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Physical Knots

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Abstract. What happens to knot theory when the knots, traditionally studied as purely one dimensional, completely flexible filaments, are given physical substance – in the form of thickness, rigidity, or some kind of self-repelling? Researchers have developed several measures of knot complexity, modeled on these kinds of physical "reality". We shall explore these ideas, see relations between different notions of complexity, and compare the "ideal" conformations of knots that arise. We also note that there are observed relationships between these measures of complexity and behavior of actual knotted DNA molecules. The development of "Physical Knot Theory" is characterized by growing understanding along with an ample supply of open questions.

1. Introduction

Knots meet science in three different ways[1]: At the most straightforward level, we can try to understand actual tangible objects that occupy space, have mass, etc. They may be large, as in Figures 1-9, or microscopic, as in Figures 10 and 11.

Next up in abstraction are the 1-dimensional knots that might occur as flow-lines in a fluid flow or other physical system (see e.g. papers by Moffatt[**Mof90**] or Cantarella-DeTurk-Gluck [**CDG00**] on knotted flux tubes, Buck on knotted n-body orbits [**Buc98b**], and Fadeev-Niemi on knotted solitons [**FN97**]). The earlier work by J. Birman and R. Williams on knotted orbits in ODE flows has continued to expand, as in the book [**GHS97**] and recent papers by R. Ghrist and several coauthors.

There is a level even more subtle than flow-lines: the most abstract connection between knots and science is the phenomenon we might call "analogous patterns", where purely mathematical definitions and relationships in abstract knot theory are echoed by definitions and relationships in physics. This is a connection developed by L. Kauffman.

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[1]This paper is a revised and expanded version of notes prepared for the January 2001 AMS Short Course on Knots in Science, and is offered as an introduction to some of the questions confronted in the present volume.

We began using the terms “physical knots” or “physical knot theory” in 1996, as the title of an AMS Special Session. One can see how the field has been developing by reviewing the lists of talks for that session[2], the IMACS2000 session on Physical Knots[3], and, of course, the present volume. The 1998 book *Ideal Knots* [**SKK98**] provides an accessible entré, with expository articles by many of the people working in this area.

In this paper, we concentrate on knots made of real physical “stuff” that one can perceive and handle, and on mathematical models that seek to capture some of the physical properties.

2. “Strength” of knots

This problem appears to be well-understood, in qualitative terms, by the engineers and others who encounter it in day to day applications. But there is not yet an overall theory to explain all that is observed and, in particular, that would give good quantitative predictions. We introduce the idea here in order to motivate various particular questions later, and also because the phenomenon is an appealing combination of easy statement, physical relevance, and mathematical subtlety.

People who enjoy fishing or sewing are familiar with the phenomenon that a string with a knot tied in it will break more readily than the same string without the knot. Some books of knots include the results of experiments on different knots, reporting the “strength of the knot” as the ratio (or percentage ratio)

$$\frac{\text{breaking strength of string with a knot tied in it}}{\text{breaking strength of same string with no knot}} .$$

This fraction appears to vary according to the type of knot. Why?

We can see in Figure 2 that the rope is bent where it emerges from the knot. Presumably this bending is one of the primary causes of weakening. There may also be an effect due to compression of the rope.

The strength also varies with the kind of string being used. One study[4] comparing different brands of fly-fishing line found that tying an overhand knot in one brand of line produced a small decrease in breaking strength, while doing the same thing to a different brand produced a much larger weakening. What geometric or physical properties of the fishing line could account for this? It appears that the line’s diameter is at least one factor.

Because the knot-strength of a particular material varies with knot type, the strength is usually defined in terms of an overhand knot. Even with knot type fixed, we are not aware of an explicit way to calculate the knot strength explicitly as a function of appropriate parameters for the particular kind of rope. The more general, and still wide open, problem is: *Given the knot-type and appropriate physical parameters of the rope, predict the percentage loss of breaking strength.*

The knot-strength phenomenon is even recognized in international trade disputes (at least one, anyway). In 1994, the Canadian International Trade Tribunal decided[5] that U.S. companies were dumping certain kinds of twine, defined in terms of knot-strength. Here are excerpts from the report:

[2]http://at.yorku.ca/d/a/a/a/03.htm

[3]http://www.haverford.edu/math/ rmanning/imacs2000.html

[4]Bill Nash, http://www.flyfishingreview.com/topics/archive/leadertest.html or http://hometown.aol.com/billsknots/ldrtst.htm

[5]http://www.tcce.gc.ca/dumping/Inquirie/Findings/nq93003e/nq93003e.htm

> The Canadian International Trade Tribunal, under the provisions of section 42 of the Special Import Measures Act, has conducted an inquiry following the issuance by the Deputy Minister of National Revenue for Customs and Excise of a preliminary determination of dumping dated December 23, 1993, and of a final determination of dumping dated March 23, 1994, respecting the importation into Canada of synthetic baler twine with a knot strength of 200 lbs or less, originating in or exported from the United States of America.
>
> ....
>
> Synthetic baler twine is used with agricultural baling equipment to bind bales of hay or straw. Baling equipment is designed specifically to produce either square or round bales. In the case of square balers, the twine is knotted. As square bales usually undergo considerable physical manipulation, the knot strength of the twine is an important consideration. In the case of round balers, the twine is merely wound around the bale a number of times, and the twine is not stressed by either knotting or the physical manipulation of the bale itself. Nevertheless, in round baling, the tensile strength of the twine is still an important consideration.
>
> ....
>
> It should be noted that knot strength and tensile strength are not interchangeable terms. Synthetic baler twine with a knot strength of 130 lbs may have a considerably higher tensile strength.

The question of knot-strength is also of interest to chemists, molecular biologists, and others working on understanding the physics, in particular breaking strength, of polymers.

In his talk at the 1996 AMS meeting in Iowa, E. Wasserman described computer simulations designed to analyze the effect of pulling tight a knot tied in a long chain molecule. A computationally intensive simulation of breaking knotted polyethylene, is reported in [**SSWK99**]. The chains were pulled until they broke, typically right at the point where the filament "enters" the knot. This led one of the authors to later say, "...it suggests that knots are topological objects that have universal properties that do not depend on their size"[**KS00**][6].

Researchers have developed laboratory techniques to manipulate individual polymer molecules. In a 1999 experiment, polysaccharide molecules were attached at their ends and stretched until they broke [**GBRCS99**]. Since the breaking strength was much less than the expected breaking strength of the polymer itself, the authors concluded that the break was happening at the points where the molecule was attached to the supports, rather than somewhere in the middle of the polymer chain. This led to a debate [**SDD$^+$99**] between the authors and another group about whether the observed low breaking strength actually might be due to knotting in the long molecules.

3. Getting to the mathematics

The act of pulling a knot tight leads to interesting mathematical questions. Modulo the transition from open-rope knots to closed loops, if we tie an overhand

[6] http://www.npaci.edu/envision/v16.2/biopolymers.html

knot (a common name for the simplest open-rope knot that we call the trefoil when we think of closed loops) in a rope and pull it tight, we always seem to get a figure that looks like Figures 8(left), 9, 12, 13, 14. The tight figure-eight knots in Figures 4, 6, and 8(right) are remarkably similar. The tight knot in a rope has something fundamental in common with conformations produced in very different settings: a living creature performing life functions, a curve given by parametric equations, a curve (actually a polygon with 100 edges, so it looks like a smooth curve) found by computer simulation to maximize the ratio of diameter to length of the "virtual rope", and a curve (100 edge polygon again) obtained from the previous one by lowering a certain self-repelling energy function (see later section).

