Möbius Energy of Thick Knots

Eric J. Rawdon

Department of Mathematics and Computer Science,
Duquesne University,
Pittsburgh, PA 15282, USA
Email: rawdon@mathcs.duq.edu

Jonathan Simon

Department of Mathematics,
University of Iowa,
Iowa City, IA 52242, USA
Email: jsimon@math.uiowa.edu

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.

Key words: Möbius energy, knot energy, ropelength, thickness, physical knots

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 [1] and studied extensively in [2,3]. We follow an overall approach suggested by G. Buck for showing that any inverse-square knot energy should be bounded by the $4/3$ power of the ropelength.

1 Corresponding author. (J. Simon) Tel: 319-335-0768, fax: 319-335-0627.
2 Research supported by Chatham College, the University of Iowa, and NSF grant #DMS0074315
3 Research supported by NSF grant #DMS9706789
We and other researchers have defined a number of different energy functions for (smooth or polygonal) knots [1–16] based on the idea of inverse-square repelling energy (so these would correspond to inverse-cube “forces”). (See also [17] for a different approach). Roughly, these energies are defined in terms of integrals over the curve $K$

$$
\int_{x \in K} \int_{y \in K} \frac{\Box}{|x - y|^2} \, dx \, dy .
$$

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). The same purpose is accomplished by defining energies as integrals of differences [1,2],

$$
\int_{x \in K} \int_{y \in K} \frac{1}{|x - y|^2} - \frac{1}{|s - t|^2} \, dx \, dy .
$$

Here $s, t$ lie on a line or circle used for a unit-speed parameterization of the curve $K$ with $s \mapsto x$ and $t \mapsto y$. The energy we study in this paper can be defined either way [1–3] 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 $E_L(K)$ [4,6,7]: this is the ratio of the arclength of the curve to the maximum radius of a uniform non-self-intersecting tube along the curve [18], i.e. the ratio of length to radius of the rope (see Section 2 for precise definitions). Variations on thickness are developed in [17,19–25].

We showed in [7] that the normal energy $E_N(K)$, which discounts tangential self-repelling, and the symmetric energy $E_S(K)$, which models self-radiation of a filament [26], 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 the form shown below in (1). Here $\text{acn}(K)$ 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 $\text{cr}(K)$, which is the minimum over all regular projections, and $\text{cr}[K]$, which considers all $K$ in a given knot type.

$$
4\pi \text{cr}[K] \leq 4\pi \text{cr}(K) < 4\pi \text{acn}(K) \leq E_S(K) \leq E_N(K) \leq c E_L(K)^{4/3} \quad (1)
$$

The coefficient $c$ varies with different proofs; the exponent $4/3$ is sharp. A related idea is the writhe of a knot, $\text{wr}(K)$, which is the average over all spatial directions of the signed crossing numbers. Since $\text{wr}(K) \leq \text{acn}(K)$, we
get the same bound on $4\pi \text{wr}(K)$. But using a different analysis of writhe, in terms of vector fields flowing in tubes around the knot, it is shown in [27] that 
\[ \text{wr}(K) \leq \frac{1}{4} E_L(K)^{4/3}, \] which is a lower coefficient than we have for acn$(K)$. The coefficient, approximately 5, that we obtain in this paper is lower than in [7], because we do a more subtle analysis. While coefficients might be improved, the exponent $4/3$ in inequality (1) is sharp, because of examples [28,29] where crossing number grows like the $4/3$ power of ropelength. Similarly, because Möbius energy also bounds crossing number [2], the same examples show that the exponent $4/3$ in Theorem 8 of this paper is sharp.

Our main result is that the Möbius energy is bounded by the $4/3$ power of the ropelength (with coefficient $\approx 5$). 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,
\[
E_{O4}(K) = \int_{x \in K} \int_{y \in K} \frac{1}{|x - y|^2} - \frac{1}{\text{arc}(x,y)^2},
\]
where \(\text{arc}(x,y)\) denotes the minimum arclength along the curve $K$ between $x$ and $y$.

We 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 [30], 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 [31], with the slight adjustment that we do not need to consider general planar convex curves as the reference curves, just circles.
Lemma 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 $x, y \in K$ and $s, t \in C$ be any points such that $\text{arc}(x, y) = \text{arc}(s, t) \leq \pi r$. Then the chord distances satisfy

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

PROOF. See Schur’s Theorem in [31]. $\square$

We also will use results on thickness of knots developed in [18]. 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 [18] assumed that as well; but in fact the definition and results there can be modified to deal with $C^{1,1}$ curves (this has been noted by R. Litherland, O. Durumeric, and [22,32]).

