Five Point Energy Minimization 0: Main

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Abstract

This is the main paper amongst a series of 7 papers which together prove the Melnyk-Knopf-Smith phase transition conjecture for 5-point energy minimization. This paper proves the main result, drawing on results proved in the other 6 papers.

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**]. See §2 for history and context. 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.

In this paper I will deduce the main result, the Phase Transition Theorem, from the results proved in the other 6 papers.

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.*

Remark: My monograph also has a result that the TBP minimizes all Riesz potentials (a.k.a. Fejes-Toth potentials) for $s \in (-2, 0)$. This is still a theorem; I am leaving it out of this account because I want to focus on one result at a time.

In §2 I will discuss some history and context for the Phase Transition Theorem. The monograph has an extended version of this chapter, where I also discuss some of the high level ideas of the proof. In §3 I will give most of the preliminary definitions. In §4 I will deduce the Phase Transition Theorem from the results of the other papers.

2 History and Context

Which configurations of points on the sphere minimize a given potential function $F:(0,2]\to \boldsymbol{R}$? The classic choice for this question is $F=R_s$, the *Riesz potential*, given by $R_s(d)=d^{-s}$. The Riesz potential is defined when $s>0$. When $s<0$ the corresponding function $R_s(d)=-d^{-s}$ is called the *Fejes-Toth potential*. The main difference is the minus sign out in front.

The case $s=1$ is specially called the *Coulomb potential* or the *electrostatic potential*. This case of the energy minimization problem is known as *Thomson's problem*. See [**Th**]. The case of $s=-1$, in which one tries to maximize the sum of the distances, is known as *Polya's problem*.

There is a large literature on the energy minimization problem. See [**Fö**] and [**C**] for some early local results. See [**MKS**] for a definitive numerical study on the minimizers of the Riesz potential for n relatively small. The website [**CCD**] has a compilation of experimental results which stretches all the way up to about $n=1000$. The paper [**SK**] gives a nice survey of results, with an emphasis on the case when n is large. See also [**RSZ**]. The paper [**BBCGKS**] gives a survey of results, both theoretical and experimental, about highly symmetric configurations in higher dimensions.

When $n=2,3$ the problem is fairly trivial. In [**KY**] it is shown that when $n=4,6,12$, the most symmetric configurations – i.e. vertices of the relevant Platonic solids – are the unique minimizers for all R_s with $s\in(-2,\infty)-\{0\}$. See [**A**] and [**Y**] respectively for the case $n=12$ and the cases $n=4,6$. The result in [**KY**] is contained in the much more general and powerful result [**CK**, Theorem 1.2] concerning the so-called sharp configurations.

The case $n=5$ has been notoriously intractable. There is a general feeling that for a wide range of energy choices, and in particular for the power law potentials (when $s>-2$) the global minimizer is either the TBP or an FP. Here is a run-down on what is known so far:

- The paper [**HZ**] has a rigorous computer-assisted proof that the TBP is the unique minimizer for the potential $F(r)=-r$. (Polya's problem).
- My paper [**S1**] has a rigorous computer-assisted proof that the TBP is the unique minimizer for R_1 (Thomson's problem) and R_2. Again $R_s(d)=d^{-s}$.
- The paper [**DLT**] gives a traditional proof that the TBP is the unique minimizer for the logarithmic potential.
- In [**BHS**, Theorem 7] it is shown that, as $s\to\infty$, any sequence of 5-point minimizers w.r.t. R_s must converge (up to rotations) to the

FP having one point at the north pole and the other 4 points on the equator. In particular, the TBP is not a minimizer w.r.t R_s when s is sufficiently large.

- In 1977, T. W. Melnyk, O. Knop, and W. R. Smith, [**MKS**] conjectured the existence of the phase transition constant, around $s = 15.04808$, at which point the TBP ceases to be the minimizer w.r.t. R_s. This is the phase transition which our Main Theorem estabishes.