So the first tempting question is whether there exists, for each knot type, a universally optimal conformation. The two Figures 13, 14 teach us that different ways of measuring the complexity of knot conformations can lead to different kinds of "ideal" conformations. The book [**SKK98**] explores this theme in many directions. Despite its provocative title, that collection of papers really shows that there is no single "ideal". Nevertheless, it remains an interesting question of philosophy, and perhaps even mathematics, to decide why all the optimum conformations look so similar. For smooth trefoil knots, we do indeed seem to have some kind of Platonic "ideal" shape around which the optimizers, i.e. minimizers of various notions of geometric complexity, seem to hover.

Given a particular measure of geometric complexity of knot conformations, we can ask basic mathematical questions:

- Does each knot type contain an optimal conformation? (Any geometric features of such an optimum conformation would be a new invariant of topological knot-type.)
- Is the optimal conformation unique? Even if there is only one absolute minimizer, are there local minima? (So one might talk about the "energy spectrum" [**Mof90**] of a knot type as a topological invariant.)

In subsequent sections, we discuss these and other questions in the context of several physically motivated ways of assigning numbers to knot conformations, attempting to measure how crumpled or crooked or otherwise complicated they are, and trying to determine which knots can arise under various kinds of physical restrictions.

(4) Thickness of knots, rope-length
(5) Energy of knots
(6) Edge number of a knot
(7) Random knotting, probability of a knot

4. Thickness of Knots, Rope-Length

How much rope does it take to make a knot? Can you make a closed-loop trefoil knot with a one foot length of one inch diameter rope?

This question was posed to the author in 1985 by L. Siebenmann. Our first partial results were announced in [**Sim**] and [**Lit92**] and improved in [**LSDR99**]. It would take more than $2.5\pi \approx 7.85$ inches of one-inch diameter rope to tie a knot. See Figure 16. In frames A and B, we use Fenchel's theorem on the total curvature of a closed curve, and then the Fary-Fenchel-Milnor theorem [**Mil50**] on the total curvature of a nontrivial knot to get initial lower bounds. In frame C, we approximate the alleged knot with a polygon to get a larger lower bound. In practice, using computer simulations or real ropes (the numbers come out about the same) it has been shown (Figure 16, frame F) that one needs a length:diameter ratio of nearly 16 to form a knot. See [**DEJvR97, KBM+96, Pie98, Buc96b, Raw97, Raw98, Raw00**], and R. Scharein's KnotPlot site. So our original theoretical minimum was around half the experimental value. The theoretical bound has been improved by J. Cantarella, R. Kusner, and J. Sullivan [**CKS99, CKS02**] to $\approx 3.42\pi \approx 10.73$, (Figure 16, frame D) by analyzing how a thick tube would have to intersect a singular disk spanning the knot. The best bound so far has been obtained by Y. Diao [**Dia01**], who did a careful analysis of the geometry of (what we might describe as) "seeing" essential crossings in a thick knot, and pushed the theoretical lower bound to just over 12 inches (Figure 16, frame E) for a trefoil knot. So the answer to Siebenmann's question is "No". However, aside from the æsthetic pleasure in stating the question that way, there is no particular magic about "one foot". The basic problem remains open: Just how much "rope" does it take to tie a knot? The best theoretical lower bound so far is still around 25% too low.

We present here some of the ideas developed in [**LSDR99**]. The first step in approaching such a problem mathematically is to agree on a model for "rope". Each smooth simple closed curve in 3-space has a tubular neighborhood with circular cross sections, and we use such a tube as our model.

Specifically, let K be a smooth simple closed curve in $\mathbb{R}^3$. For a point $p \in K$ and radius $r > 0$, let $D_r(p)$ be a circular disk of radius r, centered at p, and perpendicular to K at p. (See Figure 15.) If r is small enough, then the disks $D_r(p)$, $p \in K$, are pairwise disjoint (and their union is a solid torus neighborhood of K). We define the *thickness radius* or *rope radius* of K, denoted $r(K)$, to be the supremum of all such good radii. Intuitively, $r(K)$ measures how much one can thicken the knot before the thick tube begins to self-intersect.

With this model, we showed in [**LSDR99**] that in order to make a nontrivial knot, it must be the case that

$$\frac{\text{total length of } K}{r(K)} \geq 5\pi \quad .$$

The situation is summarized in Figure 16 (but note the criteria in Figure 16 are stated in terms of $\frac{\text{length}}{\text{diameter}}$, to be consistent with peoples' intuitive understanding of diameter as the measure of a rope's thickness). For very short lengths of thick "rope", the core curve cannot have enough total curvature to be a closed curve. For somewhat more total length, we can make closed curves, but only trivial knots, because [**Mil50**] a nontrivial knot has total curvature $> 4\pi$. With a little more length, we run out of proof that knots are impossible, but still have a ways to go to reach the experimentally determined minimum needed.

The proof to get from $L/D > 2\pi$ to $L/D \geq 2.5\pi$ (i.e. $L/r \geq 5\pi$) involves showing that if $n > \frac{\text{length of } K}{\pi \cdot r(K)}$, then inside the open tube of radius $r(K)$ about K, we can construct a polygon that is isotopic in the tube toThickTube K. So if the ratio is less than 5, then the knot K is equivalent to a 5-stick polygon; but it takes at least six edges to make a nontrivial knot [**Ran94**].

Our understanding of $r(K)$ comes from a theorem characterizing thickness in terms of two other geometric properties of the curve. The first is the minimum radius of curvature of K, which we denote $MinRad(K)$. For the second, consider the curve in Figure 17. There are two chords of the ellipse having the property that the chord is perpendicular to the curve at both of its endpoints (the major and minor axes). Any smooth closed space curve has such a chord, namely the one for which the distance between the two endpoints is maximum. Define a pair (x, y) of such points to be a *doubly critical* pair, and define the *doubly-critical self-distance* of K to be

$$\mathrm{dcsd}(K) = \min\{|(y - x)| : (x, y) \text{ is a doubly critical pair}\}$$

Continuing the ellipse example, in that case, $\mathrm{dcsd}(K)$ is the length of the minor axis.

THEOREM 4.1 (Characterizing thickness). [**LSDR99**] *For any smooth knot, K, the thickness radius $r(K)$ equals the minimum of* $\mathrm{MinRad}(K)$ *and* $\frac{1}{2}\mathrm{dcsd}(K)$.

4.1. Making a subtle but useful distinction. The *self distance* of K, a definition generally attributed to N. Kuiper, is defined like $\mathrm{dcsd}(K)$, but we only require that the chord be perpendicular to the knot at at least one endpoint; call such a pair of points (x, y) on the knot *singly critical*; and call the infimum of distances between such pairs the *singly-critical self-distance*, $\mathrm{scsd}(K)$. Typically, there are more singly critical pairs of points than doubly critical pairs (see Figure 17), and the inequality generally is strict:

$$\mathrm{scsd}(K) < \mathrm{dscd}(K) .$$

However, for measuring thickness, the two kinds of critical self-distance are equivalent.

