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 23 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

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

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'.

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 $\boldsymbol{w} \in (15, 15_+)$ such that:*

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

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

3. *For each $s \in (\boldsymbol{w}, 15_+)$ 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 $\boldsymbol{w}$.

1.3 First Result

Let $\boldsymbol{K}_4$ denote the set of configurations which have 4-fold dihedral symmetry. In this paper, we will introduce a retraction $\Upsilon \to \boldsymbol{K}_4$ which decreases the R_s-potential on $\Upsilon - \boldsymbol{K}_4$ for all $s \geq 12$. This result establishes the following fact: If some configuration in Υ has less or equal R_s energy than the TPB for some $s \geq 12$ then so does a configuration in $\boldsymbol{K}_4$. In order to state the precise result proved here, I first need to introduce some background information.

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 $\mathcal{E}_F(p_1, p_2, p_3, p_4)$ when we mean the F-potential of the corresponding 5-point configuration.

Figure 1 shows the two possible avatars (up to rotations) of the triangular bi-pyramid, first separately and then superimposed. We call the one on the left the *even avatar*, and the one in the middle the *odd avatar*. The points for the even avatar are $(\pm 1, 0)$ and $(0, \pm\sqrt{3}/3)$. When we superimpose the two avatars we see some extra geometric structure that is not relevant for our proof but worth mentioning. The two circles respectively have radii $1/2$ and 1 and the 6 segments shown are tangent to the inner one.
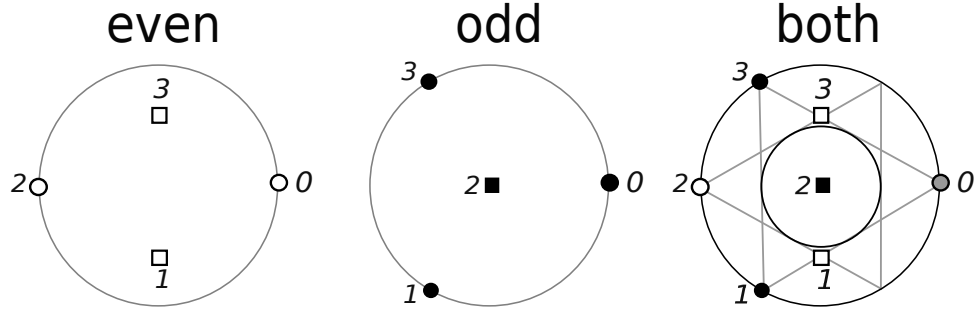
Figure 1: Even and odd avatars of the TBP.

The Special Domain: We let $\Upsilon \subset (\boldsymbol{R}^2)^4$ denote those avatars p_0, p_1, p_2, p_3 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. $512p_3 \in [-16, 16] \times [349, 464]$.

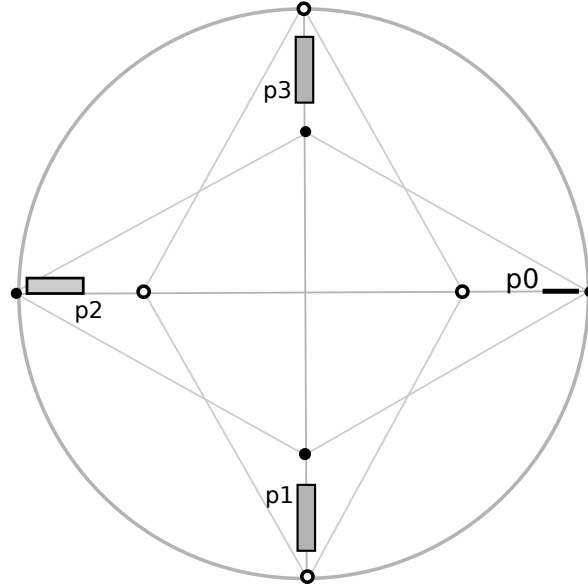As we discussed above, Υ contains the avatars that compete with the TBP near the exponent $\mathbf{w}$.

