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-repulsion? 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 strong relations between these measures of complexity and behavior of actual knotted DNA molecules. Audience members will receive a genuine piece of rope and some easy-to-understand unsolved problems.

1 Introduction

Knots meet science in three different ways: 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, 2, 3, 4, 6, 7, 8, 9, 10, or microscopic, as in Figures 11 and 12.

Next up in abstraction are the 1-dimensional knots that might occur as flow-lines in a fluid flow or other physical system (see talk by R. Ricca, also

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papers by H.K. Moffatt on knotted flux tubes [27], G. Buck on knotted n-body orbits [4], L. Faddeev and A. Niemi on knotted solitons [14], R. Ghrist and earlier work by J. Birman and R. Williams on knotted orbits in ODE flows).

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.)

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\(^1\) and the IMACS2000 session on Physical Knots \(^2\). The 1998 book *Ideal Knots* [44] provides an accessible entrée, with expository articles by many of the people working in this area.

In this talk, as in the presentations on DNA and polymers by D. Sumners, A. Stasiak, and S. Whittington, 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

Here is a physical knots problem (actually a cluster of several) whose statement is immediately accessible to all of us and to our students. The problem appears to be well-understood in qualitative terms, by the engineers and others who encounter it in day to day applications; but I believe there is not yet an overall theory (nor will this talk provide one) to explain all that is observed and, in particular, that would give good quantitative predictions. We introduce the idea here in order to motivate some particular questions later, and also just because the phenomenon is so simple and intriguing.

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

\(^1\)http://at.yorku.ca/d/a/a/a/03.htm
\(^2\)http://www.haverford.edu/math/ rmanning/imacs2000.html
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\(^3\) 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, it is usually defined in terms of an overhand knot.

The knot-strength phenomenon is even recognized in international trade disputes (at least one, anyway). In 1994, the Canadian International Trade Tribunal decided\(^4\) that U.S. companies were dumping certain kinds of twine, defined in terms of knot-strength. Here are excerpts from the report:

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.

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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

\(^3\)Bill Nash, http://www.flyfishingreview.com/topics/archive/leadertest.html or http://hometown.aol.com/billsknots/ldrtst.htm

\(^4\)http://www.tcce.gc.ca/dumping/Inquirie/Findings/nq93003e/nq93003e.htm
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 [34]. 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" [20].

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 [18]. 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 [42] 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 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 9, 10, 15, 16, 17. 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 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 16, 17 teach us that different ways of measuring the complexity of knot conformations can lead to different kinds of “ideal” conformations. The book [44] 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.

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 topological knot-type invariant.)

- 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” [27] of a knot type as a topological invariant.)

In the following sections, we discuss these and other questions in the context of two physically motivated ways of assigning numbers to knot conformations, attempting to measure how crumpled or crooked or otherwise complicated they are.
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 [38] and [24] and have been improved since then [26]. However, the answer is still unknown. In practice, it takes a length:diameter ratio of around 16 to form a knot. But the best we have been able to prove theoretically is the need for at least $2.5\pi \approx 7.85$ [26], subsequently improved [9] to around 8.58.

To approach such a problem mathematically, we first need 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 to model a closed loop of idealized “rope”.

Specifically [26], 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 18.) 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 [26] that in order to make a nontrivial knot, it must be the case that

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

The situation is summarized in Figure 13 (but note the criteria in Figure 13 are stated in terms of [length:diameter], instead of [length:radius]). 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, one can make closed curves, but only trivial knots. 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 involves showing that if $n > \frac{\text{length of } K}{\pi r(K)}$, then inside the open tube of radius $r(K)$ about $K$, we can construct a polygon edges that is isotopic in the tube to $K$. 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 [30].

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 $\text{MinRad}(K)$. For the second, consider the curve in Figure 14. 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 \textit{doubly critical} pair, and define the \textit{doubly-critical self-distance} of $K$ to be

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

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

\textbf{Theorem characterizing thickness.} The thickness radius $r(K)$ equals the minimum of $\text{MinRad}(K)$ and $\frac{1}{2}dcsd(K)$.

\textbf{A subtlety.} The \textit{self distance} of $K$, a definition generally attributed to N. Kuiper is defined like $dcsd(K)$, but we only require that the chord be perpendicular to the knot at at least one one endpoint; call such a pair of points $(x, y)$ on the knot \textit{singly critical}; and call the infimum of distances between such pairs the \textit{singly critical self distance}, $\text{scsd}(K)$. Typically, there are more singly critical pairs of points than doubly critical pairs (see Figure 14), so, in general,

$$\text{scsd}(K) \leq dcsd(K).$$

Nevertheless, we have

\textbf{Theorem re-characterizing thickness.} The thickness radius $r(K)$ equals the minimum of $\text{MinRad}(K)$ and $\frac{1}{2}\text{scsd}(K)$.

Our definition of thickness seems mathematically natural, and seems appropriate to model “rope” that is completely flexible, albeit inelastic and incompressible. It provides a way to gain insight into the shape of a tight knot as in Figure 1. However, the tight knots shown in Figures 4 and 7 look a bit different from the tight rope. The 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.
Several groups of researchers [10] [11] [17] [23] 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 $(2)(\text{MinRad}(K))$; 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 [17] 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 [26],

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

What about existence and uniqueness of tight conformations? Certainly if we pull a piece of knotted rope tight, it becomes something; 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

**Question.** Does there exist, within each knot type, a $C^2$ curve that minimized ropelength 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 [25] that within each knot type, there exists a sequence of $C^2$ representatives whose ropelengths 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 16 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 the toy one can buy.
that consists of a set of quarter-circles that can be joined end-to-end so they swivel freely.

