Five Point Energy Minimization 4: Interpolation

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Abstract

This is Paper 4 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 a construction closely related to Hermite Interpolation.

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* $\varpi \in (15, 15_+)$ *such that:*

1. *For* $s \in (0, \varpi)$ *the TBP is the unique minimizer for* R_s*.*
2. *For* $s = \varpi$ *the TBP and some FP are the two minimizers for* R_s*.*
3. *For each* $s \in (\varpi, 15_+)$ *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 The Result of This Paper

This paper deals with a technique closely related to *Hermite Interpolation*. Compare [**CK**]. Define

$$G_k(r) = (4 - r^2)^k. \tag{4}$$

$$G_5^\flat = G_5 - 25G_1, \quad G_{10}^{\sharp\sharp} = G_{10} + 28G_5 + 102G_2, \quad G_{10}^\sharp = G_{10} + 13G_5 + 68G_2 \tag{5}$$

Theorem 1.2 (Interpolation) *Let* T_0 *be the TBP. Then*

1. *Suppose* $s \in (0, 13]$ *and* T *is any* 5*-point configuration. If we have* $F(T_0) < F(T)$ *for all* $F = G_4, G_5, G_6, G_{10}^{\sharp\sharp}$ *then* $\mathcal{E}_{R_s}(T_0) < \mathcal{E}_{R_s}(T)$*.*
2. *Suppose* $s \in [13, 15^+]$ *and* T *is any* 5*-point configuration. If we have* $F(T_0) < F(T)$ *for all* $F = G_5^\flat, G_{10}^\sharp$ *then* $\mathcal{E}_{R_s}(T_0) < \mathcal{E}_{R_s}(T)$*.*

Here is a discussion of the motivation for the Interpolation Theorem. In [**T**], A. Tumanov observes that if the TBP is the unique minimizer for G_2, G_3 and G_5, then the TBP is the unique minimizer for R_s provided that $s \in (0, 2]$. This inspired me to look for other such results, and I built a graphical user interface to find them.

For the purpose of giving results about the Riesz potentials, the functions G_k lose their usefulness at $k = 7$ because the TBP is not a minimizer for $G_7, G_8, \ldots$ At the same time, the general method requires G_k for k large in order to *extend* all the way to the phase transition, a phenomenon that occurs at $\varpi = 15.04\ldots$

My program explores combinations of the form $\sum c_k G_k$ and checks whether various lists of these *energy hybrids* produce the desired results. The computer program takes a quadruple of hybrids, $\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$, and then solves a linear algebra problem to find a linear combination

$$\Lambda_s = a_0 + \sum_{i=1}^{4} a_i(s)\Gamma_i \tag{6}$$

which matches the values of R_s at the values $\sqrt{2}, \sqrt{3}, \sqrt{4}$, the distances involved in the TBP. (I will usually write 2 as $\sqrt{4}$ because then the distances involved in the TBP are easier to remember.)

Concerning Equation 6, what we need for the quadruple to "work" on the interval (s_0, s_1) is that the functions $a_1(s), a_2(s), a_3(s), a_4(s)$ are nonnegative for $s \in (s_0, s_1)$ and that simultaneously the *comparison function* $1-(\Lambda_s/R_s)$ is positive on $(0,2) - \{\sqrt{2}, \sqrt{3}, \sqrt{4}\}$. So, my computer program lets you manipulate the coefficients defining the energy hybrids and then see plots of the functions just mentioned.

At the same time as this, my program computes the energy hybrid evaluated on the space of FPs to see how it compares to the value on the TBP. I call this the *TBP/FP competition*. On intervals $(s_0, s_1) \subset (0, \text{ש})$ we want the TBP to win the competition, as judged by the given energy hybrids. Repeatedly running these competitions and looking at the plots of the coefficients and the comparison function, I eventually arrived at the energy hybrids mentioned in the Interpolation Theorem.

2 Proof of the Interpolation Theorem

2.1 Reduction to Smaller Results

Recall that $15_+ = 15 + \frac{25}{512}$. Referring to Equations 4 and 5, we define

$$P_1 = (G_4, G_6), \qquad P_2 = (G_5, G_{10}^{\sharp\sharp}), \qquad P_3 = (G_5^{\flat}, G_{10}^{\sharp}), \tag{7}$$

$$I_1 = (0, 6], \qquad I_2 = [6, 13], \qquad I_3 = [13, 15_+]. \tag{8}$$

We say that a pair (Γ_3, Γ_4) of functions *forces* the interval I if the following is true: If T is another 5-point configuration such that $\Gamma_k(T_0) < \Gamma_k(T)$ for $k = 3, 4$ then $\mathcal{E}_s(T_0) < \mathcal{E}_s(T)$ for all $s \in I$.

