THICKNESS AND CROSSING NUMBER OF KNOTS

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§1 Introduction

Knots usually have been studied as abstract mathematical objects even though the original interest in the subject seems to be based in physics. There is now interest in re-associating the mathematical abstractions with physical-like properties such as *thickness* [L] [Si1] [DEJ] [N] [St] [LSDR] or self-repelling *energy* [Fu] [O1-O4] [BS] [BO1-2] [Si2] [Lo] [DEJ]. The motivation is partly chemistry/biology [DSKC] [DC] [DC2] [Ketc] [Si3] [St] [SSC] [WC] and partly the mathematics itself.

If we try to tie a knot in a thick piece of rope, we expect the knot to be relatively simple. One standard measure of how complicated is a given knot is the number of crossings, i.e. the number of times the knot is seen to cross over itself as one looks at it from some direction. This "crossing number" can be defined as the minimum among the various directions of projection, or the average over all of them. In this paper, we obtain a relationship between *thickness* of a knot and its *average crossing number* which captures the intuition that thick rope makes simple knots.

The route we take for connecting thickness and (average or minimum) crossing number of a knot K is to use a particular notion of *energy* for a knot, defined in [BO], which we call $E_N(K)$, the *normal energy.* This energy, which is expressed as an integral over $K \times K$, relates well to the integral formulation of average crossing number [FHW], and in turn can be related to thickness.

The *thickness* of a knot has been studied in [LDSR]; the intuitive idea is that we imagine a knot as a closed solid non-self-intersecting tube of some radius and define the *thickness* to be the ratio of the radius to the length of K (this is made precise in §2). Alternatively, the *rope length* of K, $E_L(K)$, is the ratio of length-to-radius.

In §2 we summarize some of the results from [LSDR], as they are needed later. In §3 we establish two bounds on crossing number in terms of thickness: the first (obtained along the way to the second) is quadratic, the second a $\frac{4}{3}$ power expression. The higher order bound yields a smaller value (because of the coefficients) for knots of relatively short rope-length.

The existence of a quadratic bound on minimum (as opposed to average) crossing number is implicit in [LSDR], where it is shown that a smooth knot of rope-length L is equivalent to a polygon with n edges, where n is linear in L. Since the maximum number of self-crossings of an n-sided polygon depends on n^2, we have a quadratic bound on minimum crossing number in terms of L. The existence of a similar bound on average crossing

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number might not be surprizing, since we still think of the self-crossings of K depending somehow on the square of its length. To obtain the lower order bound, we introduce volumetric considerations. We are inclined to conjecture that bounds of still lower order do not exist, and have numerical evidence* indicating that a linear bound is unlikely; however the talk [St] included provocative examples suggesting that for knots that are in "ideal" thickest-possible conformations for their knot-types, there might be a linear relationship between rope-length and average crossing number.

Some of the results presented here were announced in [B] [Si4]

§2 Definitions: Thickness, Energy, and Average Crossing Number

Throughout this paper, a *knot* is a smooth (class C^2) simple closed curve in $\mathbb{R}^3$. We shall consider several functionals that associate a number $E(K)$ with a particular curve K.

In addition to the functionals discussed below, others have been proposed and studied (e.g. [BS] [O2] [DEJ] [KS] [Si2]). As noted by [DEJ], a notion of "thickness" of a knot yields an "energy" by taking the reciprocal. Various energy functions have ben implemented so one can compute energies of a given curve and flow the curve (discretized) to an apparent local minimum [Br] [Hg] [Hu] [Sc] [Wu]. Thickness has been implemented by E. Rawdon [Ra] and a experiments based on a different definition announced in [St].

The energies cited here all satisfy the following properties (among others of course):

1. $E(K)$ is invariant under Euclidean isometry and change of scale;

2. $0 < E(K) < \infty$ if K is not self-intersecting;

3. For knots of fixed total length (or lengths uniformly bounded away from 0), if parts of a knot are brought together to make the knot self-intersect, the energy tends to $+\infty$.

4. There are only finitely many knot types realized below any given energy level, and below some level, only unknots.

Property 1 tells us that E is determined by the shape of a knot, not the size. Properties 2 and 3 tell us that E separates knot-types with infinitely high "potential energy walls". Therefore we might hope to find minimum energy conformations for each knot type; we could think of these as canonical conformations for each type. Property 4 says that energy provides a reasonable taxonomy for knots.

Let the knot K be given by the parametrized curve $x(t)$. Then we denote by x, y arbitrary points $x(t), y(t)$ in K and we write $\dot{x}(t)$ for the derivative. We also use:

$\rho_{xy} = |x - y|$ (when x,y are understood, we write only ρ)

$r_{xy} = \frac{x-y}{|x-y|}$

$d\mathbf{x} = \dot{x}(t)dt$, a line element at x and

$dx = |d\mathbf{x}|$.

