MÖBIUS ENERGY OF THICK KNOTS

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Abstract. The Möbius energy of a knot is an energy functional for smooth curves based on an idea of self-repelling. If a knot has a thick tubular neighborhood, we would intuitively expect the energy to be low. In this paper, we give explicit bounds for energy in terms of the ropelength of the knot, i.e. the ratio of the length of a thickest tube to its radius.

1. Introduction

In this paper, we exhibit a bound for the Möbius energy of a knot, in terms of the amount of "rope" needed to make the knot. This is the energy introduced in [23] and studied extensively in [14, 17].

We and other researchers have defined a number of different energy functions for (smooth or polygonal) knots [3, 4, 5, 6, 13, 14, 15, 17, 21, 23, 24, 25, 26, 28, 29, 30] based on the idea of inverse-square repelling energy (so these would correspond to inverse-cube "forces"). (See also [22] for a different approach). Roughly, these energies are defined in terms of integrals over the curve K

$$\int_{x \in K} \int_{y \in K} \frac{\Box}{|x-y|^2} \, \mathrm{d}x \, \mathrm{d}y \quad .$$

Here $\Box$ is a placeholder for any of several kinds of terms that make the integral not give too much weight to the repelling of points that are close to each other in the sense of arclength along the knot (so the improper integral will converge). Alternatively [14, 23], energies are defined as integrals of differences

$$\int_{x \in K} \int_{y \in K} \frac{1}{|x(s)-x(t)|^2} \quad - \quad \frac{1}{|s-t|^2} \quad \mathrm{d}x \, \mathrm{d}y$$

where s, t lie on a line or circle used to parametrize the curve K. The energy we study in this paper can be defined either way [14, 17, 23] and we shall use the latter.

In addition to viewing a curve as self-repelling, one also can view it as self-excluding, and define the *ropelength* energy $\mathcal{E}_L(K)$ [5, 6]: this is the ratio of the arclength of the curve to the maximum radius of a uniform non self-intersecting tube along the curve [20], i.e. the ratio of length to radius of the rope (see Section 2 for precise definitions). Variations on thickness are developed in [10, 11, 12, 16, 18, 22].

We showed in [6] that the *normal* energy $\mathcal{E}_N(K)$, which discounts tangential self-repelling, and the *symmetric* energy $\mathcal{E}_S(K)$, which models self-radiation of a filament [1], are bounded by the ropelength. These energies, in turn, dominate the number of crossings in any regular projection of the knot. The inequalities are of

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the form shown below in (1). Here $\operatorname{acn}(K)$ is the *average crossing number*, that is the average over all spatial directions of the number of crossings seen from each direction. This, in turn, is larger than the crossing number $\operatorname{cr}(K)$, which is the minimum over all regular projections, and $\operatorname{cr}[K]$ which considers all K in a given knot type.

(1) $$4\pi \operatorname{cr}[K] \leq 4\pi \operatorname{cr}(K) < 4\pi \operatorname{acn}(K) \leq \mathcal{E}_S(K) \leq \mathcal{E}_N(K) \leq c\, \mathcal{E}_L(K)^{4/3}$$

The constant c was originally obtained as 11, but that can be lowered as we do in this paper to just under 5. A related idea is the *writhe* of a knot, $\operatorname{wr}(K)$, which is the average over all spatial directions of the *signed* crossing numbers. Since $\operatorname{wr}(K) \leq \operatorname{acn}(K)$, we get the same bound on $4\pi \operatorname{wr}(K)$. But using a different analysis of writhe, in terms of vector fields flowing in tubes around the knot, it is shown in [7] that $\operatorname{wr}(K) \leq \frac{1}{4}\mathcal{E}_L(K)^{4/3}$, which is a lower coefficient than an analysis of the kind in [6] produces. It should be noted that while coefficients might be improved, the exponent 4/3 in (1) is sharp [2, 8]. Similarly, because Möbius energy also bounds crossing number [14], the same examples [2, 8] show that the exponent 4/3 in Theorem 3.1 is sharp.

The main result of this paper is that the Möbius energy also is bounded by the (4/3)-power of the ropelength. This and the results cited above support our belief that ropelength is the fundamental measure of knot complexity: given a bound on ropelength, one can find a bound on any other given knot invariant.

We state the theorem for the version of the energy that equals 4 on a circle,

$$\mathcal{E}_{O4}(K) = \int_{x\in K}\int_{y\in K} \frac{1}{|x-y|^2} - \frac{1}{\operatorname{arc}(x,y)^2}\ ,$$

where $\operatorname{arc}(x,y)$ denotes the minimum arclength along the curve K between x and y.

