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Error Bounds Between the Minimum Distance Energy of an Equilateral Knot and the Mobius Energy of an Inscribed Smooth Knot

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Error Bounds Between the Minimum Distance Energy of an Equilateral Knot and the Möbius Energy of an Inscribed Smooth Knot

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Contents

Chapter 1

Introduction

If one takes a piece of string, ties it in a knot, and then glues the two ends together to form a loop, the result is a string that has no loose ends and that is truly knotted. There is no way to untangle the string without somehow cutting it. A *mathematical knot* is such a string, except that it has no thickness. Formally, a knot can be defined as a non self-intersecting closed curve in $\mathbb{R}^3$. This paper is about knots and some of their properties. In particular, we will examine ways to define an "energy" for knots and try to find bounds between different notions of energy.

1.1 Problem to Investigate

Given a knot configuration in $\mathbb{R}^3$, a knot energy is a measure of the complexity of its spatial conformation. Formally, we define a *knot energy function* as follows: Let S be a space of knots. A *knot energy* is a scale-invariant function $f : S \to \mathbb{R}^+$, where $\mathbb{R}^+$ is the set of all non-negative real numbers. Energy functions were first defined with the hopes of providing an algorithm for determining the knot type of a given closed curve. If the knot could be flowed to an energy minimum, and if this minimum were unique, one could simply compare the knot to a precomputed table of energy minima containing the different knot types. The energy functions appear to have many local minima, however, so this goal has been elusive. Still, knot energy functions have been successful at flowing very complicated unknots to the standard regular n-gon and have provided interesting relationships with physical properties of knots found in scientific studies such as DNA. Modern computers make it possible to simulate the energy-minimizing flow, but it is necessary to represent the energy function as a function on discrete knots. One problem that arises is that there are no known techniques for efficiently flowing a smooth knot to a knot energy minimum. However, polygonal analogues have been defined to simulate the flow of smooth knots by flowing polygons.

One of the most studied energy functions is the Möbius Energy [O'H91] defined by O'Hara. One discretization of the Möbius Energy is the Minimum Distance Energy [Sim96] due to Simon. While the Minimum Distance Energy (MD-Energy) has provided interesting results, it is still an open question whether the simulations with the MD-Energy truly approximate the flow of the Möbius Energy. To justify the simulations using the Minimum Distance Energy, one must show that there exist smooth knots near the polygonal-minimized knots with similar energy. This thesis will explore the extent to which a smooth knot can be inscribed in an equilateral knot so that the Möbius Energy of the smooth knot is close to the MD-Energy of the equilateral knot.

1.2 Present Status of the Proposed Problem

In [RS05], it was shown that a polygonal knot can be inscribed in a smooth knot and that the two knots have close energies. However, this does not solve the problem at hand. One of the main goals in this area is to determine the structure of the energy-minima. Computer simulations are used to flow polygons to minima, but the question of whether these polygons are close to smooth minima is still open. While it is not clear at this point whether one can find a smooth knot near a polygonal knot with its Möbius Energy close to the MD-Energy of the polygonal knot, with the information and algorithms available, it seems to be an appealing proposition. For the remainder of this chapter, we will provide background material and describe the methods that we will use to try to reach our goal. In Chapter 2, we will examine what we think are the necessary propositions that need to be proven in order to show that the Möbius Energy of a smooth knot K inscribed in an equilateral knot P is close to the MD-Energy of P, and we will prove two of them. In Chapter 3, we provide an algorithm for inscribing equilateral knots in smooth knots. Chapter 4 is the Appendix, which contains the Maple code that we wrote to inscribe equilateral knots in smooth knots.

1.3 Background

In this section we define the quantities involved in this study, and we provide the basic framework for our methods.

Definition 1. *Let $s \to x(s)$ be a unit-speed parametrization of a C^2 smooth knot K, where s and t are the same parameter with domain a circle C. Then one form of the Möbius Energy [O'H91] is*

$$E_0(K) = \int\int_{C \times C} \frac{1}{|x(s) - x(t)|^2} - \frac{1}{|s-t|^2}\ ds\ dt.$$

Since we are dealing an with arc-length preserving parametrization, the line elements $dx = ds$ and $dy = dt$, and the previous integral becomes

$$E_0(K) = \int\int_{K \times K} \frac{1}{|x-y|^2} - \frac{1}{|s-t|^2}\ dx\ dy.$$

Next we take a look at the description of a polygonal knot and its MD-Energy.

Definition 2. *An n-edge polygonal knot P is a set of ordered vertices, $v_0, v_1, \cdots, v_{n-1}$ in $\mathbb{R}^3$, connected by a set of edges $e_0, e_1, \cdots, e_{n-1}$, where $e_i = v_{i+1} - v_i$ for $i = 0, 1, \cdots, n-2$, and $e_{n-1} = v_0 - v_{n-1}$. For simplicity, we will take all subscripts modulo n.*

In particular, we will be analyzing a subset of polygonal knots, *equilateral knots*, which are polygonal knots with equal edge lengths.

Definition 3. *Let P be an equilateral knot with n edges. Then the MD-Energy [Sim96] of P is defined as follows: For each pair of nonconsecutive edges $X, Y \in P$, compute the minimum distance between the edges, denoted $MD(X,Y)$, define $U_{md}(X,Y) = \frac{(length(X))(length(Y))}{[MD(X,Y)]^2}$, and compute the sum*

$$U_{md}(P) = \sum_{X \in P} \sum_{Y \neq X \text{ or adjacent}} U_{md}(X,Y).$$

Notice that this sum counts each edge pair twice, which is analogous to the double integral over $K \times K$ in the Möbius Energy. Then we normalize the quantity by subtracting the energy of a standard regular n-gon, and compute the Minimum Distance Energy [Sim96] as

$$E_{md}(P) = U_{md}(P) - U_{md}(\text{regular } n\text{-gon}).$$

Along with these definitions we will also need to use two other knot quantities called the Ropelength and Thickness Radius [LSDR99, Raw03]. Given a C^2 knot K, with $x \in K$, the *Thickness Radius* is defined as follows: Let $D_r(x)$ be the disk of radius r centered at x lying in the plane normal to the tangent vector at x. Then the Thickness Radius is

$$R(K) = \sup\{r > 0 : \ D_r(x) \cap D_r(y) = \emptyset \text{ for all } x \neq y \in K\}.$$

In [Raw03], it has been shown that a smooth knot can be inscribed in a polygonal knot so that the Thickness Radius of the two knots are close. We define the *Ropelength* of a smooth knot K as $E_L(K) = L(K)/R(K)$, where $L(K)$ is the arclength of K [BO95, LSDR99].