Figure 2: The sets defining Υ compared with two TBP avatars.

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

$$d_{02} = 2\|p_0 - p_2\|, \qquad d_{13} = 2\|\pi_{02}(p_1 - p_3)\|. \tag{7}$$

Here π_{02} is the projection onto the subspace perpendicular to the vector $p_0 - p_2$. Finally, we define

$$p_0^* = (d_{02}, 0), \quad p_1^* = (0, -d_{13}), \quad p_2^* = (-d_{02}, 0), \quad p_3^* = (0, d_{13}). \tag{8}$$

The avatar $(p_1^*, p_2^*, p_3^*, p_4^*)$ lies in $\boldsymbol{K}_4$.

Here is the first result of this paper.

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.

The Symmetrization Theorem I is called Lemma B in the monograph.

1.4 The Second Result

We also consider a second symmetrization operation defined on an even smaller domain and for an even smaller set of exponents.

A Second Domain: Let $\Psi_4^\sharp$ denote the set of avatars $(p_1, p_2, p_3, p_4) \in \boldsymbol{K}_4$ having the form

$$(x, 0), \quad (0, -y), \quad (-x, 0), \quad (0, y), \qquad 512(x, y) \in [440, 448]. \tag{9}$$

This domain contains the avatar representing the FP which ties with the TBP at $s = \mathfrak{w}$.

A Second Symmetrization: We define

$$\sigma(x, y) = (z, z), \qquad z = \frac{x + y + (x - y)^2}{2}. \tag{10}$$

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 $\sigma(p) = p$.*

The Symmetrization Theorem II is called Lemma C1 in the monograph. The operation σ is extremely delicate. If we take the exponent $s = 13$, the operation actually seems to *increase* the energy. The magic only kicks in around exponent 13.53.

1.5 Discussion

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. Fortunately, we only need to consider such operations on the small sets Υ and $\Psi_4^\sharp$ and for exponents fairly near $\boldsymbol{v}$. I testes various symmetrization schemes experimentally until I found good ones.

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 replaces one big verification by a bunch of smaller ones, conducted over lower dimensional configuration spaces.

Proving tht the second symmetrization lowers energy is just a 2-dimensional problem, but the result is extremely delicate, as I mentioned above. The proof relies on an algebraic miracle that I discovered experimentally.

Some experts in this problem might get excited that the Symmetrization Theorem I works for *all* exponents $s \geq 12$. Might this shed light on high energy minimizers? Alas, no. When s is very large, the domain Υ does not contain the candidate minimizers. It is known that the candidate minimizers converge to 5 of the 6 points of the regular octahedron. The limiting configuration would be represented by the avatar whose points are the 4th roots of unity – the highlighted points on the unit circle in Figure 2. I guess that my symmetrization result would hold in better adapted domains as $s \to \infty$ but I don't know how to do the analysis.

1.6 Paper Organization

In §2 I will present some computational tools which will help with the analysis. In §3 I will reduce the Symmetrization Theorem to four Lemmas, Lemma B1–B4. In subsequent chapters I will prove these lemmas in turn. Following this, I will prove he Symmetrization Theorem II.

The proofs in this paper are computer-assisted. All calculations are all done using exact arithmetic in Mathematica. The reader can download and inspect the files I wrote for this.

2　Preliminaries

In this chapter we introduce some tools which we use for the proof of the Symmetrization Theorem.

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. ♠

Before our next result we discuss Descartes' Rule of Signs. 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 is a slight simplification; the full rule also says that the number of roots (counted with multiplicity) has the same parity as the number of sign changes. One proof goes through induction on the degree, and differentiation.

