Five Point Energy Minimization 6: Endgame

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Abstract

This is Paper 6 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 the end of the proof, which compares the relevant configurations which have 4-fold dihedral symmetry.

1 Introduction

1.1 Context

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

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

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

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

My monograph [S0] proves the following result.

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

- 1. For $s \in (0, \mathbf{w})$ the TBP is the unique minimizer for R_s .
- 2. For $s = \mathbf{w}$ the TBP and some FP are the two minimizers for R_s .
- 3. For each $s \in (\mathbf{v}, 15_+)$ some FP is the unique minimizer for R_s .

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

1.2 Results

This paper analyzes symmetric configurations which are very close to being either FPs or the TBP. Essentially, these are the configurations that are left over from the rest of the analysis. In order to state the precise result proved here, I first need to introduce some background information.

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

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

Here is the inverse map:

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

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

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

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

The Special Domains: Let Ψ_4 denote the set of avatars of the form

$$(x,0),$$
 $(0,-y),$ $(-x,0),$ $(0,y),$ $64(x,y) \in [43,64].$ (7)

Let Ψ_4^{\sharp} denote the set of avatars of the form

$$(x,0),$$
 $(0,-y),$ $(-x,0),$ $(0,y),$ $64(x,y) \in [55,56].$ (8)

Finally, let Ψ_8 denote the diagonal of Ψ_4 , the points where x = y. Likewise define the diagonal Ψ_8^{\sharp} of Ψ_4^{\sharp} . The tiny domain Ψ_8^{\sharp} contains the avatar for the FP which ties with the TBP at $s = \boldsymbol{v}$.

Theorem 1.2 (Endgame) Let ξ_0 denote a avatar of the TBP. There exist $\mathbf{v} \in (15, 15_+)$ such that the following is true.

- 1. $\mathcal{E}_s(\xi_0) < \mathcal{E}_s(\xi)$ for all $(\xi, s) \in (\Psi_4 \times [13, 15]) \cup ((\Psi_4 \Psi_4^{\sharp}) \times [15, 15^+]).$
- 2. $\mathcal{E}_s(\xi_0) < \mathcal{E}_s(\xi)$ for all $(\xi, s) \in \mathcal{E}_s(\xi_0) < \mathcal{E}_s(\xi)$.
- 3. For all $s \in (\mathbf{v}, 15_+)$ and some $\xi \in \Psi_8^{\sharp}$ we have $\mathcal{E}_s(\xi_0) > \mathcal{E}_s(\xi)$.

1.3 Paper Organization

Statement 1 of the Endgame Theorem is in some sense a problem in 3variable calculus and Statements 2 and 3 are in some sense problems in 2-variable calculus. I will give computationals proof that use exact integer arithmetic. Some of the proofs are done in Mathematica and some in Java. In §2 we include some preliminary material about polynomials. In §3 I give some bounds on the partial derivatives of the relevant quantities. These bounds are used variously in the proofs of all the statements of the Engame Theorem. In §4 I will deal with Statements 1. in §5 I will deal with Statements 2 and 3. The reader can download all the code I have written to prove the Endgame Theorem. I will describe the calculations in a lot of detail, and I think that a competent programmer could reproduce them in under a day.

2 Preliminaries

Here we explain a positivity criterion for polynomials. I call this tool Positive Dominance. 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:

$$G = \sum_{I} c_{I} X^{I}, \qquad X^{I} = \prod_{i=1}^{n} x_{i}^{I_{i}}.$$
(9)

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

$$G_J = \sum_{I \leq J} c_I, \qquad G_\infty = \sum_I c_I. \tag{10}$$

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

Lemma 2.1 (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 $P(x) = a_0 + a_1x + \dots$ Let $A_i = a_0 + \dots + a_i$. The proof goes by induction on the degree of P. The case $\deg(P) = 0$ is obvious. Let $x \in (0, 1]$. We have

$$P(x) = a_0 + a_1 x + x_2 x^2 + \dots + a_n x^n \ge$$
$$x(A_1 + a_2 x + a_3 x^2 + \dots + a_n x^{n-1}) = xQ(x) > 0$$

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

Now we consider the general case. We write

$$P = f_0 + f_1 x_k + \dots + f_m x_k^m, \qquad f_j \in \mathbf{R}[x_1, \dots, x_{n-1}]. \tag{11}$$

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 $x_n \in (0, 1]$.

