Five Point Energy Minimization 5: Symmetrization

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Abstract

This is Paper 5 of series of 7 self-contained papers which together prove the Melnyk-Knopf-Smith phase transition conjecture for 5-point energy minimization. (Paper 0 has the main argument.) This paper deals with symmetrization in the critical region of moduli space.

1 Introduction

1.1 Context

Let S^2 be the unit sphere in $\boldsymbol{R}^3$. Given a configuration $\{p_i\} \subset S^2$ of N distinct points and a function $F : (0,2] \to \boldsymbol{R}$, define

$$\mathcal{E}_F(P) = \sum_{1 \leq i < j \leq N} F(\|p_i - p_j\|). \tag{1}$$

This quantity is commonly called the *F-potential* or the *F-energy* of P. A configuration P is a *minimizer* for F if $\mathcal{E}_F(P) \leq \mathcal{E}_F(P')$ for all other N-point configurations P'. The question of finding energy minimizers has a long literature; the classic case goes back to Thomsom [**Th**] in 1904.

We are interested in the case $N = 5$ and the *Riesz potential* $F = R_s$, where

$$R_s(d) = d^{-s}, \qquad s > 0. \tag{2}$$

The *Triangular Bi-Pyramid* (TBP) is the 5 point configuration having one point at the north pole, one point at the south pole, and 3 points arranged in an equilateral triangle on the equator. A *Four Pyramid* (FP) is a 5-point configuration having one point at the north pole and 4 points arranged in a square equidistant from the north pole.

Define

$$15_+ = 15 + \frac{25}{512}. \tag{3}$$

My monograph [**S0**] proves the following result.

Theorem 1.1 (Phase Transition) *There exists* $\shin \in (15, 15_+)$ *such that:*

1. *For* $s \in (0, \shin)$ *the TBP is the unique minimizer for* R_s*.*

2. *For* $s = \shin$ *the TBP and some FP are the two minimizers for* R_s*.*

3. *For each* $s \in (\shin, 15_+)$ *some FP is the unique minimizer for* R_s*.*

This result verifies the phase-transition for 5 point energy minimization first observed in [**MKS**], in 1977, by T. W. Melnyk, O, Knop, and W. R. Smith. This work implies and extends my solution [**S1**] of Thomson's 1904 5-electron problem [**Th**]. To make [**S0**] easier to referee, I have broken down the proof into a series of 7 independent papers, each of which may be checked without any reference to the others.

1.2 Results

This paper discusses the region $\Upsilon \times [12, \infty)$, where Υ is the small region shown in Figure 1. This region, which looks somewhat contrived, contains those FPs which compete with the TPB for energy exponents s reasonably near $\shin$. We begin with some background definitions.

Stereographic Projection: Let $S^2 \subset \boldsymbol{R}^3$ be the unit 2-sphere. *Stereographic projection* is the map $\Sigma : S^2 \to \boldsymbol{R}^2 \cup \infty$ given by the following formula.

$$\Sigma(x, y, z) = \left(\frac{x}{1-z}, \frac{y}{1-z}\right). \tag{4}$$

Here is the inverse map:

$$\Sigma^{-1}(x, y) = \left(\frac{2x}{1+x^2+y^2}, \frac{2y}{1+x^2+y^2}, 1 - \frac{2}{1+x^2+y^2}\right). \tag{5}$$

Σ^{-1} maps circles in $\boldsymbol{R}^2$ to circles in S^2 and $\Sigma^{-1}(\infty) = (0, 0, 1)$.

Avatars: Stereographic projection gives us a correspondence between 5-point configurations on S^2 having $(0, 0, 1)$ as the last point and planar configurations:

$$\widehat{p}_0, \widehat{p}_1, \widehat{p}_2, \widehat{p}_3, (0, 0, 1) \in S^2 \iff p_0, p_1, p_2, p_3 \in \boldsymbol{R}^2, \qquad \widehat{p}_k = \Sigma^{-1}(p_k). \tag{6}$$

We call the planar configuration the *avatar* of the corresponding configuration in S^2. By a slight abuse of notation we write $\mathcal{E}_F(p_0, p_1, p_2, p_3)$ when we mean the F-potential of the corresponding 5-point configuration.

First Domain: We let $\Upsilon \subset (\boldsymbol{R}^2)^4$ denote those avatars such that

1. $\|p_0\| \geq \|p_k\|$ for $k = 1, 2, 3$.
2. $512p_0 \in [433, 498] \times [0, 0]$. (That is, $p_0 \in [433/512, 498/512] \times \{0\}$.)
3. $512p_1 \in [-16, 16] \times [-464, -349]$.
4. $512p_2 \in [-498, -400] \times [0, 24]$.
5. $512p_3 \in [-16, 16] \times [349, 464]$.

As we discussed above, Υ contains the avatars that compete with the TBP near the exponent ש. The two rhombi in Figure 1 indicate avatars associated to the TBP.

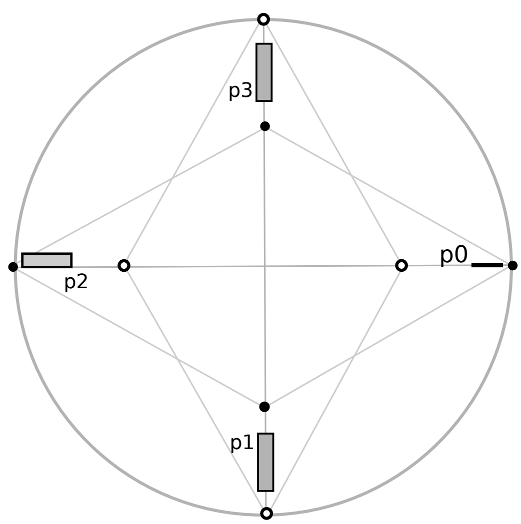

Figure 1: The sets defining Υ compared with two TBP avatars.