- Define

$$G_k(r) = (4 - r^2)^k, \qquad k = 1, 2, 3, ... \tag{4}$$

  In [**T**], A. Tumanov proves that the TBP is the unique minimizer for G_2. The minimizers for G_1 are those configurations whose center of mass is the origin. The TBP is included amongst these.

Tumanov points out that the G_2 potential does not have an obvious geometric interpretation, but it is amenable to a traditional analysis. He also mentions that his result might be a step towards proving that the TBP minimizes a range of power law potentials. Inspired by similar material in [**CK**], he 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 $s \in (0, 2]$.

We will establish other implications like this during the course of our proof of the Phase Transition Theorem. The family of potentials $\{G_k\}$ behaves somewhat like the Riesz potentials. The TBP is the unique minimizer for G_3, G_4, G_5, G_6 (as a consequence of our work here) but not a minimizer for any of G_7, G_8, G_9, G_{10}. I checked up to about $k = 100$ that the TBP does not mininize G_k when $k > 10$ and I am sure this pattern persists.

3 Preliminaries

3.1 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.

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

Here is the inverse map:

$$\Sigma^{-1}(x, y) = \left(\frac{2x}{1+x^2+y^2}, \frac{2y}{1+x^2+y^2}, 1 - \frac{2}{1+x^2+y^2}\right). \tag{6}$$

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

3.2 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:

$$\widehat{p}_0, \widehat{p}_1, \widehat{p}_2, \widehat{p}_3, (0, 0, 1) \in S^2 \iff p_0, p_1, p_2, p_3 \in \boldsymbol{R}^2, \qquad \widehat{p}_k = \Sigma^{-1}(p_k). \tag{7}$$

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.

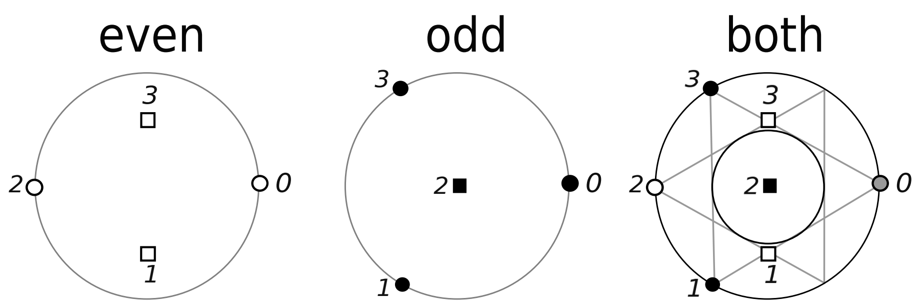

Figure 1: Even and odd avatars of the TBP.

We call 2 avatars *isomorphic* if the corresponding 5-point configurations on S^2 are isometric. Every avatar is isomorphic to an even avatar. To see this, we form a graph by joining two points in a 5-point configuration by an edge if and only if they make a far pair. As for any graph, the sum of the degrees is even. Hence there is some vertex having even degree. When we rotate so that this vertex is $(0,0,1)$, the corresponding avatar is even. By focusing on the even avatars, and further using symmetry, we arrive at a configuration space where there is just one TBP avatar.

3.3 The Big Domain

Given an avatar $\xi = (p_0, p_1, p_2, p_3)$, we write $p_k = (p_{k1}, p_{k2})$. We define a domain $\Omega \subset \boldsymbol{R}^7$ to be the set of avatars ξ satisfying the following conditions.

1. ξ is even.
2. $\|p_0\| \geq \max(\|p_1\|, \|p_2\|, \|p_3\|)$.
3. $p_{12} \leq p_{22} \leq p_{32}$ and $p_{22} \geq 0$.
4. $p_{01} \in [0,2]$ and $p_{01} = 0$.
5. $p_j \in [-3/2, 3/2]^2$ for $j = 1,2,3$.
6. $\min(p_{1k}, p_{2k}, p_{3k}) \leq 0$ for $k = 1,2$.

We define $\Omega^\flat$ to be the same domain except that we leave off Condition 6.