3 Bounds on Derivatives

3.1 A List of Results

We define

$$\Theta(x, y, s) = \mathcal{E}_s(x, y) - \mathcal{E}(1, \sqrt{3}/3).$$
(12)

Let

$$I = \left[\frac{55}{64}, \frac{56}{64}\right].$$
 (13)

In this chapter we give some bounds on Θ . Let Θ_x be the partial derivative of Θ with respect to x, etc.

Lemma 3.1 For all $(x, y, s) \in \Psi_4 \times [13, 16]$ we have $\Theta_{xx}, \Theta_{yy}, \Theta_{xy} > 0$.

Lemma 3.2

$$\Theta_{tts}(t, t, 15) < 0, \qquad \forall t \in I.$$
(14)

We say that a *block* is a rectangular solid, having the following form:

$$X = Q \times J \subset [0, 1]^2 \times [0, 16], \tag{15}$$

where Q is a square and J is an interval. We define $|X|_1$ to be the length of J and $|X|_2$ to be the side length of Q. Let v(X) denote the set of 8 vertices of X.

Lemma 3.3 For any block $X \subset \Psi_4 \times \subset [13, 16]$ we have

$$\min_{X} \Theta \ge \min_{v(X)} \Theta - (|X|_{1}^{2}/512 + |X|_{2}^{2}).$$

3.2 Proof of Lemma 3.1

We prove this for Θ_{xx} and Θ_{xy} . The case of Θ_{yy} follows from this and symmetry. Setting u = s/2 we compute

$$\mathcal{E}_s(x,y) = A(x,s) + A(y,s) + 2B(x,s) + 2B(y,s) + 4C(x,y,s), \quad (16)$$
$$A(x) = a(x)^u, \qquad B(x) = b(x)^u, \qquad C(x) = c(x)^u,$$
$$a(x) = \frac{(1+x^2)^2}{16x^2} \quad b(x) = \frac{1+x^2}{4} \quad c(x,y) = \frac{(1+x^2)(1+y^2)}{4(x^2+y^2)}$$

Hence

$$\Theta_{xx} = A_{xx} + 2B_{xx} + 4C_{xx}, \qquad \Theta_{xy} = C_{xy}.$$
 (17)

For each choice of F = A, B, C we have

$$F_{xx} = u(u-1)f^{u-2}f_x^2 + uf^{u-1}f_{xx}, \quad C_{xy} = u(u-1)c^{u-2}c_xc_y + uc^{u-1}c_{xy}.$$
 (18)

Our notation is such that f = a when F = A, etc.

We compute

$$a_{xx} = \frac{3+x^4}{8x^4} > 0, \qquad b_{xx} = \frac{1}{2}, \qquad c_{xx} = \frac{(1-y^4)(3x^2-y^2)}{2(x^2+y^2)^3} \ge 0.$$

$$c_x = \frac{x(y^4 - 1)}{2(x^2 + y^2)^2} < 0, \quad c_y = \frac{y(x^4 - 1)}{2(x^2 + y^2)^2} < 0, \quad c_{xy} = \frac{2xy(1 + x^2y^2)}{(x^2 + y^2)^3} > 0.$$

Equation 18 combines with all this to prove that $\Theta_{xx} > 0$ and $\Theta_{xy} > 0$ on $\Psi_4 \times [13, 16]$.

3.3 Proof of Lemma 3.3

We prove Lemma 3.3 through two smaller lemmas.

Lemma 3.4 $|\Theta_{xx}|, |\Theta_{yy}| \le 4 \text{ on } \Psi_4 \times [13, 16].$

Proof: By symmetry it suffices to prove this for Θ_{xx} . We already know $\Theta_{xx} > 0$ on our domain. We use the notation from the proof of Lemma 3.1. In particular, An easy exercise in calculus shows that $f \in (0, 3/5)$ on Ψ_4 for each f = a, b, c. From this bound, we see that the expression in Equation 18 is decreasing as a function of u for $u \ge 6$. (Recall that u = s/2.) Hence it suffices to prove that $4 - \Theta_{xx} \ge 0$ on $\{12\} \times [43/64, 1]^2$.