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

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

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 MinRad($K$) denote the minimum radius of curvature of $K$. We then have from [18]:

Lemma 2 The thickness of a smooth knot is bounded by the minimum radius of curvature and half the critical self-distance. In fact,

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

4
The next lemma is a consequence of Lemmas 1 and 2.

**Lemma 3** Suppose $K$ is a smooth knot of thickness $R(K) = r$. For any $x, y \in K$, such that $\text{arc}(x, y) \geq \pi r$, we must have $|x - y| \geq 2r$.

**PROOF.** Fix $x$ and consider first the two points $y \in K$ for which $\text{arc}(x, y) = \pi r$. Since, by Lemma 2, the curvature of $K$ is everywhere $\leq 1/r$, and $\text{arc}(x, y) = \pi r$, 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 $|x - y|$ is at least as large as for the corresponding points on a circle of radius $r$, i.e. $|x - y| \geq 2r$.

Now consider the arc $Y$ of $K$ consisting of those points $y$ with $\text{arc}(x, y) \geq \pi r$. Let $y_0$ be a point of $Y$ that minimizes distance to $x$. If $y_0$ is closer to $x$ than $2r$ then, from the preceding paragraph, it cannot be an endpoint of $Y$; thus it would have to be a critical point for the function $|x - y|$. But by Lemma 2, any such critical pair $(x, y)$ has distance $\geq 2r$. $\square$

In the next two lemmas, we obtain the linear bound for the energy contribution of proximal pairs, that is, points for which $\text{arc}(x, y) \leq \pi R(K)$.

**Lemma 4** For a fixed point $s$ on a circle $C$ of radius $R$,

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

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

$$
\int_{t \in C} \frac{1}{|s - t|^2} - \frac{1}{\text{arc}(s, t)^2} = 2 \int_0^{\pi R} \frac{1}{R^2(2 - 2\cos(t/R))} - \frac{1}{t^2} \, dt = \frac{2}{\pi R}.
$$

$\square$

**Lemma 5** If $K$ is a smooth knot in $\mathbb{R}^3$, then

$$
\int_{x \in K} \int_{\text{arc}(x, y) \leq \pi R(K)} \frac{1}{|x - y|^2} - \frac{1}{\text{arc}(x, y)^2} \leq \frac{2}{\pi} E_L(K).
$$
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 arclength of \( K \), which we abbreviate \( L \). By Lemma 2, the curvature of \( K \) everywhere is \( \leq \frac{1}{R(K)} = 1 \). For points \( x, y \) on \( K \) with \( \text{arc}(x, y) \leq \pi \), let \( s, t \) be points on the circle, \( C \), of radius \( 1 = R(K) \), for which \( \text{arc}(s, t) = \text{arc}(x, y) \). By Schur’s Theorem (Lemma 1), we have \( |x - y| \geq |s - t| \), so
\[
\frac{1}{|x - y|^2} - \frac{1}{\text{arc}(x, y)^2} \leq \frac{1}{|s - t|^2} - \frac{1}{\text{arc}(s, t)^2}.
\] (2)

For a fixed \( x \) on \( K \) and a fixed \( s \) on \( C \), (2) and Lemma 4 give us
\[
\int_{\text{arc}(x, y) \leq \pi} \frac{1}{|x - y|^2} - \frac{1}{\text{arc}(x, y)^2} \leq \int_{\text{arc}(s, t) \leq \pi} \frac{1}{|s - t|^2} - \frac{1}{\text{arc}(s, t)^2} \frac{2}{\pi}.
\]
Thus,
\[
\int_{x \in K} \int_{\text{arc}(x, y) \leq \pi} \frac{1}{|x - y|^2} - \frac{1}{\text{arc}(x, y)^2} \leq \int_{x \in K} \frac{2}{\pi} = \frac{2}{\pi} L.
\]

Finally, we need a lemma about measurable subsets of \( K \). When we talk about “measure”, we mean the one-dimensional Lebesgue measure on \( K \) that is just arclength when applied to intervals. We actually use only Borel sets.

We want to define subsets of \( K \) of specified measure that are closest, in terms of spatial distance, to a given point \( x \in K \). First we need a preliminary lemma about decomposing measurable sets.

**Lemma 6** Suppose \( W \) is a measurable subset of \( K \) and \( m_1, m_2 > 0 \) are numbers with \( m_1 + m_2 = \mu(W) \). Then we can partition \( W \) into measurable sets \( W_1, W_2 \), with \( \mu(W_j) = m_j \), \( j = 1, 2 \).