Our strategy will be to inscribe a smooth knot in a given polygon. Now, we provide some definitions so that we can describe the inscribing algorithm. For a vertex v_i on an n-edge polygonal knot P, let $angle(v_i)$ be the turning angle at vertex v_i. Let $|e_i|$ denote the length of e_i, and let

$$Rad(v_i) = \frac{\min\{|e_{i-1}|, |e_i|\}}{2\tan\left(\frac{angle(v_i)}{2}\right)}$$

and

$$MinRad(P) = \min_{i=0,\cdots,n-1} Rad(v_i).$$

We should note that $Rad(v_i)$ is the radius of a circular arc that can be inscribed at v_i so that the arc is tangent to both edges adjacent to v_i at their midpoints.

Definition 4. *(See Figure 1.1) Given an n-edge equilateral knot P, we will inscribe a smooth knot K in P in the following way: K has n circular arcs $\alpha_1, \alpha_2, \cdots, \alpha_n$, with each α_i spanning from the midpoint of e_i to the midpoint of e_{i+1}, and with each α_i tangent to e_i and e_{i+1} at their respective midpoints. For each α_i, the radius of α_i is*

$$Rad(v_i) = \frac{|e_i|}{2\tan\left(\frac{angle(v_i)}{2}\right)}.$$

Similar to our notation for a smooth knot K, we define the arclength of a polygonal knot P as $L(P)$. As for the thickness radius of a polygonal knot, we first need to state a couple of definitions [Raw03]. For two points $x, y \in P$, let $d_x(y) = |y - x|$. Further, we call $y \in P$ a *turning point* for $x \in P$ if d_x changes from increasing to decreasing or from decreasing to increasing at y. Let

$$DC(P) = \{(x, y) \in P \times P : x \neq y \text{ turning points of } d_y \text{ and } d_x \text{ respectively}\}.$$

Define the *doubly critical self-distance* of P as

$$dcsd(P) = \min\{||x - y|| : (x, y) \in DC(P)\}.$$

Now we define the thickness radius of a polygonal knot P as

$$R(P) = \min\left\{MinRad(P), \frac{dcsd(P)}{2}\right\}.$$

As in the smooth knot case, the ropelength of P is $E_L(P) = L(P)/R(P)$. Ropelength provides a scale-invariant measure of the knot compaction and provides us with bounds we will need when analyzing the difference between the MD-Energy of a polygonal knot and the Möbius Energy of a smooth knot.

Now that we have a method for inscribing a smooth knot in an equilateral knot, the strategy for showing that the Möbius Energy of the smooth knot is close to the MD-Energy of the polygonal knot is to take each arc on a smooth knot K inscribed in an equilateral knot P and provide an upper bound for the differences in energy in terms of $E_L(P)$ and n, where n is the number of edges of P. In other words we would like to have an error bound of the form:

$$|E_0(K) - E_{md}(P)| \;\leq\; \varphi \frac{E_L(P)^\alpha}{n^\beta}$$

for some positive constants φ, α, and β. Since $E_L(P)$ is scale-invariant, and since this proposed bound is also dependent upon n, if such a bound can be derived, then, as long as $E_L(P)$ roughly stays constant as n increases, the proposition that a polygonal

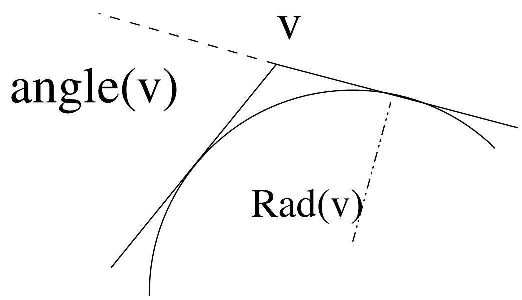

Figure 1.1: Here an arc of radius $Rad(v)$ is inscribed so that the arc is tangent to the polygonal knot at the midpoints of the adjacent edges.

knot and an inscribed smooth knot have close energies would follow immediately.

1.4 Definitions and Notation

In this section, we cover other notation that will be used in the paper. Sometimes it is necessary to talk about the Möbius Energy between two arcs on a smooth knot, and for this we use $E_0(\alpha_i, \alpha_j)$. Recall from the definition of MD-Energy of a polygonal knot P, that we normalize the quantity by subtracting the U_{md} of a regular n-gon, which we refer to as Q. We should note here that the MD-Energy of a regular n-gon is scale invariant, so for simplicity, we will always have $L(P) = L(Q)$. Also, we need a correspondence between the edges of P and Q. We do this as follows: Pick any e_i on P, and match it to any edge on Q, denoted by f_i. Then for any $e_{(i+j)}$ on P, it will correspond to $f_{(i+j)}$ on Q. We use the same correspondence between an arc on a smooth knot K and a circle C that has equal arclength as K. That is, we use β_i to denote the arc on a circle C that corresponds to α_i on a smooth knot K. Further, we will sometimes refer to the minimum length of the arc from some point $x \in K$ to another point $y \in K$ as $arc(x, y)$ and their spatial distance as $|x - y|$. The following chapter contains some lemmas and a portion of the proof that the Möbius Energy of a smooth knot K inscribed in an equilateral knot P is close to the MD-Energy of the P, and we state the lemmas that would be needed to finish the proof of that proposition.