We define $\phi(t) = (43/64)(1-t) + t$. The file LemmaC221.m computes that for s = 12 the polynomial $\Phi = \operatorname{num}_+(4 - \Theta_{xx} \circ \phi)$ is weak positive dominant and hence non-negative on $[0,1]^2$. Hence $4 - \Theta_{xx} \ge 0$ when s = 12 and $(x,y) \in \Psi_4$.

Lemma 3.5 $|\Theta_{ss}| \leq 1/64 \text{ on } \Psi_4 \times [13, 16].$

Proof: Let $\psi(s) = b^{-s}$. Let $\beta = (1.3, \sqrt{2}, \sqrt{3})$ and $\gamma = (440, 753, 4184)$. We first establish the following bound:

$$0 < \min_{b \ge \beta_j} \psi_{ss}(s, b) \le 1/\gamma_j, \qquad j = 1, 2, 3, \qquad \forall s \ge 13.$$
 (19)

As a function of s, and for b > 1 fixed, $\psi_{ss}(s,b) = b^{-s} \log(b)^2$ is decreasing. Hence, it suffices to prove Equation 19 when s = 13. Choose $b \ge 1.3$. The equation $\psi_{ssb}(13, b) = 0$ has its unique solution in $[1, \infty)$ at the value $b = \exp(2/13) < 1.3$. Moreover, the function $\psi_{ss}(13, b)$ tends to 0 as $b \rightarrow \infty$. Hence the restriction of the function $b \rightarrow \psi_{ss}(13, b)$ to $[b, \infty)$ takes its maximum value at b. Evaluating at $b = 1.3, \sqrt{2}, \sqrt{3}$ we get Equation 19.

For $x, y \in [43/64, 1]$ we easily check the inequalities

$$A(-1,x) \ge 3, \quad B(-1,x) \ge 2, \quad C(-1,x,y) \ge (1.3)^2.$$

The quantities on the left are the square distances of the various pairs of points in the corresponding configuration on S^2 . From this analysis we conclude that the 10 distances associated to a 5-point configuration parametrized by a point in Ψ_4 exceed 1.3, and at least 6 of them exceed $\sqrt{2}$, and at least 2 of them exceed $\sqrt{3}$. The same obviously holds for the TBP.

Now, 10 of the 20 terms comprising $\Theta_{ss}(x, y, s)$ are positive and 10 are negative. Also, for the terms of the same sign, all 10 of them are less than 1/440, and at least 6 of them are less than 1/753, and at least 2 of them are less than 1/4184. Hence, by Equation 19, we have the final bound $|\Theta_{ss}| \leq (4/440) + (4/753) + (2/4184) < 1/64$.

Write $I = [s_0, s_1]$ and $Q = [x_0, x_1] \times [y_0, y_1]$. Choose $(x, y, s) \in X = I \times Q$. Taylor's Theorem with remainder tells that for any function $f : [a, b] \to \mathbf{R}$ and any $x \in [a, b]$ we have

$$f(x) \ge \min(f(a), f(b)) - \frac{1}{8} \max_{[a,b]} |f''|.$$

Applying this result 3 times and using the bounds in our two lemmas, we have

$$\Theta(x, y, s) \ge \min_{i} \Theta(x, y, s_{i}) - |I|/512 \ge$$
$$\min_{i,j} \Theta(x_{j}, y, s_{i}) - |I|/512 - |x_{0} - x_{1}|/2 \ge$$
$$\min_{i,j,k} \Theta(x_{j}, y_{j}, s_{i}) - |I|/512 - |x_{0} - x_{1}|/2 - |y_{0} - y_{1}|/2 =$$
$$\min_{v(X)} \Theta - |X|_{1}/512 - |X|_{2}.$$

This completes the proof of Lemma 3.3.

3.4 Proof of Lemma 3.2

The file LemmaC3.m does the calculations for this proof. We use the notation from previous sections.