THEOREM 4.2 (Re-characterizing thickness). [**LSDR99**] *The thickness radius $r(K)$ equals the minimum of* $\mathrm{MinRad}(K)$ *and* $\frac{1}{2}\mathrm{scsd}(K)$.

Our definition of thickness seems mathematically natural, and seems appropriate to model "rope" that is completely flexible, albeit inelastic and incompressible. It provides a beginning way to gain insight into the shape of a tight knot as in Figure 2. However, the tight knots shown in Figures 4, 6, and 7 look different from the tight rope. One key is that the mouse cable and the chain cannot bend very much; their curvature is bounded by physical properties. One can define thickness in a way that takes this into account.

4.2. Alternative definitions of thickness. Several groups of researchers [**DEJvR97, DEJvR99, GM99, KS98**] have developed variations on the definition of thickness, sometimes by using the above characterization theorem as a starting point. For example, one can minimize with $\frac{1}{2} \times MinRad(K))$, which models (as Y. Diao once suggested) a rope that can bend only so much as to wrap around itself. Or one can minimize $|x - y|$ over points that are constrained to lie at least a certain distance apart in arclength along the knot. Our definition started with straightforward geometric thickness, and deduced a relationship to curvature; it is possible [**GM99**] to start with curvature as the primitive concept, and extend it globally to recover the combination of local curvature and doubly-critical self-distance that characterizes thickness.

The ratio

$$E_L(K) = \frac{\text{length of } K}{r(K)}$$

is invariant under change of scale. To define an invariant of knot type, we minimize this ratio over all smooth representatives K of a given knot type.

We use the notation E_L because this ratio can be viewed as an *energy function* on knots (see next section). In particular, the ratio becomes infinite as curves pass through themselves, and there are only finitely many knot types that occur below any given "energy" level. Specifically [**LSDR99**],

$E_L(K) <$ some given number $\implies$ bound on number of edges needed to make a polygon of the same knot type $\implies$ bound on minimum crossing number of the knot type.

4.2.1. *Be careful with polygons.* Here is one more example to illustrate the principle that things sometimes get tricky when we try to make an intuitive concept mathematically precise. In order to do computer simulations of thickness, it is useful to develop an analogous idea for polygons, since computer simulations have to deal with discrete objects. Here is the most obvious notion of thickness for a polygon: for small enough radius $r > 0$, we can construct a system of cylinders, one for each edge of the polygon, where the axes are the edges, the radii are r, the heights are the lengths of the edges, such that cylinders about nonconsecutive edges do not intersect. So we could define the thickness radius of the polygon to be the supremum of such "good" radii. Apply this construction to regular polygons inscribed in the unit circle. The thickness radius of the unit circle is 1. But as the number of edges of the inscribed polygons increases, the polygon thickness approaches 1/2. This example, and a correct definition of thickness for polygons were developed by E. Rawdon [**Raw97, Raw98, Raw00**]. The approach of [**GM99**] also handles polygons in a way that gives converging thickness for converging polygons.

4.3. Existence and uniqueness of tight conformations. Certainly if we pull a piece of knotted rope tight, it becomes <u>something</u>; but once we commit to a precise mathematical definition, the answer is less obvious. For example, we originally developed the theory of thickness for knots that are C^2 smooth. So one formulation of the existence problem would be the following.

Question: Does there exist, within each knot type, a C^2 curve that minimized rope-length over all C^2 curves of that knot type?

This is another one of those subtle points that seems to haunt (or enrich) this topic. Using the Arzela-Ascoli theorem, one can show [**Lit96**] that within each knot type, there exists a sequence of C^2 representatives whose rope-lengths converge to the infimum for the knot type, and such that the curves themselves converge to a C^1 knot of that type. But it is not known if C^2 optimizers exist for any nontrivial knot. The knot in Figure 13 illustrates the problem: the knot seems to have "bumps", where it appears that arcs meet in a way that is C^1 but not C^2. This is much like a toy one can buy that consists of a set of quarter-circles that can be joined end-to-end so they swivel freely. Because the curves are joined end-to-end, the curve is continuous; because the "curves" actually are thick tubes whose flat ends have to meet flush, the core curve is C^1 smooth. The curvatures are all numerically equal, since the plastic pieces are congruent to each other; but the vector curvature directions change abruptly at the junctions (unless one is content to build only planar curves), so the core curve is not C^2 smooth.

This method of building C^1 knots led us to think about whether there could be an analogous "building kit" from which one could indeed make C^2 smooth knots of constant scalar curvature. This is indeed the case [**McA01**]: Each knot type can be realized as a C^2 smooth curve in $\mathbb{R}^3$ having constant scalar curvature. Furthermore, there exists a finite set of "elementary pieces" such that every knot type can be built by assembling copies of these pieces.

A number of people have noted that there are simple links that indeed seem to be optimizers having the non-C^2 property, but the question of C^1 vs. C^2 for knots remains open. The simplest link example (proven in [**CKS02**]) consists of three curves: two round circles having the same radius, each simply linking a third component that has the shape of a "stadium curve" (two semi-circles connected by straight line segments).

Question: Are rope-length optimizing conformations unique? If we tie a loose figure eight knot, and pull it tight, will we always end up with the same tight conformation?

Here again, we have a clear answer for links: Some link types have different rope-length minimizing conformations; in fact, we can find continuous families of them! This sounds surprising until we see the example [**Buc96a**]: Construct the example above of two round circles linked by a stadium-curve. Now swing together the two circles, like halves of a clam or leaves of a hinge, keeping the thick circle tubes tangent to each other and to the thick tube around the stadium curve. We get a continuous family of non-congruent links with the same rope-length, which is optimal for that link type.

For composite knots, it is easy to construct examples that seem to be distinct isolated local minima, though the individual critical rope-lengths appear to be slightly different: Tie a sequence of knots such as [trefoil,figure-eight,trefoil,figure-eight] and pull it tight so the factors remain in that order. Alternatively, while the knot is loose, exchange the factors to make trefoil, trefoil, figure-eight, figure-eight], and pull that tight. It is clear that once pulled tight, it is impossible to change one conformation into the other without first lengthening the rope. (We have to be careful here; this is intuitively clear, but I am not aware of anyone having written a proof.) It *seems* clear that one can construct examples of different local optima for prime knots along the lines of the composite knot example, e.g. by a satellite construction such as doubling or cabling; but, as always, there is a difference between "intuitively obvious" and "proven".

The two pictures of tight figure-eight knots made of chain (Figures 6 and 7) suggest that even for a knot as simple as a figure-eight, there might exist distinct local minima for rope-length. When we cut a closed loop knot in two different places, as in Figure 18, and pull it tight, we do sometimes get what appear to be two different stable minima. This also works with rope. But in physical experiments, there is always the question of whether friction is playing a role. Are we observing a phenomenon that is genuinely caused by the geometry alone?

Several investigators have done experiments (see e.g. [**DEJvR97, KBM⁺96, Pie98, Buc96b, Raw97, Raw98, Raw00**], and R. Scharein's KnotPlot site[7]), either by hand or by computer, to estimate $E_L(K)$ for various knot types. While these are experiments and not theoretical calculations, the data is generally consistent from one experiment to another (with occasional differences that have prompted some lively discussions).