**PROOF.** Orient \( K \), fix a point \( z_0 \in K \), and consider the intersections of \( W \) with intervals \( I_z = [z_0, z] \) as \( z \) ranges over \( K \). Since the measure of a subset of an interval is bounded by the length of the interval, the function \( \mu(W \cap I_z) \) is continuous in \( z \). The measure \( \mu(W \cap I_z) \) is arbitrarily small when \( z \approx z_0 \), is monotonically nondecreasing as \( z \) moves around \( K \), and eventually exceeds \( m_1 \) as \( z \) approaches \( z_0 \) from the “back”. Thus there must be a value of \( z \) for which \( \mu(W \cap I_z) = m_1 \). \( \square \)

In the next lemma, and the proof of the main theorem, we use the following notation. For \( x \in K \) fixed, \( a \leq b \), let \( S(a, b], S[a, b], S[a] \) denote spherical shells of radius from \( a \) to \( b \), and the sphere of radius \( a \), all centered at \( x \).
Lemma 7 Suppose $K$ is a smooth knot with $R(K) = 1$. Fix $x \in K$ and let $Y$ be the subset of $K$ consisting of all points $y$ with $\text{arc}(x, y) \geq \pi$. Let $\nu_1, \nu_2, \ldots, \nu_m > 0$ be numbers such that $\nu_1 + \nu_2 + \cdots + \nu_m = L - 2\pi$ (i.e. $\mu(Y)$). Then there exists a sequence of radii

$$2 \leq \rho_1 \leq \rho_2 \leq \cdots \leq \rho_m$$

and a partition of $Y$ into measurable sets $W_1, W_2, \ldots, W_m$ such that

(a) for each $j$, $\mu(W_j) = \nu_j$, and

(b) $W_1 \subseteq Y \cap S[2, \rho_1]$ and for each $j > 1$, $W_j \subseteq Y \cap S[\rho_{j-1}, \rho_j]$.

PROOF. The proof is nearly straightforward. There is a slight complication because the knot $K$ might intersect some spheres $S[\rho]$ in sets of positive length.

Since $R(K) = 1$ and $y \in Y$ has $\text{arc}(x, y) \geq \pi$, by Lemma 3, $|x - y| \geq 2$, so $Y \subseteq S[2, L/2]$. We define the radius $\rho_m \leq L/2$ to be the smallest radius $\rho$ for which $Y$ is contained in $S[2, \rho]$.

We construct radii $\rho_j$ and sets $W_j$ inductively, with a slight variation at the final step. For the degenerate case $m = 1$, of course, $W_1 = Y$ and $\rho_1 = \rho_m$ is as above.

We now begin the induction. Suppose first that $\mu(Y \cap S[2]) \geq \nu_1$. By Lemma 6, we can partition $Y \cap S[2]$ into sets $W_1 \cup V$, where $\mu(W_1) = \nu_1$; let $\rho_1 = 2$.

Now suppose $\mu(Y \cap S[2]) < \nu_1$. Let

$$R_{\text{low}} = \{\rho : \mu(Y \cap S[2, \rho]) < \nu_1\}$$

and $r_1 = \sup(R_{\text{low}})$. Similarly, let

$$R_{\text{high}} = \{\rho : \mu(Y \cap S[2, \rho]) \geq \nu_1\}$$

and let $r'_1 = \inf(R_{\text{high}})$. Here $R_{\text{low}} \neq \emptyset$ because $\mu(Y \cap S[2]) < \nu_1$, so $2 \in R_{\text{low}}$, and $R_{\text{high}} \neq \emptyset$ because $\rho_m \in R_{\text{high}}$.

We claim $r_1 = r'_1$. Each element of $R_{\text{low}}$ is $< \rho$ each element of $R_{\text{high}}$. Thus, $r_1 \leq r'_1$. If the inequality is strict, then for each $\rho \in (r_1, r'_1)$, $\mu(Y \cap S[2, \rho]) \geq \nu_1$, which contradicts $\rho < r_1$.

Now define $\rho_1 = r_1 = r'_1$. The set $Y \cap S[2, r_1]$ is a monotone union of sets, each with measure $< \nu_1$. Thus, $\mu(Y \cap S[2, \rho_1]) \leq \nu_1$. On the other hand, $Y \cap S(r'_1, \infty)$ is a monotone union of sets, each with measure $< \mu(Y) - \nu_1$. Thus, $\mu(Y \cap S(\rho_1, \infty)) \leq \mu(Y) - \nu_1$, so $\mu(Y \cap S[2, \rho_1]) \geq \nu_1$. 


Using Lemma 6, we extract a subset of \( Y \cap S[\rho_1] \) whose measure is whatever \( \mu(Y \cap S[2, \rho_1]) \) may lack to make \( \nu_1 \), and let \( W_1 \) be the union of this set with \( Y \cap S[2, \rho_1] \).