First Symmetrization: Let (p_0, p_1, p_2, p_3) be an avatar with $p_0 \neq p_2$. Define

$$-p_2^* = p_0^* = (x, 0), \quad -p_1^* = p_3^* = (0, y), \qquad x = \frac{\|p_0 - p_2\|}{2}, \quad y = \frac{\|\pi_{02}(p_1 - p_3)\|}{2}. \tag{7}$$

Here π_{02} is the projection onto the subspace perpendicular to $p_0 - p_2$. The avatar $(p_1^*, p_2^*, p_3^*, p_4^*)$ lies in $\boldsymbol{K}_4$, the set of avatars which are invariant under reflections in the coordinate axes.

Theorem 1.2 (Symmetrization I) *Let $s \geq 12$ and $(p_0, p_1, p_2, p_3) \in \Upsilon$. Then*

$$\mathcal{E}_{R_s}(p_0^*, p_1^*, p_2^*, p_3^*) \leq \mathcal{E}_{R_s}(p_0, p_1, p_2, p_3)$$

with equality if and only if the two avatars are equal.

Second Domain: Let $\Psi_4^\sharp$ denote the set $(p_0, p_1, p_2, p_3) \in \boldsymbol{K}_4$ with

$$-p_2 = p_0 = (x, 0), \qquad -p_1 = p_3 = (0, y), \qquad 512(x, y) \in [440, 448]. \tag{8}$$

$\Psi_4^\sharp$ contains the avatar representing the FP which ties with the TBP at $s = \boldsymbol{\varpi}$.

Second Symmetrization: We define

$$\sigma(x, y) = (z, z), \qquad z = \frac{x + y + (x - y)^2}{2}. \tag{9}$$

Theorem 1.3 (Symmetrization II) *If $s \in [14, 16]$ and $p \in \Psi_4^\sharp$ then we have $\mathcal{E}_s(\sigma(p)) \leq \mathcal{E}_s(p)$ with equality if and only if $\sigma(p) = p$.*

Symmetrization operations like those above will *in general* surely fail, due to the vast range of possible configurations. However, certain operations might work well in very specific parts of the configuration space and for limited ranges of exponents. I found the operation that works after a ton of experimentation. Proving that the first symmetrization lowers the energy seems to involve studying what happens on the tiny but still 7-dimensional moduli space Υ. The secret to the proof is that, within Υ, the symmetrization operation is so good that it reduces the energy in pieces. What I mean is that the 10 term sum for the energy can be written as

$$e_1 + ... + e_{10} = (e_1 + e_2) + (e_3 + e_4) + (e_5 + e_6 + e_7) + (e_8 + e_9 + e_{10})$$

so that the symmetrization operation decreases each bracketed sum separately. This reduces us to establishing some lower-dimensional inequalities. Proving that the second symmetrization lowers energy is a delicate 2-dimensional problem. The proof relies on an algebraic miracle.

1.3 Paper Organization

In §2 I will present some computational tools which will help with the analysis. In §3 I will prove the Symmetrization Theorem II, because this is shorter. In §4 I will prove the Symmetrization Theorem I. The proofs in this paper are computer-assisted. All calculations are done using exact arithmetic in Mathematica. The reader can download and inspect the files I wrote for this.

2 Preliminaries

2.1 Exponential Sums

We begin with two easy and well-known lemmas about exponential sums.

Lemma 2.1 (Convexity) *Suppose that* $\alpha, \beta, \gamma \geq 0$ *have the property that* $\alpha + \beta \geq 2\gamma$. *Then* $\alpha^s + \beta^s \geq 2\gamma^s$ *for all* $s > 1$, *with equality iff* $\alpha = \beta = \gamma$.

Proof: This is an exercise with Lagrange multipliers. ♠

Given a real single-variable polynomial $f(x)$, the number of positive roots of f (counted with multiplicity) is at most the number of changes in the signs of the coefficients. This statement is included in a more precise result known as Descartes' Rule of Signs.

Lemma 2.2 (Descartes) *Let* $0 < r_1 \leq ... \leq r_n < 1$ *be a sequence of positive numbers. Let* $c_1, ..., c_n$ *be a sequence of nonzero numbers and let* $\sigma_1, ..., \sigma_n$ *be the corresponding sequence of signs of these numbers. Define*

$$E(s) = \sum_{i=1}^{n} c_i \ r_i^s. \tag{10}$$

Let K *denote the number of sign changes in the sign sequence. Then* E *changes sign at most* K *times on* $\boldsymbol{R}$.