Chapter 2

Error Bounds for Inscribed Smooth Knots

Given an equilateral knot P, we would like to know if the inscribed smooth knot K has Möbius Energy close to the MD-Energy of P. As of now, this is an open question. As we started this endeavor, we thought that it would be a good idea to use the same method that was used to prove that the MD-Energy of a polygonal knot P is close to the Möbius Energy of a smooth knot K when P is inscribed in K. When the latter was proven [RS05], the strategy was to break the knot down into different zones and analyze each zone separately. This chapter contains all progress that we made towards our goal.

2.1 Zones

In order to prove our main result, we will need to divide the knot into *zones*. In order to see the need for different zones, we first define the quantity θ_{max} as the maximum turning angle on P. Also, we need to state Schur's theorem, a definition, and a theorem concerning the thickness radius of a given knot.

Lemma 5. *(Schur's Theorem for piecewise smooth curves) Let C and C^* be two piecewise smooth curves of the same length, such that C, together with the chord connecting its endpoints, forms a simple convex plane curve. Let s be the arclength parameter for C and C^*. Let $k(s)$ be the curvature of C at a regular point, $a(s)$ the angle between the oriented tangents at a vertex, and denote corresponding quantities for C^* by the same notations with asterisks. Let d and d^* be the distances between the endpoints of C and C^*, respectively. Then, if*

$$k^*(s) \leq k(s) \text{ and } a^*(s) \leq a(s),$$

we have $d^* \geq d$.

Proof. See Schur's Theorem in [Che67]. □

The implication of Schur's Theorem is that a polygonal knot that curves less than a planar knot of equal length will have a higher distance between endpoints than the corresponding endpoints on the planar curve. This is useful in analyzing Möbius Energy and MD-Energy since the MD-Energy of a polygonal knot depends heavily upon the minimum distance between the endpoints of its edges and the Möbius Energy of a smooth knot depends on the distance between its points as well.

Definition 6. *Let P be a polygonal knot, and let p, q be two points on P. We define $vb(p, q)$ as the minimum number, over the two arcs of edges containing p and q, of vertices between p and q, including p and/or q if either is a vertex. For edges e_i, e_j on P, let $vb(e_i, e_j)$ be the minimum number of vertices between the midpoints of e_i and e_j.*

Lemma 7. *The thickness of an equilateral knot P is the minimum of MinRad and half of the minimum distance between points in $VB(P)$ where*

$$VB(P) = \{(p, q) : vb(p, q) \geq \pi/\theta_{max}\}.$$

Proof. See [CPR05]. □

When evaluating the distance between edges on a polygonal knot and arcs on the inscribed smooth knot, depending on how many arcs (or edges) are separating the two in question, there are different bounds for the minimum distance. For instance, Schur's theorem gives us a nice way to bound the distance between vertices x, y on an equilateral knot where $vb(x,y) < \frac{\pi}{\theta_{max}}$. Further, by definition, we do not even consider edges on a polygon that are adjacent, but for smooth knots, we do consider such adjacent arcs. Then there is the situation when we are comparing two edges (x, y) where $vb(x,y) \geq \frac{\pi}{\theta_{max}}$. If that is the case, then from Lemma 7 and [CPR05], $|x - y| \geq 2R(P)$. In our analysis, finding bounds for the minimum distance between points on a smooth knot and edges on a polygonal knot will depend on the amount of accumulated curvature on the knot between the two points or edges, so we need a way to tie together the curvature of a smooth knot, and the maximum turning angle of a polygonal knot. For these reasons, we need to divide the knot into *zones*, and analyze each zone individually. Now we will define the zones.

1. The *Adjacent Zone*: This zone is for comparing adjacent arcs on the smooth knot, that is, comparing α_i with α_{i-1} and α_{i+1}. By definition, there is no Adjacent Zone for polygonal knots, so here we will bound $\sum_{i,j} E_0(\alpha_i, \alpha_j)$.

2. The *Near Zone*: This zone is for non-adjacent edges (and their corresponding arcs) where for any two points p, q we have $vb(p,q) \leq \frac{\pi}{\theta_{max}}$. We define the integer m, where $m = \lfloor \frac{\pi}{\theta_{max}} \rfloor$, and note that the Near Zone for each e_i will contain the first m edges in either direction from e_i, excluding the adjacent edges.

   Within the Near Zone, we break the knot down into two different *sub-zones*.

   (a) The *Very Near Zone*: Here, we define the integer $p = \lfloor m^{\frac{3}{4}} \rfloor$. The Very Near Zone contains, for each e_i, the edges $e_{i+2}, e_{i+3}, \cdots, e_{i+p}$. Here we will bound $\sum_{i,j} E_0(\alpha_i, \alpha_j)$, and $\sum_{i,j}(U_{md}(e_i, e_j) - U_{md}(f_i, f_j))$.

(b) The *Moderately Near Zone*: The Moderately Near Zone contains, for each e_i, the edges $e_{i+p+1}, e_{i+p+2}, \cdots, e_{i+m}$. In the Moderately Near Zone, it is sufficient to bound $\sum_{i,j}(E(\alpha_i, \alpha_j) - U_{md}(e_i, e_j))$ and $\sum_{i,j}(E(\beta_i, \beta_j) - U_{md}(f_i, f_j))$.

3. The *Far Zone*: Edges that are not contained in either the Near Zone or Adjacent Zone are contained in the Far Zone. Similar to the Moderately Near Zone, it is sufficient to bound $\sum_{i,j}(E(\alpha_i, \alpha_j) - U_{md}(e_i, e_j))$ and $\sum_{i,j}(E(\beta_i, \beta_j) - U_{md}(f_i, f_j))$.

These zones are slightly different from the zones defined for the proof that the error bound of the Möbius Energy of a smooth knot and the MD-Energy of a polygonal knot inscribed in the smooth knot are close. Each zone should be analyzed separately, and an error bound derived for each one. The idea is that for the Far Zone and Moderately Near Zone on the polygon, there is a corresponding zone on the the inscribed smooth knot that would be close in energy. In the Adjacent Zone and Very Near Zone, the polygonal knot and smooth knot are analyzed separately, and it is shown that the contributions are small.