To continue the induction, let \( Y_1 = Y - W_1 \). Note \( Y_1 \subseteq Y \cap S[\rho_1, \infty). \)

Suppose \( \rho_1, \ldots, \rho_{j-1} \) and \( W_1, \ldots, W_{j-1} \) have been chosen as required in the statement of the lemma and the set \( Y_{j-1} = Y - (W_1 \cup \cdots \cup W_{j-1}) \subseteq S[\rho_{j-1}, \infty) \).

Note that since \( W_1, \ldots, W_{j-1} \subseteq Y \cap S[2, \rho_{j-1}], Y \cap S(\rho_{j-1}, \infty) \subseteq Y_{j-1} \). So for any \( \rho, \rho' \) with \( \rho_{j-1} < \rho < \rho' \), we have \( Y_{j-1} \cap S[\rho, \rho'] = Y \cap S[\rho, \rho'] \).

Now proceed much like the initial case. If \( j = m \), we finish by taking \( W_j = Y_{j-1} \) and \( \rho_m \) as above.

There are two cases: If \( \mu(Y_{j-1} \cap S[\rho_{j-1}]) \geq \nu_j \), then let \( W_j \) be a subset of \( Y_{j-1} \cap S[\rho_{j-1}] \) of measure \( \nu_j, \rho_j = \rho_{j-1} \), and \( Y_j = Y_{j-1} - W_j \).

Suppose now \( \mu(Y_{j-1} \cap S[\rho_{j-1}]) < \nu_j \). Define
\[
R_{low} = \{ \rho : \mu(Y_{j-1} \cap S[\rho_{j-1}, \rho]) < \nu_j \}
\]
and \( r_j = \sup(R_{low}) \). Similarly, let
\[
R_{high} = \{ \rho : \mu(Y_{j-1} \cap S[\rho_{j-1}, \rho]) \geq \nu_j \}
\]
and let \( r'_j = \inf(R_{high}) \). Here \( R_{low} \neq \emptyset \) because \( \rho_{j-1} \in R_{low} \) and \( R_{high} \neq \emptyset \) because \( \rho_m \in R_{high} \).

As in the initial case, we have \( r_j = r'_j \), and we define \( \rho_j = r_j = r'_j \). Also, \( \mu(Y_{j-1} \cap S[\rho_{j-1}, \rho_j]) \leq \nu_j \) and \( \mu(Y_{j-1} \cap S[\rho_{j-1}, \rho_j]) \geq \nu_j \).

Let \( W_j \) be the union of \( Y_{j-1} \cap S[\rho_{j-1}, \rho_j] \) with a subset of \( Y_{j-1} \cap S[\rho_j] \) of however much additional measure is needed to reach \( \nu_j \). Finally, let \( Y_j = Y_{j-1} - W_j \). Note then \( Y_j \subseteq Y \cap S[\rho_j, \infty) \).  

3 Thick knots have bounded energy

In this section, we prove that the Möbius energy of a knot is bounded by 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 8** If \( K \) is a smooth knot in \( \mathbb{R}^3 \) then
\[
E_{O4}(K) < 4.57 E_L(K)^{4/3}.
\]
Theorem 9 If $K$ is a smooth knot in $\mathbb{R}^3$ then

$$E_{O4}(K) \leq \frac{1}{4} E_L(K)^2. \quad (4)$$

Remark For short knots, the quadratic bound is better than the $4/3$ power bound. Comparing (3) to (4), we see that one needs ropelengths over 79 before the advantage of the lower exponent is evident. If one uses the actual bound (12) we obtain in the proof, which is a complicated expression dominated by a $4/3$ power term, then that bound is lower than (4) for ropelengths $> 41$. Computer simulations suggest [33,34] the only knots that can be realized with a ropelength $\leq 41$ are the unknot and the trefoil.

PROOF. [of Theorems 8 and 9] We will obtain the quadratic bound en route to the $4/3$ power bound.

We follow an overall plan similar to [6,7], but introduce a limit process in the main argument. Since $E_{O4}$ and $E_L$ are both invariant under change of scale, we begin by rescaling $K$ to have thickness $R(K) = 1$, so that $E_L(K)$ is just the total arclength of $K$, which we abbreviate $L$.

The energy $E_{O4}(K)$ 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 $\text{arc}(x, y) \leq \pi R(K) = \pi$, and the integral over the rest of $K \times K$.