*provided by E. Rawdon

We define four energy functions, each of which have properties 1-4 above, bound the crossing number, and are independent of parametrization. The first three (E_N, E_S, E_O) are given by integrals taken over $K \times K$ and are implemented in [Br]. The fourth, E_L, is defined more geometrically

The *normal energy* is (equivalent to [BO1]):

$$E_N(K) = \int\int \frac{|d\mathbf{x} \times r|^2}{\rho^2} \quad .$$

We sometimes write $d\mathbf{x} \times r$ as $\sin\alpha$, where α is the angle between the chord $(y - x)$ and the tangent direction $d\mathbf{x}$ or as $\cos\theta$, where θ is the angle between $(y - x)$ and the normal plane to K at x.
The *symmetric energy* is:

$$E_S(K) = \int\int \frac{|d\mathbf{x} \times r||d\mathbf{y} \times r|}{\rho^2} \quad .$$

The *O'Hara energy* (also called the *Möbius energy* or the *conformal energy* [O1] [BHW] [KS]) is:

$$E_O(K) = \int\int \frac{1}{\rho^2} - \frac{1}{|x - y|^2_{S^1}} \quad .$$

($|x - y|_{S^1}$ denotes the arclength distance between x and y along K; we may think of a unit-speed parametrization with a circle S^1 of some radius as parameter space).

We next define the *thickness* $R(K)$ and *rope length* $E_L(K)$. The definition and results summarized below are taken from [LSDR]. We introduce theorem numbers here for later use.

Let $N(K; \mathbb{R}^3)$ be the normal bundle of K in $\mathbb{R}^3$ and let $e : N(K; \mathbb{R}^3) \to \mathbb{R}^3$ be the standard projection map. Since we are assuming K is a C^2 embedding, we know that for sufficiently small $\epsilon > 0$, the map e is a C^1 diffeomorphism of the tube around $K \times 0$ in $N(K; \mathbb{R}^3)$ of radius ϵ to a neighborhood of K in $\mathbb{R}^3$. We define $R(K)$ to be the supremum of such ϵ. It may be shown that the following more naive definition is equivalent.

For each $x \in K$, let N_x denote the normal plane to K at x; and let $D(x, R)$ denote the solid disk of radius R centered at x contained in N_x. Then

$$R(K) = sup\{\, R : D(x, R) \cap D(y, R) = \emptyset \; \forall x \neq y \in K \,\} \quad .$$

The *rope length* or *length energy* of K is defined as:

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

Results in [LSDR] on thickness (hence on E_L if one normalizes the knot to have total length =1) include the following.

Theorem T1. *Maximum curvature of $K \leq R(K)$.*

There actually is a complete characterization of $R(K)$. Define a pair of points (x, y) of K to be *critical* if the chord vector $(x - y)$ is perpendicular to the tangent at x or perpendicular at y, and let $R_2(K)$ be half the minimum of all distances $|x - y|$ for such pairs. Then we have:

Theorem T2. *$R(K)$ equals the minimum of the minimum radius of curvature of K and $R_2(K)$. In particular, $R(K) \leq$ each of these.*

Remark. It is clear that $R(K)$ cannot exceed half the *doubly critical* self-distance, that is between pairs of points where the chord is perpendicular to both tangents; however [LSDR] goes on to establish the result for half the *singly critical* self-distance. This may be a bit surprizing, as the minimum singly-critical self-distance of a curve is, in general, smaller than the minimum doubly-critical self-distance (e.g. any ellipse that isn't a circle). But when self-distance is "in control" of thickness, then the two minima coincide. Because this detail is needed later in Theorem 2, we repeat the proof below.

Proof of part of Theorem T2. We show here that the thickness $R(K)$ is at most half the singly-critical self-distance of K. Let x, y be points realizing the minimum singly-critical self-distance: so the chord vector $(x - y)$ is perpendicular to the tangent to K at x, and the points x, y have minimum distance $|x - y|$ for this property. Suppose $|x - y|$ is strictly less than $2R(K)$. Let z be the midpoint of the segment between x and y. If the chord vector $(x - y)$ were also perpendicular to the tangent to K at y, this would place z in the intersection of two normal disks to K of radius $= \frac{|x-y|}{2} < R(K)$, a contradiction. So the tangent at y is not perpendicular to the chord; thus there exist points of K closer to z than the point y. Let y_2 be a point of K closest to z. Then either $y_2 = z$ or there is a chord vector $(z - y_2)$ perpendicular to K at y_2. In either case, we have that the normal disks to K at x and y_2 of radius $= \frac{|x-y|}{2} < R(K)$ meet at z. □

Theorems T1 and T2 are needed later. There also is a relation between thickness and the ratios of chord length to arclength along K that may be of interest. For points x, y on K, let $arc(x, y)$ denote the minimum arclength along K between the two points.