Lemma 2.2 (Descartes) *Let $0 < r_1 \leq r_1 ... \leq r_n < 1$ 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*

$$E(s) = \sum_{i=1}^{n} c_i \ r_i^s. \tag{11}$$

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 Positive Dominance

Our main tool is what we call Positive Dominance. This is a positivity certificate for polynomials on the unit cube. The works [**S2**] and [**S3**] give more details about this criterion. I developed the Positive Dominance criterion myself, though I would not be surprised to learn that it has turned up elsewhere in the vast field of computational algebra.

Let $G \in \mathbf{R}[x_1, ..., x_n]$ be a multivariable polynomial:

$$G = \sum_I c_I X^I, \qquad X^I = \prod_{i=1}^n x_i^{I_i}. \qquad (12)$$

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

$$G_J = \sum_{I \preceq J} c_I, \qquad G_\infty = \sum_I c_I. \qquad (13)$$

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

$$P = f_0 + f_1 x_k + ... + f_m x_k^m, \qquad f_j \in \mathbf{R}[x_1, ..., x_{n-1}]. \qquad (14)$$

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 $x_n \in (0, 1]$. ♠

2.3 Operations on Polynomials and Rational Functions

Here are two more operations we perform on polynomials and rational functions.

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

$$S_{x_j, k}(P)(x_1, ..., x_n) = P(x_1, ..., x_{j-1}, x_j^*, x_{j+1}, ..., x_n), \quad x_j^* = \frac{k}{2} + \frac{x_j}{2}. \quad (15)$$

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

Positive 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 $\mathrm{num}_+(f) = f_1$.

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3 The Symmetrization Theorem I

In this chapter we reduce the Symmetrization Theorem I to smaller steps. Recall that the domain Υ is defined in §1.3 and shown in Figure 1. Let $X = (p_1, p_2, p_3, p_4)$ be an avatar in Υ. We will perform successive operations on X to arrive at $X' = (p'_1, p'_2, p'_3, p'_4)$ and $X'' = (p''_1, ...)$, etc.

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. We call this operation *rotation*. Let Υ' denote the domain of avatars X' such that

1. $\|p'_0\| \geq \|p'_k\|$ for $k = 1, 2, 3$.

2. $512p'_0 \in [432, 498] \times [-16, 16]$. (Compare $[433, 498] \times [0, 0]$.)

3. $512p'_1 \in [-32, 32] \times [-465, -348]$. (Compare $[-16, 16] \times [-464, -349]$.)

4. $512p'_2 \in [-498, -400] \times [-16, 16]$. (Compare $[-498, -400] \times [0, 24]$.)

5. $512p'_3 \in [-32, 32] \times [348, 465]$. (Compare $[-16, 16] \times [349, 464]$.)

6. $p'_{02} = p'_{22}$. (Compare $p_{02} = 0$.)

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

Lemma 3.1 (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. $512p''_0 \in [416, 498] \times [-16, 16]$ and $(p''_{21}, p''_{22}) = (-p''_{01}, p''_{02})$.

2. $-512p_1, 512p''_3 \in [0, 0] \times [348, 465]$.

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. A typical term is:

$$R_s(p_i, p_j) = \frac{1}{\|\Sigma^{-1}(p_i) - \Sigma^{-1}(p_j)\|^s}. \qquad (16)$$

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. Thus, for instance

$$L = \{(0,2), (0,4), (2,4)\} \implies \mathcal{E}_s(P, L) = R_s(p_0, p_2) + R_s(p_0, p_4) + R_s(p_2, p_4).$$

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 lower $\mathcal{E}_s(P, L)$ unless the operation fixes P. When we make this definition we mean to take the appropriate domains.

Lemma 3.2 (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 3.3 (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 3.4 (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.*

The Symmetrization Theorem I follows immediately from Lemmas B1, B2, B3, and B4. We prove these results in subsequent chapters.

4 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. This is a tedious exercise in trigonometry.

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

$$512 \cos(\theta) \in [0, 1], \qquad 512 \sin(\theta) \in [0, 16]. \tag{17}$$

From Equation 17, 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.