Proof: Suppose we have a counterexample. By continuity, perturbation, and taking mth roots, it suffices to consider a counterexample of the form $\sum c_i t^{e_i}$ where $t = r^s$ and $r \in (0, 1)$ and $e_1 > ... > e_n \in \boldsymbol{N}$. As s ranges in r, the variable t ranges in $(0, \infty)$. But $P(t)$ changes sign at most K times on $(0, \infty)$ by Descartes' Rule of Signs. This gives us a contradiction. ♠

2.2 Polynomial Operations

1. Positive Dominance: The works [**S2**] and [**S3**] give more details about positive dominance. Here I explain the basics. Let $G \in \boldsymbol{R}[x_1, ..., x_n]$ be a multivariable polynomial:

$$G = \sum_I c_I X^I, \qquad X^I = \prod_{i=1}^{n} x_i^{I_i}. \tag{11}$$

Given two multi-indices I and J, we write $I \preceq J$ if $I_i \leq J_i$ for all i. Define

$$G_J = \sum_{I \preceq J} c_I, \qquad G_\infty = \sum_I c_I. \tag{12}$$

We call G *weak positive dominant* (WPD) if $G_J \geq 0$ for all J and $G_\infty > 0$. We call G *positive dominant* if $G_J > 0$ for all J.

Lemma 2.3 (Weak Positive Dominance) *If G is weak positive dominant then $G > 0$ on $(0,1]^n$. If G is positive dominant then $G > 0$ on $[0,1]^n$.*

Proof: We prove the first statement. The second one has almost the same proof. Suppose $n = 1$. Let $P(x) = a_0 + a_1 x + ...$ Let $A_i = a_0 + ... + a_i$. The proof goes by induction on the degree of P. The case $\deg(P) = 0$ is obvious. Let $x \in (0,1]$. We have

$$P(x) = a_0 + a_1 x + x_2 x^2 + \cdots + a_n x^n \geq$$

$$x(A_1 + a_2 x + a_3 x^2 + \cdots a_n x^{n-1}) = xQ(x) > 0$$

Here $Q(x)$ is WPD and has degree $n-1$.

Now we consider the general case. We write

$$P = f_0 + f_1 x_k + ... + f_m x_k^m, \qquad f_j \in \boldsymbol{R}[x_1, ..., x_{n-1}]. \tag{13}$$

Since P is WBP so are the functions $P_j = f_0 + ... + f_j$. By induction on the number of variables, $P_j > 0$ on $(0,1]^{n-1}$. But then, when we arbitrarily set the first $n-1$ variables to values in $(0,1)$, the resulting polynomial in x_n is WPD. By the $n = 1$ case, this polynomial is positive for all $x_n \in (0,1]$. ♠

2. Subdivision: Let $P \in \boldsymbol{R}[x_1, ..., x_n]$ as above. For any x_j and $k \in \{0,1\}$ we define

$$S_{x_j,k}(P)(x_1, ..., x_n) = P(x_1, ..., x_{j-1}, x_j^*, x_{j+1}, ..., x_n), \qquad x_j^* = \frac{k}{2} + \frac{x_j}{2}. \tag{14}$$

If $S_{x_j,k}(P) > 0$ on $(0,1]^n$ for $k = 0, 1$ then we also have $P > 0$ on $(0,1]^n$.

3. Numerator selection: If $f = f_1/f_2$ is a bounded rational function on $[0,1]^n$, written in so that f_1, f_2 have no common factors, we always choose f_2 so that $f_2(1, ..., 1) > 0$. If we then show, one way or another, that $f_1 > 0$ on $(0,1]^n$ we can conclude that $f_2 > 0$ on $(0,1]^n$ as well. The point is that f_2 cannot change sign because then f blows up. But then we can conclude that $f > 0$ on $(0,1]^n$. We write $\text{num}_+(f) = f_1$.

3 The Symmetrization Theorem II

Our symmetrization is the map σ from Equation 9, and we always write $(z,z)=\sigma(x,y)$. Let $\phi:[0,1]^2\to\Psi_4^\sharp$ be the affine isomorphism whose linear part is a positive diagonal matrix. We use variables $(a,b)\in[0,1]^2$ so that $(x,y)=\phi(a,b)\in\Psi_4^\sharp$. For any rational function $F:\Psi_4^\sharp\to\boldsymbol{R}$ we define

$$N_F=\frac{\mathrm{num}_+((F-F\circ\sigma)\circ\phi)}{q},\qquad q(a,b)=(a-b)^2. \tag{15}$$

For all the choices of F we make, N_F will be a polynomial.

Recall that $\Sigma^{-1}(p_4)=(0,0,1)$, and define

$$r_{ij}=\frac{1}{\|\Sigma^{-1}(p'_i)-\Sigma^{-1}(p'_j)\|}. \tag{16}$$

We write $\mathcal{E}_s(x,y)=G_s(x,y)+H_s(x,y)$, where

$$G_s=r_{02}^s+r_{13}^s,\qquad H_s=2p_{04}^s+2p_{14}^s+4p_{01}^s. \tag{17}$$

The file `LemmaC1.m` computes that N_{G_2} is a WPD polynomial. This combines with the Convexity Lemma to show $G_s-G_s\circ\sigma>0$ on $\Psi_4^\sharp\times(2,\infty)$. To finish the proof, we need to show $H_s-H_s\circ\sigma\geq 0$ on $\Psi_4^\sharp\times[14,16]$.

Suppose that there is some $(x,y)\in\Psi_4^\sharp$ and some $s\in[14,16]$ such that $h(s)=H_s(x,y)-H_s(z,z)<0$. The file `LemmaC21.m` computes that $-N_{H_2}$ and $N_{H_{14}}$ and $N_{H_{16}}$ are all WPD polynomials. Hence $h(2)<0$ and $h(14)>0$ and $h(16)>0$. Hence h has at least 3 roots in $[2,16]$.