Theorem T3. *Suppose K is a (C^2) knot of total length 1 and thickness R. Then for any x, y on K,*

$$\frac{arc(x, y)}{|x - y|} \leq \frac{1}{4R} \quad .$$

Remark. In terms of the rope-length $E_L(K)$, Theorem T3 says

$$\frac{arc(x, y)}{|x - y|} \leq \frac{1}{4} E_L \quad .$$

The supremum of this ratio over all pairs of points of K is called the *distortion* of K [G] [O2].

The following is how one shows that the energy $E_L(K)$ satisfies Property 4 above.

Theorem T4. *We assume K is normalized to have total length $= 1$. Given a lower bound on $R(K)$ (i.e. an upper bound on $E_L(K)$), one can deduce an upper bound on the bridge number of K (from curvature); the number of sticks needed to represent K as a polygon (from a close analysis of local behavior); and the minimum crossing number of the knot type $[K]$ (from stick number).*

We next define the *average crossing number*, $acn(K)$. When a knot in 3-space is projected into a plane, for almost all choices of direction, the projected curve is immersed and one can count the number of self-crossings. This can be averaged (as an integral over the unit sphere) over all directions to produce the average crossing number. M. Freedman *et al* showed [FHW] that $acn(K)$ can be computed as double integral over $K \times K$, which facilitates comparison with energies.

The integral is a modification of Gauss's formula for the linking number of two space curves. The integrand for the average crossing number measures, in some sense, the probability that the line elements $d\mathbf{x}, d\mathbf{y}$ appear to cross from an arbitrary perspective. The formula is:

$$acn(K) = \frac{1}{4\pi} \iint_{S \times S} \frac{||[d\mathbf{x}, d\mathbf{y}, r]||}{\rho^2} dxdy \ ,$$

where the numerator of the integrand is the norm of the triple scalar product of the three vectors.

The number $acn(K)$, being an average, bounds the minimum crossing number of the knot type, denoted here c([K]). Therefore $acn(K)$ is another reasonable measure of the complexity of the conformation K. However, $acn(K)$ does not provide any barrier to the changing of knot-types, and so is not much use as an energy. On the other hand, an energy function which does blow up on self-intersection and also bounds the crossing number would both measure complexity and have canonical minima. Note that bounding the crossing number is in itself a worthy goal, since this invariant of knots seems difficult to analyze.

In the next section we connect the energies $E_N(K)$, $E_S(K)$, $E_L(K)$, and $acn(K)$.

§3 Comparison Theorems for Energies and Average Crossing Number

Theorem 1.

$$E_N(K) \geq E_S(K) \geq 4\pi acn(K) \geq 4\pi c([K]) \ .$$

Remark. A similar inequality between $E_O(K)$ and $acn(K)$ is established in [FHW]. Once we obtain (Theorem 2) a relation between E_N and E_L then we can deduce a bound for $acn(K)$ in terms of E_L as well (Corollary 2.1). One cannot hope for a converse saying that some energy is bounded by a function of acn: Draw a planar curve modeled on part of the graph $y = sin\frac{1}{x}$; such a curve will have $acn(K) = 0$ since it is planar, but arbitrarily high energy (of all kinds) since it is packed tightly**.

**R. Randell pointed out this example

Proof of Theorem 1. Assume a unit-speed parametrization. The numerator of the integrand for $acn(K)$ is the magnitude of the triple scalar product of unit vectors: $|[d\mathbf{x}, d\mathbf{y}, r]|$. For some angles α, β , we have $\sin\alpha = |d\mathbf{x} \times r|$, and $\sin\beta = |d\mathbf{y} \times r|$. Then $|[d\mathbf{x}, d\mathbf{y}, r]| \leq \sin\alpha \sin\beta$, since the angle from the line of $d\mathbf{y}$ to the plane of $d\mathbf{x}$ and r is $\leq$ either of the angles from $d\mathbf{y}$ to $d\mathbf{x}$ or to r, so $E_S(K) \geq 4\pi acn(K)$. Moreover,

$$2E_N(K) = \int\int \frac{|d\mathbf{x} \times r|^2}{\rho^2} + \frac{|d\mathbf{y} \times r|^2}{\rho^2} = \int\int \frac{\sin^2\alpha + \sin^2\beta}{\rho^2} ,$$

since this counts every element twice. But $\sin^2\alpha + \sin^2\beta \geq 2\sin\alpha\sin\beta$, so $E_N(K) \geq E_S(K)$. □

We now wish to relate the energy $E_N(K)$ to the rope-length $E_L(K)$. Theorem 2 will say that if E_L is small then E_N is small.