5 Proof of Lemma B2

5.1 A More General Result

The significance of the number

$$s_3 = \frac{\sqrt{3}}{3}. \tag{18}$$

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 $b_u \le a_u$ and $b_v \le a_v$. Let

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

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

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:

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

$$\|\widehat{p}_u - \widehat{p}_v\|^{-s} + \|\widehat{p}_u - (0, 0, 1)\|^{-s} + \|\widehat{p}_v - (0, 0, 1)\|^{-s} \tag{19}$$

for all $s \ge 2$, with equality iff $(r_u, r_v) = (p_u, p_v)$ up to rotation about the origin. The rest of this chapter establishes Equation 19.

5.2   The Main Arguments

We will establish Equation 19 in two steps.

Lemma 5.1 (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

$$p_u = (-x + h, y), \quad p_v = (x + h, y), \quad q_u = (-x, 0), \quad q_v = (x, 0). \quad (20)$$

We compute

$$A_2 = \frac{h^4 + y^2(2 + 2x^2 + y^2) + 2h^2(1 - x^2 + y^2)}{16x^2}, \quad B_2 = \frac{y^2 + h^2}{2}. \quad (21)$$

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

Define

$$F_s(a_u, a_v) = \|\widehat{q}_u - \widehat{q}_v\|^{-s} + \|\widehat{q}_u - (0,0,1)\|^{-s} + \|\widehat{q}_v - (0,0,1)\|^{-s}, \quad (22)$$

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

$$E(s) = F_s(a_u, a_v) - F_s(b_u, b_v). \quad (23)$$

Lemma 5.2 (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

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$\widehat{\zeta}_u, \widehat{\zeta}_v$ 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 $s \geq 2$. ♠

6 Proof of Lemma B3

6.1 Setting up the Calculations

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

$$q'_0 = \left(\frac{q_{01} - q_{21}}{2}, q_{02} \right), \qquad q'_1 = (0, q_{21}), \qquad q'_2 = \left(\frac{q_{21} - q_{01}}{2}, q_{22} \right), \tag{24}$$

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 $(q_0, q_1, q_2) \in (\mathbf{R}^2)^3$ 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 $\mathbf{R}^6$ that contains D. Note that D is really a 5 dimensional set, because $q_{21} = q_{01}$. We will use parameters a, b, c, d, e to parametrize a subset of $\mathbf{R}^6$ that contains D.

We define

$$[u, v]t = u(1 - t) + vt. \tag{25}$$

The map $t \to [u, v]t$ maps $[0, 1]$ to $[u, v]$.

For all 4 choices of signs we define $\phi_{\pm, \pm} : [0, 1]^5 \to (\mathbf{R}^2)^3$ as follows:

$$\phi_{\pm, \pm}(a, b, c, d, e) = q_0(a, d, \pm b), q_1(\pm e, c), q_2(a, d, \pm b), \tag{26}$$

where

$$512 q_0(a, d, \pm b) = ([416, 498]a + 49e, \pm 16b).$$

$$512 q_1(\pm d, c) = (\pm 32d, [348 + 465]c)$$

$$512 q_2(a, d, \pm b) = ([-416, -498]a + 49e, \pm 16b).$$

In these coordinates, horizontal symmetrization is the map

$$(a, b, c, d, e) \to (a, b, c, 0, 0). \tag{27}$$

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.

6.2 Checking the Parametrization

We first show how to parametrize a superset of D.

Lemma 6.1 (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 (q_{01}, q_{21}) satisfying all the conditions for inclusion in D lies in the triangle Δ with vertices $(498, -498)$ and $(498, -400)$ and $(432, -400)$. 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

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

We have $\Delta \subset \Delta^*$ because

$$(432, -400) = (416, -416) + (16, 16), \qquad (498, -400) = (449, -449) + (49, 49).$$

This completes the proof. ♠

6.3 Checking the Energy Decrease

Using our coordinates above, we define

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

$$\Phi_{\pm,\pm}(a, b, c, d, e) = \text{num}_+(F_{\pm,\pm}(a, b, c, d, e) - F_{\pm,\pm}(a, b, c, 0, 0)). \qquad (28)$$

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.