Let (p_0,p_1,p_2,p_3) and (p'_0,p'_1,p'_2,p'_3) respectively be the configurations corresponding to (x,y) and $(z,z)=\sigma(x,y)$. Without claiming to have the terms in order, we have

$$h(s)=+2r_{04}^s-4(r'_{04})^s+2r_{14}^s+4r_{01}^s-4(r'_{01})^s. \tag{18}$$

By Descartes Lemma, the sign sequence for h changes sign at least 3 times. Looking at the signs above (two minuses and three pluses) we see that there must be exactly 3 sign changes (when the terms are put in the correct order) and moreover the largest sign in the sequence must (+). Otherwise h eventually goes negative and thus would have a large positive root. Noting that $x\in(0,1)$ we compute

$$r_{01}^2-r_{04}^2=\frac{1-x^4}{4(x^2+y^2)}>0.$$

Hence $r_{04}<r_{01}$. Likewise $r_{14}<r_{01}$. We conclude that r_{01} must contribute the final (+) to the sign sequence. But the file `LemmaC22.m` computes that $-N_{r_{01}^2}$ is a WPD polynomial. Hence $r'_{01}\geq r_{01}$, a contradiction.

4 The Symmetrization Theorem I

4.1 Reduction to Four Lemmas

The domain Υ is defined in §1.2. Let $X = (p_0, p_1, p_2, p_3)$ be an avatar in Υ. We perform successive operations on X to arrive at $X' = (p'_0, p'_1, p'_2, p'_3)$ and $X'' = (p''_0, ...)$, etc. We write $I_r = [-r, r]$.

We let X' be the planar configuration which is obtained by rotating X about the origin so that p'_0 and p'_2 lie on the same horizontal line, with p'_0 lying on the right. Let Υ' denote the domain of avatars X' such that

1. $\|p'_0\| \geq \|p'_k\|$ for $k = 1, 2, 3$.
2. $512p'_0 \in [432, 498] \times I_{16}$. (Compare $[433, 498] \times I_0$.)
3. $512p'_1 \in I_{32} \times [-465, -348]$. (Compare $I_{16} \times [-464, -349]$.)
4. $512p'_2 \in [-498, -400] \times I_{16}$. (Compare $[-498, -400] \times [0, 24]$.)
5. $512p'_3 \in I_{32} \times [348, 465]$. (Compare $I_{16} \times [349, 464]$.)
6. $p'_{02} = p'_{22}$. (Compare $p_{02} = 0$.)

The comparisons are with Υ. In the next section we prove:

Lemma 4.1 (B1) *If $X \in \Upsilon$ then $X' \in \Upsilon'$.*

Given an avatar $X' \in \Upsilon'$, there is a unique configuration X'', invariant under under reflection in the y-axis, such that p'_j and p''_j lie on the same horizontal line for $j = 0, 1, 2, 3$ and $\|p''_0 - p''_2\| = \|p'_0 - p'_2\|$. We call this *horizontal symmetrization*. In a straightforward way we see that horizontal symmetrization maps Υ' into Υ'', the set of avatars $p''_0, p''_1, p''_2, p''_3$ such that

1. $-512p''_2, 512p''_0 \in [416, 498] \times I_{16}$
2. $-512p''_1, 512p''_3 \in I_0 \times [348, 465]$.
3. $p''_{02} = p''_{22}$.

Let **K4** denote the set of configurations invariant under reflections in the coordinate axes. Given a configuration $X'' \in \Upsilon''$ there is a unique configuration $X'' \in$ **K4** such that p''_j and p'''_j lie on the same vertical line for $j = 0, 1, 2, 3$. We call this operation *vertical symmetrization*. The configuration X''' coincides with the configuration X^* defined in Lemma B.

In summary (and using obvious abbreviations) we have

$$\Upsilon \quad \overrightarrow{\text{Rot}} \quad \Upsilon' \quad \overrightarrow{\text{HS}} \quad \Upsilon'' \quad \overrightarrow{\text{VS}} \quad \mathbf{K_4}.$$

Symmetrization, as an operation on Υ', is the composition of vertical and horizontal symmetrization.

Each avatar corresponds to a 5-point configuration on S^2 *via* stereographic projection. The energy of the 5 point configuration involves 10 pairs of points. Referring to Equation 16, a typical term is r_{ij}^s. Given a list L of pairs of points in the set $\{0,1,2,3,4\}$ we define $\mathcal{E}_s(P,L)$ to be the sum of the R_s-potentials just over the pairs in L. E.g. $L = \{(0,2),(0,4)\} = r_{02}^s + r_{04}^s$.

We call the subset L *good* for the parameter s, and with respect to one of the operations, if the operation does not increase the value of $\mathcal{E}_s(P,L)$. We call L *great* if the operation strictly lowers $\mathcal{E}_s(P,L)$ unless the operation fixes P. We mean to take the appropriate domains in all cases. The Symmetrization Theorem I follows immediately from Lemma B1 and from the 3 lemmas below.