The proof of this theorem follows the same model as the proof in [6]. The paradigm is to use one kind of analysis to bound the energy contribution coming from pairs of points (x, y) where x and y are near each other in arclength along the knot, and a different analysis for pairs where x and y are relatively far apart. The analysis of proximal pairs will be special for each particular energy function, and yields typically a *linear* bound on energy in terms of ropelength. The analysis of distal pairs is identical for the various energy functions: with little work, we can get a bound on energy that is *quadratic* in ropelength; and with more work, we obtain a bound that is (4/3)-power in the ropelength. We add the proximal and distal contributions to get the overall bound.

In a recent book [31], many ideas of energy and thickness for knots are discussed. Many of us interested in such ideas thought that knots should have "ideal" forms. It has turned out that the knot conformations that minimize the various ideas of energy differ from one another. The similarities and differences are equally provocative.

2. The Lemmas

The first lemma is a version of a theorem of Schur. This is taken from [9], with the slight adjustment that we do not need to consider general planar convex curves as the reference curves, just circles.

Lemma 2.1. *Let K be a C^2 smooth curve in $\mathbb{R}^3$ whose curvature everywhere is $\leq$ some number k. Let C be a circle of curvature k, i.e. of radius $r = \frac{1}{k}$. Let $x, y \in K, s, t \in C$ such that* $\mathrm{arc}(x,y) = \mathrm{arc}(s,t) \leq \pi r$. *Then the chord distances satisfy*

$$|x-y| \geq |s-t|.$$

Proof. See Schur's Theorem in [9].

□

We also will use results on thickness of knots developed in [20]. Let K be a smooth knot in $\mathbb{R}^3$, a simple closed curve that is at least C^2 smooth. We assume C^2 smoothness throughout this paper, and the work in [20] assumed that as well; but in fact the definition and results there can be modified to deal with $C^{1,1}$ curves.

For each $x \in K$, let $D(x,r)$ denote the disk of radius r centered at x and orthogonal at x to K. For sufficiently small $r > 0$, the disks are pairwise disjoint, their union forming a tubular neighborhood of K. We define the *injectivity radius* of K, $R(K)$, to be the supremum of such good radii. The radius $R(K)$ measures the maximum thickness of "rope" that could be used to form the curve K. Of course, $R(K)$ changes with scale. We define the scale-invariant *ropelength* or *length energy* of K to be

$$E_L(K) = \frac{\mathrm{arclength}(K)}{R(K)} \quad .$$

The radius $R(K)$ is affected by curvature and by points of K that are far apart in the sense of arclength but close in space. For the latter kinds of points, distances will be minimized at pairs of points (x,y) that are critical points for the distance function $|x-y|$. Specifically, define the *critical self-distance* of K to be the minimum of $|x-y|$ over all pairs $(x,y) \in K \times K$, $x \neq y$, for which the chord $x-y$ is perpendicular to K at either or both of its endpoints. Let $\mathrm{MinRad}(K)$ denote the minimum radius of curvature of K. We then have from [20]:

Lemma 2.2. *The thickness of a smooth knot is bounded by the minimum radius of curvature and half the critical self-distance. In fact,*

$$R(K) = \min\left\{\mathrm{MinRad}(K), \frac{1}{2}\text{ critical self distance}(K)\right\}.$$

The next lemma is a consequence of Lemmas 2.1 and 2.2.

Lemma 2.3. *Suppose K is a smooth knot of thickness $R(K) = r$. For any $x, y \in K$, such that $arc(x,y) \geq \pi r$, we must have $|y-x| \geq 2r$.*

Proof. Fix x and consider first the two points $y \in K$ for which $\mathrm{arc}(x,y) = \pi r$. Since, by Lemma 2.2, the curvature of K is everywhere less than $1/r$, and $\mathrm{arc}(x,y) = \pi r$, so in particular it is $\leq \pi r$, we can apply Schur's Theorem to the arc from x to such y to conclude that $|y-x|$ is at least as large as for the corresponding points on a circle of radius r, i.e. $|y-x| \geq 2r$.

Now consider the arc Y of K consisting of those points y with $\mathrm{arc}(x,y) \geq \pi r$. If any of these is closer to x than $2r$ then, from the preceding paragraph, it cannot be an endpoint; thus it would be a critical point for the function $|y-x|$. But by Lemma 2.2, any such critical pair (x,y) has distance $\geq 2r$.

□

In the next two lemmas, we obtain the linear bound for the energy contribution on proximal pairs.