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Lemma 6.2 (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 $[0,1]^5$. ♠

7 Proof of Lemma B4

7.1 Setting up the Calculation

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 $(\mathbf{R}^2)^3$. We parametrize a superset of $D_\pm$ in a manner similar to what we did in the proof of Lemma B3. As in Equation 25, let $[u, v]t = u(1 - t) + vt$. We define

$$\phi_\pm(a, b, c, d) = (q_0(b, d), q_1(a, c), q_3(a, c)),$$

$$512q_0(b, d) = ([416, 498]b, 16d).$$

$$512q_1(a, c) = (0, -[348, 465]a \pm 59c).$$

$$512q_3(a, c) = (0, +[348, 465]a \pm 59c).$$

In these coordinates, the symmetrization operation is $(a, b, c, d) \to (a, b, 0, 0)$.

7.2 The Main Calculations

Lemma 7.1 (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

$$F_{s,\pm}(a, b, c, d) = \|\Sigma^{-1}(q_0) - \Sigma^{-1}(q_1)\|^{-s} + \|\Sigma^{-1}(q_0) - \Sigma^{-1}(q_3)\|^{-s}, \quad (29)$$

$$\Phi_{s,\pm}(a, b, c, d) = \text{num}_+(F_{s,\pm}(a, b, c, d) - F_{s,\pm}(a, b, 0, 0)). \quad (30)$$

The points on the right side of Equation 29 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.

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Lemma 7.2 (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 7.3 (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 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

$$f|_{c=0}, \qquad f|_{d=0} \qquad 4f_c + f_d, \qquad\qquad (31)$$

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 §2.3, we check that the two subdivisions $S_{b,0}(h)$ and $S_{b,1}(h)$ are WPD. This proves $h \geq 0$ on $[0,1]^2$. ♠

8 The Symmetrization Theorem II

We use the notation from §1.4. We write

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

$$G_s(x,y) = \|\widehat{p}_0, \widehat{p}_2\|^{-s} + \|\widehat{p}_1, \widehat{p}_3\|^{-s},$$

$$H_s(x,y) = 2\|\widehat{p}_0, (0,0,1)\|^{-s} + 2\|\widehat{p}_1, (0,0,1)\|^{-s} + 4\|\widehat{p}_0, \widehat{p}_1\|^{-s}. \qquad (32)$$

The Symmetrization Lemma II is an immediate consequence of Lemmas C1 and C2 proved below.

Lemma 8.1 (C1) $G_s(x,y) \geq G_s(z,z)$ *for* $s \geq 2$ *and* $(x,y) \in \Psi_4^{\sharp}$. *When* $s > 2$ *we get equality if and only if* $x = y$.

Proof: By the Convexity Lemma from §2.1 it suffices for us to prove that $G_2(x,y) \geq G_2(z,z)$ for all $x,y \in \Psi_4$. Let $\phi : [0,1]^2 \to \Psi_4^{\sharp}$ be the affine isomorphism whose linear part is a positive diagonal matrix. Define

$$\Phi = \operatorname{num}_+(G_2 \circ \phi - G_2 \circ \sigma \circ \phi). \qquad (33)$$

The file `LemmaC1.m` computes that $\Phi(a,b) = (a-b)^2 \Phi^*$, where Φ^* is weak positive dominant. Hence $\Phi^* > 0$ on $(0,1)^2$. This does it. ♠

Lemma 8.2 (C2) $H_s(x,y) \geq H_s(z,z)$ *for* $s \in [14,16]$ *and* $(x,y) \in \Psi_4^{\sharp}$.

Proof: We fix an arbitrary point $(x,y) \in \Psi_4^{\sharp}$ with $x \neq y$ and make all definitions relative to this point. We let $h(s) = H_s(x,y) - H_s(z,z)$.