Because the *s*-energy of the TBP does not depend on the *t*-variable, we have

$$\Theta_{stt}(t,t,15) = 2A_{stt}|_{s=15} + 4B_{stt}|_{s=15} + 4C_{stt}|_{s=15}.$$
(20)

Call the three functions on the right $\alpha(t)$, $\beta(t)$, and $\gamma(t)$. To finish the proof, we just need to see that each of these is negative in I. We write $f \sim f^*$ if

$$\frac{f}{f^*} = 2^u t^v (1+t^2)^w (2+t^2+t^{-2})^x$$

for exponents $u, v, w, x \in \mathbf{R}$. In this case, f and f^* have the same sign.

Lemma 3.6 $\beta < 0$ on *I*.

Proof: Taking
$$(u, v, w, x) = (-14, 0, 11/2, 0)$$
 we have $\beta \sim -\beta^*$,
 $\beta^*(t) = (-2 + 30 \log(2)) + t^2(-58 + 420 \log(2)) - 15(1 + 14t^2) \log(1 + t^2)$

Noting that $\log(2) = 0.69...$ we eyeball β^* and see that it is positive for $t \in I$. The term $+420 \log(2)t^2$ dominates. Hence $\beta < 0$ on I.

Lemma 3.7 $\gamma < 0$ on *I*.

Proof: Taking
$$(u, v, w, x) = (-41/2, -16, 12, 1/2)$$
 we have $\gamma \sim -\gamma^*$,
 $\gamma^*(t) = (-31 + 360 \log(2)) + \underline{t^2(56 - 585 \log(2))} + t^4(-29 + 315 \log(2)) + 15(-8 + 13t^2 - 7t^4) \log(2 + t^2 + t^{-2}).$

We have $\gamma^*(55/64) > 2^4$ and we estimate easily that $\gamma_t^* > -2^{10}$ on *I*. Only the underlined term has negative derivative in *I*. Noting that *I* has length 2^{-6} , we see that γ^* cannot decrease more than 2^4 as we move from x_0 to any other point of *I*. Hence $\gamma^* > 0$ on *I*. Hence $\gamma < 0$ on *I*.

Lemma 3.8 $\alpha < 0$ on *I*.

Proof: Taking (u, v, w, x) = (-29, -14, 10, 3/2) we have $\alpha \sim -\alpha *$, $\alpha^*(t) = \gamma^*(t) + \delta^*(t), \qquad \delta^*(t) = 15 \log 2 \times (8 - 13t^2 + 7t^4).$

We see easily that $\delta^* > 0$ on I. So, from Lemma C33, we have $\alpha^* > 0$ on I. Hence $\alpha < 0$ on I.

4 Proof of Statement 1

4.1 Rational Approximation

We first explain our calculation and then we give a record of its performance.

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 (<). We call this the *expanding out method*.

More generally, we will want to verify inequalities like

$$\sum_{i=1}^{10} b_i^{-s} - \sum_{i=1}^{10} a_i^{-s/2} > C.$$
(21)

where all a_i belong to the set $\{2,3,4\}$, and b_i, c, s are all rational. more specifically $s \in [13, 15_+]$ will be a dyadic rational and c will be positive. The expression on the left will be $\mathcal{E}_s(p) - \mathcal{E}_s(p_0)$ for various choices of p, and the constant C is related to the error term we define below.

Here is how we handle expressions like this. For each index $i \in \{1, ..., 10\}$ we produce rational numbers A_i and B_i such that

$$A_i^{s/2} > a_i \qquad B_i^s < b_i. \tag{22}$$

We use the expanding out method to check these inequalities. We then check that

$$\sum_{i=1}^{10} B_i - \sum_{i=1}^{10} A_i > C.$$
(23)

This last calculation is again done with integer arithmetic. Equations 22 and 23 together imply Equation 21. Logically speaking, the way that we produce the rational A_i and B_i does not matter, but let us explain how we find them in practice. For A_i we compute $2^{32}a_i^{-s/2}$ and round the result up to the nearest integer N_i . We then set $A_i = N_i/2^{32}$. We produce B_i in a similar way. When we have verified Equation 21 in this manner we say that we have used the *rational approximation method* to verify Equation 21. We will only need to make verifications like this on the order of 20000 times.