3.4 The Definite Neighborhood of the TBP

We specially treat avatars very near the TBP. When we string out the points of ξ_0, we get $(1,\ 0, -u, -1, 0, 0, u)$ where $u = \sqrt{3}/3$. The space indicates that we do not record $p_{02} = 0$. We let Ω_0 denote the cube of side-length 2^{-17} centered at ξ_0.

3.5 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 ϖ.

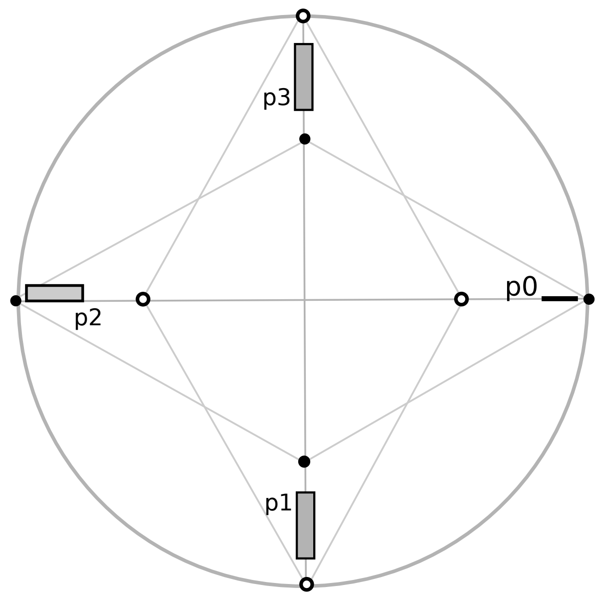

Figure 2: The sets defining Υ compared with two TBP avatars.

3.6 The Special Potentials

Rather than work with the Riesz potentials, we work with potentials that have a more polynomial flavor.

$$G_k(r) = (4 - r^2)^k. \tag{8}$$

Also define

$$G_5^\flat = G_5 - 25G_1,$$
$$G_{10}^{\sharp\sharp} = G_{10} + 28G_5 + 102G_2,$$
$$G_{10}^{\sharp} = G_{10} + 13G_5 + 68G_2 \tag{9}$$

4 Proof of the Phase Transition Theorem

4.1 A Resume of Papers

The other 6 papers I have written all have names of the form "5 Point Energy Minimization: X" where "X" stands for some facet of the proof. Here are the 6 topics:

- Energy Lemma
- Big Calculation
- Local Analysis
- Interpolation
- Symmetrization
- Endgame

I will refer to the papers by these names in the arguments below.

4.2 Energy Lemma

The Energy Bound Paper establishes a certain energy bound, which we call Lemma E. Lemma E plugs into a divide-and-conquer scheme which establishes the theorem below which we call the Containment Theorem. We will not describe Lemma E here because it is a rather technical result.

4.3 Big Calculation

Let Ω and Ω_0 and Υ be as in the previous chapter. Here we explain the results from the Big Calculation Paper. Here is the first result.

Theorem 4.1 (Containment) *The following is true:*

1. *Let $F = G_4, G_6, G_{10}^\sharp$. If ξ is not equivalent to any avatar in Ω then then ξ does not minimize $\mathcal{E}_F$.*
2. *Let $F = G_5^\flat$. If ξ is not equivalent to any avatar in $\Omega^\flat$ then then ξ does not minimize $\mathcal{E}_F$.*

Here is the second and main result.

Theorem 4.2 (Calculation) *Assuming Lemma E, the following is true.*

1. *The TBP is the unique minimizer for $G_4, G_5^\flat, G_6$ amongst 5-point configurations which have avatars in $\Omega - \Omega_0$.*

2. *The TBP is the unique minimizer for $G_{10}^\sharp$ among 5-point configurations which have avatars in $\Omega - \Omega_0 - \Upsilon$.*

3. *The TBP is the unique minimizer for $G_{10}^{\sharp\sharp}$ among 5-point configurations which have avatars in Υ.*

Since Lemma E is true, and proved in the Energy Bound Paper, the Calculation Theorem holds unconditionally. Now we can state the main corollary of the Big Computation paper in an unconditional way that does not mention Lemma E.