Lemma 2.4. *For a fixed point s on a circle C of radius R,*

$$\int_{t\in C} \frac{1}{|s-t|^2} - \frac{1}{\operatorname{arc}(s,t)^2} = \frac{2}{\pi R} .$$

Proof. Fix s on a circle C of radius R. Note that if $\operatorname{arc}(s,t) = \theta$, then $|s-t|^2 = R^2(2 - 2\cos\theta)$. Thus,

$$\begin{aligned} \int_{t\in C} \frac{1}{|s-t|^2} - \frac{1}{\operatorname{arc}(s,t)^2} &= 2\int_0^{\pi R} \frac{1}{R^2(2-2\cos(t/R))} - \frac{1}{t^2}\,\mathrm{d}t \\ &= \frac{2}{\pi R} . \end{aligned}$$

□

Lemma 2.5. *If K is a smooth knot in $\mathbb{R}^3$, then*

$$\int_{x\in K}\int_{\operatorname{arc}(x,y)\le \pi R(K)} \frac{1}{|x-y|^2} - \frac{1}{\operatorname{arc}(x,y)^2} \le \frac{2}{\pi} E_L(K) .$$

Proof. We begin by rescaling K to have $R(K) = 1$; note this leaves each side of the inequality unchanged. Then $E_L(K)$ is just the new total arc length of K, which we abbreviate L. By Lemma 2.2, the curvature of K everywhere is $\ge \frac{1}{R(K)} = 1$. For points x, y on K with $\operatorname{arc}(x,y) \le \pi$, let s, t be points on the circle, C, of radius $1 = R(K)$, for which $\operatorname{arc}(s,t) = \operatorname{arc}(x,y)$. By Schur's Theorem (Lemma 2.1), we have $|x-y| \ge |s-t|$, so

$$\frac{1}{|x-y|^2} - \frac{1}{\operatorname{arc}(x,y)^2} \le \frac{1}{|s-t|^2} - \frac{1}{\operatorname{arc}(x,y)^2} = \frac{1}{|s-t|^2} - \frac{1}{\operatorname{arc}(s,t)^2} . \tag{2}$$

For a fixed x on K and a fixed s on C, (2) and Lemma 2.4 gives us that

$$\begin{aligned} \int_{\operatorname{arc}(x,y)\le \pi R(K)} \frac{1}{|x-y|^2} - \frac{1}{\operatorname{arc}(x,y)^2} &\le \int_{\operatorname{arc}(s,t)\le \pi R(K)} \frac{1}{|s-t|^2} - \frac{1}{\operatorname{arc}(s,t)^2} \\ &= \frac{2}{\pi\, R(K)} \\ &= \frac{2}{\pi} . \end{aligned}$$

Thus,

$$\int_{x\in K}\int_{\operatorname{arc}(x,y)\le \pi R(K)} \frac{1}{|x-y|^2} - \frac{1}{\operatorname{arc}(x,y)^2} \le \int_{x\in K} \frac{2}{\pi} = \frac{2}{\pi} L .$$

□

3. Thick knots have bounded energy

In this section, we prove that the Möbius energy of a knot is bounded by the the ropelength. Our goal is partly the theorem itself and partly the paradigm: any "energy" defined in terms of inverse-square distances should have an analogous bound, with the proof following this model.

Theorem 3.1. *If K is a smooth knot in $\mathbb{R}^3$ then*

$$\mathcal{E}_{O4}(K) < 4.57\,\mathcal{E}_L(K)^{\frac{4}{3}}, \tag{3}$$

Remark. The theorem is stated this way to emphasize the (4/3)-power relationship. The bound we obtain is more complicated, but dominated by the (4/3)-power and less than 4.57 times that. If the knot is very long, it requires less of the (4/3)-power to dominate the lower order terms, so the coefficient 4.57 can be reduced towards an asymptotic limit of $2\sqrt[3]{6} < 3.64$ for very long knots.

Theorem 3.2. *If K is a smooth knot in $\mathbb{R}^3$ then*

$$\mathcal{E}_{O4}(K) \leq \frac{1}{4}\mathcal{E}_L(K)^2 - \frac{\pi}{2}\mathcal{E}_L(K) + 4\,. \tag{4}$$

Remark. For short knots, the quadratic bound is better than the (4/3)-power bound. Specifically, for $E_L(K) \lessapprox 87$, (4) is less than (3).

Proof of Theorems 3.1 and 3.2. We will obtain the quadratic bound en route to the (4/3)-power bound.

We follow the same plan as used in [5, 6]. Since $\mathcal{E}_{O4}$ and $\mathcal{E}_L$ are both invariant under change of scale, we begin by rescaling K to have thickness $R(K) = 1$, so that $\mathcal{E}_L(K)$ is just the total arc length of K, which we abbreviate L.