The following result implies the Interpolation Theorem.

Lemma 2.1 (A2) *The following is true.*

1. *The pair* (G_4, G_6) *forces* $(0, 6]$.
2. *The pair* $(G_5, G_{10}^{\sharp\sharp})$ *forces* $[6, 13]$.
3. *The pair* $(G_5^{\flat}, G_{10}^{\sharp})$ *forces* $[13, 15_+]$.

We use this notation to keep consistent with the monograph.

Let R_s be the Riesz s-potential. We say that a pair of functions (Γ_3, Γ_4) *specially forces* $s \in \boldsymbol{R} - \{0\}$ if there are constants $a_0, ..., a_4$ (depending on s) such that

$$\Lambda_s = a_0 + a_1 G_1 + a_2 G_2 + a_3 \Gamma_3 + a_4 \Gamma_4, \tag{9}$$

1. $\Lambda_s(x) = R_s(x)$ for $x = \sqrt{2}, \sqrt{3}, \sqrt{4}$.
2. $a_1, a_2, a_3, a_4 > 0$.
3. $\Lambda_s(x) \le R_s(x)$ for all $x \in (0, 2]$.

We say that (Γ_3, Γ_4) *specially forces* the interval I if this pair specially forces all $s \in I$.

Lemma 2.2 (A21) *If* (Γ_3, Γ_4) *specially forces* I *then* Γ *forces* I.

Proof: Let T_0 be the TBP and let T be some other 5-point configuration. We simplify the notation and write $F(T) = \mathcal{E}_F(T)$. We assume

$$\Gamma_j(T_0) < \Gamma_j(T)$$

for $j = 3, 4$ and we want to show that that $R_s(T_0) < R_s(T)$ for all $s \in I$. It is well known that $\Gamma_1(T_0) \le \Gamma_1(T)$ and, by Tumanov's result [**T**], $\Gamma_2(T_0) \le \Gamma_2(T)$. Let $a_j = a_j(s)$ for $s \in I$. The quantities $\sqrt{2}, \sqrt{3}, \sqrt{4}$ are the distances which appear between pairs of points in T_0. Therefore $\Lambda_s(T_0) = R_s(T_0)$. But then

$$R_s(T) \ge \Lambda_s(T) = a_0 + \sum_{j=1}^{4} a_j \Gamma_j(T) > a_0 + \sum_{j=1}^{4} a_j \Gamma_j(T_0) = \Lambda_s(T_0) = R_s(T_0).$$

This completes the proof. ♠

Lemma 2.3 (A22) *For each $i = 1, 2, 3$ the pair P_i specially forces I_i.*

Lemma A2 is an immediate consequence of Lemma A21 and Lemma A22.

2.2 Proof of Lemma A22

Referring to Equation 9 we solve the equations

$$\Lambda_s(\sqrt{m}) = R_s(\sqrt{m}), \quad m = 2, 3, 4, \qquad \Lambda'_s(\sqrt{m}) = R'_s(\sqrt{m}), \quad m = 2, 3. \tag{10}$$

Here f' denotes the derivative of f, a function defined on $(0, 2]$. We don't need to constrain $f'(2)$. For each s this gives us a linear system with 5 variables and 5 equations. In all cases, our solutions have the following structure

$$(a_0, a_1, a_2, a_3, a_4) = M(2^{-s/2}, 3^{-s/2}, 4^{-s/2}, s2^{-s/2}, s3^{-s/2}) \tag{11}$$

We will list M below for each of the 3 cases.

Lemma 2.4 (A221) *For each $i = 1, 2, 3$ the following is true. When M is defined relative to the pair P_i then the coefficients a_1, a_2, a_3, a_4 are positive functions on the interval I_i.*

We want to see that the function

$$H_s = 1 - \frac{\Lambda_s}{R_s}. \tag{12}$$

takes its minima at $r = \sqrt{2}, \sqrt{3}$ on $(0, 2]$. Differentiating with respect to $r \in (0, 2]$ we have

$$H'_s(r) = r^{s-1}(s\Lambda_s(r) + r\Lambda'_s(r)). \tag{13}$$

Using the general equation $rG_k'(r) = 2kG_k(r) - 8kG_{k-1}(r)$, we see that

$$\psi_s = s\Lambda_s(r) + r\Lambda_s'(r) \tag{14}$$

is a polynomial in $t = 4 - r^2$.