4.4. DNA knots. Given that we seem to be measuring something fundamental about each knot type, it is not entirely surprising that such data correlates well

[7] http://www.cs.ubc.ca/nest/imager/contributions/scharein/KnotPlot.html

with actual physical behavior of knotted DNA loops in certain laboratory experiments. This is discussed in [**SKB+96**] and a similar relationship (though not as carefully calibrated) for knot energies in [**Sim96**]. We can see in Figure 12 why more complicated knots ought to move faster in some kind of obstruction field: for different knots made from filaments of the same length and thickness, more complicated knots will tend to be more compact in their overall shapes.

To avoid claiming that the situation is a lot simpler than it really is, we should remember that in the DNA loops experiments, one is dealing with flexible knots that are constantly changing shape. Figure 10 illustrates the sizes involved; in this picture, the DNA has been coated to make it 10 times thicker and so make the configuration easier to see. The original filament was quite thin relative to its length. Also, the double-helix was nicked before the knot was run in the gel, so there was little stiffness: overall, the loop was extremely flexible in the gel and the actual conformation varied widely. Thus notions such as "size" or "more compact" have to be understood as time-averaged properties of the statistical ensemble of actual conformations.

Even with this caveat, it still seems intuitively plausible that there should be some relation between complexity of knot type and average size, and so gel velocity. However the quantitative relationship that seems to hold between minimum rope-length of a knot type and relative gel mobility *in certain experiments* remains impressive and not fully understood.

The stipulation "*in certain experiments*" is necessary. S. Levine and H. Tsen showed [**LT96**] that we may see one knot type moving faster than another (5_1 vs. 5_2) under certain conditions (voltage) and the order reversed under different conditions. Recently, A. Stasiak announced an experiment in which a collection of knots types exhibited one ordering for low voltage and exactly the opposite ordering for a higher voltage. From these observations, we are forced to conclude that the relation between knot type and gel velocity in not some simple (even qualitative) correlation. The open problem here is to develop a model of agarose-gel electrophoresis of DNA loops that accounts for all of this. We have begun developing a graphical computational model of loops moving through obstructions to help understand this process [**HS99a, HS99b**].

5. Energy of Knots

Around the time people were beginning to speculate on thickness of knots, we also were considering the following "thought-experiment": Suppose you make a knot out of string, spread an electric charge on it, and let go; what would happen? Presumably the knot would spring apart, trying to get as far from itself (whatever that means) as possible. We would expect knots to achieve conformations that are as "wide open" as possible, so perhaps the same conformations as we see for thickened knots.

In addition to its intrinsic mathematical appeal, this question is relevant to the behavior of knotted molecules such as Figures 10 or 11. Electrostatic self-repelling is an important factor in synthesis and understanding conformations. For example, in laboratory experiments in which DNA strands formed loops [**SW94a, SW94b**] by random cyclization, it was found that the concentration of knots produced (rare, compared to the concentration of unknotted loops in these experiments) increased in the presence of positive ions to buffer the self-repelling of the DNA molecules.

When trying to get filaments to tie themselves in knots, there is an additional energy cost if the filaments are self-repelling.

5.1. Simplest definition of knot energy does not work. (See [**BS93**] for more details.) If X and Y are points in $\mathbb{R}^3$, then the standard definition of electrostatic repelling energy is (in some units)

$$E_{\text{points}} = \frac{q^2}{\|X - Y\|} \quad ,$$

where each point carries a charge q. If we had more than two points, we would compute the pairwise potentials and add them up.

Imagine next two line segments X, Y in space, with a uniform unit charge density (i.e. $dq = dx$) on each. It seems a natural extension of the discrete charge case to define the electrostatic potential energy of the ensemble of two charged sticks to be

$$\int_{x \in X} \int_{y \in Y} \frac{dxdy}{\|x - y\|} \quad .$$

This does not have one of the basic mathematical properties we want for knot energies: to provide an infinite energy barrier to changing knot type. In particular, the double integral above remains finite if we move the segments X, Y so that one passes through the other.

Suppose for a moment that we were willing to accept the preceding situation. Let K be a knot in space and imagine spreading a charge along K. We would be tempted to define

$$E_{\text{why not?}} = \int_{x \in K} \int_{y \in K} \frac{dxdy}{\|x - y\|} \quad .$$

Unfortunately, this integral is infinite for all curves. The problem is that it gives too much weight to near-neighbor interactions. And, as with the disjoint sticks example, it gives too little weight to the non-near-neighbor interactions: an arc of the knot could pass through another part, changing knot-type, without the energy blowing up.

5.2. Knot energies with good mathematical properties. In order to obtain a notion of energy for knots that is finite for embedded curves and infinite for self-intersecting ones, we want to

- Increase the power of $\|x - y\|$ in the denominator to cause the energy to become infinite if one part of the knot tries to pass through the other. (Increasing to power 2 has the added advantage that the resulting energy will be scale-invariant.)
- Find a way to cancel the near-neighbor effect, so the energy will be finite for embedded knots. This can be done for smooth curves either by subtracting an appropriate term from the integrand, or by paying attention to the direction of $(x - y)$ as well as its length.

Investigators have developed many energy functionals $E(K)$ for smooth or polygonal knots, e.g. [**BO95, BS93, BS97, BS99, DEJvR97, FHW94, Fuk88, KS97, Mof90, O'H91, O'H92b, O'H92a, O'H94, Sim96, Sim94**], all having the basic properties:

(1) $E(K)$ is finite for embedded knots.
(2) $E(K)$ is a continuous function on the (appropriate) space of knots.

(3) $E(K)$ becomes infinite if a knot is moved so as to approach crossing itself.
(4) $E(K)$ is invariant under change of scale in $\mathbb{R}^3$.

As the theory has been developing, some common themes have emerged. Often one can prove theorems such as those listed below. For particular energy functions, some of these are open conjectures. One grand problem remaining is to develop an overall theory of knot energies. Suppose one postulates a function $u(K)$ having the four properties listed above. Must u be some function of the energies already defined? What other fundamental properties (e.g. from among the theorems listed below) should we add to u in order to make this true? Can some of the theorems below be proven axiomatically, that is just from assuming one is working with an energy function satisfying conditions (1) - (4)?

- Given a bound on energy, one can deduce bounds on other measures of knot complexity, e.g. crossing number. This leads to ...
- Only finitely many knot types appear below a given energy level.
- Within each knot type, there is a particular curve that achieves minimum energy for that knot type. (This is a contrast to *total curvature* of a knot [**Mil50**]). Sometimes one must distinguish between prime knot types and composite knot types for this result. Also one needs to be careful about "knot type" here, e.g. C^2 vs. C^1 smooth, or polygons with a fixed number of edges vs. all polygons of a given topological knot type.
- A standard circle (or regular n-gon) is the overall global minimum energy conformation.
- The given energy is bounded by (some function of) the rope-length $E_L(K)$.

Several of the energies have been implemented for computer simulation of gradient flow or other energy minimization methods, and the programs are available for downloading e.g. [**Bra89, Hun, Sch, Wu**].

In the next section, we give some of the particular energy definitions and indicate some of the computer implementations. In the subsequent section, we present theorems to illustrate several of the general principles listed above.