Lemma 4.2 (B2) *The lists* $\{(0,2),(0,4),(2,4)\}$ *and* $\{(1,3),(1,4),(3,4)\}$ *are both great for all* $s \geq 2$ *and with respect to symmetrization.*

Lemma 4.3 (B3) *The lists* $\{(0,1),(1,2)\}$ *and* $\{(0,3),(3,2)\}$ *are both good for all* $s \geq 2$ *and with respect to horizontal symmetrization.*

Lemma 4.4 (B4) *The lists* $\{(0,1),(0,3)\}$ *and* $\{(2,1),(2,3)\}$ *are both good for all* $s \geq 12$ *and with respect to vertical symmetrization.*

4.2 Proof of Lemma B1

We want to prove that if $X \in \Upsilon$ then $X' \in \Upsilon'$. Rotation about the origin does not change the norms, so X' satisfies Condition 1. Moreover, Condition 6 holds by construction. We must check Conditions 2,3,4,5.

Let ρ_θ denote the counterclockwise rotation through the angle θ. Since p_0 lies on the x axis and p_2 lies on or above it, we have to rotate by a small amount counterclockwise to get p_0' and p_2' on the same horizontal line. That is, the rotation moves the right point up and the left one down. Hence $\theta \geq 0$. This angle is maximized when p_0 is an endpoint of its segment of constraint and p_2 is one of the two upper vertices of rectangle of constaint. Not thinking too hard which of the 4 possibilities actually realizes the max, we check for all 4 pairs (p_0, p_2) that the second coordinate of $\rho_{1/34}(p_0)$ is larger than the second coordinate of $\rho_{1/34}(p_0)$. From this we conclude that $\theta < 1/34$. This yields

$$512\cos(\theta) \in [0,1], \qquad 512\sin(\theta) \in [0,16]. \tag{19}$$

From Equation 19, the map $512p_0 \to 512p_0'$ changes the first coordinate by $512\delta_{01} \in [0,16]$ and $512\delta_{02} \in [-1,0]$. This gives (something stronger than) Condition 2 for Υ'. At the same time, we have $p_{21}' = p_{01}'$ and the change $512p_2 \to 512p_2'$ changes the second coordinate by $512\delta_{21} \in [0,1]$. This gives Condition 4 for Υ' once we observe that $|p_{21}'| \leq |p_{01}'|$.

For Condition 3 we just have to check (using the same notation) that $512\delta_{11} \in [0,16]$ and $512\delta_{12} \in [-1,1]$. The first bound comes from the inequality $512\sin(\theta) < 16$. For the second bound we note that the angle that p_1 makes with the y-axis is maximized when p_1 is at the corners of its constraints in Υ. That is,

$$p_1 = \left(\frac{\pm 16}{512}, \frac{349}{512}\right).$$

Since $\tan(1/21) > 16/349$ we conclude that this angle is at most $1/21$. Hence

$$|512\delta_{12}| \leq \max_{|x| \leq 1/21} \left|\cos\left(x + \frac{1}{34}\right) - \cos(x)\right| < 1.$$

This gives Condition 3. The same argument gives Condition 5.

4.3 Proof of Lemma B2

Let $s_3 = \sqrt{3}/3$. The significance of this number is that inverse stereographic projection maps the triangle with vertices $(\pm s_3, 0)$ and ∞ to an equilateral triangle on S^2 having a vertex at $(0,0,1)$.

Let (u,v) stand for either $(0,2)$ or $(1,3)$. For the points associated with $\{(u,v),(u,4),(v,4)\}$. We make the following definitions for $a_u, a_v, b_u, b_v > 0$.

1. Start with p_u, p_v so that $\|p_u\|, \|p_v\| < 1$ and let $a_u = a_v$ be such that

   $$\|p_u - p_v\|/2 = s_3 + a_u = s_3 + a_v.$$

   Let $q_u = (-s_3 - a_u, 0)$ and $q_v = (s_3 + a_v, 0)$.

2. Choose b_u, b_v with $b_u \leq a_u$ and $b_v \leq a_v$. Let

   $$r_u = (-s_3 - b_u, 0), \qquad r_v = (s_3 + b_v, 0).$$

   Note that $\|r_u - r_v\| \leq \|q_u - q_v\|$.

3. Let p_u^*, p_v^* be images of r_u, r_v under any rotation about the origin.

We start with $(p_1, p_2, p_3, p_4) \in \Upsilon$. This guarantees that $a_u, b_u, a_v, b_v > 0$. For the points (p_u, p_v) our symmetrization operation is a special case of the map

$$(p_u, p_v) \to (p_u^*, p_v^*),$$

for suitable choice of constants and a suitable rotation.

Recall that $\widehat{p}$ is the image of p under inverse stereographic projection. Lemma B2 is implied by:

$$\|\widehat{r}_u - \widehat{r}_v\|^{-s} + \|\widehat{r}_u - (0,0,1)\|^{-s} + \|\widehat{r}_v - (0,0,1)\|^{-s} \leq$$

$$\|\widehat{p}_u - \widehat{p}_v\|^{-s} + \|\widehat{p}_u - (0,0,1)\|^{-s} + \|\widehat{p}_v - (0,0,1)\|^{-s} \tag{20}$$

for all $s \geq 2$, with equality iff $(r_u, r_v) = (p_u, p_v)$ up to rotation about the origin.

We will establish Equation 20 in two steps.

Lemma 4.5 (B21) *Let $s \geq 2$ and*

$$A_s = \|\widehat{p}_u - \widehat{p}_v\|^{-s} - \|\widehat{q}_u - \widehat{q}_v\|^{-s},$$

$$B_s = \|\widehat{p}_u - (0,0,1)\|^{-s} + \|\widehat{p}_v - (0,0,1)\|^{-s} - \|\widehat{q}_u - (0,0,1)\|^{-s} - \|\widehat{q}_v - (0,0,1)\|^{-s}.$$

Then $A_s, B_s \geq 0$, with equality iff $p_u = q_u$ and $p_v = q_v$ up to a rotation.

