..., j = 1, 2, ..., d_k\}$ is a complete set of orthonormal basis on the space $L^2(S^{n-1})$.

Let $\mathrm{Proj}_k : L^2(S^{n-1}) \to \mathcal{H}_k$ be the orthogonal projection onto the component $\mathcal{H}_k$, and write

$$\mathrm{Proj}_k\psi(x) = \sum_{k=1}^{d_k} \langle \psi, Y_{k,j} \rangle_{S^{n-1}} Y_{k,j}^n(x) = \int_{S^{n-1}} \sum_{j=1}^{d_k} Y_{k,j}^n(x) Y_{k,j}^n(y) \psi(y) d\sigma(y).$$

The projection Proj_k becomes an integral operator with the (reproducing) kernel

$$q_k^n(x, y) = \sum_{j=1}^{d_k} Y_{k,j}^n(x) Y_{k,j}^n(y).$$

Note that the polynomial $q_k^n(x, y)$ is invariant under the rotation, that is, $q_k^n(gx, gy) = q_k^n(x, y)$ for any $g \in \mathcal{O}(n)$. We can replace the function $q_k^n(x, y)$ by $Q_k^n(\langle x, y \rangle)$, which only depends on the inner product of $x, y \in S^{n-1}$.

By changing the variables to the spherical coordinate, the integral of the rotationally invariant function reads

$$\int_{S^{n-1}} q_k^n(x, y) d\sigma(x) = \frac{\omega_{n-1}}{\omega_n} \int_{-1}^{1} Q_k^n(t)(1 - t^2)^{(n-3)/2} dt,$$

where ω_n is the surface area of S^{n-1}. In conjunction with the orthogonality of each subspace $\mathcal{H}_k^n \subset L^2(S^{n-1})$, we have

$$\begin{aligned}
\langle Q_i^n(\cdot, y), Q_j^n(\cdot, y)\rangle_{S^{n-1}} &= \int_{S^{n-1}} Q_i^n(\langle x, y\rangle) Q_j^n(\langle x, y\rangle) d\sigma(x) \\
&= \frac{\omega_{n-1}}{\omega_n} \int_{-1}^{1} Q_i^n(t) Q_j^n(t)(1-t^2)^{(n-3)/2} dt \\
&= \frac{\omega_{n-1}}{\omega_n} \langle Q_i^n, Q_j^n\rangle_{\omega_t}
\end{aligned}$$

Therefore, $\{Q_k^n\}_{k=0}^{\infty}$ is the family of orthogonal polynomials on the interval $[-1, 1]$ with respect to the inner product $\langle\ ,\ \rangle_{\omega_t}$ with weight $\omega(t) = (1-t^2)^{(d-3)/2}$, which is known as the Gegenbauer polynomials. For the unit sphere S^2, the functions are the Legendre polynomials. For the unit circle S^1, the corresponding functions are the Chebyshev polynomials of the first kind, given by $T_k(\cos\theta) = \cos(k\theta)$.

By a slight abuse of notation, we denote Q_k^n as the normalized Gegenbauer polynomials with $Q_k^n(1) = 1$ in the rest of the thesis. Additionally, we sometimes write $Q_k^n(x, y)$ to represent $Q_k^n(\langle x, y\rangle)$, emphasizing the points rather than their inner product. We finish this section by proving the equivalence of (ii) and (iii) in Theorem 2.1.1.

Theorem 2.1.2 (*Linear Programming Bound*)**.** *Let $f \in C[-1, 1]$ be a rotationally invariant potential on S^{n-1}, and $h \in C[-1, 1]$ be a positive definite function on S^{n-1}. That is, $h(t) = \sum_{k=0}^{\infty} h_k Q_k^n(t)$ and $h_k \geqslant 0$ for all $k \geqslant 1$. If $h(t) \leq f(t)$ for all $t \in [-1, 1]$, then for any $\mu \in \mathcal{P}(\Omega)$,*

$$I_{n,f}(\mu) \geqslant h_0 = I_{n,h}(\sigma),$$

where σ is the uniform measure on S^{n-1}. The equality holds if and only if f and h are identical.

Proof. Note that for $\mu \in \mathcal{P}(\Omega)$, we have

$$I_{n,f}(\mu) \geqslant I_{n,h}(\mu) \geqslant I_{n,h}(\sigma) = h_0.$$

The second inequality follows from the positive definiteness of Q_k^n in (2.1):

$$\begin{aligned} I_{n,h}(\mu) &= \int_{S^{n-1}} \int_{S^{n-1}} \sum_{k=0}^{\infty} h_k Q_k^n(x,y) d\mu(x) d\mu(y) \\ &= h_0 + \sum_{k=1}^{\infty} h_k \int_{S^{n-1}} \int_{S^{n-1}} Q_k^n(x,y) d\mu(x) d\mu(y) \\ &\geqslant h_0, \end{aligned}$$

and the equality follows the direct computation

$$I_{n,h}(\sigma) = \frac{\omega_{n-1}}{\omega_n} \int_{-1}^{1} h(t) Q_0^n(t)(1-t^2)^{(n-3)/2} dt = h_0.$$

□

2.2 Riesz s-Energy with Euclidean and Geodesic Distance

In this section, we recall the phase transition of the Riesz s-potential $f_s(x,y) = \rho(x,y)^s$ in the case when s is positive, and $\rho(x,y)$ is the Euclidean or the geodesic distance. Although these two metrics on the sphere have the same topology, their maximizers differ in the range $1 < s < 2$.

For the power $s > 0$, we consider the maximization of the energy $\mathcal{I}(n, f_s)$ instead of the minimum. Otherwise, the optimizer will be clustered into a single point, resulting in zero energy. Therefore, when applying the theorem, we'll consider the potential $-f(x,y)$, so we don't need to change the sign in the theorem.