Let

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

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

and

$$E_{\text{reg}} = \int_{x \in K} \int_{\text{arc}(x,y) \geq \pi} \frac{1}{\text{arc}(x,y)^2}.$$

So we have

$$E_{O4} = E_{\text{prox}} + E_{\text{dist}} - E_{\text{reg}}.$$

By Lemma 5,

$$E_{\text{prox}} \leq 2 \pi L.$$
Also, by symmetry of the circle,

\[ E_{\text{reg}} = \int_{x \in K} \left( 2 \int_{t^2}^{L} \frac{1}{t^2} \, dt \right) \, dx = L \left( 2 \int_{\pi}^{L} \frac{1}{t^2} \, dt \right) = \frac{2}{\pi} L - 4 , \]

so

\[ E_{04} \leq E_{\text{dist}} + 4 . \tag{5} \]

We now bound \( E_{\text{dist}} \). 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

\[ I_{\text{dist}}^x = \int_{\text{arc}(x,y) \geq \pi} \frac{1}{|x - y|^2} . \]

Here first is the quadratic bound.

By Lemma 3, and our rescaling to \( R(K) = 1 \), we have for each point \( y \in K \),

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

Thus,

\[ I_{\text{dist}}^x \leq \frac{1}{2^2} (L - 2\pi) . \]

Multiplying by \( L \), we get

\[ E_{\text{dist}} \leq \frac{1}{4} L^2 - \frac{\pi}{2} L . \tag{6} \]

Combine (6) with (5) to complete a quadratic polynomial bound:

\[ E_{04}(K) \leq \frac{1}{4} L^2 - \frac{\pi}{2} L + 4 . \tag{7} \]

Because \( K \) is a smooth closed curve with maximum curvature \( \leq 1 \) (by Lemma 2 and the fact that we have normalized \( K \) to have thickness radius = 1), the total curvature of \( K \) is at most \( L \). But by Fenchel’s theorem, the total curvature of a closed curve is at least \( 2\pi \). Thus \( L \geq 2\pi > 8/\pi \), so the linear part of (7) is negative, and we have

\[ E_{04}(K) \leq \frac{1}{4} L^2 . \tag{8} \]

We now develop the \( 4/3 \) power bound. If \( L < \frac{104}{3} + 2\pi \approx 41 \), i.e. \( L - 2\pi < \frac{4}{3} (3^3 - 1^3) \), then our proof stops here. The quadratic bound (4) is valid and certainly (4) < (3), so (3) is valid as well. We continue under the assumption that \( E_L(K) \geq \frac{104}{3} + 2\pi \).
The first observation is that for any \( \rho > 0 \), 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 \( \pi \) 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 packed within any given distance from \( x \).

Fix \( x \) on \( K \). Let \( Y_{\text{dist}} \) denote the set on which we integrate to compute \( I^x_{\text{dist}} \), that is \( Y_{\text{dist}} = \{ y \in K : \operatorname{arc}(x, y) \geq \pi \} \). The arclength of \( Y_{\text{dist}} \) is just \( L - 2\pi \).

Let \( S(\rho, \sigma] \) denote the half-open spherical shell centered at \( x \) with radius from \( \rho \) to \( \sigma \). Let \( Y(\rho, \sigma] = Y_{\text{dist}} \cap S(\rho, \sigma] \), a measurable set, and let \( \ell(\rho, \sigma] \) denote its 1-dimensional measure, i.e. the measure of the length of \( K \) lying in \( S(\rho, \sigma] \). Let \( T(\rho, \sigma] \) be the solid tube with axis \( Y(\rho, \sigma] \), that is, the portion of the unit radius tube about \( K \) consisting of disks centered at points \( y \in Y(\rho, \sigma] \). The 3-dimensional measure, i.e. volume, of \( T(\rho, \sigma] \) is \( \pi \ell(\rho, \sigma] \). Define \( S[\rho, \sigma], Y[\rho, \sigma], \ell[\rho, \sigma], T[\rho, \sigma] \) analogously. Note that \( Y_{\text{dist}} \subset S[2, L/2] \). The subset of \( Y_{\text{dist}} \) lying at distance exactly 2 from \( x \) plays a special role in the analysis, so we also define \( S[2], Y[2], \ell[2], T[2] \).

Let \( P = \left( \frac{3}{4}L - \frac{3\pi}{2} + 1 \right)^{1/3} - 1 \). The constant \( P \) is the radius required so that a spherical shell from \( r = 1 \) to \( r = P + 1 \) has the same volume as a tube of radius 1 about a set of length \( L - 2\pi \).