Proof: Note that if $A_2 > 0$ then $A_s > 0$ for all $s > 0$. If $B_2 > 0$ then the Convexity Lemma implies that $B_s > 0$ for all $s > 2$. So, it suffices to prove that $A_2, B_2 > 0$. We rotate so that

$$p_u = (-x+h, y), \quad p_v = (x+h, y), \quad q_u = (-x, 0), \quad q_v = (x, 0). \tag{21}$$

We compute

$$A_2 = \frac{h^4 + y^2(2 + 2x^2 + y^2) + 2h^2(1 - x^2 + y^2)}{16x^2}, \qquad B_2 = \frac{y^2 + h^2}{2}. \tag{22}$$

Since $x \in (0,1)$ we have $A_2, B_2 > 0$ unless $h = y = 0$. ♠

Define

$$F_s(a_u, a_v) = \|\widehat{q}_u - \widehat{q}_v\|^{-s} + \|\widehat{q}_u - (0,0,1)\|^{-s} + \|\widehat{q}_v - (0,0,1)\|^{-s}, \tag{23}$$

Likewise define $F_s(b_u, b_v)$. Finally, define

$$E(s) = F_s(a_u, a_v) - F_s(b_u, b_v). \tag{24}$$

Lemma 4.6 (B22) *$E(s) \geq 0$ with equality iff $b_u = a_u$ and $b_v = a_v$.*

Proof: It suffices to prove this result in the intermediate case when $a_u = b_u$ or $a_v = b_v$ because then we can apply the intermediate result twice to get the general case. Without loss of generality we consider the case when $a_v = b_v$ and $b_u < a_u$. With the file `LemmaB22.m` – see below – we compute that $\partial F_2/\partial a_u$ and $-\partial F_{-2}/\partial a_u$ are both rational functions of a_u, a_v with all positive coefficients. Hence $E(2) > 0$ and $E(-2) < 0$.

Consider the sign sequence for $E(s)$. When $a_u = b_u$, the expression $E(s)$ is an exponential sum with 4 terms. When $a_u = a_v = 0$ the points $\widehat{\zeta}_u, \widehat{\zeta}_v$ and $(0, 0, 1)$ make an equilateral triangle on a great circle. Hence, when $a_u, a_v, b_u, b_v > 0$ the point $\widehat{\zeta}_u$ is closer to $(0, 0, 1)$ than it is to $\widehat{\zeta}_v$ both in its old location and in its new location. The inward motion of the point ζ_u increases the shorter (corresponding spherical) distance and decreases the longer (corresponding spherical) distance. More to the point, our move decreases the longer inverse-distance and increases the shorter inverse-distance. Thus the sign sequence (§2.1) for $E(s)$ is $+, -.-, +$.

By Descartes' Lemma, $E(s)$ changes sign at most twice and also $E(s) > 0$ when $|s|$ is sufficiently large. Since $E(-2) < 0$ as see that E changes sign on $(-\infty, -2)$. If E has a root in $(2, \infty)$ then in fact E has at least 2 roots (counted with multiplicity) because it starts and ends positive on this interval. But then E has at least 3 roots, counting multiplicity. This is contradiction. Hence $E(s) > 0$ for $s \geq 2$. ♠

4.4 Proof of Lemma B3

The domain Υ' is symmetric with respect to reflection in the X-axis. Thanks to this symmetry, it suffices to prove Lemma B3 for the list $\{(0, 1), (1, 2)\}$. We set $q_j = p'_j$ and $q'_j = p''_j$.

We introduce the notation $q_1 = (q_{10}, q_{11})$, etc. The horizontal symmetrization operation is given by

$$(q_0, q_1, q_2) \to (q'_0, q'_1, q'_2),$$

where

$$q'_0 = \left(\frac{q_{01} - q_{21}}{2}, q_{02}\right), \qquad q'_1 = (0, q_{21}), \qquad q'_2 = \left(\frac{q_{21} - q_{01}}{2}, q_{22}\right), \tag{25}$$

Note that $\|q_0' - q_1'\| = \|q_2' - q_1'\|$. This means that the kind of inequality we are trying to establish has the form $2A^s \leq B^s + C^s$ for choices of A, B, C which depend on the points involved. Therefore, by the Convexity Lemma, it suffices to prove that $\{(0,1),(1,2)\}$ is good for the parameter $s = 2$.

Let D denote the set of triples of points $(q_0, q_1, q_2) \in (\boldsymbol{R}^2)^3$ such that there is some q_3 such that $q_0, q_1, q_2, q_3 \in \Upsilon'$. Most of our proof involves finding a concrete parametrization of a subset of $\boldsymbol{R}^6$ that contains D. Note that D is really a 5 dimensional set, because $q_{22} = q_{02}$. We will use parameters a, b, c, d, e to parametrize a subset of $\boldsymbol{R}^6$ that contains D.