Theorem 2.2.1 (Björck [7]). *Let $f_s(x,y) = \|x-y\|^s$ be the potential on the sphere S^{n-1}. Then, for any dimension $n \geq 2$, the continuous energy $\mathcal{I}(n, f_s)$ is maximized as follows:*

(i) For $0 < s < 2$, the uniform measure on the sphere is the unique maximizer.

(ii) For $s = 2$, it is maximized by all barycentric measures, i.e., measures with center of mass at the origin

$$\int_{S^{n-1}} x d\mu(x) = 0.$$

(iii) For $s > 2$, the discrete measure $\frac{1}{2}(\delta_x + \delta_{-x})$ for $x \in S^{n-1}$ is the unique maximizer.

Theorem 2.2.2 (Bilyk-Dai [3]). *Let $f_s(x,y) = \arccos(\langle x, y\rangle)^s$ be the potential on the sphere S^{n-1}. Then, for any dimension $n \geq 2$, the continuous energy $\mathcal{I}(n, f_s)$ is maximized as follows:*

(i) For $0 < s < 1$, the uniform measure on the sphere is the unique maximizer.

(ii) For $s = 1$, it is maximized by all centrally symmetric measures, in other words, $d\mu(x) = d\mu(-x)$.

(iii) For $s > 1$, the discrete measure $\frac{1}{2}(\delta_x + \delta_{-x})$ for $x \in S^{n-1}$ is the unique maximizer.

Instead of checking the Gegenbauer coefficients of the potentials for each dimension n, it's enough to consider the Maclaurin series of the potential on $[-1, 1]$ at once. Suppose that the potential has the expansion $f(t) = \sum_{k=0}^{\infty} a_n t^n$ with $a_k \geq 0$ for all k, then the mth Gegenbauer coefficient becomes

$$\int_{-1}^{1} f(t) Q_m^n(t)(1-t^2)^{(n-3)/2} dt = \sum_{k=0}^{\infty} a_k \int_{-1}^{1} t^k Q_m^n(t)(1-t^2)^{(n-3)/2} dt$$

Using the Rodrigues' formula for Gegenbauer polynomials and integration by parts, each term in the right-hand side is non-negative

$$\int_{-1}^{1} t^k \, Q_m^n(t) \, (1-t^2)^{(n-3)/2} \, dt = \begin{cases} > 0, & \text{if } k \geq m \text{ and } k-m \text{ is even,} \\ 0, & \text{otherwise.} \end{cases}$$

Therefore, by Theorem 2.1.1, the energy $\mathcal{I}(n, f)$ is minimized by the uniform measure and is independent of the dimension n. Moreover, the converse holds and was proved by Schoenberg.

Theorem 2.2.3 (Schoenberg [18])**.** *A potential $f : [-1, 1] \to \mathbb{R}$ is positive definite on S^{n-1} for all dimensions n if and only if all the coefficients a_n in the Maclaurin series*

$$f(t) = \sum_{k=0}^{\infty} a_k t^k$$

are non-negative.

Now, we are ready to prove Theorem 2.2.1 and 2.2.2 by calculating the Maclaurin series of the potentials. For the Riesz s-energy with Euclidean distance, we have

$$(2 - 2\langle x, y\rangle)^{s/2} = 2^{s/2}(1 - \langle x, y\rangle)^{s/2} = 2^{s/2} + 2^{s/2} \sum_{k=1}^{\infty} c_k(s/2)\langle x, y\rangle^k,$$

where we use the notation

$$c_k(x) = \frac{-x(1-x)(2-x)\cdots(k-1-x)}{k!}$$

for variable x. It is clear that the Taylor coefficients are strictly negative only as $s \in (0, 2)$, so the uniform measure is the unique maximizer. For the interval $s \in (2, \infty)$, we first note that the discrete measure $\frac{1}{2}(\delta_x + \delta_{-x})$ is also an energy maximizer as $s = 2$.

Thus, for any pair of points $x, y \in S^{n-1}$, we can rescaling the energy

$$f_2(x,y) \geq 2^{2-s} f_s(x,y)$$

with equality only as x, y are antipodal. As a result, for any $\mu \in \mathcal{P}(S^{n-1})$, the energy $I_{n,s}(\mu)$ is bounded above

$$2^{2-s} I_{n,s}(\mu) \leq I_{n,2}(\mu) \leq I_{n,2}(\sigma) \tag{2.3}$$

where the equality holds only as $\mu = \frac{1}{2}(\delta_x + \delta_{-x})$.

For the case of geodesic distance, we have

$$\arccos \langle x, y\rangle = \frac{\pi}{2} - \sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{4^n(2n+1)} \langle x, y\rangle^{2n+1} =: \frac{\pi}{2} - A(\langle x, y\rangle).$$

Note that all the coefficients in $A(t)$ are positive and bounded $|A(t)| \leq \pi/2$, so the geometric series gives

$$\arccos(\langle x, y\rangle)^s = (\pi/2)^s \left(1 - \frac{A(\langle x, y\rangle)}{\pi/2}\right)^s = (\pi/2)^s + (\pi/2)^s \sum_{k=1}^{\infty} c_k(s) \left(\frac{A(\langle x, y\rangle)}{\pi/2}\right)^k$$

Again, the signs of the coefficient and are all non-negative only as $0 < s < 1$, and the case $s > 1$ follows from the same argument as in (2.3).

2.3 Mixed Potential and its Phase Transitions

Based on the difference in the phase transition occurring in the previous section, we consider the mixed potential

$$F_{\gamma,s}(x,y) = \left(\gamma\sqrt{2 - 2\langle x, y\rangle} + (1-\gamma) \arccos\langle x, y\rangle\right)^s \tag{2.4}$$

constituted by the convex combination of Euclidean and geodesic distances, where the parameter $\gamma \in [0,1]$ and $s \in (0,\infty)$.