5.3. Examples of knot energies. The first energy below is the most directly geometric, and (as one might expect from that characterization) seems to be one that can control all the others. The next two energies offer two solutions to the problem of how to "fix" the obvious-but-doesn't-work extension of discrete repelling charges to smooth curves. The fourth functional is defined explicitly for polygons.

Rope-length of a knot: [**BO95, BS97, BS99**]. As discussed in Section 4, the ratio

$$E_L(K) = \frac{\text{length of } K}{r(K)}$$

has the properties we require of a knot energy. Computational studies include [**MR, Pie98, Raw97, Raw98, Raw00, SDKK98**], and a provocative example in [**GM99**].

Möbius energy : (regularized to be zero for a round circle)] [**O'H91, FHW94, KS97**]. Let $t \to x$ be a length-preserving parametrization of K, where the domain is a circle C whose total arclength is the same as K.

$$E_O(K) = \int_{s\in C}\int_{t\in C} \frac{1}{\|x(s)-x(t)\|^2} - \frac{1}{\|s-t\|^2}\, ds\, dt \ .$$

This energy is implemented in [**Bra89**].

REMARK 5.1. The other widely used regularization for the Möbius energy uses the minimum arclength between s and t instead of the chord $\|s-t\|$. This produces energy $= 4$ for a standard round circle. When two statements of theorems about the Möbius energy seem different, because there is some ± 4 term, it probably is just that the writer is using the "other" regularization.

Normal energy and Symmetric energy: [**BO95, BS97, BS99**]

For each pair of points x, y on K, let α be the angle between the chord $(y-x)$ and the tangent to the knot at x. Let β be the angle between the chord and the tangent at y. We define

$$E_N(K) = \int_{x\in K}\int_{y\in K} \frac{|\sin(\alpha)|^2}{\|x-y\|^2}$$

and

$$E_S(K) = \int_{x\in K}\int_{y\in K} \frac{|\sin(\alpha)\sin(\beta)|}{\|x-y\|^2}$$

These functionals have been implemented in [**Bra89**] and [**Sch**].

Knot energy for polygons: Minimum-Distance energy: [**Sim96, Sim94**]

This energy for polygonal knots treats each pair of edges as if there is a uniform density of "charge", so the total for each segment is proportional to its length, but pretends that for any given pair of segments, the "charge" is concentrated at the points where the two segments are closest to each other. Since consecutive segments are touching, we do not include these in summing the contributions of the various pairs of segments.

For disjoint line segments in space, e_i, e_j, let $MD(e_i, e_j)$ denote the minimum distance between e_i and e_j and

$$U_{MD}(e_i, e_j) = \frac{|e_i|\,|e_j|}{MD(e_i, e_j)^2}\ .$$

Suppose P is a polygon with edges (numbered cyclically) $e_1, \cdots, e_n$.

$$E_{MD}(P) = \sum_{i=1}^{n} \sum_{j\neq i-1,i,i+1} U_{MD}(e_i, e_j).$$

This energy works fine for polygons with a fixed number of edges, but when we want to study polygonal approximations of smooth curves, we need to "regularize" the sum in much the same way as the Möbius energy is regularized. Let R_n denote a regular planar polygon with n edges, where n is the number of edges of P. Then we define

$$\widetilde{E}_{MD}(P) = E_{MD}(P) - E_{MD}(R_n).$$

The energy E_{MD} has been implemented in [**Hun**] [**Sch**] [**Wu**], and the subject of a challenging computer experiment in [**KHG98**] which might show that there can exist distinct conformations of a knot-type with the same *global* minimum energy, something we would conjecture does not happen.

The energy U_{MD} and the others have proven surprisingly effective in untangling complicated looking curves. For example, using a gradient-descent type algorithm (so no intelligent help along the way from the user, and no "heating" as in simulated annealing), the program $MING$ [**Wu**] completely untangled the complicated unknot shown in figure 19.

The functions $\widetilde{E}_{MD}$ and E_O look somewhat similar - there ought to be a theorem saying that the polygonal energy for polygons inscribed in some smooth curve K are approximations of $E_O(K)$. The principle holds provided the polygons do not have too much distortion in their edge-lengths. Here is one version:

THEOREM 5.2. [**SR**] *Suppose K is a smooth knot and P_n is a sequence of polygons inscribed in K, where the vertices of P_n are n points spaced equally along K in terms of arclength along K. Then*

$$\lim_{n\to\infty} \widetilde{E}_{MD}(P) = E_O(K) \ .$$

5.4. Energies dominate crossing-number, and rope-length dominates them all. We have established theorems [**BS97, BS99, RS**] which justify the belief that rope-length is the most fundamental "energy": For any smooth knot K, if we are given an upper bound on $E_L(K)$, then we can calculate upper bounds on other knot-energies, as well as bounds on the crossing-number of the knot and (so) bounds on traditional algebraic measures of knot-complexity.

Let $\mathrm{cr}(K)$ denote the minimum crossing number of some particular curve K, that is we count the crossings when we view K from whatever direction produces a regular projection with the smallest number of crossings. Let $\mathrm{cr}[K]$ be the minimum crossing number of the knot-type, that is the minimum of $\mathrm{cr}(K)$, taken over all curves representing this particular knot-type. Alternatively, we can view a particular curve K from all directions, count the number of crossings seen from each direction, and average them over the S^2 of directions. This is called the *average crossing number of* K, denoted $\mathrm{acn}(K)$. Clearly

$$\mathrm{cr}[K] \leq \mathrm{cr}(K) \leq \mathrm{acn}(K) \ .$$

It is shown in [**FHW94**] that $\mathrm{acn}(K)$ can be expressed as an integral (similar to Gauss's double integral formula for the linking number of two loops). Specifically,

$$\mathrm{acn}(K) = \frac{1}{4\pi} \int_{x\in K} \int_{y \in K} \frac{| < T_x \, , T_y \, , x-y > |}{|x-y|^3} \quad ,$$

where T_x, T_y are the unit tangents at x, y and $< u, v, w >$ is the triple scalar product $(u \times v)\cdot w$ of the three vectors u, v, w.

This integral formula allows us to compare $\mathrm{acn}(K)$ to energies of K.

THEOREM 5.3. *For any smooth knot K,*

[**BS97, BS99**] c_1 acn(K) $\leq E_S(K) \leq E_N(K)$ $\leq \{c_2 \ E_L(K)^2, c_3 \ E_L(K)^{4/3}\}$
c_4 acn(K) $\leq$ [**FHW94**] $E_O(K)$ $\leq$ [**RS**] $c_5 \ E_L(K)^{4/3}$

The theorems are stated in the papers with particular constants c_1, c_2, etc. But the we want to emphasize the exponents here. The reason we mention both quadratic and 4/3 power bounds is that for relatively simple knots, the quadratic bound is lower than the 4/3 bound because of those coefficients. The coefficients can be improved (e.g. [**Dia01**] for the quadratic bound on $\mathrm{cr}[K]$, [**RS**] compared to [**BS97, BS99**] for both bounds on $\mathrm{acn}(K)$) and we do not know what is "best possible" for them. But the exponent 4/3 is sharp. There are examples [**Buc98a, CKS98**] of homologous families (borrowing a term from our chemist colleagues) of knots and links where the minimum crossing numbers grow like the 4/3 power of the rope-lengths, so the energies are trapped between.