Remarks. There cannot be a converse. This (family of) example(s) is based on an example given in [FHW], used there to show that finite energy E_O does not imply C^2 smooth. For each n, construct a C^2 curve K_n as follows: Start with a round unit circle K_0. Replace a small arc of K_0 with a bump that is an arc (representing $\leq \frac{1}{n}$ degrees) of a circle of small radius $r \leq \frac{1}{n}$. Smooth the corners to make a C^2 curve K_n. The minimum radius of curvature of K_n is $\leq r$. Thus, from Theorem T2, the thickness $R(K_n) \leq r$, i.e. $E_L(K_n) \gtrapprox 2\pi n$. As we let n aproach ∞, the energies $E_N, E_S, and E_O$ of K_n approach the energies of a circle, while E_L is unbounded. Incidentally, this example also shows that E_L is not C^1-continuous; it is [L2] C^2-continuous.

Regarding the formula below, it would be especially interesting if one could reduce the power $\frac{4}{3}$. Based on computer experiments, it appears that there might be linear inequlities relating the energies E_O and E_L for certain special conformations. Also there may be linear inequalities relating the energies for minimum-energy conformations under several energies [KS] [St] [B]. But it seems less likely that linear bounds exist for general conformations. We state two bounds: the quadratic bound has smaller coefficient than the ($\frac{4}{3}$) power bound, so it is smaller for low energy situations.

Theorem 2.

$$11E_L(K)^{4/3} \geq E_N(K)$$
$$\frac{1}{4}E_L(K)^2 \geq E_N(K)$$

Corollary 2.1.

$$11E_L(K)^{4/3} \geq 4\pi acn(K)$$
$$\frac{1}{4}E_L(K)^2 \geq 4\pi acn(K)$$

Proof of 2.1. This follows directly from Theorems 1 and 2. □

This bound on $acn(K)$ is very large relative to our intuitive sense of what a knot having certain E_L looks like. Incidentally, Corollary 2.1 becomes an improvement on the bound for $c([K])$ implicit in [LDSR] when E_L is large, e.g. $E_L \geq 94$.

Proof of Theorem 2. This proof, which includes discussion and several lemmas, occupies the rest of the paper.

To begin, normalize the curve so it has thickness $R = 1$ and, therefore, $E_L(K) = L$, the actual arclength of K.

The energy $E_N(K) =$

$$\int_{x\in K}\int_{y\in K}\frac{|d\mathbf{x}\times r|^2}{\rho^2} \quad .$$

Let I^x denote the inner integral; we shall obtain a bound on I^x in terms of $E_L(K) = L$ and then multiply by the length L to get our bound on E_N.

For each $x \in K$, define two sets (recall $arc(x, y) =$ minimum arclength along K between x and y):

$$L_x = \{y \in K | arc(x, y) \leq \pi\}$$

and

$$G_x = \{y \in K | arc(x, y) \geq \pi\} \quad .$$

Define "local" and "global" integrals as follows:

$$I^x = I_{loc} + I_{glob} = \int_{y\in L_x}\frac{|d\mathbf{x}\times r|^2}{\rho^2} \quad + \quad \int_{y\in G_x}\frac{|d\mathbf{x}\times r|^2}{\rho^2} \quad .$$

We first seek to bound I_{loc}. (This part of the argument also will yield the overall quadratic bound.) Each point in $\mathbb{R}^3$ lies on a circle tangent to K at x, having some radius $\sigma > 0$. (The tangent line to K may be viewed as $\sigma = \infty$.) The contribution of a point $y \in K$ to I^x depends (see Lemma 2b below) on the radius σ for that y. We show in Lemma 2a that $\sigma \geq 1$ for all $y \in K$.

At the given point $x \in K$, for each radius $\sigma \geq 1$, let $Q_x(\sigma)$ be the union of circles of radius σ that are tangent to K at x. In particular, let Q_x denote $Q_x(1)$. The set $Q_x(\sigma)$ is a singular torus (it is pinched at the point x). Define W_x to be the interior of Q_x, and let V_x denote $R^3 - (Q_x \cup W_x)$.

Lemma 2a. *For each $y \in K$ (in particular $y \in L_x$), $y \in V_x \cup Q_x$. That is, K cannot turn enough to get inside W_x.*

Proof of 2a. Let B be a closed 3-ball of radius $= 1$ whose boundary is tangent to K at x. The union of all such 3-balls equals the pinched solid torus $\overline{W}_x$. Thus it suffices to show that for each such ball B, $K \cap int(B) = \emptyset$. Suppose $K \cap int(B) \neq \emptyset$. The we can replace B by a ball B' of some radius $\delta < 1$, tangent to K at x, whose interior still meets K.