From the previous section, we know that $\mathcal{I}(n, F_{\gamma,s})$ is uniquely maximized by the uniform measure on S^{n-1} as $s \in (0,1]$, and by $\frac{1}{2}(\delta_x + \delta_{-x})$ as $s \in [2,\infty)$. It is interesting to ask how the phase transition behaves when the two distinct maximizers compete with each other. In this section, we use the linear programming bound to obtain an upper bound, and apply the *conjugate gradient descent* to find a numerical lower bound. At first glance, we thought that there should be a single phase transition moving from $s = 1$ to $s = 2$ gradually as the parameter γ decreases. However, a bunch of discrete measures other than the antipodal pair or the uniform measure turn out to be maximizers in the current range of s.

power s	maximizer μ	$I_{3,F_{0.5,s}}(\mu)$	$I_{3,F_{0.5,s}}(\frac{1}{2}(\delta_x + \delta_{-x}))$	$I_{3,F_{0.5,s}}(\sigma)$
1.28	antipodal pair	1.67439	1.67439	1.66061
1.27	octahedron	1.661502	1.65865	1.65239
1.26	octahedron	1.65188	1.64307	1.644233
1.25	octahedron	1.64232	1.62763	1.63614
1.24	octahedron	1.63282	1.61233	1.62810
1.23	octahedron	1.62340	1.59718	1.62012
1.22	cube	1.61407	1.58216	1.612198
1.21	icosahedron	1.60560	1.56730	1.60434
1.198	14 points	1.59560	1.54964	1.59498
1.195	dodecahedron	1.59317	1.54526	1.59265
1.19	22 points	1.58918	1.53798	1.58878

Table 2.1: Numerical lower bounds for $\mathcal{I}(3, F_{\gamma,s})$ as $\gamma = 0.5$

The following are the numerical experiments we have conducted, especially for the case $\gamma = 0.5$ and dimensions $n = 2, 3$.

(1) We first guess that the phase transition of each γ happens at some point $s_{\gamma,n} \in [1,2]$ such that the energy of the antipodal point is equal to the uniform measure. Thus, we consider the case of $\gamma = 0.5$, where $s_{0.5,3} \approx 1.26$. However, by applying

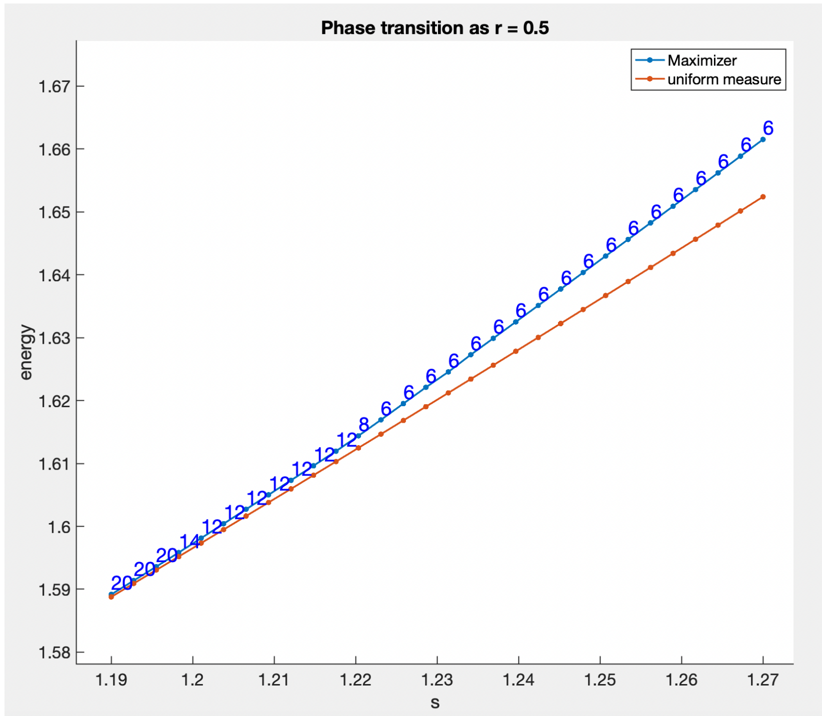

Figure 2.1: In the case $n = 3$, $\gamma = 0.5$, and $s \in [1.19, 1.27]$, several discrete numerical maximizers are found by the conjugate gradient descent method. These measures supported on a finite set of S^2 exhibit greater energy than the uniform measure and other discrete measures of small size (see Table 2.1). In the figure, the number next to each point indicates the support size of the discrete maximizer. In particular, the numbers 6, 8, 12, and 20 correspond to the octahedron, cube, icosahedron, and dodecahedron, respectively.

Theorem 2.1.2, the linear program for the mixed energy gives the upper bound $\mathcal{I}(3, F_{0.5,1.26}) \leq 1.6542$, where the degree of the auxiliary function is set to be 25. From Table 2.1, we see that the LP bound is closer to the energy of a discrete measure that is uniformly distributed on the six vertices of the octahedron.

(2) Based on the observation in (1), we implement the *conjugate gradient descent* method to find the numerical maximizers whose energy is greater than the one given by the uniform measure on S^2 and $\frac{1}{2}(\delta_x + \delta_{-x})$ as $s \leq s_{\gamma,3}$. The result of

the case $(\gamma, n) = (0.5, s)$ and $s \in [1.19, 1.28]$ are listed in the Table 2.1 and Figure 2.1. Surprisingly, as s decreases from $s_{0.5,3}$ to 1, the maximizer remains discrete, but the size of its support grows drastically as $s \to 1$.

(3) By checking the Gegenbauer coefficients of the potential $F_{\gamma,s}$ numerically, it appears that the function $-F_{\gamma,s}$ is not positive definite in the region $s \in (1, 2)$ and exhibits a sequence of negative coefficients at high orders.