Lemma 2.5 (A222) *For each choice P_j and each $s \in I_j$ the following is true. The function ψ_s has 4 simple roots in $[0,4]$. Two of the roots are 1 and 2 and the other two respectively lie in $(0,1)$ and $(1,2)$.*

Let us deduce Lemma A2. Our construction and Lemma A221 immediately take care of Conditions 1 and 2 of special forcing. Condition 3: The roots of ψ_s in $[0,4)$ are in bijection with the roots of H_s' in $(0,2]$ and their nature (min, max, simple) is preserved under the bijection. We check for one parameter in each of the three cases that the roots 1 and 2 correspond to local minima and the other two roots correspond to local maxima. Since these roots remain simple for all s in the relevant interval, the nature of the roots cannot change as s varies. Hence H_s has exactly 2 local minima in $(0,2]$, at $r = \sqrt{2}, \sqrt{3}$. But then $H_s \geq 0$ on $(0,2]$. This completes the proof.

2.3 A Positivity Algorithm

In our proofs of Lemmas A221 and A222 we need to deal with expressions of the following form:

$$F(s) = \sum c_i s^{t_i} b_i^{s/2}, \tag{15}$$

where $b_i, c_i \in \boldsymbol{Q}$ and $t_i \in \boldsymbol{Z}$ and $b_i > 0$. Here we explain how we deal with such expressions.

For each summand we compute a floating point value, x_i. We then consider the floor and ceiling of $2^{32}x_i$ and divide by 2^{32}. This gives us rational numbers x_{i0} and x_{i1} such that $x_{i0} \leq x_i \leq x_{i1}$. Since we don't want to trust floating point operations without proof, we formally check these inequalities with what we call the *expanding out method*.

Expanding Out Method: Suppose we want to establish an inequality like $(\frac{a}{b})^{\frac{p}{q}} < \frac{c}{d}$, where every number involved is a positive integer. This inequality is true iff $b^p c^q - a^p d^q > 0$. We check this using exact integer arithmetic. The same idea works with $(>)$ in place of $(<)$.

To check the positivity of F on some interval $[s_0, s_1]$ we produce, for each term, the 4 rationals $x_{i00}, x_{i10}, x_{i01}, x_{i01}$. Where x_{ijk} is the approximation computed with respect to s_k. We then let y_i be the minimum of these expressions. The sum $\sum y_i$ is a lower bound for Equation 15 for all $s \in [s_0, s_1]$. On any interval exponent I where we want to show that Equation 15 is positive, we pick the smallest dyadic interval $[0, 2^k]$ that contains I and then run the following subdivision algorithm.

1. Start with a list L of intervals. Initially $L = \{[0, 2^k]\}$.
2. If L is empty, then **HALT**. Otherwise let Q be the last member of L.
3. If either $Q \cap I = \emptyset$ or the method above shows that Equation 15 is positive on Q we delete Q from L and go to Step 2.
4. Otherwise we delete Q from L and append to L the 2 intervals obtained by cutting Q in half. Then we ago to to Step 2.

If this algorithm halts then it constitutes a proof that $F(s) > 0$ for all $s \in I$.

2.4 Proof of Lemma A221 and part of Lemma A222

Referring to Equation 11 we first list out the matrices in all 3 cases. For P_1 we get

$$792M = \begin{bmatrix} 0 & 0 & 792 & 0 & 0 \\ 792 & 1152 & -1944 & -54 & -288 \\ -1254 & -96 & 1350 & 87 & 376 \\ 528 & -312 & -216 & -39 & -98 \\ -66 & 48 & 18 & 6 & 10 \end{bmatrix} \qquad (16)$$

For P_2 and P_3 we list $368536M$ in each case.

$$\begin{bmatrix} 0 & 0 & 268536 & 0 & 0 \\ 88440 & 503040 & -591480 & -4254 & -65728 \\ -77586 & -249648 & 327234 & 2361 & 65896 \\ 41808 & -19440 & -22368 & -2430 & -9076 \\ -402 & 264 & 138 & 33 & 68 \end{bmatrix} \qquad (17)$$

$$\begin{bmatrix} 0 & 0 & 268536 & 0 & 0 & 0 \\ 982890 & 116040 & -1098930 & -52629 & -267128 & 0 \\ -91254 & -240672 & 331926 & 3483 & 68208 & 0 \\ 35778 & -15480 & -20298 & -1935 & -8056 & 0 \\ -402 & 264 & 138 & 33 & 68 & 0 \end{bmatrix} \qquad (18)$$

Now we turn to the analysis of the coefficients. For Cases 2 and 3 (meaning $j = 2, 3$) we get Lemma A22 by running the positivity algorithm for a_1, a_2, a_3, a_4 on the intervals I_j. The algorithm halts and we are done. For $j = 1$ the situation is trickier because these coefficients vanish at the endpoint $s = 0$ of the interval $I_1 = (0, 6]$.