We define

$$[a,b,t] = \frac{a(1-t)}{512} + \frac{bt}{512}. \tag{26}$$

Here $F_{512}(a, b, \cdot)$ maps the interval $[0, 1]$ onto the interval $[a, b]/512$. Given $(a, b, c, d, e) \in [0, 1]^5$ and $\sigma_1, \sigma_2 \in \{-, +\}$ we define

$$\begin{aligned} p0 &= ([+416, +498, a] + [0, 49, e], [0, 16\sigma_1, b]);\\ p1 &= ([0, 32\sigma_2, d], [348, 465, c]);\\ p2 &= ([-416, -498, a] + [0, 49, e], [0, 16\sigma_1, b]); \end{aligned} \tag{27}$$

We call this map ϕ_{σ_1,σ_2}. In these coordinates, horizontal symmetrization is the map

$$(a, b, c, d, e) \to (a, b, c, 0, 0). \tag{28}$$

We have two steps we need to take. First we really need to show that we have parametrized a superset of D. Second, we need to calculate the energy change as a function of a, b, c, d, e and check at it decreases.

Lemma 4.7 (B31) *We have*

$$D \subset \phi_{+,+}([0,1]^5) \cup \phi_{+,-}([0,1]^5) \cup \phi_{-,+}([0,1]^5) \cup \phi_{-.-}([0,1]^5).$$

Proof: Recall that $q_i = (q_{i1}, q_{i2})$. Let D_{ij} denote the set of possible coordinates q_{ij} that can arise for points in D. Thus, for instance

$$D_{01} = [-16, 16]/512.$$

Let D^*_{ij} denote the set of possible coordinates q_{ij} that can arise from the union of our parametrizations. By construction $D_{i2} \subset D^*_{i2}$ for $i = 0, 1, 2$ and $D_{11} \subset D^*_{11}$.

Remembering that we have $q_{01} \geq |q_{21}|$, we see that the set of pairs $512(q_{01}, q_{21})$ satisfying all the conditions for inclusion in D lies in the triangle Δ with vertices

$$(498, -498), \quad (498, -400), \quad (432, -400).$$

At the same time, the set of pairs $(512)(p^*_{01}, p^*_{21})$ that we can reach with our parametrization is the rectangle Δ^* with vertices

$$(498,-498), \quad (416,-416), \quad (498,-498)+(49,49), \quad (416,-416)+(49,49).$$

One checks easily that hence $\Delta \subset \Delta^*$. Indeed, Δ is inscribed in Δ^*. ♠

Using our coordinates above, we define

$$F_{\pm,\pm}(a,b,c,d,e) = \|\widehat{q}_0 - \widehat{q}_1\|^{-2} + \|\widehat{q}_2 - \widehat{q}_1\|^{-2},$$

$$\Phi_{\pm,\pm}(a,b,c,d,e) = \mathrm{num}_+(F_{\pm,\pm}(a,b,c,d,e) - F_{\pm,\pm}(a,b,c,0,0)). \qquad (29)$$

Here q_0, q_1, q_2 are the points which correspond to (a,b,c,d,e) under our map $\phi_{\pm,\pm}$ and $\widehat{q}_0, \widehat{q}_1, \widehat{q}_2$ are their images under inverse stereographic projection. To finish our proof, we just have to show that $\Phi_{\pm,\pm}(a,b,c,d,e) \geq 0$ on $[0,1]^5$. The following lemma, and continuity, gives us this result.

Lemma 4.8 (B32) *For any sign choice,* $\Phi_{\pm,\pm} > 0$ *on* $(0,1)^5$.

Proof: We let $\Phi_a = \partial\Phi/\partial a$, and likewise for the other variables. Iterating this notation, we let Φ_{aa}, etc., denote the second partials.

Let Φ be any of the 4 polynomials. The file `LemmaB32.m` – see below – computes that

1. Φ and Φ_d and Φ_e are zero when $d = e = 0$.
2. Φ_{dd} and Φ_{ee} are weak positive dominant, hence nonnegative on $[0,1]^5$.
3. $\Phi_d + 2\Phi_e$ is weak positive dominant, hence nonnegative on $[0,1]^5$.

Let $Q_d \subset [0,1]^5$ be the sub-cube where $d = 0$. We fix (a,b,c) and consider the single variable function $\phi(d) = \Phi(a,b,c,d,0)$. From Items 1 and 2 above, $\phi(0) = \phi'(0) = 0$ and $\phi''(d) \geq 0$. Hence $\phi(d) \geq 0$ for $d \geq 0$. Hence $\Phi \geq 0$ on Q_d. A similar argument shows that likewise $\Phi \geq 0$ on Q_e.

Any point in $(0,1)^5$ can be joined to a point in $Q_d \cup Q_e$ by a line segment L which is parallel to the vector $(0,0,0,1,2)$. From Item 3 above, Φ increases along such a line segment as we move out of $Q_d \cup Q_e$. Hence $\Phi \geq 0$ on $[0,1]^5$. ♠

4.5 Proof of Lemma B4

The set Υ'' is symmetric with respect to reflections in both coordinate axes. Thanks to these symmeties, it suffices to prove that $\{(0,1),(0,3)\}$ is good for all $s \geq 12$, and it suffices to consider the case when $p''_{02} \geq 0$. That is, the point p_0 lies on or above the X-axis. For ease of notation set $q_k = p''_k$ and $q'_k = p'''_k$. We are considering the case when $q_{02} \geq 0$.

Let D be the set of configurations (q_0, q_1, q_3) such that $q_{02} \geq 0$ and $(q_0, q_1, q_2, q_3) \in \Upsilon''$ when q_2 is the reflection of q_0 in the Y-axis. Let $D_\pm \subset D$ denote those configurations with $\pm(q_{12}+q_{32}) \geq 0$. Obviously $D = D_+ \cup D_-$.