6. Edge number of a knot

This is, at first glance, a numerical measure of knot-complexity that is very different from "energy". In some ways it is geometrically more like crossing number than like something having to do with self-repelling or self-excluding: Given n sticks (of the same length, or allowed to vary) (allowed to lie any way in space, or restricted to the lie on some lattice such as the grid with vertices $\mathbb{Z}^3$) one cannot make a polygonal knot with n edges whose minimum crossing number is greater than n^2 (simply because each pair of sticks can only create at most one crossing). So as knot complexity rises, the number of edges needed to realize the knots also has to rise. But it need not rise as fast as we might first think: The result of [**Neg91**] says that the minimum edge-number of a knot type is on the order of its minimum crossing number n; we don't need to go to n^2 to realize the knot.

What is the minimum edge number of a given knot-type? Are there essentially different conformations for a particular knot-type and a particular number of edges? Is the space of (for example) 7-stick figure-eight knots connected? These kinds of questions may connect to behavior of smaller macrocyclic molecules, or polymers with some rigidity. For example, standard laboratory experiments with knotted DNA loops have involved filament lengths on the order of 30-50 Kuhn statistical segments. So some of the physical behaviors of these loops may resemble behaviors of polygons rather than smooth curves. And of course smaller molecules behave in various ways like ensembles of rigid components.

This topic is naive, in the sense that the definition is immediate. But the theorems can be subtle or complicated. G. Buck has noted that the minimum edge-number for a knot-type on the integer lattice is similar to rope-length: The nonconsecutive edges are at least one unit apart from each other, and we can round the corners to get a smooth knot with $r(K) = 1/2$. So the rope-length of the knot type is at most twice the edge number on the integer lattice.

Here are some papers that contend with questions about edge-number and properties of knots made of a specified number or kind of edges: [**CM98, CJ98, Dia93, JVR98, Jin97, McC98, Mei97, Mei98, Mil94a, Mil94b, MR, Neg91, Ran88, Ran94, Ran98**].

Just to keep connected to the various energy ideas, we may note that, as indicated in Section 4, we have from [**LSDR99**]:

THEOREM 6.1.

$$\text{edge} - \text{number of } [K] \leq \frac{E_L(K)}{\pi} + 1 \, .$$

The bound is sharp, because of the example of a standard round circle C. We have $E_L(C) = 2\pi$, it takes 3 edges to make a simple closed curve.

7. Random knotting, probability of a knot

Here is another informal question that has lead to a lot of computational and mathematical study, with a strong promise of physical applications: *What is the probability of a knot?* To make sense of this, one needs to agree on some particular "experiment", that is to assume some particular method of generating simple closed curves, and then ask what is the expected rate of production of one particular knot type. (The probability of producing nontrivial knots in general is then just $1 - \text{prob}[\text{unknot}]$.)

Perhaps the major theoretical result is that knots happen, in a sense inevitably [**SW88, DPS94**]: If a filament is spun out by a random walk, then as the length grows without bound, the probability that the filament is tied in a knot grows exponentially (with the number of steps) close to 1. The proof actually shows that composite knots are inevitable, since what are shown to exist are knots in the filament that are tight in the sense that there is no room for the (ever growing) filament to run back through the knots and untie them.

At the next level of understanding, we might ask how different filament lengths favor one knot type over another: Granted that knots are inevitable as the randomly generated filament gets longer, it should be the case that relatively simple knots should appear sooner than more complicated ones. On the other hand, as the filaments get even longer, it becomes harder to maintain having just a simple knot, as more complicated knots and composites become frequent. This intuition is born out by the study [**DT94**] and many since then.

8. Additional references

The article [**O'H98**] is a technical survey of many of the energy functions that have been developed. We have cited several times here the book [**SKK98**] containing that article; it is an accessible introduction to many of the topics introduced in this paper as well as some we have not discussed.

9. Historical note

I learned last summer (thanks to E. Rawdon) of a paper [**KV76**] published in 1976 that began exploring a number of ideas about mathematically modeling physical knots that many of us have subsequently rediscovered. It appears that those of us who subsequently began working in the area have been unaware of this paper. The paper explores, for example, the questions of how long a smooth tube, or how many sticks in a polygon, or how many steps on any of several lattices, does it take to make a knot.

10. Acknowledgement

The author is happy to acknowledge the help of colleagues in various aspects of research and exposition for this paper, in particular G. Buck and E. Rawdon.

FIGURE 1. Rope Knot Loose

FIGURE 2. Rope Knot Pulled Tight

Figure 3. Loose Knot Made of Mouse Cable

Figure 4. Tight Knot Made of Mouse Cable

FIGURE 5. Loose Knot Made of Chain

FIGURE 6. Tight Knot Made of Chain

FIGURE 7. Alternate Conformation of Tight Knot Made of Chain

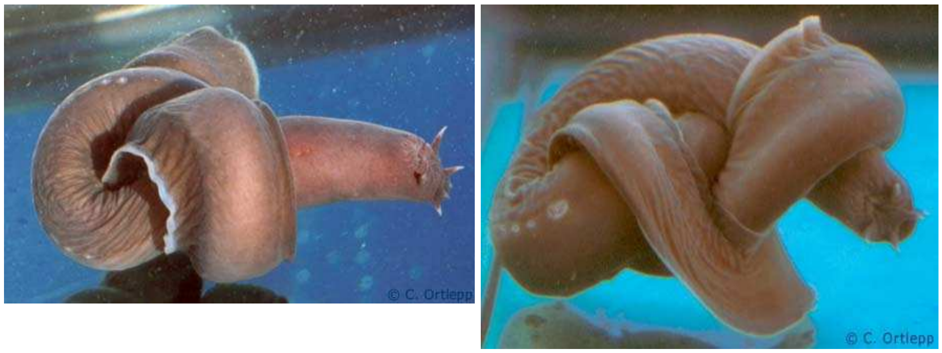

FIGURE 8. Hagfish tying itself into an overhand knot(left) and a figure-eight knot(right). Figures provided by C. Ortlepp, Dept. Zoology, UBC. See http://www.zoology.ubc.ca/labs/biomaterials/slime.html

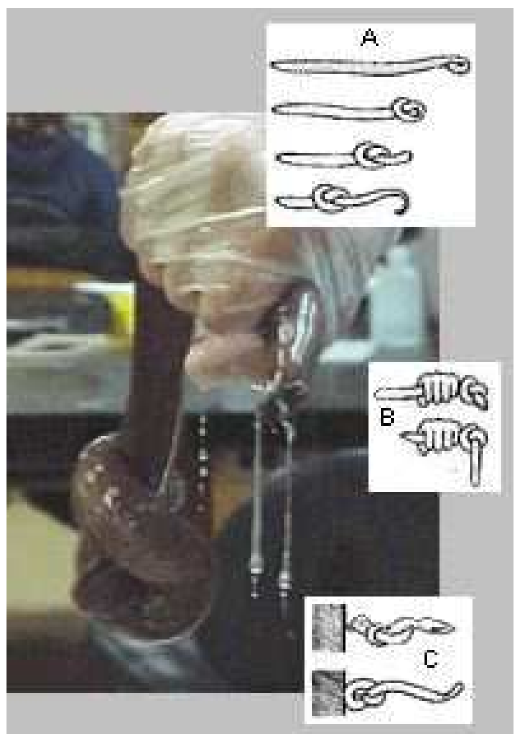

FIGURE 9. Actual hagfish knotting
http://oceanlink.island.net/oinfo/hagfish/hagfish.html