Corollary 4.3 *The following is true.*

1. *The TBP is the unique minimizer for $G_4, G_5^\flat, G_6, G_{10}^{\sharp\sharp}$ among configurations which are not represented by avatars in Ω_0.*

2. *The TBP is the unique minimizer for $G_{10}^\sharp$ among 5-point configurations which have are not represented by avatars in $\Upsilon \cup \Omega_0$.*

Proof: The only non-obvious point is the statement about $G_{10}^{\sharp\sharp}$. Since the TBP is a global minimizer for G_1 and (uniquely so) for $G_5^\flat$ on $\Omega - \Omega_0$, we see that the TBP is the unique minimizer for G_5 on $\Omega - \Omega_0$. Since the TBP is the unique minimizer for $G_{10}^\sharp$ and G_5 and (by Tumanov's result [**T**]) G_2 on $\Omega - \Omega_0 - \Upsilon$ we see that the TBP is the unique minimizer for $G_{10}^{\sharp\sharp}$ on $\Omega - \Omega_0 - \Upsilon$. This combines with Statement 3 of the Calculation Theorem to show that the TBP is the unique minimizer for $G_{10}^{\sharp\sharp}$ on $\Omega - \Omega_0$. ♠

4.4 Local Analysis

The Local Analysis paper deals with configurations having avatars in Ω_0. Here is the main result.

Theorem 4.4 (Local Convexity) *For $F = G_4, G_6, G_5^\flat, G_{10}^\sharp$, the Hessian of $\mathcal{E}_F$ is positive definite at every point of Ω_0.*

Let $\xi \in \Omega_0$ be other than ξ_0. The Local Convexity Theorem combines with the vanishing gradient to show that the restriction of $\mathcal{E}_F$ to the line segment γ joining ξ_0 to ξ is convex and has 0 derivative at ξ_0. Hence $\mathcal{E}_F(\xi) > \mathcal{E}_F(\xi_0)$.

Corollary 4.5 *Let F be any of $G_4, G_5^\flat, G_5, G_6, G_{10}^\sharp, G_{10}^{\sharp\sharp}$. Then ξ_0 is the unique minimizer for $\mathcal{E}_F$ inside Ω_0.*

Proof: Let F be any of the functions from the Local Convexity Theorem. Let $\xi \in \Omega_0$ be other than ξ_0. The Local Convexity Theorem combines with the vanishing gradient to show that the restriction of $\mathcal{E}_F$ to the line segment γ joining ξ_0 to ξ is convex and has 0 derivative at ξ_0. Hence $\mathcal{E}_F(\xi) > \mathcal{E}_F(\xi_0)$.

It remains to deal with $F = G_5$ and $F = G_{10}^{\sharp\sharp}$. As is well known, ξ_0 is a minimizer for G_1. Since ξ_0 is the unique minimizer for $G_5^\flat$ in Ω_0, we see that ξ_0 is also the unique minimizer for $G_5 = G_5^\flat + 25G_1$ in Ω_0.

By the main result in [**T**], ξ_0 is the unique global minimizer for G_2. With this in mind, we see that the same kind of argument we just gave for G_5 also works for $G_{10}^{\sharp\sharp} = G_{10}^\sharp + 15G_5 + 34G_2$. ♠

Combining this result with Corollary 4.3 we get the following result.

Corollary 4.6 *The following is true.*

1. *The TBP is the unique minimizer for $G_4, G_5^\flat, G_6, G_{10}^{\sharp\sharp}$ amongst all configurations.*
2. *The TBP is the unique minimizer for $G_{10}^\sharp$ among 5-point configurations which are not represented by avatars isomorphic to those in Υ.*

4.5 Interpolation

The results above do not deal with the Riesz potentials at all. The main result in the Interpolation paper bridges the gap. Here is the main result.