Before we launch into Case 1, we add two quantities we test, namely $\psi_s(0)$ and $\psi_s(4)$. We have

$$11\psi_s(0) = \begin{bmatrix} -88 \\ -128 \\ +216 \\ +6 \\ +32 \\ +11 \end{bmatrix} \cdot \begin{bmatrix} 2^{-s/2} \\ 3^{-s/2} \\ 4^{-s/2} \\ s2^{-s/2} \\ s3^{-s/2} \\ s4^{-s/2} \end{bmatrix}, \qquad \frac{11}{s}\psi_s(4) = \begin{bmatrix} -2112 \\ +1664 \\ +459 \\ +219 \\ 288 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 2^{-s/2} \\ 3^{-s/2} \\ 4^{-s/2} \\ s2^{-s/2} \\ s3^{-s/2} \\ s4^{-s/2} \end{bmatrix}$$

In other words, these quantities have the same form as the functions $a_j(s)$ for $j = 1, 2, 3, 4$. We run the positivity algorithm and show that all 6 quantities are positive on $[1/4, 6]$.

Now we deal with the interval $(0, 1/4]$. Note that

$$\sup_{m=2,3,4} \sup_{s \in [0,1]} \left| \frac{\partial^6}{\partial s^6} m^{-s/2} \right| < \frac{1}{8}. \tag{19}$$

All our (scaled) expressions have the form $Y \cdot V(s)$,

$$V(s) = (2^{-s/2}, 3^{-s/2}, 4^{-s/2}, s2^{-s/2}, s3^{-s/2}, s4^{-s/2}).$$

For an integer vector Y. Moreover the sum of the absolute values of the coefficients in each of the Y vectors is at most 5000. This means that, when we take the 5th order Taylor series expansion for $Y \cdot V(s)$, the error term is at most

$$5000 \times \frac{1}{8} \times \frac{1}{6!} < 1.$$

We compute each Taylor series, set all non-leading positive terms to 0, and crudely round down the other terms:

$$\begin{aligned}
792a_1(s): &\quad 98s - 69s^2 + 0s^3 - 6s^4 + 0s^5 - 1s^6 \\
792a_2(s): &\quad 14s - 3s^2 - 2s^3 + 0s^4 - 1s^5 - 1s^6. \\
792a_3(s): &\quad 1s + 0s^2 - 1s^3 + 0s^4 + 0s^5 - 1s^6. \\
792a_4(s): &\quad .03s + 0s^2 + 0s^3 - .01s^4 + 0s^5 - 1s^6. \\
11\psi_s(0): &\quad .08s + 0s^2 - .02s^3 + 0s^4 - .01s^5 - 1s^6. \\
(11/s)\psi_s(4): &\quad 11 + 0s + 0s^2 - 1s^3 - 1s^4 + 0s^5 - 1s^6.
\end{aligned}$$

These under-approximations are all easily seen to be positive on $(0, 1/4]$. My computer code does these calculations rigorously with interval arithmetic, but it hardly seems necessary.

2.5 Proof of Lemma A222

Case 1: In Case 1 we compute that

$$\psi_s(t) = t^6 - \frac{48}{12+s}t^5 + ... \tag{20}$$

We don't care about the other terms. Since ψ_s has degree 6 we conclude that ψ_s has at most $N = 6$ roots, counting multiplicity. By construction $H_s(\sqrt{m}) = H_s'(\sqrt{m}) = 0$ for $m = 2, 3$ and $H_s(\sqrt{4}) = 0$. This means that H_s has extrema at $r_2 = \sqrt{2}$ and $r_3 = \sqrt{3}$ and at points $r_{23} \in (\sqrt{2}, \sqrt{3})$ and $r_{34} \in (\sqrt{3}, \sqrt{4})$. Correspondingly ψ_s has roots $t_1 = 1$ and $t_2 = 2$ and $t_{01} \in (0, 1)$ and $t_{12} \in (1, 2)$. The sum of all the roots of ψ_s is $48/(12+s) < 4$. Since $t_1 + t_2 + t_{01} + t_{12} > 4$ we see that not all roots can be positive. Hence $N < 6$. Since ψ_s is positive at $t = 0, 4$ we see that N is even. Hence $N = 4$. This means that the only roots of ψ_s in $(0, 4)$ are the 4 roots we already know about. Since these roots are distinct, they are simple roots.