2.2 Bounds for the Zones

Now we set up a lemma that proves part of what is necessary in order to show that the Möbius Energy of a smooth knot inscribed in an equilateral knot and the MD-Energy of that equilateral knot are close.

Recall that in the Very Near Zone, we are interested in comparing an edge e_i on P with non-adjacent edge e_j such that $vb(e_i, e_j) \leq p$. As previously mentioned, here we bound $\sum_{i,j}(U_{md}(e_i, e_j) - U_{md}(f_i, f_j))$. Thus, for E_{md} in the Very Near Zone, we

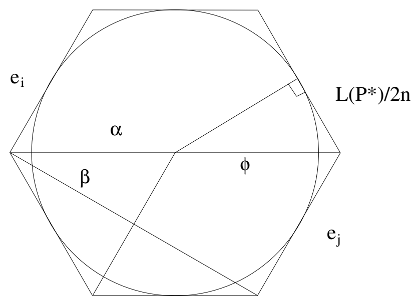

Figure 2.1: Here we illustrate Lemmas 8 and 9. In regard to Lemma 9, $k = 2$.

would like a bound for

$$E_{md} = 2\sum_{i=1}^{n}\sum_{j=i+2}^{i+p}\frac{|e_i||e_j|}{MD(e_i,e_j)^2} - \frac{|f_i||f_j|}{MD(f_i,f_j)^2}.$$

We should note that we start the count at $i+2$ because we do not consider adjacent edges. Further, we can bound the sums uniformly in i and multiply that bound by $2n$, that is, we will bound

$$2n\sum_{k=1}^{p}\left|\frac{|e_i||e_{i+k+1}|}{MD(e_i,e_{i+k+1})^2} - \frac{|f_i||f_{i+k+1}|}{MD(f_i,f_{i+k+1})^2}\right|.$$

In order to do this, we will find a positive upper bound and a negative lower bound for the difference term. Then we can take the difference of the two bounds, and we will have a bound for the absolute value. In order to find an upper bound, our strategy is to find a lower bound for $MD(e_i, e_{i+k+1})$. This is both necessary and sufficient since both P and Q are equilateral, and $|e_i|$ and $|f_i|$ are known quantities. Further, since Q is a regular n-gon, we can also easily derive $MD(f_i, f_{i+k+1})$. To find a lower bound for $MD(e_i, e_{i+k+1})$, it is necessary to state some lemmas first.

Lemma 8. *Given a regular n-gon P^* and a circle C inscribed in P^*, the length of a line segment drawn from the center of C to any vertex of P^* has length*

$$\frac{L(P^*)}{2n\sin(\frac{\pi}{n})}.$$

Proof. (See Figure 2.1) Construct a line segment ϕ from the center of C to any vertex of P^*. Then

$$\sin\left(\frac{\pi}{n}\right) = \frac{\frac{L(P^*)}{2n}}{|\phi|},$$

which implies that

$$|\phi| = \frac{L(P^*)}{2n\sin(\frac{\pi}{n})}.$$

□

Lemma 9. *Given a regular n-gon knot P^* and a circle C inscribed in P^*, then*

$$MD(e_i, e_{i+k+1}) = \frac{L(P)\sin(\frac{k\pi}{n})}{n\sin(\frac{\pi}{n})},$$

for $k = 1, \cdots, m$.

Proof. (See Figure 2.1) First construct a line segment β connecting the closest endpoints of e_i and e_{i+k+1}. Then, from the center of C, construct a line segment in one of two ways. If k is even, make the line segment from the center of C go through the vertex at $e_{i+\frac{k}{2}}$ and $e_{i+\frac{k}{2}+1}$. If k is odd, make the line segment from the center of C go through the midpoint of $e_{i+\frac{k+1}{2}}$. Then construct a line segment α from the center of C to the vertex of e_i and e_{i+1}. Then,

$$\sin\frac{k\pi}{n} = \frac{\frac{1}{2}|\beta|}{|\alpha|},$$

so, (using Lemma 8)

$$MD(e_i, e_{i+k+1}) = |\beta| = \frac{L(P)\sin(\frac{k\pi}{n})}{n\sin(\frac{\pi}{n})}.$$

□

Recall that Schur's Theorem says that a lower bound for $MD(e_i, e_{i+k+1})$ on P can be determined by finding the distance between edges in the plane that are connected by a set of vertices, where the turning angle at each vertex is the maximum turning angle on P.

Lemma 10. *Let P be an equilateral planar knot with edges $e_0, e_1, \cdots, e_{n-1}$, where the turning angle at each vertex is θ_{max}, then*

$$MD(e_i, e_{i+k+1}) = \frac{L(P)\sin(\frac{k\theta_{max}}{2})}{n\sin(\frac{\theta_{max}}{2})} = \frac{|e_i|\sin(\frac{k\theta_{max}}{2})}{\sin(\frac{\theta_{max}}{2})},$$

for $k = 1, \cdots, m$.

Proof. This follows immediately from Lemma 9. □

Now we prove our bound for E_{md} in the Very Near Zone.