The energy $\mathcal{E}_{O4}(K)$ is defined as a double-integral over $K \times K$. We bound separately the integral over the portion of $K \times K$ consisting of pairs (x, y) with $\operatorname{arc}(x, y) \leq \pi R(K) = \pi$, and the integral over the rest of $K \times K$.

Let

$$\mathcal{E}_{\text{prox}} = \int_{x\in K}\int_{\operatorname{arc}(x,y)\leq\pi} \frac{1}{|x-y|^2} - \frac{1}{\operatorname{arc}(x,y)^2}\;,$$

$$\mathcal{E}_{\text{dist}} = \int_{x\in K}\int_{\operatorname{arc}(x,y)\geq\pi} \frac{1}{|x-y|^2}\;,$$

and

$$\mathcal{E}_{\text{reg}} = \int_{x\in K}\int_{\operatorname{arc}(x,y)\geq\pi} \frac{1}{\operatorname{arc}(x,y)^2}\;.$$

So we have

$$\mathcal{E}_{O4} = \mathcal{E}_{\text{prox}} + \mathcal{E}_{\text{dist}} - \mathcal{E}_{\text{reg}}\;.$$

By Lemma 2.5,

$$\mathcal{E}_{\text{prox}} \leq \frac{2}{\pi}\,L\,. \tag{5}$$

Also,

$$\mathcal{E}_{\text{reg}} = 2\int_{\pi}^{\frac{L}{2}} \frac{1}{t^2}\,\mathrm{d}t = \frac{2}{\pi}\,L - 4\,. \tag{6}$$

We next bound $\mathcal{E}_{\text{dist}}$. We shall bound the inner integral and then multiply by the length of K to bound the energy. The inner integral, for each x, is

$$I^x_{\text{dist}} = \int_{\text{arc}(x,y)\geq\pi} \frac{1}{|x-y|^2} \ .$$

Here first is the easy quadratic bound.

By Lemma 2.3, and our rescaling to $R(K) = 1$, we have for each point $y \in K$,

$$\text{arc}(x,y) \geq \pi \Rightarrow |y-x| \geq 2 \ .$$

Thus,

$$I^x_{\text{dist}} \leq \frac{1}{2^2}(L-2\pi) \ .$$

Multiplying by L, we get

$$\mathcal{E}_{\text{dist}} \leq \frac{1}{4}L^2 - \frac{\pi}{2}L \ . \tag{7}$$

Combine (7) with (5) and (6) to complete the quadratic bound:

$$\mathcal{E}_{O4}(K) \leq \frac{1}{4}L^2 - \frac{\pi}{2}L + 4 \ .$$

We now develop the (4/3)-power bound. This bound is approximately half of what could be obtained by combining Lemma 2.5 above with the estimates in [5, 6].

The first observation is that if $|x-y| \geq \rho$, then the integrand $\frac{1}{|x-y|^2} \leq \frac{1}{\rho^2}$. In obtaining the quadratic bound, we stopped here, allowing the idea that with respect to each point $x \in K$, the whole knot (except for the arc around x of length π in each direction) lies just at distance 2 from x. But *the knot is thick*: a piece w of K of length $\ell(w)$ carries along with it a solid tube W of volume $\pi\ell(w)$ (we still are assuming $R(K) = 1$). Furthermore, such a tube W cannot intersect any other part of K nor any of the rest of the tube around K. This restricts how much length of K can be located at any given distance from x.

Fix x on K. Let Y_{dist} denote the set on which we integrate to compute I^x_{dist}, that is $\{y \in K : \text{arc}(x,y) \geq \pi\}$. The arc length of Y_{dist} is just $L - 2\pi$. Let $S(\rho)$ denote the sphere centered at x with radius ρ and $S[\rho,\sigma]$ the spherical shell between radii ρ and σ. Let $Y(\rho)$ denote $Y_{\text{dist}} \cap S(\rho)$ and $Y[\rho,\sigma] = Y_{\text{dist}} \cap S[\rho,\sigma]$, and let $\ell(\rho)$, $\ell[\rho,\sigma]$ denote the corresponding lengths of K lying in $S(\rho)$, $S[\rho,\sigma]$. Note by Lemma 2.3, $Y(\rho) = \emptyset$ for $\rho < 2$.