Cases 2 and 3: First of all, the functions H_s are the same in Cases 2 and 3. This is not just a computational accident. In both cases we are building H_s from the functions G_1, G_2, G_5, G_{10}. So, we combine Cases 2 and 3 by proving that the common polynomial ψ_s just has 4 roots for each $s \in [6, 16]$. I will describe a proof which took me quite a lot of experimentation to find. One tool I will use is *positive dominance*. Here I will just explain the easy case we need in this section: A real polynomial $a_0 + a_1 t + ... a_n t^n$ is positive on $[0, 1]$ provided that the sums $a_0, a_0 + a_1, a_0 + a_1 + a_2, ..., a_0 + ... + a_n$ are all positive.

The same analysis as in Case 1 shows that ψ_s has roots at $1, 2$, and in $(0, 1)$ and in $(1, 2)$. We just want to see that there are no other roots.

We can factor ψ_s as $(t-1)(t-2)\beta_s$ where β_s is a degree 8 polynomial. Taking derivatives with respect to t, we notice that

1. $\gamma_s = 268536 \times 12^{s/2} \times (\beta_s'' - \beta_s')$ is positive for $s \times t \in [6, 16] \times [0, 4]$.
2. $-\beta_s'(0) > 0$ for all $s \in [6, 16]$.
3. $\beta_s'(4) > 0$ for all $s \in [6, 16]$.

Statement 1 shows in particular that β_s' never has a double root. This combines with Statements 2 and 3 to show that the number of roots of β_s' in $[0, 4]$ is independent of $s \in [6, 16]$. We check explicitly that β_6' has only one root in $[0, 4]$. Hence β_s' always has just one root. But this means that

β_s has at most 2 roots in $[0,4]$. This, in turn, means that ψ_s has at most 4 roots in $[0,4]$. This completes the proof modulo the 3 statements.

Now we establish the 3 statements. We first give a formula for γ_s. Define matrices M_3, M_4, M_6 respectively as:

$$\begin{bmatrix} -546840 & -1800480 & 99720 & -397440 & -234600 & -33120 & 173880 & -22080 \\ 18366 & 17112 & 80766 & 24288 & 18630 & 11592 & 4830 & -1104 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} -345600 & -1576320 & -509760 & -760320 & -448800 & -63360 & 332640 & -42240 \\ -199296 & -698784 & 75216 & -149376 & -79960 & 5856 & 94920 & -12992 \\ 7104 & 8432 & 33960 & 11968 & 9180 & 5712 & 2380 & -544 \end{bmatrix}$$

$$\begin{bmatrix} 892440 & 3376800 & 410040 & 1157760 & 683400 & 96480 & -506520 & 64320 \\ -73350 & -246888 & -228942 & -165792 & -110370 & -41688 & 27510 & -2064 \\ 1473 & 4092 & 10557 & 5808 & 4455 & 2772 & 1155 & -264 \end{bmatrix}$$

Define 3 polynomials P_3, P_4, P_6 by the formula:

$$P_k(s,t) = (1, s, s^2) \cdot M_k \cdot (1, ..., t^7) = \sum_{i=0}^{2} \sum_{j=0}^{7} (M_k)_{ij} s^i t^j, \qquad k = 3, 4, 6. \quad (21)$$

We have

$$\gamma = P_3 3^{s/2} + P_4 4^{s/2} + P_6 6^{s/2}. \quad (22)$$

To check the positivity of γ_s we check that each of the 16 functions

$$\gamma_s(v/4 + 1/4) = a_{v,0} + a_{v,1} t + ... a_{v,7} t^7 \quad (23)$$

satisfies the following condition: $A_{v,k} = a_{v,0} + ... + a_{v,k}$ is positive for all $k = 0, ..., 7$ and all $s \in [6,16]$. This shows that the corresponding polynomial is positive on $[0,1]$.

For each $v = 0, ..., 15$ and each $k = 0, ..., 7$ we have a 3×3 integer matrix $\mu_{v,k}$ such that

$$A_{v,k} = (1, s, s^2) \cdot \mu_{v,t} \cdot (3^{s/2}, 4^{s/2}, 6^{s,2}). \quad (24)$$

This gives 128 matrices to check. We get two more such matrices from the conditions $-\beta_s'(0) > 0$ and $\beta_s'(4) > 0$. All in all, we have to check that 130 expressions of the form in Equation 24 are positive for $s \in [6,16]$. These expressions are all special cases of Equation 15, and we use the method discussed above to show positivity in all 130 cases. The program runs in several hours.

3 References

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See Paper 0 for an extended bibliography.