Lemma 11. *Let P be an equilateral knot. Then, in the Very Near Zone,*

$$|E_{md}(P)| = |U_{md}(P) - U_{md}(Q)| \leq 0.66\left(\frac{E_L(P)^{\frac{5}{4}}}{n^{\frac{1}{4}}}\right).$$

Proof. In the Very Near Zone, we have

$$E_{md}(\text{very near}) = 2\sum_{i=1}^{n}\sum_{j=i+2}^{i+p}\frac{|e_i||e_j|}{MD(e_i,e_j)^2} - \frac{|f_i||f_j|}{MD(f_i,f_j)^2}.$$

As stated before,

$$2\sum_{i=1}^{n}\sum_{j=i+2}^{i+p}\frac{|e_i||e_j|}{MD(e_i,e_j)^2} - \frac{|f_i||f_j|}{MD(f_i,f_j)^2} \leq 2n\sum_{k=1}^{p}\left|\frac{|e_i||e_{i+k+1}|}{MD(e_i,e_{i+k+1})^2} - \frac{|f_i||f_{i+k+1}|}{MD(f_i,f_{i+k+1})^2}\right|.$$

In order to obtain an upper bound for this summand, we need to find lower bound for the denominatior of the first term, as the other denominator and numerators are known quantities. By Schur's Theorem and Lemma 10

$$MD(e_i, e_{i+k+1})^2 \geq \frac{|e_i|^2\sin^2(\frac{k\theta_{max}}{2})}{\sin^2(\frac{\theta_{max}}{2})}.$$

Using Lemma 9, for an upper bound we have

$$\left|\frac{|e_i||e_{i+k+1}|}{MD(e_i,e_{i+k+1})^2}-\frac{|f_i||f_{i+k+1}|}{MD(f_i,f_{i+k+1})^2}\right|\leq\frac{|e_i|^2}{\frac{|e_i|^2\sin^2\left(\frac{k\theta_{max}}{2}\right)}{\sin^2\left(\frac{\theta_{max}}{2}\right)}}-\frac{|e_i|^2}{\frac{|e_i|^2\sin^2\left(\frac{k\pi}{n}\right)}{\sin^2\left(\frac{\pi}{n}\right)}}.$$

If we take a look at the denominators of each term in our upper bound, we can see that the denominator of the first term is the minimum distance between edges on a planar knot that curves more than Q. Thus, by Schur's Theorem,

$$\frac{\sin^2\left(\frac{k\theta_{max}}{2}\right)}{\sin^2\left(\frac{\theta_{max}}{2}\right)}<\frac{\sin^2\left(\frac{k\pi}{n}\right)}{\sin^2\left(\frac{\pi}{n}\right)},$$

which implies that

$$\frac{\sin^2\left(\frac{\theta_{max}}{2}\right)}{\sin^2\left(\frac{k\theta_{max}}{2}\right)}>\frac{\sin^2\left(\frac{\pi}{n}\right)}{\sin^2\left(\frac{k\pi}{n}\right)}.$$

Further, if we simplify our upper bound we obtain

$$\frac{|e_i|^2}{\frac{|e_i|^2\sin^2\left(\frac{k\theta_{max}}{2}\right)}{\sin^2\left(\frac{\theta_{max}}{2}\right)}}-\frac{|e_i|^2}{\frac{|e_i|^2\sin^2\left(\frac{k\pi}{n}\right)}{\sin^2\left(\frac{\pi}{n}\right)}}=\frac{\sin^2(\frac{\theta_{max}}{2})}{\sin^2(\frac{k\theta_{max}}{2})}-\frac{\sin^2(\frac{\pi}{n})}{\sin^2(\frac{k\pi}{n})},$$

and thus our upper bound is positive. For the lower bound, we simply find an upper bound for $MD(e_i, e_{i+k+1})$ by straightening out all of the edges separating e_i and e_{i+k+1} and taking the length of the resulting line segment. This gives us

$$\left|\frac{|e_i||e_{i+k+1}|}{MD(e_i,e_{i+k+1})^2}-\frac{|f_i||f_{i+k+1}|}{MD(f_i,f_{i+k+1})^2}\right|\geq\frac{|e_i|^2}{k^2|e_i|^2}-\frac{|e_i|^2}{\frac{|e_i|^2\sin^2(\frac{k\pi}{n})}{\sin^2(\frac{\pi}{n})}}.$$

We can use the same argument as for our upper bound to show that this lower bound is negative. That is, we see that the minimum distance between the edges of a knot that has less curvature than that of a planar knot of the same length is greater than the minimum distance between the edges on the planar knot. Thus,

$$k^2 > \frac{\sin^2(\frac{k\pi}{n})}{\sin^2(\frac{\pi}{n})},$$

giving us

$$\frac{1}{k^2} < \frac{\sin^2(\frac{\pi}{n})}{\sin^2(\frac{k\pi}{n})}.$$

Simplifying our lower bound, we obtain

$$\left|\frac{|e_i||e_{i+k+1}|}{MD(e_i, e_{i+k+1})^2} - \frac{|f_i||f_{i+k+1}|}{MD(f_i, f_{i+k+1})^2}\right| \geq \frac{1}{k^2} - \frac{\sin^2(\frac{\pi}{n})}{\sin^2(\frac{k\pi}{n})},$$

and thus our lower bound is negative. Taking the difference between the upper and lower bounds, we have

$$\left|\frac{|e_i||e_{i+k+1}|}{MD(e_i, e_{i+k+1})^2} - \frac{|f_i||f_{i+k+1}|}{MD(f_i, f_{i+k+1})^2}\right| \leq \frac{\sin^2(\frac{\theta_{max}}{2})}{\sin^2(\frac{k\theta_{max}}{2})} - \frac{1}{k^2}.$$

Using the Taylor Series expansions for the numerator and denominator of the first term of our bound, and letting $x = \frac{\theta_{max}}{2}$, we have $\sin^2(x) \leq x^2$ and $\sin^2(kx) \geq k^2x^2 - \frac{1}{3}k^4x^4$, since $x \in (0, \frac{\pi}{2})$, which gives us

$$2n\sum_{k=1}^{p}\left|\frac{|e_i||e_{i+k+1}|}{MD(e_i, e_{i+k+1})^2} - \frac{|f_i||f_{i+k+1}|}{MD(f_i, f_{i+k+1})^2}\right| \leq 2n\sum_{k=1}^{p}\frac{x^2}{k^2x^2 - \frac{1}{3}k^4x^4} - \frac{1}{k^2}.$$