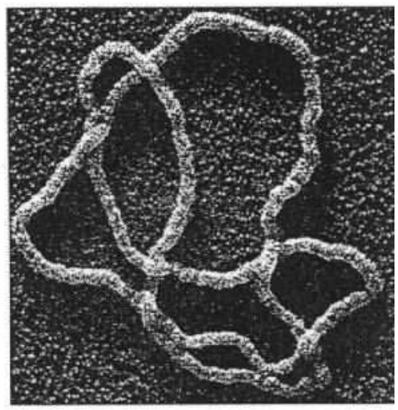

FIGURE 10. DNA Knot [**Sum95**]

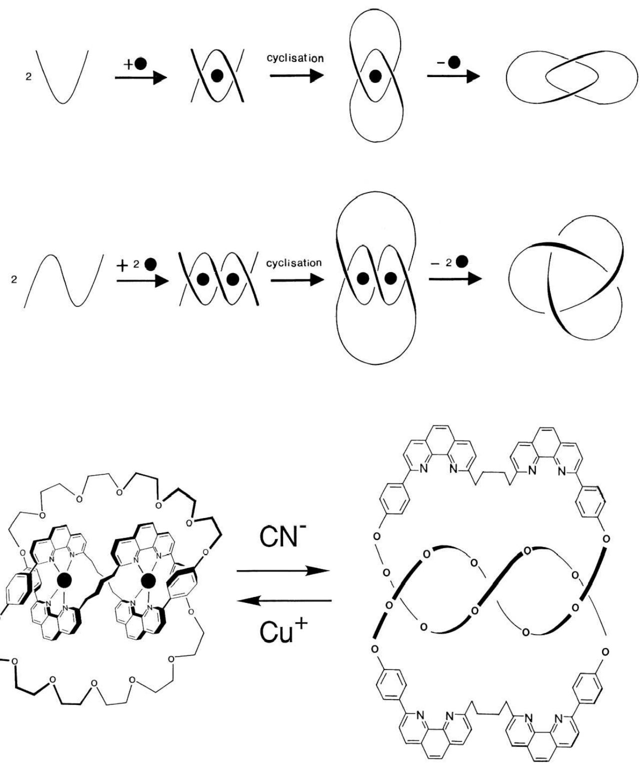

FIGURE 11. Synthesis of molecular trefoil knot. (Figures provided by J.-P. Sauvage and C.O. Dietrich-Buchecker), [**DBS89, DBRS97**]

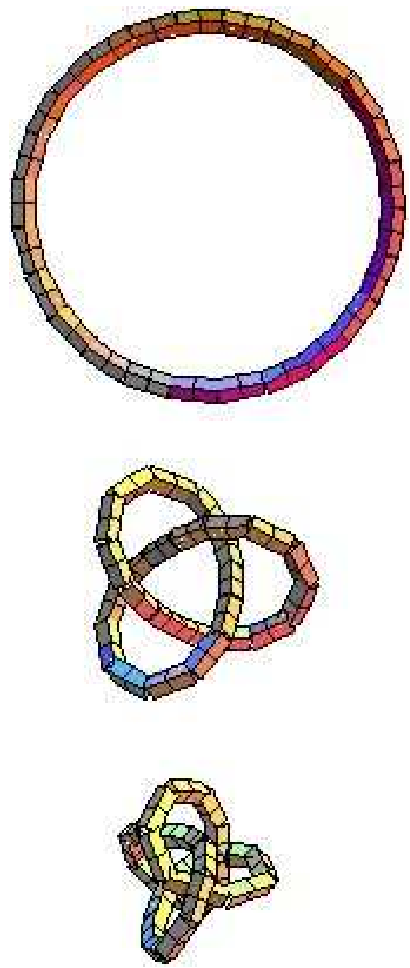

Figure 12. Different knots made from the same length and thickness of "rope" have different overall/average sizes. This is why different DNA knots travel at different speeds in gel electrophoresis.

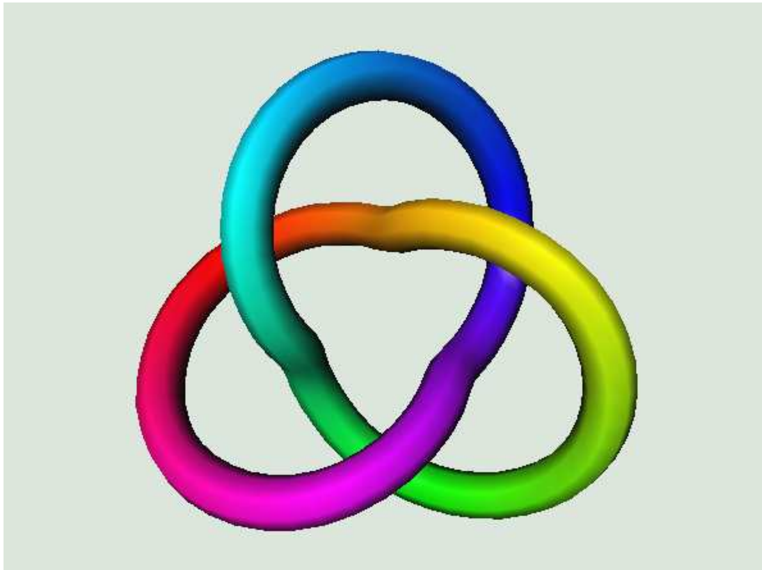

FIGURE 13. This conformation of the trefoil knot has maximum thickness for a given length (equivalently, minimum length for a given thickness). For a given length of string, it admits a uniform tube of maximum radius. The tube shown here is thinner than maximum, so that we can see certain features of the shape of the core knot. Original data 100 stick polygon provided by E. Rawdon)

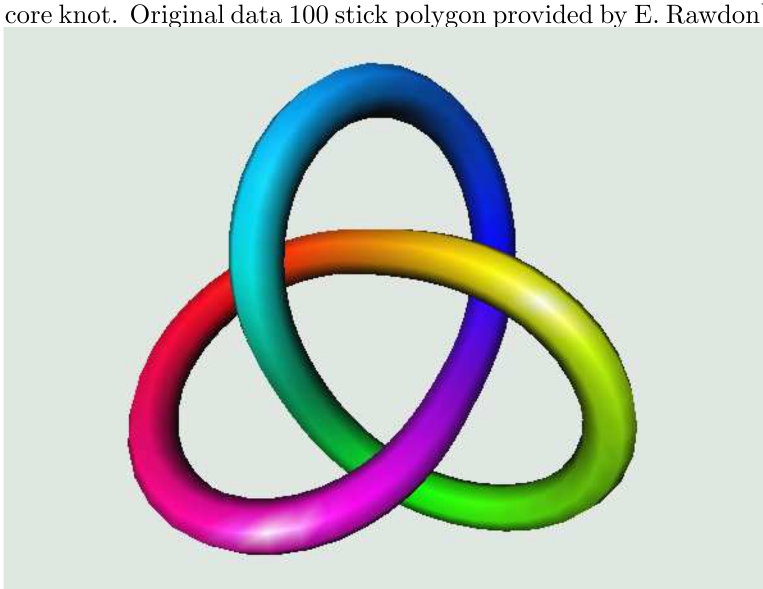

FIGURE 14. This conformation was obtained from the previous one by lowering the *minimum distance energy*, using the program MING. The curvature is now more uniform, but the maximum tube-thickness is smaller.