Theorem 4.7 (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 $\mathcal{E}_{R_s}(T_0) < \mathcal{E}_{R_s}(T)$.*

The Interpolation Theorem and Corollary 4.6 combine to prove the following result.

Corollary 4.8 *Let T_0 be the TBP. Then*

1. *Suppose $s \in (0,13]$ and T is any 5-point configuration. Then we have $\mathcal{E}_{R_s}(T_0) < \mathcal{E}_{R_s}(T)$.*
2. *Suppose $s \in [13, 15^+]$ and T is any 5-point configuration not represented by an avatar isomorphic to one in Υ. Then $\mathcal{E}_{R_s}(T_0) < \mathcal{E}_{R_s}(T)$.*

4.6 Symmetrization

Let $\boldsymbol{K}_4$ denote the set of avatars which are invariant under reflections in the coordinate axes. We describe a symmetrization operation which maps Υ into $\boldsymbol{K}_4$. Let (p_0, p_1, p_2, p_3) be an avatar with $p_0 \neq p_2$. Define

$$-p_2^* = p_0^* = (x, 0), \quad -p_1^* = p_3^* = (0, y), \qquad x = \frac{\|p_0 - p_2\|}{2}, \quad y = \frac{\|\pi_{02}(p_1 - p_3)\|}{2}. \tag{10}$$

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 $\boldsymbol{K}_4$. Here is the first result in the Symmetrization paper.

Theorem 4.9 (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.

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

$$-p_2 = p_0 = (x, 0), \qquad -p_1 = p_3 = (0, y), \qquad 512(x, y) \in [440, 448]. \tag{11}$$

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

We define

$$\sigma(x, y) = (z, z), \qquad z = \frac{x + y + (x - y)^2}{2}. \tag{12}$$

Here is the second result in the Symmetrization paper.

Theorem 4.10 (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 $\sigma(p) = p$.*

4.7 Endgame

Let Ψ_4 denote the set of avatars of the form

$$(x,0), \qquad (0,-y), \qquad (-x,0), \qquad (0,y), \qquad\qquad 64(x,y) \in [43,64]. \tag{13}$$

Let $\Psi_4^\sharp$ denote the set of avatars of the form

$$(x,0), \qquad (0,-y), \qquad (-x,0), \qquad (0,y), \qquad\qquad 64(x,y) \in [55,56]. \tag{14}$$

Finally, let Ψ_8 denote the diagonal of Ψ_4, the points where $x=y$. Likewise define the diagonal $\Psi_8^\sharp$ of $\Psi_4^\sharp$. To relate Ψ_4 to the discussion above, we have

$$\Upsilon \cap \boldsymbol{K}_4 \subset \Psi_4$$

and (obviously)

$$\Psi_8^\sharp \subset \Psi_4^\sharp \subset \Psi_4.$$

The tiny domain $\Psi_8^\sharp$ contains the avatar for the FP which ties with the TBP at $s = \varpi$.

Here is the result of the Endgam Paper.

Theorem 4.11 (Endgame) *Let ξ_0 denote a avatar of the TBP. There exist $\varpi \in (15, 15_+)$ 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 $s \in (\varpi, 15_+)$ and some $\xi \in \Psi_8^\sharp$ we have $\mathcal{E}_s(\xi_0) > \mathcal{E}_s(\xi)$.*

Combining the Endgame Theorem with the two Symmetrization Theorems we get the following corollary.

Corollary 4.12 *Let ξ_0 denote a avatar of the TBP. There exist a number $\varpi \in (15, 15_+)$ such that the following is true:*

1. *$\mathcal{E}_s(\xi_0) < \mathcal{E}_s(\xi)$ for all $(\xi, s) \in \Upsilon \times [13, \varpi)$.*
2. *For all $x \in (\varpi, 15^+)$ there is some $\xi \in \Upsilon$ such that $\mathcal{E}_s(\xi_0) > \mathcal{E}_s(\xi)$.*

The Phase Transition Theorem follows immediately from Corollary 4.8 and Corollary 4.12.

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