(4) This phenomenon also appears in the case of the unit circle. See Table 2.2 and Figure 2.2 for the numerical results.

power s	maximizer μ	$I_{2,F_{0.5,s}}(\mu)$	$I_{2,F_{0.5,s}}(\frac{1}{2}(\delta_x + \delta_{-x}))$	$I_{2,F_{0.5,s}}(\sigma)$
1.28	antipodal pair	1.67439	1.67439	1.65825
1.27	square	1.66079	1.65865	1.64877
1.26	square	1.64967	1.64306	1.63937
1.25	square	1.63864	1.62762	1.63006
1.24	square	1.62769	1.61232	1.62082
1.23	square	1.61683	1.59717	1.61167
1.22	square	1.60606	1.58216	1.60260
1.21	hexagon	1.59613	1.56730	1.59360
1.20	hexagon	1.58642	1.55257	1.58468
1.19	octagon	1.57697	1.53797	1.57584
1.18	decagon	1.56778	1.52352	1.56708

Table 2.2: Numerical lower bounds for $\mathcal{I}(2, F_{\gamma,s})$ as $\gamma = 0.5$

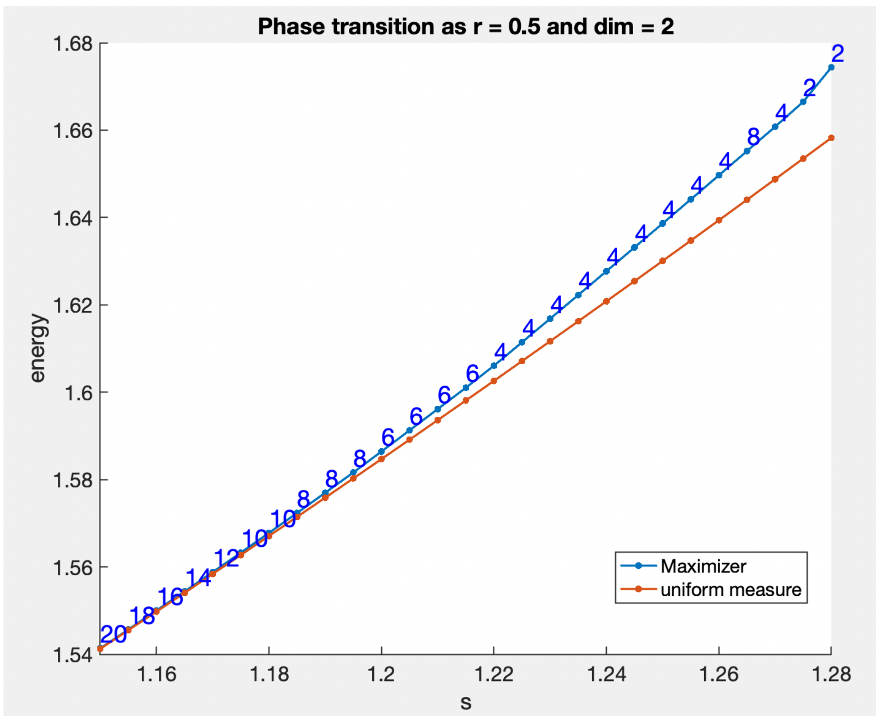

Figure 2.2: In the case $n = 2$, $\gamma = 0.5$, and $s \in [1.15, 1.28]$, several discrete numerical maximizers (regular m-gon) are found by the conjugate gradient descent method. These maximizers exhibit greater energy than both $\frac{1}{2}(\delta_x + \delta_{-x})$ and the uniform measure on S^1 (see Table 2.2). The number next to each point indicates the support size of the discrete maximizer.

Chapter 3

Three-point Energy and Semidefinite Programming Bound

As a generalization of Riesz s-energy, the continuous energy minimization of the multivariate geometric potential

$$A_s(x, y, z) = \text{area}(x, y, z)^s$$

is first considered in the paper [6], where $\text{area}(x, y, z)$ is the area of the triangle spanned by the three vertices $x, y, z \in S^{n-1}$. To address the potential involving three points, the semidefinite programming bound is the most common approach at present and generalizes the two-point bound discussed in the previous section.

The semidefinite programming bound, or the SDP bound, was first developed by Bachoc and Vallentin [1] in 2008 in their seminal paper on the kissing number problem. The idea of considering matrix-valued positive definite kernels was inspired by Schrijver's work on maximal separation codes in coding theory [19], in which a family of positive semidefinite matrices was extracted from the Terwilliger algebra of the Hamming graphs.

The Bachoc-Vallentin SDP bound for discrete energy minimization was initially used by Cohn and Woo [9] to demonstrate the universal optimality of the rhombic dodecahedron code in the projective space $\mathbb{R}\mathrm{P}^2$. The continuous version of the SDP bound was explored in the papers [5] and [6], where it was shown that the uniform measure serves as a maximizer for the three-point energy $\mathcal{I}(n, A_2)$ and is relevant for the three-point generalization of the p-frame potential and the packing problem of spherical codes.

In this section, we first review the semidefinite programming bound and its variation for the continuous energy minimization, and then implement it for the potential A_s.