For integers $k = 2, 14, 16$ define

$$\Phi_k = \operatorname{num}_+(H_k \circ \phi - H_k \circ \sigma \circ \phi). \qquad (34)$$

An algebraic miracle happens. The file `LemmaC21.m` computes that

1. $-\Phi_2(x,y) = (x-y)^2 \Phi_2^*(x,y)$ and Φ_2^* is weak positive dominant.

2. $\Phi_{14}(x,y) = (x-y)^2 \Phi_{14}^*(x,y)$ and Φ_{14}^* is weak positive dominant.

3. $\Phi_{16}(x,y) = (x-y)^2 \Phi_{16}^*(x,y)$ and Φ_{16}^* is weak positive dominant.

We conclude that $h(2) < 0$ and $h(14) > 0$ and $h(16) > 0$. Hence h has a root in $(2, 14)$. If $h(s_0) < 0$ for some $s_0 \in (14, 16)$ then h has at least 3 roots in $(2, 16)$. We conclude from the Descartes Lemma that the sign sequence for h changes sign at least 3 times. Moreover, if the sign sequence for h changes sign exactly 3 times then $h(s) > 0$ on $(16, \infty)$.

We contradict this situation. 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). We have

$$h(s) = +2r_0^s - 4(r_0')^s + 2r_1^s + 4r_{01}^s - 4(r_{01}')^s, \tag{35}$$

where

1. $r_{01} = \|\Sigma^{-1}(p_0) - \Sigma^{-1}(p_1)\|^{-1}$.

2. $r_0 = \|\Sigma^{-1}(p_0) - (0, 0, 1)\|^{-1}$ and $r_1 = \|\Sigma^{-1}(p_1) - (0, 0, 1)\|^{-1}$.

3. $r_{01}' = \|\Sigma^{-1}(p_0') - \Sigma^{-1}(p_1')\|^{-1}$.

4. $r_0' = \|\Sigma^{-1}(p_0') - (0, 0, 1)\|^{-1} = \|\Sigma^{-1}(p_1') - (0, 0, 1)\|^{-1}$.

Assuming that

$$r_0, r_1, r_0' < 1/\sqrt{2} < r_{01}, r_{01}', \qquad r_{01} < r_{01}', \tag{36}$$

the sign sequence has at most 3 sign changes. Also, the final inequality says that $h(s) < 0$ for s large. This is a contradiction. To finish our proof, we establish Equation 36.

We have $x, y, z \in (0, 1)$. We compute

$$(1/2) - r_0^2 = \frac{1 - x^2}{4} > 0, \quad (1/2) - r_1^2 = \frac{1 - y^2}{4} > 0, \quad (1/2) - (r_0')^2 = \frac{1 - z^2}{4} > 0,$$

$$(r_{01})^2 - (1/2) = \frac{(1 - x^2)(1 - y^2)}{4(x^2 + y^2)} > 0, \quad (r_{01}')^2 - (1/2) = \frac{(1 - z^2)^2}{8z^2} > 0.$$

This proves the first string of inequalities in Equation 36. For the second inequality, we define $J = \|\widehat{p}_0 - \widehat{p}_1\|^{-2} = r_{01}^2$ and then define Φ in terms of J just as in Equation 34. The file `LemmaC22.m` computes that

$$\Phi(a, b) = -(a - b)^2 \Phi^*(a, b)$$

where Φ^* is weak positive dominant. Hence $\Phi^* > 0$ on $(0, 1)^2$. Hence $\Phi < 0$ on $(0, 1)^2$. Hence $J(z, z) > J(x, y)$. But this implies that $r_{01} < r_{01}'$. This establishes Equation 36. ♠

Remark: A further analysis of h would show that terms in Equation 35 are correctly ordered with respect to the size of the exponent, provided that (x, y) is chosen so that $r_0 < r_1$.

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See Paper 0 for an extended bibliography.