We bound the total amount of length that can lie in each spherical shell by a function \( \ell^* \) (see (9) below). Let \( \ell^*[2] = \frac{4}{3}(3^3 - 1^3) = \frac{104}{3} \). For \( 2 \leq a < b \), let

\[
\ell^*(a, b) = \frac{4}{3} \left( (\min\{b, P\} + 1)^3 - (\min\{a, P\} + 1)^3 \right).
\]

In particular, when \( 2 \leq a < b \leq P \), this simplifies to

\[
\ell^*(a, b) = \frac{4}{3} \left( (b + 1)^3 - (a + 1)^3 \right).
\]

Let

\[
\ell^*[2, b] = \ell^*[2] + \ell^*(2, b).
\]

For \( b \leq P \), \( \ell^*[2, b] = \frac{4}{3} ((b + 1)^3 - 1^3) \). For \( b > P \), notice that \( \ell^*(2, b) = \ell^*(2, P] \) so \( \ell^*[2, b] = \ell^*[2, P] = L - 2\pi \).

We now show that

\[
\ell[2, r] \leq \ell^*[2, r] \text{ for all } 2 \leq r.
\] (9)
The tube $T[2, r]$ has volume $\pi \ell[2, r]$. But $T[2, r]$ lies entirely within $S[1, r + 1]$, whose volume is $\frac{4}{3} \pi ((r + 1)^3 - 1^3)$. Thus, when $2 \leq r \leq P$,

$$\pi \ell[2, r] \leq \frac{4}{3} \pi ((r + 1)^3 - 1^3) = \pi \ell^*[2, r].$$

If $r > P$, then $\ell^*[2, r] = \ell^*[2, P] = L - 2\pi \geq \ell[2, r]$. Thus, we have (9).

We next partition $Y_{\text{dist}}$ into sets $W_j$ whose distance to $x$ is controlled, and express $I^*_{\text{dist}}$ as the sum of the contributions from these sets.

Let $n \in \mathbb{N}$ and $\delta = \frac{P-2}{n}$. Then,

$$\ell^*[2, P] = \ell^*[2] + \ell^*(2, 2 + \delta) + \ell^*(2 + \delta, 2 + 2\delta) + \cdots + \ell^*(P - \delta, P)$$

We define a sequence of sets $\{W_j\}$ using Lemma 7 as follows. Let $\nu_0 = \ell^*[2]$ and $\nu_j = \ell^*(2 + (j-1)\delta, 2 + j\delta)$ for $1 \leq j \leq n$. Note that $\nu_n = \ell^*(2 + (n-1)\delta, 2 + n\delta) = \ell^*(P - \delta, P)$. Since $\nu_0 + \nu_1 + \cdots + \nu_n = L - 2\pi = \mu(Y_{\text{dist}})$, by Lemma 7, there exists a sequence $2 \leq \rho_0 \leq \rho_1 \leq \cdots \leq \rho_n$ and a partition of $Y_{\text{dist}}$ into measurable sets $W_0, \ldots, W_n$ such that: for $1 \leq j \leq n$, we have $\mu(W_j) = \nu_j$ and $W_j \subseteq Y_{\text{dist}} \cap S[\rho_{j-1}, \rho_j]$; for $j = 0$, we have $\mu(W_0) = \nu_0$ and $W_0 \subseteq Y_{\text{dist}} \cap S[2, \rho_0]$.

We want to know how far each $W_j$ is from $x$, so we next bound the radii $\rho_j$ (from below) in terms of $j$ and $\delta$. If $y \in W_0$, then $|x - y| \geq 2$ by Lemma 3. For $1 \leq j \leq n$, we claim $|x - y| > 2 + (j - 1)\delta$ for all $y \in W_j$, except perhaps a set of measure 0. Suppose $M$ is a non-zero measure subset of $W_1$ such that for all $y \in M$, we have $|x - y| \leq 2$. Then $W_0 \cup M \subseteq Y[2]$ and $\ell[2] \geq \mu(W_0) + \mu(M) > c \mu(W_0) = \ell^*[2]$, which contradicts (9). We continue using induction. Suppose for all $0 \leq k < j \leq n$, we have $|x - y| > 2 + (k - 1)\delta$.