4.2 The Grading Step

We say that a rational number p/q is *dyadic* if q is a power of 2. We say that a block (defined in the previous chapter) is *dyadic* if all coordinates of all the block vertices are dyadic rationals.

We perform the following pass/fail evaluation of X.

- 1. If $I \subset [0, 13]$ or $I \subset [15_+, 16]$ or $Q \cap \Psi_4 = \emptyset$, we pass X because X is irrelevant to the calculation.
- 2. If $s_0 \ge 15$ and $Q \subset \widehat{\Psi}_4$ we pass X.
- 3. $s_0 < 13$ and $s_1 > 13$ we fail X because we don't want to make any computations which involve exponents less than 13.
- 4. If X has not been passed or failed, we try to use the rational approximation method to verify that $\Theta(v) > |X|_1^2/512 |X|_2^2$ for each vertex v of X. If we succeed at this, then we pass X. Otherwise we fail X.

To prove Statement 1 of the Endgame Theorem it suffices to find a partition of $[0, 16] \times [0, 1]^2$ into blocks which all pass the evaluation.

Subdivision: Let $X = I \times Q$. Here is the rule we use to subdivide X: If $16|X|_2 > |X|_1$ we subdivide X along Q dyadically, into 4 pieces. Otherwise we subdivide X along I, into two pieces. This method takes advantage of the lopsided form of Lemma C22 and produces a small partition.

4.3 Running the Algorithm

We perform the following algorithm.

- 1. We start with a list L of blocks. Initially L has the single member $\{0, 16\} \times \{0, 1\}^2$.
- 2. We let *B* be the last block on *L*. We grade *B*. If *B* passes, we delete *B* from *L*. If $L = \emptyset$ then **HALT**. If *B* fails, we delete *B* from *L* and append to *L* the subdivision of *B*. Then we go back to Step 1.

For the calculation, I used a 2017 iMac Pro with a 3.2 GHz Intel Zeon W processor, running the Mojave operating system. The Java version is **Java 8 Update 201**. When I run the algorithm, it halts with success after 21655 steps and in about 1 minute. The partition it produces has 14502 blocks. This proves Statement 1 of the Endgame Theorem.

5 Proof of Statements 2 and 3

We carry over the notation from the previous two chapters. In particular, we define Θ as in Equation 12. Our parameter interval is I = [55, 56]/64. The left endpoint is

$$t_0 = \frac{55}{64}.$$
 (24)

Lemma 5.1 For any $\xi \in \widehat{\Psi}_8$ let $\Theta(s,\xi) = \mathcal{E}_s(\xi) - \mathcal{E}_s(\xi)$. Then for $s \in [15, 15_+]$ we have $\partial \Theta / \partial s < 0$.

Proof: We compute that

$$\Theta_{st}(t_0, t_0, 15) < 0, \qquad \Theta_s(t_0, t_0, 15) < -2^{-7},$$
(25)

and these conditions combine with Equation 14 to show that

$$\Theta_s(15,t,t) < -2^{-7}. \qquad \forall t \in I.$$
(26)

Lemma 3.5 gives us $|\Theta_{ss}| \leq 2^{-6}$ on $[13, 16] \times \Psi_4$. Hence

$$|\Theta_{ss}| \times |15_{+} - 15| \le 2^{-6} \times \frac{25}{512} < 2^{-7}.$$
(27)

Hence $\Theta_s(s,t,t)$ varies by less than 2^{-7} as s ranges in $[15,15_+]$. Hence $\Theta_s(s,t,t) < 0$ for all $s \in [15,15_+]$ and all $t \in I$.

Now we deduce Statements 2 and 3. By Statement 1, we have $\Theta > 0$ on $\widehat{\Psi}_8 \times \{15\}$. We compute that $\Theta(x, x, 15^+) < 0$ for

$$x = 445/512 \in [55, 56]/64.$$

Combining this with Lemma 5.1, we see that there exists a smallest parameter $\boldsymbol{w} \in (15, 15_+)$ such that $\Theta(\boldsymbol{w}, p^*) = 0$ for some $p^* \in \widehat{\Psi}_8$. For $s > \boldsymbol{w}$, Lemma 5.1 now says that $\Theta(s, p^*) < 0$. This establishes Statements 2 and 3 at the same time.

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