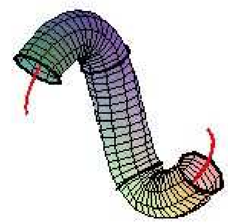

FIGURE 15. Modeling thick "rope" as a smooth curve with a normal-disk tubular neighborhood.

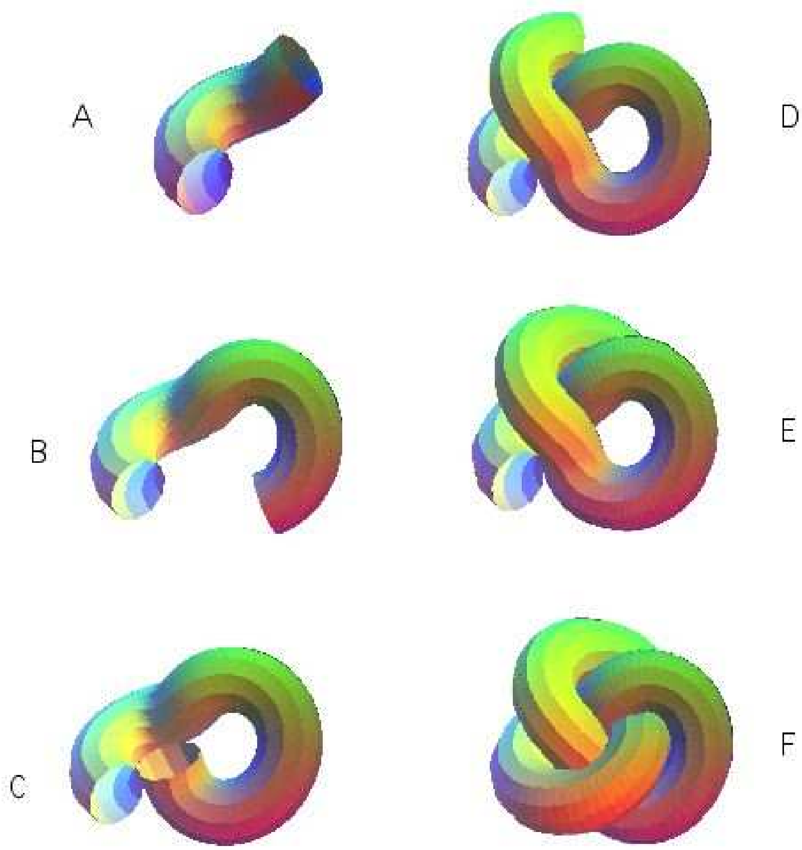

FIGURE 16. How much "rope" is needed to tie a knot? See page 4. (A) $L/D \geq \pi$. (B)$L/D > 2\pi$. (C) $L/D \geq 2.5\pi$. (D) $L/D > 10.7$. (E) $L/D > 12$. (F)$L/D \approx 16.3$.

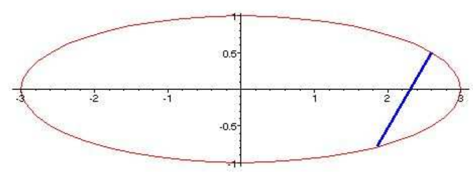

FIGURE 17. Doubly-Critical Self-Distance may be strictly larger than Singly-Critical Self-Distance

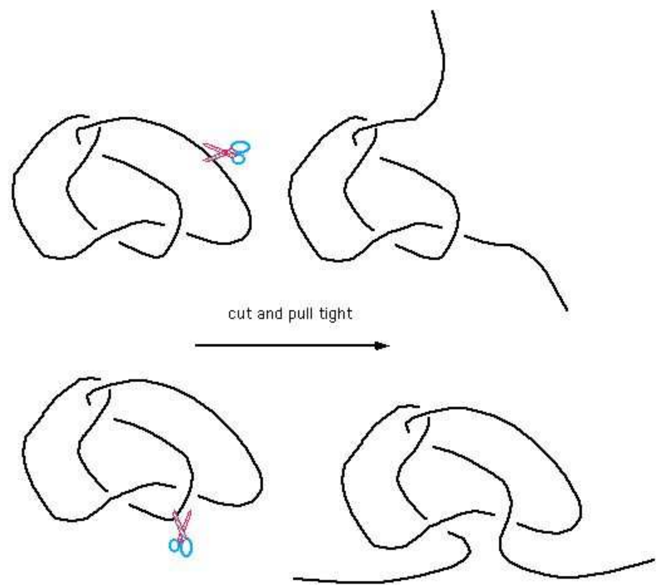

FIGURE 18. Cut in different places and then tighten

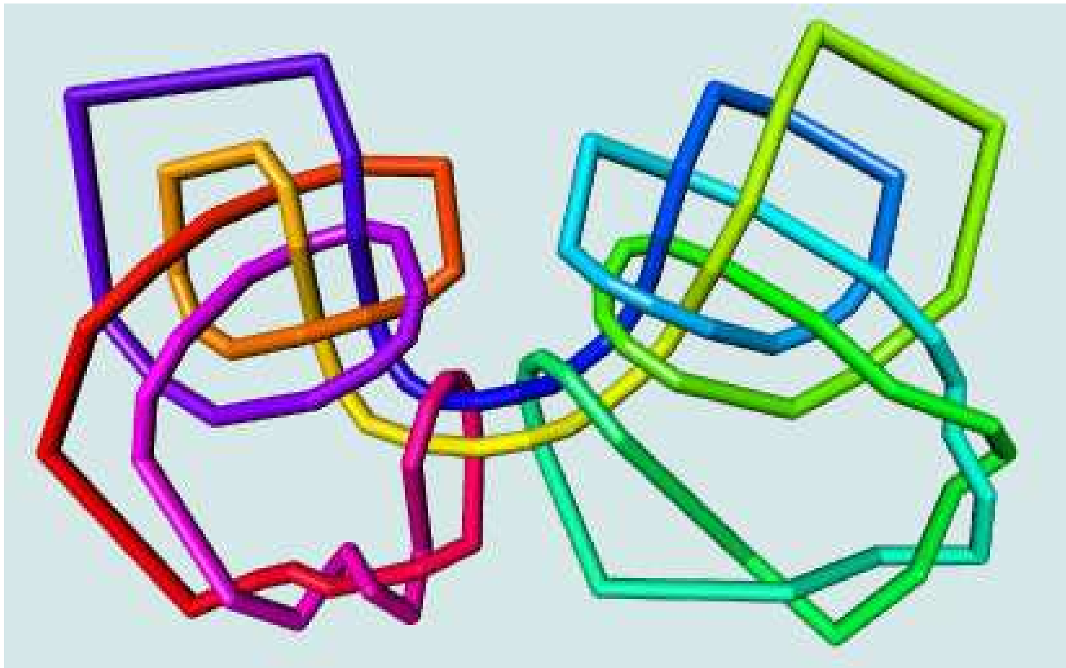

FIGURE 19. A complicated unknot that is successfully simplified by knot energy

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