A number of people have noted that there are simple links that indeed seem to be optimizers having this non-$C^2$ property; but the question of $C^1$ vs. $C^2$ for knots remains open. The simplest link example consists of three curves: two round circles with the same radius, located one above the other in parallel planes, with the third component a “stadium curve” (two semicircles connected by straight line segments) linking the two circles.

**Question.** Are ropelength 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: there can exist different local minima for some link types, in fact continuous families of them! This sounds surprising until we see the example [2]: Construct the example above of two parallel circles linked by a stadium-curve. Now open apart 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 of distinct local minima: 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. (But 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 optimia 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 7 and 8) 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 5, and pull it tight, we do seem to get two different stable minima. This seems also to work with rope, but there is always the question in physical experiments of whether friction is playing a
role, or is what we are observing really being caused by the geometry.

Various people have done experiments (see e.g. [10] [19] [29] [3] [33] (based on [31], summary in [32]), and R. Scharein’s KnotPlot site \(^6\) 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). Given that we seem to be measuring something fundamental about each knot type, it is not entirely surprising that such data correlates well with actual physical behavior of knotted DNA molecules in certain laboratory experiments. This is discussed in [43] and a similar relationship (though not as carefully calibrated) for knot energies in [39]. See also A. Stasiak’s talk in this mini-course. We can see in Figure 15 why more complicated knots ought to move faster in some kind of obstruction field; but the quantitative relationship that seems to hold between rope-length of a knot type and relative gel mobility remains impressive and not fully understood.

Another subtlety. 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 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 in [31] [32] [33]. The approach of [17] also handles polygons in a way that gives converging thickness for converging polygons.

\(^6\)http://www.cs.ubc.ca/nest/imager/contributions/scharein/KnotPlot.html
5 Energy of Knots

Around the time people were beginning to speculate on thickness of knots, they also were thinking about the following “cocktail party” thought-question: 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. One would expect the knot to achieve a conformation that is as “wide open” as possible, so perhaps the same conformations as we see in thick knots.

In addition to its intrinsic appeal, this question was felt to be, and should still be, relevant to the behavior of knotted molecules such as Figures 11 or 12. Electrostatic self-repulsion is an important factor in synthesis and understanding conformations. For example, in laboratory experiments in which DNA strands formed loops [36] [37] 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-repulsion of the DNA molecules.

5.1 Discuss why naive definition of self-repelling energy does not work.

reference [7]

If $X$ and $Y$ are points in $\mathbb{R}^3$ then the standard definition of electrostatic repelling energy, in some units, assuming each point carries a unit charge $q$, is

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

If we had more than two points, we would compute the pairwise potentials and add them up. If we consider two line segments $X, Y$ with a uniform unit charge density on each, it then seems natural to define the electrostatic potential energy of the ensemble of two charged sticks to be

$$\int_{x \in X} \int_{y \in Y} \frac{dx\,dy}{\|x - y\|}.$$ 

This does not have one of the basic properties that 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.
Now suppose we have a knot $K$ in space and we imagine spreading a charge along $K$. We would be led to defining

$$E_{\text{doesn’t work}} = \int_{x \in K} \int_{y \in K} \frac{dxdy}{\|x - y\|}.$$  

Unfortunately, this integral is infinite for all curves. The problem is that it gives too much weight to near-neighbor interactions.

In order to obtain a notion of energy for knots, 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.

5.2 Define Möbius energy, Normal energy, Symmetric energy; note relation of $E_S$ to radiating tubes

References [28] [15] [22] [5] [8]

Möbius energy (regularized to be zero for a round circle) Let $t \rightarrow x$ be a length-preserving parametrization of $K$, where the domain is a circle $C$.

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

Normal energy and Symmetric energy For each pair of points $x, y$ on $K$, let $\alpha$ be the angle between the chord $(y - x)$ and the tangent to the knot at $x$. Let $\beta$ 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

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

implemented in [1] [35]
5.3 Knot energy for polygons: Minimum-Distance energy

ref [41], implemented in [35] [46]
( also cite early work of [16] )

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

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

5.4 Rope-length dominates all the other energies.

ref [8] [6]

5.5 Minimum Distance energy for polygons approximates Möbius energy for smooth curves provided the inscribed polygons are reasonable and the energies are regularized the right way.

ref [40]
6 Historical note

I learned last summer (thanks to E. Rawdon) of a paper [21] 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.
Figure 3: Loose Knot Made of Mouse Cable

Figure 4: Tight Knot Made of Mouse Cable
Figure 5: Cut in different places and then tighten

Figure 6: Loose Knot Made of Chain
Figure 7: Tight Knot Made of Chain

Figure 8: Alternate Conformation of Tight Knot Made of Chain
Figure 9: Drawing of a hagfish.
http://www.zoology.ubc.ca/labs/biomaterials/slme.html

Figure 10: Actual hagfish knotting
http://oceanlink.island.net/oinfo/hagfish/hagfish.html
Figure 11: DNA Knot [45]

Figure 12: DNA Knot [13] [12]
Figure 13: Thick Tubes [26]
Figure 14: Doubly-Critical Self-Distance may be strictly larger than Singly-Critical Self-Distance

Figure 15: 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 16: 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.)

Figure 17: This conformation was obtained from the above one by lowering the minimum distance energy. The curvature is now more uniform, but the maximum tube-thickness is smaller.
To define the THICKNESS $r(K)$, increase radius of meridian disks until they touch.

Figure 18: Defining the thickness of a knot

References