3.1 Semidefinite Programming Bound for Continuous Energy Minimization

For convenience, we denote $u = \langle x, z\rangle$, $v = \langle y, z\rangle$, $t = \langle x, y\rangle$ to be the three inner products of the triples $x, y, z \in S^{n-1}$. The SDP bound in [1] states that the three-point matrix-valued function $S_k^n(u, v, t)$ and $Y_k^n(u, v, t)$ with the (i, j)-entry defined by

$$S_k^n(u, v, t) = \frac{1}{6}\sum_{\pi\in S_3} Y_k^n(\pi(x), \pi(y), \pi(z)) \tag{3.1}$$

$$(Y_k^n)_{i+1,j+1}(x, y, z) = Q_i^{n+2k}(u)Q_j^{n+2k}(v)P_k^n(u, v, t) \tag{3.2}$$

are positive definite in the sense that

$$\sum_{(x,y,z)\in X^3} (Y_k^n)(x, y, z) \succeq 0 \quad \text{for all} \quad X \subset S^{n-1}, \tag{3.3}$$

where Q_k^n is the Gegenbauer polynomial of degree k on S^{n-1} introduced in Section 2.1 and

$$P_k^n(u,v,t) = ((1-u^2)(1-v^2))^{k/2} Q_k^{n-1}\left(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}\right). \tag{3.4}$$

The construction of (3.1) relies on the stabilizer subgroup $\mathcal{O}(n-1) \subset \mathcal{O}(n)$, which fixes the point z while acting on the function $(Y_k^n)(x,y,z)$. This action is described by the equation $(Y_k^n)(h.x, h.y, h.z) = (Y_k^n)(x,y,z)$ for all $h \in \mathcal{O}(n-1)$ and any $x, y \in S^{n-1}$. This property allows for the decomposition of $\mathcal{H}_k^n$ in (2.2) into a more refined $\mathcal{O}(n-1)$-irreducible subspace

$$\mathcal{H}_k^n \cong \bigoplus_{i=0}^{k} \mathcal{H}_{i,k}^{n-1}, \qquad \mathcal{H}_{i,k}^{n-1} \cong \mathcal{H}_i^{n-1}.$$

In this case, $Q_i^{n+2k}(u)$ appears in the orthonormal basis on $\mathcal{H}_{k,k+i}^{n-1}$, and a similar process in Section 2.1 is used to deduce 3.1. Through the weak* density of discrete measures in $\mathcal{M}(S^{n-1})$, the following statement is equivalent to the positive definiteness in (3.3).

Theorem 3.1.1 (Bachoc-Vallentin [1], Bilyk et al. [6]). *For any dimension $n \geq 3$ and degree $k \geq 0$, the three-point matrix-valued function $S_k^n(x,y,z)$ is positive definite, that is,*

$$I_{n,S_k^n}(\mu) = \int_{S^{n-1}} \int_{S^{n-1}} \int_{S^{n-1}} S_k^n(x,y,z) d\mu(x) d\mu(y) d\mu(z) \geq 0$$

for all signed finite regular Borel measures $\mu \in \mathcal{M}(S^{n-1})$.

Using this theorem, we can prove the SDP bound for continuous energy minimization of three-point potentials. In the statement, the auxiliary function is expressed by the Frobenius inner product of matrices.

Theorem 3.1.2 (*Semidefinite Programming Bound*). *Let $F(u,v,t)$ be the potential on*

S^{n-1}, and $H(u,v,t)$ be a multivariate polynomial with the expression

$$H(u,v,t) = h_0 + \sum_{k=0}^{\infty} \langle H_k, S_k^n(u,v,t) \rangle.$$

Assume that

(i) $H_k \succeq 0$ for all k,

(ii) $F(u,v,t) \geqslant H(u,v,t)$ for all triples (u,v,t) in the domain

$$\Omega = \{(u,v,t) \in [-1,1]^3 : 1 + 2uvt - u^2 - v^2 - t^2 \geqslant 0\},$$

(iii) The $(0,0)$-entry of H_0 is zero.

Then, for any $\mu \in \mathcal{P}(\Omega)$,

$$I_{n,F}(\mu) \geqslant h_0.$$

Proof. Note that

$$I_{n,F}(\mu) \geq I_{n,H}(\mu) \geqslant h_0,$$

where the first inequality is clear due to condition (ii), and the second one follows from Theorem 3.1.1:

$$\begin{aligned}
I_H(\mu) &= h_0 + \int_{S^{n-1}} \int_{S^{n-1}} \int_{S^{n-1}} \sum_{k=0}^{\infty} \langle H_k, S_k^n(x,y,z) \rangle d\mu(x) d\mu(y) d\mu(z) \\
&= h_0 + \sum_{k=0}^{\infty} \left\langle H_k, \int_{S^{n-1}} \int_{S^{n-1}} \int_{S^{n-1}} S_k^n(x,y,z) d\mu(x) d\mu(y) d\mu(z) \right\rangle \\
&\geqslant h_0 + H_0(0,0) \\
&= h_0.
\end{aligned}$$

□

Remark 3.1.1. *By the same argument used in proving 2.2.3, we can substitute the matrix* $S_k^n(u,v,t)$ *in Theorem 3.1.2 with the simpler matrix defined as*

$$(S_k(u,v,t))_{i,j} = u^i v^j (t-uv)^k \qquad (i,j \geq 0).$$

This substitution ensures that the SDP bound is independent of the dimension, which aligns with the case of our energy $I(n, A_s)$ *as* $s = 4, 6, 8$ *discussed in the next section.*

3.2 Numerical SDP Bound for Three-point Potential

In this section, we introduce the three-point potential $A_s(x,y,z)$, defined by the area of the triangle formed by the three vertices $x, y, z \in S^{n-1}$, and subsequently apply the SDP bound provided in the previous section.