The volume of the solid tube associated to $Y(2)$ is $\pi\ell(2)$; this tube is contained in $S[1,3]$, so the tube has volume $\pi\ell(2) \leq \frac{4}{3}\pi(3^3 - 1^3)$, and we see that $\ell(2) \leq \frac{104}{3}$. If the total length of K is less than $2\pi + \frac{104}{3} \approx 41$, then our analysis stops here and we have just the quadratic bound from Theorem 3.2. Assuming K has total length $> 2\pi + \frac{104}{3}$, we continue. (As a curiosity, we note that any knot other than a trefoil or an unknot apparently has length bigger than 41, see e.g. [31, p. 6].)

Assume the knot is in an idealized "densest possible" packing around x, so in particular $\ell(2) = \frac{104}{3}$, and the contribution of $Y(2)$ to $\mathcal{E}_{\text{dist}}$ is $\left(\frac{104}{3}\right)\left(\frac{1}{2^2}\right)$. After this initial large hypothetical amount of length located at distance 2 from x, the rest of our analysis deals with density of length at each distance, rather than a discrete amount as is done in [5, 6]. The function $\ell(\rho)$ for $\rho > 2$ will be controlled by its derivative.

Consider how much length of Y can be contained in a thin shell $S(2, 2+\Delta\rho]$. The length $\ell(2, 2+\Delta\rho]$ gives rise to a volume contained in $S(1, 2+\Delta\rho+1]$. But the volume of shell $S[1,3]$ already is assumed to be covered by the tube around $Y(2)$.

Thus only the volume of $S(3, 3 + \Delta\rho]$ is available for the volume of the additional tube. This gives

$$\pi\ell(2, 2 + \Delta\rho] \leq \frac{4}{3}\pi((3 + \Delta\rho)^3 - 3^3) \ .$$

We apply the same reasoning to any shell $(\rho, \rho + \Delta\rho]$. Assuming always that the knot is packed around x in the hypothetical densest way, we have that for $\rho > 2$, the distribution of length relative to ρ is given by

$$\mathrm{d}\ell = 4(\rho + 1)^2 \mathrm{d}\rho \ .$$

Let P denote the radius needed to engulf all of Y_{dist}. Then the total length of Y_{dist} is given by

$$\ell(Y_{\mathrm{dist}}) = \frac{104}{3} + \int_{\rho=2}^{P} 4(\rho + 1)^2 \mathrm{d}\rho \ . \tag{8}$$

and the (hypothetical highest) energy integrand by

$$\text{maximum } I^x_{\mathrm{dist}} = \frac{104}{12} + \int_{\rho=2}^{P} 4\frac{(\rho + 1)^2}{\rho^2} \mathrm{d}\rho \ . \tag{9}$$

We can use (8) to find P in terms of L and plug this into (9).
We have

$$L - 2\pi = \frac{104}{3} + \int_{\rho=2}^{P} 4(\rho + 1)^2 \mathrm{d}\rho,$$

which gives

$$P = \left(\frac{3}{4}L - \left(\frac{3}{2}\pi - 1\right)\right)^{1/3} - 1; . \tag{10}$$

Meanwhile, from (9) we have

$$\text{maximum } I^x_{\mathrm{dist}} = 4P + 8\ln P - 4\frac{1}{P} + \left(\frac{8}{3} - 8\ln(2)\right) \ . \tag{11}$$

Multiply (11) by L to bound E_{dist} and combine with (5) and (6) to obtain.

$$\mathcal{E}_{O4}(K) \leq L\left(4P + 8\ln P - 4\frac{1}{P} + \left(\frac{8}{3} - 8\ln(2)\right)\right) + 4 \ . \tag{12}$$

It is evident from (10) that P is on the order of $L^{1/3}$. So from (12), our bound for $\mathcal{E}_{O4}$ is on the order of $L^{4/3}$.

To get a simple bound of the form $cL^{4/3}$ we can estimate each of the terms above, or more easily (and yielding a smaller coefficient c) we can use an algebra-graphing tool to substitute (10) into (12) and measure the ratio of the result to $L^{4/3}$. The ratio increases to approximately 4.563 as L increases to around 1115, and then decreases towards the asymptotic limit of $2\sqrt[3]{6} < 3.64$. Recall from the derivation that the bound in (12) only applies if $L \geq 2\pi + \frac{104}{3} \approx 41$. For $2\pi \leq L \leq 2\pi + \frac{104}{3}$, the quadratic bound (4) applies, and this is also less than $4.57\, L^{\frac{4}{3}}$. Thus we can say for all L,

$$\mathcal{E}_{O4}(K) < 4.57\, \mathcal{E}_L(K)^{4/3} \ .$$

The coefficient can be reduced below 4 if the length is enormous (around 376,000). □

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