Suppose $M$ is a non-zero measure subset of $W_j$ such that for all $y \in M$, we have $|x - y| \leq 2 + (j - 1)\delta$. Then $W_0 \cup W_1 \cup \cdots \cup W_{j-1} \cup M \subseteq Y[2, 2 + (j-1)\delta]$. Thus,

$$\pi \ell[2, 2 + (j-1)\delta] \geq \mu(W_0) + \mu(W_1) + \cdots + \mu(W_{j-1}) + \mu(M)$$

$$> \mu(W_0) + \mu(W_1) + \cdots + \mu(W_{j-1})$$

$$= \pi \left( \ell^*[2] + \ell^*(2, 2 + \delta) + \cdots + \ell^*(2 + (j-2)\delta, 2 + (j-1)\delta) \right)$$

$$= \pi \ell^*[2, 2 + (j-1)\delta],$$

which contradicts (9).
Since $Y_{\text{dist}} = W_0 \cup W_1 \cup \cdots \cup W_n$,

$$I_{\text{dist}}^x = \int_{y \in W_0} \frac{1}{|x-y|^2} + \int_{y \in W_1} \frac{1}{|x-y|^2} + \cdots + \int_{y \in W_n} \frac{1}{|x-y|^2} < \frac{1}{2^2} \ell^*(2) + \frac{1}{2^2} \ell^*(2, 2 + \delta) + \cdots + \frac{1}{(P - \delta)^2} \ell^*(P - \delta, P). \quad (10)$$

The first term of (10) is $\frac{104}{12}$. The rest is

$$\sum_{j=1}^n \frac{1}{(2 + (j-1)\delta)^2} \ell^*(2 + (j-1)\delta, 2 + j\delta),$$

which equals

$$\sum_{j=1}^n \frac{1}{r_j^2} \left(4(r_j + 1)^2 \Delta r + 4(r_j + 1) \Delta r^2 + \frac{4}{3} \Delta r^3\right),$$

where $r_j = 2 + (j-1)\delta$ and $\Delta r = \delta$. This is a Riemann sum for $\int_2^P \frac{4(r+1)^2}{r^2} \, dr$ plus terms of higher order in $\Delta r$ whose contribution approaches 0 as $\Delta r \to 0$.

The bound (10) holds for all choices of $n$, so as $n \to \infty$, we get

$$I_{\text{dist}}^x \leq \frac{104}{12} + \int_2^P \frac{4(r+1)^2}{r^2} \, dr = \frac{8}{3} + 4P - \frac{4}{P} + 8 \ln(P) - 8 \ln(2).$$

We then multiply by $L$ to get

$$E_{\text{dist}} \leq L \left(\frac{8}{3} + 4P - \frac{4}{P} + 8 \ln(P) - 8 \ln(2)\right). \quad (11)$$

Combining (5) with (11) yields

$$E_{O4}(K) \leq L \left(\frac{8}{3} + 4P - \frac{4}{P} + 8 \ln(P) - 8 \ln(2)\right) + 4. \quad (12)$$

We substitute $P = \left(\frac{3}{4}L - \frac{3\pi}{2} + 1\right)^{1/3} - 1$ to obtain our final bound.

This bound is messy, but on the order of $L^{4/3}$. We use a computer algebra system to plot the bound divided by $L^{4/3}$. The ratio achieves its maximum of $\approx 4.5626$ near $L = 1115$. Thus, for all $L$ we have

$$E_{O4}(K) \leq 4.57L^{4/3}.$$

For some values of $L$, in particular as $L$ gets very large, the coefficient 4.57 can be further reduced. If $\frac{104}{3} + 2\pi < L < 128$ or $L > 376,000$, we have $E_{O4}(K) \leq 4L^{4/3}$. As $L$ tends to infinity, the constant decreases to $3^{1/4}4^{3/4} \approx 3.63$. 

\[\square\]
References

[1] J. O’Hara, Energy of a knot, Topology 30 (2) (1991) 241–247.

[2] M. H. Freedman, Z.-X. He, Z. Wang, Möbius energy of knots and unknots, Ann. of Math. (2) 139 (1) (1994) 1–50.

[3] R. B. Kusner, J. M. Sullivan, Möbius energies for knots and links, surfaces and submanifolds, in: Geometric topology (Athens, GA, 1993), Amer. Math. Soc., Providence, RI, 1997, pp. 570–604.

[4] G. Buck, J. Orloff, A simple energy function for knots, Topology Appl. 61 (3) (1995) 205–214.

[5] G. Buck, J. Simon, Knots as dynamical systems, Topology Appl. 51 (3) (1993) 229–246.

[6] G. Buck, J. Simon, Energy and length of knots, in: Lectures at KNOTS ’96 (Tokyo), World Sci. Publishing, River Edge, NJ, 1997, pp. 219–234.

[7] G. Buck, J. Simon, Thickness and crossing number of knots, Topology Appl. 91 (3) (1999) 245–257.

[8] Y. Diao, K. Ernst, E. Janse Van Rensburg, Energies of knots, preprint (March 1995).

[9] S. Fukuhara, Energy of a knot, in: A fête of topology, Academic Press, Boston, MA, 1988, pp. 443–451.