Since x is a fixed value, $\frac{x^2}{k^2x^2 - \frac{1}{3}k^4x^4} - \frac{1}{k^2}$ is a function of k and decreasing on the interval $(0, p]$, and

$$2n\sum_{k=1}^{p}\frac{x^2}{k^2x^2 - \frac{1}{3}k^4x^4} - \frac{1}{k^2} \leq 2n\int_0^p \frac{x^2}{k^2x^2 - \frac{1}{3}k^4x^4} - \frac{1}{k^2}\, dk.$$

Integrating with respect to k, we have

$$2n\int_0^p \frac{x^2}{k^2x^2-\frac{1}{3}k^4x^4}-\frac{1}{k^2}\,dk \;=\; 2n\left(\frac{1}{\sqrt{3}}x\tanh^{-1}\left(\frac{1}{\sqrt{3}}xp\right)\right)$$
$$=\; 2nx\left(\frac{1}{\sqrt{3}}\tanh^{-1}\left(\frac{1}{\sqrt{3}}x^{1/4}x^{3/4}p\right)\right).$$

Using our definitions of integers m and p, we have that $p^{4/3}\theta_{max} \leq m\theta_{max} \leq \pi$. Thus, $p(\theta_{max})^{3/4} \leq \pi^{3/4}$ so $px^{3/4} \leq (\pi/2)^{3/4}$. Since $\tanh^{-1}$ is increasing on $(0,1)$, we have

$$2n\int_0^p \frac{x^2}{k^2x^2-\frac{1}{3}k^4x^4}-\frac{1}{k^2}\,dk \leq 2nx\left(\frac{1}{\sqrt{3}}\tanh^{-1}\left(\frac{1}{\sqrt{3}}\left(\frac{\pi}{2}\right)^{3/4}x^{1/4}\right)\right).$$

Since $\tanh^{-1}$ is only defined on the interval $(-1,1)$, and specifically, we are only interested in the interval $(0,1)$, we need to be sure that our argument for $\tanh^{-1}$ is always a number that is less than one. However, since it is not possible for θ_{max} to be greater than π, and since $\left(\frac{1}{\sqrt{3}}\left(\frac{\pi}{2}\right)^{3/4}x^{1/4}\right)$ is an increasing function, we only need to be sure that letting $x = \frac{\theta_{max}}{2} = \frac{\pi}{2}$ is a valid argument. If we plug in $\frac{\pi}{2}$ for x in $\frac{x^{1/4}\pi^{3/4}}{2^{3/4}\sqrt{3}}$, we get 0.90689, so we are in the domain of $\tanh^{-1}$. In order to bound our expression, we need to find some constant β so that $\tanh^{-1}\left(\frac{1}{\sqrt{3}}xp\right) \leq \beta x^{1/4}$. Since $\frac{\tanh^{-1}\left(\frac{1}{\sqrt{3}}\left(\frac{\pi}{2}\right)^{3/4}x^{1/4}\right)}{x^{1/4}}$ is increasing on $\mathbb{R}^+$, and since $\theta_{max} \leq \pi$, we have

$$\frac{\tanh^{-1}\left(\frac{1}{\sqrt{3}}\left(\frac{\pi}{2}\right)^{3/4}x^{1/4}\right)}{x^{1/4}} \leq 1.35.$$

So we know that for $0 < x \leq \frac{\pi}{2}$, that $\tanh^{-1}(\frac{1}{\sqrt{3}}xp) \leq 1.35x^{1/4}$. Further, from [LSDR99, Raw03], we know that

$$R(P) \leq MinRad(P) = \frac{L(P)}{2n\tan(\frac{\theta_{max}}{2})},$$

which implies that

$$\tan\left(\frac{\theta_{max}}{2}\right) \leq \frac{L(P)}{2nR(P)}.$$

So, since $\arctan(x)$ is increasing over its entire domain,

$$\arctan\left[\tan\left(\frac{\theta_{max}}{2}\right)\right] = \frac{\theta_{max}}{2} \leq \arctan\left(\frac{L(P)}{2nR(P)}\right).$$

We also know, by Taylor Series, that $\arctan(x) \leq x$ for all x, so

$$x = \frac{\theta_{max}}{2} \leq \arctan\left(\frac{L(P)}{2nR(P)}\right) \leq \frac{L(P)}{2nR(P)} = \frac{E_L(P)}{2n}.$$

Putting this all together we have

$$\begin{aligned}
2n\sum_{k=1}^{p}\left|\frac{|e_i||e_{i+k+1}|}{MD(e_i,e_{i+k+1})^2} - \frac{|f_i||f_{i+k+1}|}{MD(f_i,f_{i+k+1})^2}\right| &\leq 2n\sum_{k=1}^{p}\frac{\sin^2(\frac{\theta_{max}}{2})}{\sin^2(\frac{k\theta_{max}}{2})} - \frac{1}{k^2} \\
&\leq 2n\sum_{k=1}^{p}\frac{x^2}{k^2x^2 - \frac{1}{3}k^4x^4} - \frac{1}{k^2} \\
&\leq 2n\int_0^p \frac{x^2}{k^2x^2 - \frac{1}{3}k^4x^4} - \frac{1}{k^2}\,dk \\
&\leq 2nx\left(\frac{1}{\sqrt{3}}\tanh^{-1}\left(\frac{1}{\sqrt{3}}\left(\frac{\pi}{2}\right)^{3/4}x^{1/4}\right)\right) \\
&\leq 2nx\left(\frac{1}{\sqrt{3}}\right)1.35x^{1/4} \\
&\leq 2n\frac{E_L(P)^{5/4}}{(2n)^{5/4}}\left(\frac{1.35}{\sqrt{3}}\right) \\
&< 0.66\left(\frac{E_L(P)^{5/4}}{n^{1/4}}\right).
\end{aligned}$$

□

Next, we bound $\sum_{i,j} E_0(\alpha_i,\alpha_j)$ in the Adjacent and Very Near Zones.