Let z be the center of B'. Because K is tangent to the boundary of B' at x, we know that the normal disk to K at x of radius $= \delta$ just hits z. Let A be the closure of a component A^o of $K \cap int(B')$; so A^o is an open arc, and the endpoints a_1, a_2 of A lie on the boundary of B' (One of the endpoints might or might not be x; that does not matter).

Let p be a point of A for which the distance to z is minmum. Then $|z-p| < \delta$ whereas $|a_1 - z| = |a_2 - z| = 1$; thus the point p must lie in A^o (so $p \neq x$), and hence be a critical point of the distance function. So the line-segment $\overline{pz}$ is perpendicular to K at p. Thus z is contained in two different normal disks to K, one at p and one at x, each of radius $\leq \delta < 1$. This contradicts the normalization to $R(K) = 1$, and so we must have that the component A^o cannot exist. This completes the proof of Lemma 2a. □

Lemma 2b. *Let $y \in K$ lie on a circle of radius σ tangent to K at x. Then* $\frac{|d\mathbf{x} \times r|^2}{\rho^2} = \frac{1}{4\sigma^2}$

Proof of 2b. [BO1] Let p be the center of the circle; express $\frac{|d\mathbf{x} \times r|^2}{\rho^2}$ in terms of sines and cosines of the angles of the triangle pxy. □

Remark. If we multiply the above constant integrand by $(2\pi\sigma)(2\pi\sigma)$, we obtain the result [BO1] that if C is a round circle (of any radius) then the energy $E_N(C) = \pi^2$.

We can now obtain the bound on I_{loc} and the overall quadratic bound for E_N. From Lemma 2a, we have that each point $y \in K$ lies on a circle of radius $\sigma \geq 1$ tangent to K at x (and so contributes $\leq \frac{1}{4}$ to the integrand) or lies on the tangent line to K at x (and so contributes zero to the integrand). Thus

$$I_{loc} \leq \int_{-\pi}^{\pi} \frac{1}{4} = \frac{\pi}{2} \quad .$$

Similarly,

$$I^x \leq \int_0^L \frac{1}{4} = \frac{L}{4} \quad .$$

Thus

$$E_{N(K)} = \int_{x \in K} I^x \leq \frac{L^2}{4} \quad .$$

We now proceed towards the $(\frac{4}{3})$ power bound by analyzing I_{glob}.

The first observation is that for points $y \in G_x$, $|x - y| \geq 2$ (that is for $y \in G_x$, the integrand $\frac{|d\mathbf{x} \times r|^2}{\rho^2}$ is $\leq \frac{1}{4}$ because of the distance between x and y, regardless of the angle.

Lemma 2c. *If K is a C^2 knot normalized to have $R(K) = 1$, then for each $x, y \in K$, $|x - y| < 2 \implies arc(x, y) < \pi$. That is $y \in G_x \implies |x - y| \geq 2$.*

Proof of 2c. Let B^o be the interior of the closed ball B of radius $= 1$ centered at x. Then $B^o \cap K$ is an open subset of K, so its components are open arcs. Let A be the component of $B^o \cap K$ containing x.

We first claim that there are no other components of $B^o \cap K$. Suppose A' is another component. Since points of A' have distance to x strictly < 2, in particular a point p of A' closest to x must exist in in the open set A'. Thus p is a critical point of the distance function to x, so the line segment $\overline{xp}$ is perpendicular to the tangent to K at p. Thus x lies in a normal disk to K (centered at p) of some radius $\delta < 2$. But the self-distance bound on thickness of K (see Theorem T2 in Section 2) would then be $\leq \delta/2$ and so strictly < 1. Thus A is the only component of $B^o \cap K$.

The next ingredient for Lemma 2c we need is a theorem of Schur; this is the version stated in [Ch]. In our application, the plane arc C below will be a semicircle of radius $= 1$, and the curve C^* will be either of the two arcs of K starting at x having length π. Schur's theorem formalizes the intuitively appealing idea that if two curves are launched from the same point, then the curve of lower curvature has to end up (for at least some amount of arclength) farther in space from the beginning point.

