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

During the past decade I have written several versions of a proof that rigorously 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. See [**S0**] for the latest version. This work implies and extends my solution [**S1**] of Thomson's 1904 5-electron problem [**Th**]. Unfortunately, after a number of attempts I have not been able to publish my work on this. Even though I have taken great pains to make the proof modular and checkable, the monograph still gives the impression of being too difficult to referee.

Now I am taking a new approach. 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. The longest of the papers is 20 pages. The drawback of this approach is twofold. First, there will necessarily be some redundancy in these papers. Second, none of the papers has a blockbuster result in itself. To help offset the second drawback, I will state the main result in full in each paper, and I will try to explain how the small result proved in each paper relates to the overall goal.

1.2 The Phase Transition Result

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

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

This quantity is commonly called the *F-potential* or the *F-energy* of P. A configuration P is a *minimizer* for F if $\mathcal{E}_F(P) \le \mathcal{E}_F(P')$ for all other N-point configurations P'.

We are interested in the *Riesz potentials*:

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

R_s is also called a *power law potential*, and R_1 is specially called the *Coulomb potential* or the *electrostatic potential*. The question of finding the N-point minimizers for R_1 is commonly called *Thomson's problem*.

We consider the case $N = 5$. 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

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

Theorem 1.1 (Phase Transition) *There exists $\mathfrak{w} \in (15, 15_+)$ such that:*

1. *For $s \in (0, \mathfrak{w})$ the TBP is the unique minimizer for R_s.*

2. *For $s = \mathfrak{w}$ the TBP and some FP are the two minimizers for R_s.*

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

The proof has many moving parts. The largest part involves eliminating all the configurations and energy exponents outside a set of the form $\Upsilon \times [13, 15^+]$ using a computer-assisted divide-and-conquer algorithm. This paper discusses the region $\Upsilon \times [12, \infty)$. This region, which looks somewhat contrived, contains those FPs which compete with the TPB for energy exponents s reasonably near $\mathfrak{w}$.

1.3 Results

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.

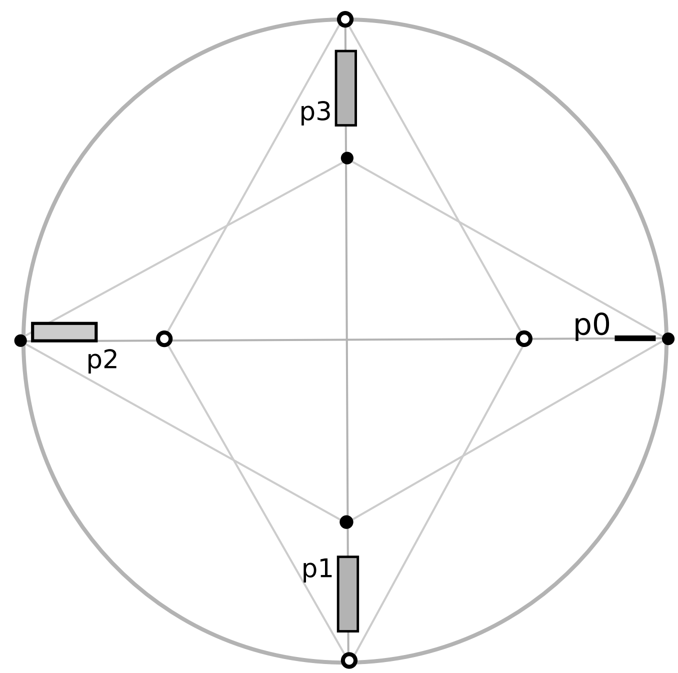

Figure 1: The sets defining Υ compared with two TBP avatars.

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 $s = \mathfrak{w}$.

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 $\mathcal{E}_s(\sigma(p)) \le \mathcal{E}_s(p)$ 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. For example, the operation σ is extremely delicate. If we take the exponent $s=13$, the operation actually seems to *increase* the energy. I tested various symmetrization schemes experimentally until I found ones adapted to the critical regimes defined above.

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.

Some experts in this problem might get excited that the Symmetrization Theorem I works for *all* exponents $s \ge 12$. Might this shed light on high energy minimizers? Alas, no. When s is very large, the domain Υ does not contain the candidate minimizers.

1.4 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

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

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 §1.3. 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:

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

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

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

We compute

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

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

Define

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

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

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

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

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

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

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.