Let $x, y, z \in S^{n-1}$ and denote u, v, t to be the inner products among them. By using the parallelogram formula, we can write

$$\begin{aligned} A_s(x,y,z) &= \left(\frac{1}{4} \det \begin{pmatrix} \langle y-x, y-x \rangle & \langle y-x, z-x \rangle \\ \langle z-x, y-x \rangle & \langle z-x, z-x \rangle \end{pmatrix} \right)^{s/2} \\ &= \left(\frac{3}{4} - \frac{1}{2}(u+v+t) + \frac{1}{2}(uv+ut+vt) - \frac{1}{4}(u^2+v^2+t^2) \right)^{s/2} \end{aligned}$$

When s is an even number, A_s is a multivariate polynomial in variables u, v, t. In particular, as $s = 2$, it can be expressed exactly by the matrices S_k^n:

$$\begin{aligned} A_2(u, v, t) = \frac{3(d-1)}{4d} &- \left\langle \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{3(d-1)}{4d} \end{pmatrix}, S_0 \right\rangle \\ &- \left\langle \begin{pmatrix} 3/2 & 0 \\ 0 & 3/2 \end{pmatrix}, S_1 \right\rangle - \left\langle \begin{pmatrix} \frac{3(d-2)}{4(d-1)} & 0 \\ 0 & 0 \end{pmatrix}, S_2 \right\rangle \end{aligned} \tag{3.5}$$

By Theorem 3.1.2, we know that $\mathcal{I}(n, A_2)$ is maximized by the uniform measure for each $n \geq 3$, and the power $s = 2$ is the only case proved in the paper [6]. For other values of s, the potential A_s is no longer a polynomial, which makes the application of Theorem 3.1.2 more difficult.

The primary challenge in applying Theorem 3.1.2 is verifying condition (ii). While it is possible to sample within the domain Ω and convert the condition into linear constraints, this approach yields poor performance and does not result in the feasible solution we desire. Fortunately, for even powers $s = 2, 4, 6, \ldots$, the condition (ii) in Theorem 3.1.2 guarantees that the difference between the potential and the auxiliary function is a non-negative polynomial over the compact domain Ω. According to Putinar's Theorem in real algebraic geometry [17], we can express this difference as a sum of squares of polynomials on Ω. Therefore, it can be reformulated as semidefinite constraints in our program.

Consequently, the SDP approach is sufficient in the case $s = 2, 4, 6, 8$, and the numerical upper bounds on $\mathcal{I}(n, A_s(x, y, z))$ are listed in Table 3.1. The following are observations and hypotheses deduced from the numerical experiment.

(1) Let Δ_k be the discrete measure that is uniformly distributed on the vertices of the regular k-simplex inscribed on S^{k-1}, which exists on the sphere S^{n-1} for all $n \geq k$.

s	dim n	SDP bound
2	3	0.5
2	4	0.5625
2	5	0.6
2	6	0.625
4	$3-6$	2/3
6	$3-6$	1.0679
8	$3-6$	1.802

Table 3.1: SDP bound for $\mathcal{I}(n, A_s)$

The numerical SDP bound on $\mathcal{I}(n, A_s)$ with $s = 2, 4, 6, 8$ are listed in Table 3.1. To derive this table, we used CVX, a package for specifying and solving convex programs [10], [13]. For $s = 2$, the bound is achieved by the uniform measure on S^{n-1}, which appears as the scalar term in the expression (3.5). For $s = 4, 6, 8$, the bound is attained by the discrete measure $\Delta_3, \Delta_3, \Delta_2$, respectively.

(2) As the dimension $n = 3$ and the power s increase from 2 to 6, the energy of the discrete measure given by the three vertices of an equilateral triangle

$$I_{3,A_s}(\Delta_2) = \frac{2}{9}\left(\frac{3\sqrt{3}}{4}\right)^s$$

begins to exceed that of the regular tetrahedron

$$I_{3,A_s}(\Delta_3) = \frac{3}{8}\left(\frac{2\sqrt{3}}{3}\right)^s.$$

This crossover point occurs at $s^* = \log(\frac{27}{16})/\log(\frac{9}{8}) \approx 4.44247$. Based on this observation and the numerical results of conjugate gradient descent, we conjecture that the three-point energy $\mathcal{I}(3, A_s)$ is maximized by the regular tetrahedron Δ_3 when $s \in [2, s^*]$ and by the equilateral triangle Δ_2 when $s \in [s^*, \infty)$.

(3) For each dimension $n \geq 3$, the sequence of energy

$$I_{n,A_s}(\Delta_2), I_{n,A_s}(\Delta_3), ..., I_{n,A_s}(\Delta_n)$$

is monotone increasing for all $s \in [2, 2+\varepsilon]$ and some small ε, which implies that Δ_n should be the discrete maximizer of the energy $\mathcal{I}(n, A_s)$ in that range. Moreover, by comparing the energy of each $I_{n,A_s}(\Delta_k)$ as the power s varies, we can partition the interval $[2, \infty)$ into $n-1$ non-overlapping segments

$$[2, \infty) = [2, s^*_{n-1}] \cup [s^*_{n-1}, s^*_{n-2}] \cup \cdots \cup [s^*_2, \infty).$$

In this partitioning, the discrete measure Δ_k exhibits the greatest energy within the segment $[s^*_k, s^*_{k-1}]$ for all k (set $s^*_1 := \infty$). Here, s^*_k represents the phase transition point where the energy $I_{n,A_s}(\Delta_{k+1}) = I_{n,A_s}(\Delta_k)$.

(4) Based on the observation in (3), we conjecture that for each dimension $n \geq 3$ and $2 \leq k \leq n$, the discrete measure Δ_k is the energy maximizer of $\mathcal{I}(n, A_s)$ in the region $s \in [s^*_k, s^*_{k-1}]$.