Schur's Theorem. *Let C be a plane arc with curvature $k(s)$ which forms a convex curve with its chord. Let C^* be an arc of the same length referred to the same parameter s such that its curvature $k^*(s) \leq k(s)$. If d^* and d denote the lengths of the chords joining their endpoints, then $d \leq d^*$.*

Since K has $R(K) = 1$, we know (Theorem T1 in Section 2) that the curvature of K is ≤ 1. Now use Schur's Theorem to compare an arc C^* of K of length π starting at x with a planar semi-circle C of radius $= 1$ starting at x, both arcs parametrized by arclength. When we reach the end of the semicircle, we are at a point q with $|q - x| = 2$; thus the far endpoint of C^*, call it q^*, has $|q^* - x| \geq 2$. So if we trace along K from x in both directions, we must leave the open unit ball B^o at or before the endpoints of L_x since those two endpoints are not in B^o. By the previous claim, once K leaves B^o, it cannot return. So $y \in K \cap B^o \implies arc(x, y) < \pi$. This completes the proof of Lemm 2c. □

In analyzing I_{glob}, we shall ignore $|d\mathbf{x} \times r|$, which is ≤ 1, and bound $\int_{G_x} \frac{1}{\rho^2}$. The basic idea in the rest of our argument is that the condition $R(K) = 1$ prevents too much arclength of K from being too close to the point $x \in K$. We shall consider spherical shells (of thickness =1) about a point x and bound the amount of K that can lie within a given shell. The maximum energy contribution would occur if the hypothetical maximum packing in each case actually occurred; assuming that (unattainable) shape were attained, we get a bound for the energy contribution from each shell, along with a bound on the number of shells (since we have only the given total length L available).

For a (measurable) set $A \subseteq K$, let $\ell(A)$ denote the total arclength (i.e. measure) of A. For a given point $x \in K$, and $0 \leq a < b \in \mathbb{R}$, let

$$B[a, b) \;=\; \{p \in \mathbb{R}^3 \;:\; a \leq |x - p| < b\,\},$$

$$G_x[a, b) = G_x \cap B[a, b)\ , \quad \text{and}$$

$$\ell[a, b) = \text{total arclength of } G_x[a, b)\ .$$

We also need notation for the solid tube about K, or some part A of K, that is the union of all the normal disks $D(y, 1)$ to K of radius $R(K) = 1$, where y ranges over A. For a set $A \subseteq K$, denote this union $tube(A)$. When A is measurable, Pappus' theorem (i.e. a special case of Fubini's theorem) tells us that the volume of $tube(A)$ is defined, and equals $\ell(A)$ multiplied by the (perpendicular) cross-sectional area $\pi(1)^2$, i.e.

$$vol(tube(A)) = \pi \times \ell(A)\ .$$

We note that $B[0, b)$ is just the open ball of radius $= b$ centered at x and that the sets $K[a, b)$ are Borel sets in K so we may talk about their measure or arclength.

Lemma 2d. *(Using the preceeding notation:)*

$$\ell[0,2) = 0 \ ,$$

and for $a \geq 1$,

$$\ell[a,b) \leq \frac{4}{3}[(b+1)^3 - (a-1)^3] \ .$$

Proof. The statement $\ell[0,2) = 0$ is just Lemma 2c. For the second part, if $y \in K$ is contained in $B[a,b)$ then for each point $p \in D(y,1)$, $|p-y| \leq 1 \implies (a-1) \leq |p-x| < |b+1|$. so $D(y,1) \subset B[a-1,b+1)$. Thus $tube(G_x[a,b)) \subset B[a-1,b+1)$ and comparing the volumes gives the desired inequality. □

Remark. In using Lemma 2d for the argument below, we shall have a special situation in which the shell $B[a-1,a)$ already has been filled from some source other than $tube(G_x[a,b))$; so the only available new volume will be from $B[a,b+1)$. This will give the bound $\ell[a,b) \leq \frac{4}{3}[(b+1)^3 - (a)^3]$.

We know $\ell[0,2) = 0$, and we next find bounds for $\ell[2,3)$, $\ell[3,4)$, etc.

From Lemma 2d, $\ell[2,3) \leq \frac{4}{3}[(4)^3 - (1)^3] = 84$. Assume that $\ell[2,3)$ actually equals this upper bound (which would represent the maximum possible contribution to I_{glob}). Then, as in the *Remark* following Lemma 2d, we have that $\ell[3,4) \leq \frac{4}{3}[(5)^3 - (4)^3]$ and, in general, for each $n \geq 3$, $\ell[n,n+1) \leq \frac{4}{3}[(n+2)^3 - (n+1)^3]$. Here we are assuming that for each $n \geq 3$, $\ell[n,n+1)$ equals this upper bound, which in turn restricts the available volume for the next tube. The questions remaining are: What is a bound on the energy contribution from each of these shells, and how many shells does it require to exhaust K (or rather G_x)?