Lemma 12. *Let K be a smooth knot inscribed in an equilateral knot P. Then, in the*

Adjacent and Very Near Zones,

$$\left|\sum_{i,j} E_0(\alpha_i, \alpha_j)\right| < 1.42\,\frac{E_L(P)^{5/4}}{n^{1/4}}.$$

Proof. Let $r = MinRad(K)$, (and thus, $r = MinRad(P) \geq R(P)$) and let $a = arc(x, y)$. Let C be a circle where $L(C) = L(K)$, and with radius R. Let $s, t \in C$ such that $arc(s, t) = arc(x, y)$. Thus, we will bound

$$\left|\int_{x\in K}\int_{y\in K,(\text{Adjacent and Very Near})} \frac{1}{|x-y|^2} - \frac{1}{|s-t|^2}\right|.$$

Since the choice of x is arbitrary, we can bound

$$\left|\int_{x\in K}\int_{y\in K,(\text{Adjacent and Very Near})} \frac{1}{|x-y|^2} - \frac{1}{|s-t|^2}\right| \leq 2L(K)\int_x^{x+(p+1)r\theta_{max}} \frac{1}{|x-y|^2} - \frac{1}{|s-t|^2}\,dy.$$

First, we find an upper bound. From [RS05],

$$\frac{1}{|s-t|^2} = \frac{1}{R^2(2-2\cos(\frac{a}{R}))}.$$

Note: In this case, $a = arc(s, t)$, since $arc(s, t) = arc(x, y)$. Thus, from [RS05], and using Schur's Theorem,

$$|x-y|^2 \geq r^2\left(2 - 2\cos\left(\frac{a}{r}\right)\right).$$

and

$$\frac{1}{|x-y|^2} - \frac{1}{|s-t|^2} \leq \frac{1}{r^2(2-2\cos(\frac{a}{r}))} - \frac{1}{R^2(2-2\cos(\frac{a}{R}))}.$$

Since $r^2 \leq R^2$ [RS05], this upper bound is nonnegative. Next, we find a lower bound. First, we note that on any curve that arclength is greater than or equal to chordlength, so $|x-y|^2 \leq a^2$. Thus,

$$\frac{1}{|x-y|^2} - \frac{1}{|s-t|^2} \geq \frac{1}{a^2} - \frac{1}{|s-t|^2} = \frac{1}{a^2} - \frac{1}{R^2(2-2\cos(\frac{a}{R}))},$$

which is negative since $|s-t|^2 < a^2$. Now, we take the difference between the upper and lower bounds:

$$\left|\frac{1}{|x-y|^2} - \frac{1}{|s-t|^2}\right| \leq \left[\frac{1}{r^2(2-2\cos(\frac{a}{r}))} - \frac{1}{R^2(2-2\cos(\frac{a}{R}))}\right] - \left[\frac{1}{a^2} - \frac{1}{R^2(2-2\cos(\frac{a}{R}))}\right]$$

$$= \frac{1}{r^2(2-2\cos(\frac{a}{r}))} - \frac{1}{a^2}.$$

So

$$2L(K)\int_x^{x+(p+1)r\theta_{max}} \frac{1}{|x-y|^2} - \frac{1}{|s-t|^2}\, dy \leq 2L(K)\int_0^{x+(p+1)r\theta_{max}} \frac{1}{r^2(2-2\cos(\frac{a}{r}))} - \frac{1}{a^2}\, da,$$

which is a function of a real variable. From [RS05] we have

$$2L(K)\int_x^{x+(p+1)r\theta_{max}} \frac{1}{r^2(2-2\cos(\frac{a}{r}))} - \frac{1}{a^2}\, da \leq 2L(K)(p+1)r\theta_{max}\left(\frac{1}{4} - \frac{1}{\pi^2}\right)\frac{1}{r^2}.$$

Combining the quantities, we have

$$
\begin{aligned}
2L(K)\int_x^{x+(p+1)r\theta_{max}} & \frac{1}{|x-y|^2}-\frac{1}{|s-t|^2}\,dy \\
&\leq 2L(K)\int_x^{x+(p+1)r\theta_{max}} \frac{1}{r^2(2-2\cos(\frac{a}{r}))}-\frac{1}{a^2}\,da \\
&\leq 2L(K)(p+1)r\theta_{max}\left(\frac{1}{4}-\frac{1}{\pi^2}\right)\frac{1}{r^2}\ \text{[RS05]} \\
&\leq \frac{2L(K)2p\theta_{max}(0.15)}{r}\ (\text{since for } p\geq 2,\ 2p\geq p+1) \\
&\leq \frac{2L(P)2p\theta_{max}(0.15)}{r}\ (\text{since } L(K)\leq L(P)) \\
&\leq 0.60\,\frac{L(P)p\theta_{max}^{3/4}\theta_{max}^{1/4}}{R(P)} \\
&\leq 0.60\,\frac{L(P)\pi^{3/4}\theta_{max}^{1/4}}{R(P)}\ (\text{since } p\theta_{max}^{3/4}\leq\pi^{3/4}) \\
&= 0.60\,\frac{L(P)\pi^{3/4}}{R(P)}\left(\frac{L(P)^{1/4}}{R(P)^{1/4}n^{1/4}}\right) \\
&< 1.42\,\frac{E_L(P)^{5/4}}{n^{1/4}}.
\end{aligned}
$$

□

This particular proof is very similar to the proposition that was necessary in order to prove that the MD-Energy of a polygonal knot inscribed in a smooth knot was close to the Möbius Energy of the smooth knot. This proposition is appropriate here because whether the equilateral knot is inscribed in the smooth knot, or vice versa, we are only comparing the smooth knot to itself, and the equilateral knot is not involved. We were not able to complete the necessary proofs for the Moderately Near Zone and Far Zone, but the idea would be to find bounds for $|E_0(K)-E_{md}(P)|$ and $|E_0(C)-E_{md}(Q)|$.

Chapter 3

Creating Equilateral Knots

In this chapter, we shift our attention to creating equilateral knots. For smooth knots, an equilateral knot can be inscribed so that the MD-Energy will be a good approximation of the Möbius Energy of the smooth knot. We thought that it would be useful to create a list of MD-Energies for the equilateral knots that were inscribed in each chosen smooth knot.