3.3 Exact Solution for $\mathcal{I}(n, A_6)$

In this section, we give a full solution to the energy maximization $\mathcal{I}(n, A_s(x, y, z))$ in the range $s \geq 6$ by deriving a family of exact auxiliary functions from the numerical

SDP bound of $\mathcal{I}(n, A_6)$, where we choose the auxiliary function H_6 of the form

$$\begin{aligned} H_6(u,v,t) &= \langle H_0, S_0(u,v,t)\rangle + \langle H_1, S_1(u,v,t)\rangle + h_0 \\ &= \left\langle \begin{pmatrix} 0 & 0 \\ 0 & 3^7/2^{11} \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & A \end{pmatrix} \right\rangle + \left\langle \begin{pmatrix} a & b \\ b & c \end{pmatrix}, \begin{pmatrix} B & C \\ C & D \end{pmatrix} \right\rangle - \frac{3^7}{2^{11}} \end{aligned} \tag{3.6}$$

where

$$\begin{aligned} A &= \frac{1}{3}(tu+tv+uv) \\ B &= \frac{1}{3}(t+u+v) - \frac{1}{3}(tu+tv+uv) \\ C &= \frac{1}{3}(tu+tv+uv) - \frac{1}{6}(t^2u+t^2v+u^2v+u^2t+v^2u+v^2t) \\ D &= tuv - \frac{1}{3}(t^2u^2+t^2v^2+u^2v^2) \\ a &= 715/357,\ b = -293/122,\ c = 991/265, \end{aligned}$$

and the two positive semidefinite matrices H_0, H_1 are obtained by solving the SDP in CVX using MOSEK [14]. Thus, the auxiliary function has a clear expression

$$\begin{aligned} H_6(u,v,t) = & \frac{a}{3}(t+u+v) + \left(\frac{3^7}{2^{11}} - a + 2b\right)\frac{1}{3}(tu+tv+uv) \\ & + ctuv - \frac{b}{3}(t^2u+t^2v+u^2v+u^2t+v^2u+v^2t) \\ & - \frac{c}{3}(t^2u^2+t^2v^2+u^2v^2) - \frac{3^7}{2^{11}}. \end{aligned} \tag{3.7}$$

To derive the exact value of a, b, c, we may assume that the polynomial $H_6(u,v,t)$ satisfies the following linear constraints

- $-A_6(u,v,t) = H_6(u,v,t)$ at $(u,v,t) = (-1/2,-1/2,1)$ or $(-1/2,-1/2,-1/2)$
- $-\frac{d}{du}A_6(u,u,1) = \frac{d}{du}H_6(u,u,1)$ at $(u,v,t) = (-1/2,-1/2,1)$ or $(1,1,1)$

- $-\frac{d}{du}A_6(u,u,u) = \frac{d}{du}H_6(u,u,u)$ at $(u,v,t) = (-1/2,-1/2,-1/2)$ or $(1,1,1)$

These constraints arise naturally from the inner-product triples of the equilateral triangle, which is the support of the suspected discrete maximizer. It is equivalent to solving the linear system

$$\begin{pmatrix} -1 & 1 & -1/4 \\ 2 & 1 & -1 \\ 1 & 2 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \frac{3^7}{2^{11}} \begin{pmatrix} -5 \\ -2 \\ 2 \end{pmatrix}$$

which has a unique solution $(a,b,c) = \frac{3^7}{2^{11}} \cdot (2,-2,4)$. Surprisingly, in comparison with the potential $A_6(x,y,z)$, the resulting auxiliary function

$$\begin{aligned} H_6(u,v,t) = \; & \frac{3^7}{2^{11}}\bigg(\frac{2}{3}(u+v+t) - \frac{5}{3}(ut+vt+uv) \\ & + 4uvt + \frac{2}{3}(t^2u + t^2v + u^2v + u^2t + v^2u + v^2t) \\ & - \frac{4}{3}(t^2u^2 + t^2v^2 + u^2v^2) - 1\bigg) \end{aligned} \tag{3.8}$$

satisfies the requested properties

- $-A_6(u,v,t) \geqslant H_6(u,v,t)$ for all triples $(u,v,t) \in \Omega$.
- $-A_6(u,v,t) = H_6(u,v,t)$ only at $(1,1,1)$, $(1,-1/2,-1/2)$, and $(-1/2,-1/2,-1/2)$ in Ω.

Moreover, if we replace the coefficient $3^7/2^{11}$ in (3.8) by the energy $I_{3,A_s}(\Delta_2) = \frac{2}{9}\left(\frac{3\sqrt{3}}{4}\right)^s$, the corresponding auxiliary function

$$\begin{aligned} H_{6,s}(u,v,t) = \; & \frac{2}{9}\left(\frac{3\sqrt{3}}{4}\right)^s \Big(\frac{2}{3}(u+v+t) - \frac{5}{3}(ut+vt+uv) \\ & + 4uvt + \frac{2}{3}(t^2u + t^2v + u^2v + u^2t + v^2u + v^2t) \\ & - \frac{4}{3}(t^2u^2 + t^2v^2 + u^2v^2) - 1\Big) \end{aligned}$$

or, equivalently,

$$H_{6,s}(u,v,t) = \frac{2}{9}\left(\frac{3\sqrt{3}}{4}\right)^s \left(\left\langle \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & A \end{pmatrix} \right\rangle + \left\langle \begin{pmatrix} 2 & -2 \\ -2 & 4 \end{pmatrix}, \begin{pmatrix} B & C \\ C & D \end{pmatrix} \right\rangle - 1\right)$$

is still feasible for all $s \geq 6$. However, the perturbed auxiliary function stops working for some range in the interval $[s^*, 6)$. Since $H_{6,s}(u,v,t)$ meets all the conditions in Theorem 3.1.2, we can draw the following conclusion:

Theorem 3.3.1. *For any dimension $n \geq 3$ and power $s \geq 6$, the energy*

$$\mathcal{I}(n, A_s) = \frac{2}{9}\left(\frac{3\sqrt{3}}{4}\right)^s$$

is maximized by the discrete measure that is uniformly distributed over the vertices of an equilateral triangle on the equator of S^2.