For the first shell, $y \in G_x[2,3) \implies$

$$\int_{G_x[2,3)} \frac{1}{\rho^2} \leq \frac{1}{2^2}(84) \ = 21 \ .$$

For points $y \in G_x[n,n+1)$, we have $\frac{1}{\rho^2} \leq \frac{1}{n^2}$. So,

$$\int_{G_x[n,n+1)} \frac{1}{\rho^2} \leq \frac{1}{n^2}\frac{4}{3}[(n+2)^3 - (n+1)^3] \ = 4 + \frac{12}{n} + \frac{28}{3n^2} \ .$$

Since $n \geq 3$, this is less than 9.04, which is the bound we shall use for the contribution from each shell for $n \geq 3$. So if $B[N,N+1)$ is the last shell needed to cover G_x, we have

$$I_{glob} \leq 21 + 9.04(N-2) = 2.92 + 9.04N$$

To bound the number of shells, recall that we are assuming the maximum contribution from each one, that is

$$\ell[2,3) = 84$$

and for each $n \geq 3$,

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

We need to determine a number N for which

$$84 + \sum_{n=3}^{N} \frac{4}{3}[(n+2)^3 - (n+1)^3] \ \geq \ell(G_x) \ \ .$$

Expand the sum and substitute $\ell(G_x) = L - 2\pi$ to see that we need N to satisfy

$$2\pi + 4 + 4N + 4(N+1)^2 + \frac{4}{3}(N+1)^3 \geq L \ \ .$$

If N is the greatest integer $[(\frac{3}{4}L)^{1/3}]$ then the $(N+1)^3$ term makes it clear that the above sum is greater than L. Consequently, we only need to consider shells up to that value of N. So

$$I_{glob} \leq 2.92 + 9.04N \leq 2.92 + 9.04[(\frac{3}{4}L)^{1/3}] \leq 2.92 + 9.04(\frac{3}{4}L)^{1/3} \ \ .$$

Now let us combine and simplify the bounds (For relatively short curves, one might want to avoid this simplification, as well as others made in the preceeding arguments, to obtain sharper bounds; however, so long as one uses this kind of analysis, it appears that all one can gain is improved coefficients, not an improvement in the exponent $\frac{4}{3}$). We have

$$I_{loc} \leq \frac{\pi}{2} \ \text{ and}$$

$$I_{glob} \leq 2.92 + 9.04(\frac{3}{4}L)^{1/3} \ \ .$$

Because $L \geq 2\pi$, it follows that

$$I^x = I_{loc} + I_{glob} \leq 11L^{1/3} \ \ .$$

Multiplying by the length L to bound the outer integral, we obtain

$$E_N(K) = \int_{x \in K} I^x \leq 11L^{4/3} \ \ .$$

This completes the proof of Theorem 2. □

References

[Br] K. Brakke (further devel. by J. Sullivan), *EVOLVER*, Geometry Center, University of Minnesota, http://www.geom.umn.edu/software/download/evolver.html, Program for visualizing and energy minimizing knots.

[B] G. Buck, *On the energy and length of a knot*, talk in Special Session on Physical Knot Theory, Amer. Math. Soc., Iowa City, March 1996.

[BO1] G. Buck and J. Orloff, *A simple energy function for knots*, Topology and its Appl. **61**, 205-214.

[BO2] G. Buck and J. Orloff, *Computing canonical conformations of knots*, Topology and its Appl. **51**, 246–253.

[BS] G. Buck and J. Simon, *Knots as dynamical systems*, Topology and its Appl. **51** (1993), 229-246.

[BS2] G. Buck and J. Simon, *Energy and length of knots*, sub. to Proc. of Intl. Conf. Knot Theory, Tokyo, July 1996.

[Ch] S.S. Chern, *Curves and surfaces in euclidean space*, Studies in global Geometry and Analysys, MAA Studies in Mathematics vol. 4, 1967.

[DSKC] F.B.Dean, A. Stasiak, T. Koller, and N.R. Cozzarelli, *Duplex DNA knots produced by escherichia coli topoisomerase I*, J. Biological Chemistry **260** (1985), 4975–4983.

[DEJ] Y. Diao, K. Ernst, and E.J.J. VanRensburg, *Energies of knots*, (preprint, 3/95); *Knot energies by ropes*, (preprint 4/96).

[DC] P. Dröge and N.R. Cozzarelli, *Recombination of knotted substrates by Tn3 resolvase*, Proc. Nat. Acad. Sci. U.S.A. **86** (1989), 6062–6066.

[DC2] P. Dröge and N.R. Cozzarelli, *Topological structure of DNA knots and catenanes*, Methods in Enzymology **212** (1992), 120–130.