The sets $D_\pm$ are 4-dimensional subsets of $(\boldsymbol{R}^2)^3$. We parametrize a superset of $D_\pm$ much as we did in the proof of Lemma B3. As in Equation 26 we define

$$[a,b,t] = \frac{(1-t)a}{512} + \frac{bt}{512}.$$

Given $(a,b,c,d) \in [0,1]^4$ and $\sigma \in \{+,-\}$ we define

$$\begin{aligned} p_0 &= ([416, 498, b], [0, 16, d]); \\ p_1 &= (0, -[348, 465, a] + [0, 59\sigma, c]); \\ p_3 &= (0, +[348, 465, a] + [0, 59\sigma, c]); \end{aligned} \tag{30}$$

We call this map ϕ_σ. In these coordinates, the symmetrization operation is $(a,b,c,d) \to (a,b,0,0)$.

Lemma 4.9 (B41) $D_\pm \subset \phi_\pm([0,1]^4)$.

Proof: This is just like the proof of Lemma B31. The only non-obvious point is why every pair (p_{12}, p_{32}) is reached by the map $\phi_\pm$. The essential point is that for configurations in $D_\pm$ we have $512|p_{12}+p_{32}| \leq 2 \times 59$. ♠

Following the same idea as in the proof of Lemma B3, we define

$$F_{s,\pm}(a,b,c,d) = \|\Sigma^{-1}(q_0) - \Sigma^{-1}(q_1)\|^{-s} + \|\Sigma^{-1}(q_0) - \Sigma^{-1}(q_3)\|^{-s}, \tag{31}$$

$$\Phi_{s,\pm}(a,b,c,d) = \mathrm{num}_+(F_{s,\pm}(a,b,c,d) - F_{s,\pm}(a,b,0,0)). \tag{32}$$

The points on the right side of Equation 31 are coordinatized by the map $\phi_\pm$. We can finish the proof by showing that $\phi_{2,+} \geq 0$ and $\phi_{12,-} \geq 0$ on $[0,1]^4$. The Convexity Lemma then takes care of all exponents greater than 2 on D_+ and all exponents greater than 12 on D_-. Notice the asymmetry in the calculation. The $(+)$ side is much less delicate.

Lemma 4.10 (B42) $\Phi_{2,+} \geq 0$ *on* $[0,1]^4$.

Proof: Let $\Phi = \Phi_{2,+}$. Let $\Phi|_{c=0}$ denote the polynomial we get by setting $c = 0$. Etc. Let $\Phi_c = \partial\Phi/\partial c$, etc. The Mathematica file `LemmaB42.m` computes that $\Phi|_{c=0}$ and $\Phi|_{d=0}$ and $\Phi_c + \Phi_d$ are weak positive dominant. Hence $\Phi \geq 0$ when $c = 0$ or $d = 0$ and the directional derivative of Φ in the direction $(0,0,1,1)$ is non-negative. This suffices to show that $\Phi \geq 0$ on $[0,1]^4$. ♠

Lemma 4.11 (B43) $\Phi_{12,-} \geq 0$ *on* $[0,1]^4$.

Proof: The file `LemmaB43.m` has the calculations. Let $\Phi = \Phi_{12,-}$. This monster has 102218 terms.

Step 1: Let M denote the maximum coefficient of Φ. We let Φ^* be the polynomial we get by taking each coefficient of c of Φ and replacing it with $\text{floor}(10^{10}c/M)$. Note that if Φ^* is nonnegative on $[0,1]^4$ then so is Φ.

Step 2: Now Φ^* has 37760 monomials in which the coefficient is -1. We check that each such monomial is divisible by one of c^2 or d^2 or cd. Let

$$\Psi = \Phi^{**} - 37760(c^2 + d^2 + cd),$$

where Φ^{**} is obtained from Φ^* by setting all the (-1) monomials to 0. We have $\Psi \leq \Phi^*$ on $[0,1]^4$. Hence, if Ψ is non-negative on $[0,1]^4$ then so is Φ^*. The polynomial Ψ has 5743 terms.

Step 3: We check that Ψ_{aaa} is WPD and hence non-negative on $[0,1]^4$. This massive calculation reduces us to showing that the restrictions $\Psi|_{a=0}$ and $\Psi_a|_{a=0}$ and $\Psi_{aa}|_{a=0}$ are all non-negative on $[0,1]^3$. Consider

$$f|_{c=0}, \qquad f|_{d=0} \qquad 4f_c + f_d, \tag{33}$$

We show that all three functions are WPD when either $f = \Psi_a|_{a=0}$ or $f = \Psi_{aa}|_{a=0}$. This shows that $\Psi_a|_{a=0}$ and $\Psi_{aa}|_{a=0}$ are non-negative on $[0,1]^3$. Also, we show that the first two functions are WPD when $f = \Psi|_{a=0}$.

Step 4: Let $g = 4f_c + f_d \geq 0$ on $[0,1]^3$ when $f = \Psi|_{a=0}$. We check that g_d is WPD and hence non-negative on $[0,1]^3$. This reduces us to showing that $h = g|_{d=0}$ is non-negative on $[0,1]^2$. here h is a 2-variable polynomial in b, c. Referring to the operation in §2.2, we check that the two subdivisions $S_{b,0}(h)$ and $S_{b,1}(h)$ are WPD. This proves $h \geq 0$ on $[0,1]^2$. ♠

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See Paper 0 for an extended bibliography.