The idea is that if we can inscribe a sequence of *nearly* equilateral knots, (a sequence of increasing n values) then we can derive a close approximation of the Möbius Energy of the smooth knot and verify the theorem that says that there is a bounded error for $|E_0(K) - E_{md}(P)|$. The word nearly is necessary because for computational purposes, we chose an error of varying values from 10^{-5} to 10^{-13}. In this study, we consider three ellipses and seven knots of varying complexity. Our hope was to build a table of polygonal knots that could be used to approximate the Möbius Energy of the smooth knots. Also, we wanted to see if there might be any evidence that the bound known to be true could be improved. Further, once these equilateral knots are created, one could inscribe smooth knots in them and see if there is any evidence that the Möbius Energy of the inscribed smooth knot is converging to the MD-Energy of the equilateral knot. The reason for using the ellipses is that the program ran quite slowly on the 3-dimensional knots, and the ellipses were a good test case.

3.1 Algorithm

In order to inscribe an equilateral knot in a smooth knot, we simply need the parametrization of the smooth knot with period 2π, and a program that can solve algebraic equations, in our case *Maple*. The algorithm for inscribing an equilateral knot in the smooth knot with parametrization $(x(t), y(t), z(t))$ is as follows: (Note: In the case of an ellipse, $z(t) = 0$.)

1: Take a positive ϵ.

2: Find the arclength of the knot.

3: Let $upperbound = arclength/n$, where n is the number of edges on the polygon.

4: Let $lowerbound = 0.5(upperbound)$.

5: Let $edgelength = 0.5(upperbound + lowerbound)$.

6: $d \leftarrow edgelength$.

7: Compute $x(0), y(0)$, and $z(0)$.

8: $OldPointX \leftarrow x(0),\ OldPointY \leftarrow y(0),\ OldPointZ \leftarrow z(0)$.

9: Solve for t in $(x(t) - OldPointX)^2 + (y(t) - OldPointY)^2 + (z(t) - OldPointZ)^2 = d^2$.

10: $newt \leftarrow t$.

11: $OldPointX \leftarrow x(newt),\ OldPointY \leftarrow y(newt),\ OldPointZ \leftarrow z(newt)$.

12: Repeat steps $9, 10$, and 11 $(n - 1)$ times.

13: Evaluate $a = |t - 2\pi|$.

14: If $a < \epsilon$, stop.

15: If $a \geq \epsilon$, then if $t < 2\pi$, $d \leftarrow lowerbound$. Otherwise, $d \leftarrow upperbound$, and $d = 0.5(upperbound + lowerbound)$, and repeat process starting with step 7.

Chapter 4

Appendix

4.1 Code for Inscribing Equilateral Knots in Smooth Knots

The following is the Maple code that we wrote in order to generate nearly equilateral knots. In the near future, the results of this program will be displayed on a website. The results will include tables listing each ellipse and knot that we used along with their respective thickness radius and arclength, and they will also include the MD-Energies of each equilateral knot that was inscribed in them.

```
> x:=t->x(t);
> y:=t->y(t);
> z:=t->z(t);
> xp:=unapply(diff(x(t),t),t);
> yp:=unapply(diff(y(t),t),t);
> zp:=unapply(diff(z(t),t),t);
> g:=int(sqrt((xp(t))^2+(yp(t))^2+(zp(t))^2),t=0..2*Pi);
> w:=evalf(g);
> epsilon:=0.00001;
> for j from 600 to 601 do
>    filename:="knotfile." ||j|| ".txt";
>    filename1:="knotfile1." ||j|| ".txt";
```

```
>     fd:=fopen(filename,WRITE);
>     fd1:=fopen(filename1,WRITE);
>     upBound:=w/j;
>     lowBound:=upBound*0.5;
>     d:=0.5*(lowBound+upBound);
>     Error:=1.0;
>     OldPointX:=x(0);
>     OldPointY:=y(0);
>     OldPointZ:=z(0);
>     newt:=0.0;
>     while Error>=epsilon do
>        newt := 0.0;
>        for i from 1 to j do
>           eq1:=(x(t)-OldPointX)^2+(y(t)-OldPointY)^2+(z(t)-OldPointZ)^2-d^2;
>           newt:=fsolve(eq1,t,t=newt..newt+(0.5*Pi));
>           OldPointX:=x(newt):
>           OldPointY:=y(newt):
>           OldPointZ:=z(newt):
>        end do:
>        Error:=evalf(abs((2*Pi)-newt));
>        if Error<epsilon then
>           fprintf(fd,"{%d}\n",j);
>           newt:=0.0:
>           OldPointX:=x(newt):
>           OldPointY:=y(newt):
>           OldPointZ:=z(newt):
>           for k from 1 to j do
>           eq2:=(x(t)-OldPointX)^2+(y(t)-OldPointY)^2+(z(t)-OldPointZ)^2-d^2;
>           newt:= fsolve(eq2,t,t=newt..newt+(0.5*Pi));
>           OldPointX:=x(newt):
>           OldPointY:=y(newt):
>           OldPointZ:=z(newt):
>           fprintf(fd,"%f, %f, %f\n",OldPointX,OldPointY,OldPointZ);
>           end do:
>           fprintf(fd1,"%f, %g\n",d,epsilon);
>        else
```

```
>           if newt<evalf(2*Pi) then
>              lowBound:=d;
>           else
>              upBound:=d;
>           end if;
>           d:=0.5*(upBound+lowBound);
>           Error:=evalf(abs(2*Pi-newt));
>           filename2:="knotData." ||j|| ".txt";
>           fd2:=fopen(filename2,WRITE);
>           fprintf(fd2,"%f, %f, %f\n",upBound,lowBound,d);
>           fclose(fd2);
>        end if:
>           OldPointX:=x(0):
>           OldPointY:=y(0):
>           OldPointZ:=z(0):
>        end do:
>        fclose(fd);
>        fclose(fd1);
>  end do:
```

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