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

[Fu] S. Fukuhara, *Energy of a knot*, A Fête of Topology: Papers Dedicated to Itiro Tamura (Y.T. Matsumoto and S. Morita, ed.), Academic Press, New York, 1988, pp. 443–451.

[G] M. Gromov, *Filling Riemannian manifolds*, J. Diff. Geom. **18** (1983), 1–147, (see p. 113).

[Hg] M. Huang, Univ. Illinois-Chicago, http://www.eecs.uic.edu/ mhuang/research.html, Program for visualizing and energy minimizing knots.

[Hu] K. Hunt, *KED*, University of Iowa, http://www.cs.uiowa.edu/ hunt/, Program for visualizing, manipulating, and energy minimizing polygonal knots.

[Ketc] R. Kanaar, A. Klippel, E. Shekhtman, J.M. Dungan, R. Kahmann, and N.R. Cozzarelli, *Processive recombination by the phage Mu Gin system: Implications for the mechanisms of DNA strand exchange, DNA site alignment, and enhancer action*, Cell **62** (1990), 353–366.

[KS] R. Kusner and J. Sullivan, *Möbius energies for knots and links, surfaces and manifolds*, Geometry Center Research Report GCG64 (1993 rev. 1994), University of Minnesota, to appear in Proc. of 1993 Georgia Top. Conf..

[L] R. Litherland, *Thickness of knots*, talk in Workshop on 3-Manifolds, Univ. Tennessee, 1992.

[L2] R. Litherland, *Thickness of knots*, talk in Special Session on Physical Knot Theory, Amer. Math. Soc., Iowa City, March 1996.

[LSDR] R. Litherland, J. Simon, O. Durumeric, and E. Rawdon, *Thickness of knots*, preprint 6/96 (based on [L] [Si1]).

[Lo] S. Lomonaco, *The modern legacies of Thompson's atomic vortex theory in classical electrodynamics*, (preprint, 4/95).

[N] Alexander Nabutovsky, *Non-recursive functions, knots "with thick ropes", and self-clenching "thick" hyperspheres*, Comm. Pure Appl. Math. **48(4)** (1995), 381-428.

[O1] J. O'Hara, *Energy of a knot*, Topology **30** (1991), 241–247.

[O2] J. O'Hara, *Family of energy functionals of knots*, Topology Appl. **48** (1992), 147–161.

[O3] J. O'Hara, *Energy functionals of knots*, Topology-Hawaii (K. H. Doverman, ed.), (Proc. of 1991 Conference), World Scientific, 1992, pp. 201–214, (Computer program by K. Ahara).

[O4] J. O'Hara, *Energy functionals of knots II*, Topology and its Appl. **56** (1994), 45–61.

[Ra] E. Rawdon, Univ. Iowa, http://www.math.uiowa.edu/ rawdon/thick.html, Program for visualizing and maximizing thickness of knots (work in progress).

[Sc] R. Scharein, *Knot-Plot*, Univ. British Columbia, www.cs.ubc.ca/spider/scharein/, Program for drawing, visualizing, manipulating, and energy minimizing knots.

[Si1] J. Simon, *Thickness of Knots*, talk in Special Session on Knotting Phenomena in the Natural Sciences, American Mathematical Society, Santa Barbara, Nov. 1991; *Lecture Notes on Physical Knot Theory*, (notes by H. Naka), 1993, from summer 1991 course, Kwansei Gakuin University.

[Si2] J. Simon, *Energy functions for polygonal knots*, J. Knot Theory and its Ramif. **3** (1994), 299–320.

[Si3] J. Simon, *Energy functions for knots: beginning to predict physical behavior*, preprint 11/94, to appear 1996 in Proc. of 1994 IMA Conference on Geometry and Topology of DNA.

[Si4] J. Simon, *Thickness and energy of knots*, talks at IMA Conf. on Polymers (Minneapolis 6/96) and Intl. Conf. on Knot Theory (Tokyo, 7/96)..

[SSC] S. Spengler, A. Stasiak, and N.R. Cozzarelli, *The stereostructure of knots and catenanes produced by phage λ integrative recombination: implications for mechanism and DNA structure*, Cell **42** (1985), 325–334.

[St] A. Stasiak, *Ideal forms of knots*, talk in Special Session on Physical Knot Theory, Amer. Math. Soc., Iowa City, March 1996.

[WC] S. Wasserman and N.R. Cozzarelli, *Supercoiled DNA-directed knotting by T4 topoisomerase*, J. Biol. Chem. **266** (1991), 73–95.

[Wu] Y.-Q. Wu, *MING*, University of Iowa, http://www.math.uiowa.edu/ wu/, Program for visualizing, manipulating, and energy minimizing polygonal knots.

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