[10] S. J. Lomonaco, Jr., The modern legacies of Thomson’s atomic vortex theory in classical electrodynamics, in: The interface of knots and physics (San Francisco, CA, 1995), Amer. Math. Soc., Providence, RI, 1996, pp. 145–166.

[11] J. O’Hara, Energy functionals of knots, in: Topology Hawaii (Honolulu, HI, 1990), World Sci. Publishing, River Edge, NJ, 1992, pp. 201–214.

[12] J. O’Hara, Family of energy functionals of knots, Topology Appl. 48 (2) (1992) 147–161.

[13] J. O’Hara, Energy functionals of knots. II, Topology Appl. 56 (1) (1994) 45–61.

[14] J. Simon, Energy functions for knots: beginning to predict physical behavior, in: Mathematical approaches to biomolecular structure and dynamics (Minneapolis, MN, 1994), Springer, New York, 1996, pp. 39–58, reprinted with update in [30].

[15] J. Simon, Energy and thickness of knots, in: Topology and geometry in polymer science (Minneapolis, MN, 1996), Springer, New York, 1998, pp. 49–65.

[16] J. K. Simon, Energy functions for polygonal knots, J. Knot Theory Ramifications 3 (3) (1994) 299–320, random knotting and linking (Vancouver, BC, 1993).
[17] H. K. Moffatt, The energy spectrum of knots and links, Nature 347 (1990) 367–369.

[18] R. A. Litherland, J. Simon, O. Durumeric, E. Rawdon, Thickness of knots, Topology Appl. 91 (3) (1999) 233–244, (based on [35] [36]).

[19] Y. Diao, C. Ernst, E. J. Janse van Rensburg, Knot energies by ropes, J. Knot Theory Ramifications 6 (6) (1997) 799–807.

[20] Y. Diao, C. Ernst, E. J. Janse van Rensburg, Properties of knot energies, in: Topology and geometry in polymer science (Minneapolis, MN, 1996), Springer, New York, 1998, pp. 37–47.

[21] Y. Diao, C. Ernst, E. J. Janse van Rensburg, Thicknesses of knots, Math. Proc. Cambridge Philos. Soc. 126 (2) (1999) 293–310.

[22] O. Gonzalez, J. H. Maddocks, Global curvature, thickness, and the ideal shapes of knots, Proc. Natl. Acad. Sci. USA 96 (9) (1999) 4769–4773 (electronic).

[23] R. B. Kusner, J. M. Sullivan, On distortion and thickness of knots, in: Topology and geometry in polymer science (Minneapolis, MN, 1996), Springer, New York, 1998, pp. 67–78.

[24] E. J. Rawdon, Approximating the thickness of a knot, in: Ideal knots, World Sci. Publishing, River Edge, NJ, 1998, pp. 143–150.

[25] E. J. Rawdon, Approximating smooth thickness, J. Knot Theory Ramifications 9 (1) (2000) 113–145.

[26] G. Buck, Four-thirds power law for knots and links, Nature 392 (1998) 238–239.

[27] J. Cantarella, D. DeTurk, H. Gluck, Upper bounds for the writhing of knots and the helicity of vector fields, in: Proceedings of the Conference in Honor of the 70th Birthday of Joan Birman, International Press, 2000.

[28] G. Buck, Most smooth closed space curves contain approximate solutions of the n-body problem, Nature 395 (1998) 51–53.

[29] J. Cantarella, R. Kusner, J. Sullivan, Tight knot values deviate from linear relations, Nature 392 (1998) 237–238.

[30] A. Stasiak, V. Katritch, L. H. Kauffman (Eds.), Ideal knots, World Scientific Publishing Co. Inc., River Edge, NJ, 1998.

[31] S. S. Chern, Curves and surfaces in Euclidean space, in: Studies in Global Geometry and Analysis, Math. Assoc. Amer. (distributed by Prentice-Hall, Englewood Cliffs, N.J.), 1967, pp. 16–56.

[32] J. Cantarella, R. Kusner, J. Sullivan, On the minimum ropelength of knots and links, preprint (2001).

[33] A. Stasiak, J. Dubochet, V. Katritch, P. Pierański, Ideal knots and their relation to the physics of real knots, in: Ideal knots, World Sci. Publishing, River Edge, NJ, 1998, pp. 1–19.
[34] K. Millett, E. Rawdon, Energy, ropelength, and other physical aspects of
equilateral knots, preprint (2001).

[35] R. Litherland, Thickness of knots, talk in Workshop on 3-Manifolds, Univ.
Tennessee (1992).

[36] J. Simon, Thickness of knots, talk in Special Session on Knotting Phenomena
in the Natural Sciences, American Mathematical Society, Santa Barbara, Nov.
1991.