3.4 Exact Solution for $\mathcal{I}(n, A_4)$

In this section, we give a exact solution to the energy maximization $\mathcal{I}(n, A_4)$, where we choose the auxiliary function H_4 of the form

$$
\begin{aligned}
H_4(u,v,t) &= \langle H_0, S_0(u,v,t)\rangle + \langle H_1, S_1(u,v,t)\rangle + h_0 \\
&= \left\langle \begin{pmatrix} 0 & 0 \\ 0 & 2/3 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & A \end{pmatrix} \right\rangle + \left\langle \begin{pmatrix} a & b \\ b & c \end{pmatrix}, \begin{pmatrix} B & C \\ C & D \end{pmatrix} \right\rangle - \frac{2}{3}
\end{aligned} \tag{3.9}
$$

where $a = 451/250, b = -507/466$ and $c = 377/305$ are obtained by solving the SDP in CVX using MOSEK [14], and A, B, C, D are the same polynomials listed in the previous section. Thus, the auxiliary function has a clear expression

$$
\begin{aligned}
H_4(u,v,t) = &\ \frac{a}{3}(t+u+v) + \left(\frac{2}{3} - a + 2b\right)\frac{1}{3}(tu+tv+uv) \\
&+ ctuv - \frac{b}{3}(t^2u + t^2v + u^2v + u^2t + v^2u + v^2t) \\
&- \frac{c}{3}(t^2u^2 + t^2v^2 + u^2v^2) - \frac{2}{3}.
\end{aligned} \tag{3.10}
$$

To derive the exact values of a, b, and c in our auxiliary function $H_4(u,v,t)$, we may assume that H_4 meets the following linear constraints.

- $-A_4(u,v,t) = H_4(u,v,t)$ at $(u,v,t) = (-1/3, -1/3, -1/3)$
- $-\frac{d}{du}A_4(u,u,1) = \frac{d}{du}H_4(u,u,1)$ at $(u,v,t) = (-1/3,-1/3,1)$ and $(1,1,1)$.

These constraints naturally emerge from the inner product triples of the regular tetrahedron, which is the conjectured maximizer. It turns into the linear system

$$\begin{pmatrix} -4/9 & 8/27 & -4/81 \\ 2/9 & 4/9 & -14/81 \\ -2/3 & -4/3 & -2/3 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \frac{2}{3} \begin{pmatrix} -16/9 \\ -4/9 \\ -4/3 \end{pmatrix}$$

which has a unique solution $(a, b, c) = \frac{2}{3} \cdot (11/4, -3/2, 9/4)$. Surprisingly, in comparison with the potential $A_4(x, y, z)$, the resulting auxiliary function

$$\begin{aligned} H_4(u, v, t) = \; & \frac{2}{3}\bigg(\frac{11}{12}(u + v + t) - \frac{19}{12}(ut + vt + uv) \\ & + \frac{9}{4}uvt + \frac{1}{2}(t^2u + t^2v + u^2v + u^2t + v^2u + v^2t) \\ & - \frac{3}{4}(t^2u^2 + t^2v^2 + u^2v^2) - 1\bigg) \end{aligned} \tag{3.11}$$

satisfies the requested properties

- $-A_4(u, v, t) \geqslant H_4(u, v, t)$ for all triples $(u, v, t) \in \Omega$.
- $-A_4(u, v, t) = H_4(u, v, t)$ only at $(1, 1, 1)$, $(1, -1/3, -1/3)$, and $(-1/3, -1/3, -1/3)$ in Ω.

As $H_4(u, v, t)$ satisfies all the conditions in Theorem 3.1.2, we conclude that the uniform distribution on the vertices of the regular tetrahedron on S^{n-1} minimizes the energy $\mathcal{I}(n, A_4)$ for all dimensions $n \geq 3$. However, the function H_4 does not extend to any feasible auxiliary function for other values of s near 4.

Since $H_4(u, v, t)$ meets all the conditions in Theorem 3.1.2, we can draw the following conclusion:

Theorem 3.4.1. *For any dimension* $n \geq 3$*, the energy*

$$\mathcal{I}(n, A_4) = \frac{2}{3}$$

is maximized by the discrete measure that is uniformly distributed over the vertices of the regular tetrahedron on S^2*.*

Chapter 4

Conclusion and Discussion

Our two main results for the continuous energy maximization on the sphere S^{n-1} are as follows:

- In Section 3.2, we compute the numerical upper and lower bounds of the energy $\mathcal{I}(n, F_{\gamma,s})$ for the two-point potential

$$F_{\gamma,s}(x,y) = \left(\gamma\sqrt{2-2\langle x,y\rangle} + (1-\gamma)\arccos\langle x,y\rangle\right)^s.$$

  using the linear program outlined in Theorem 2.1.2 and the conjugate gradient descent method, particularly when the parameter $\gamma = 0.5$, the power $1 < s < 2$, and the dimension $n = 2, 3$. The conjectured phase transitions are listed in Table 2.1 and 2.2, where a bunch of new discrete measures appear as maximizers.

- In Section 3.3 and 3.4, we derive the exact SDP bound for the three-point potential

$$A_s(x,y,z) = \text{area}(x,y,z)^s$$

  as $s = 4$ and $s \geq 6$, where $\text{area}(x,y,z)$ is the area of the triangle spanned by the three vertices x, y, z on the sphere. Explicitly, we show that the energy $\mathcal{I}(n, A_s)$ is maximized by a discrete measure that is uniformly distributed over the vertices of a regular tetrahedron for $s = 4$ and over an equilateral triangle for $s \geq 6$. For dimension $n = 3$, we conjecture that the former remains the maximizer on the interval $[2, s^*]$, while the latter remains the maximizer on the interval $[s^*, \infty)$. Hence, there's only a single phase transition $s^* = \frac{\log(27/16)}{\log(9/8)} \approx 4.44247$ in the whole region $(2, \infty)$. The version of the conjecture of dimension $n > 3$ is remarked in the end of Section 3.2, where each discrete measure Δ_k formed by the vertices of k-simplex with $2 \leq k \leq n$ become energy maximizers of $\mathcal{I}(n, A_s)$ for s in some subinterval in $(2, \infty)$.

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