Role of flexibility in entanglement

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Entanglement is essential to the function of many physical systems. Flexibility and length determine the extent to which the system can become entangled. Given a perfectly flexible unit-radius tube, several researchers have studied the minimum length needed to tie different types of knots. Can one obtain the same configurations with less flexible tubing? Does more flexibility always yield tighter knots? We demonstrate a phase change in flexibility beyond which more flexibility adds very little entanglement. This level of flexibility is surprisingly low and appears to have a global bound. Since tensile strength and flexibility act inversely, this level of flexibility provides the maximal tensile strength for materials that need to pack tightly. This is a basic design principle that should be observable in nature.

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I. INTRODUCTION

Polymer materials derive a great deal of their properties from the entanglement of the polymer strands. This is just one category of the large number of materials made of woven or tangled strands. In general, for a filament there is a trade-off between tensile strength and flexibility—stronger materials (such as wire rope) tend to be less flexible. In this paper we ask: how is entanglement affected by flexibility? We find a phase change. There is a regime in which increased flexibility dramatically increases entanglement possibilities, but then, once the threshold is passed, increasing flexibility gives small if any increase in entanglement. The phase change takes place well short of the flexibility required for a tube to double back on itself. We expect that both natural and designed systems take advantage of this phase change—maximizing strength by requiring only the flexibility needed for the entanglements of the system.

We study this phenomenon by asking how much flexibility is required to achieve "tight" conformations for various entanglement patterns. We find that the flexibility varies—in fact we find patterns that require arbitrarily little flexibility to tighten—but we find that all patterns, including the most common mathematical knots, can be tightened to within 1.5% of perfectly tight with a flexibility of 0.50, the phase change threshold.

II. RESULTS

In this paper, we explore tight knot conformations of idealized rope with different flexibilities. In particular, we find minimal length-to-radius knot conformations with an infinite energy barrier at specific flexibility values. This is done through the use of a discretized ropelength function [1,2] that has been shown to finely approximate the mathematical behavior of ropelength for smooth curves [3]. This approach can be used to analyze the behavior of tight knots on the macroscopic level, such as stiff ropelike materials, or at the microscopic level, such as hard bounds on bond angles in molecules or the study of polymer chains. Alternate approaches for fully flexible materials have been explored in Refs. [4–8].

Consider tying a knot with a piece of steel cable. The inherent inflexibility of the material makes it impossible to construct a circular conformation whose ropelength is 2π (as is the case with a perfectly flexible material). Given a knot-making material with a uniform radius, we compute the flexibility constant f by dividing 2π by the length-to-radius ratio needed to construct a circular conformation. The resulting flexibility values lies in the range $0 < f \leq 1.00$. Thus, a fully flexible material has $f = 1.00$ and can fully double back on itself. A flexibility of $f = 0.50$ is the minimum flexibility re-

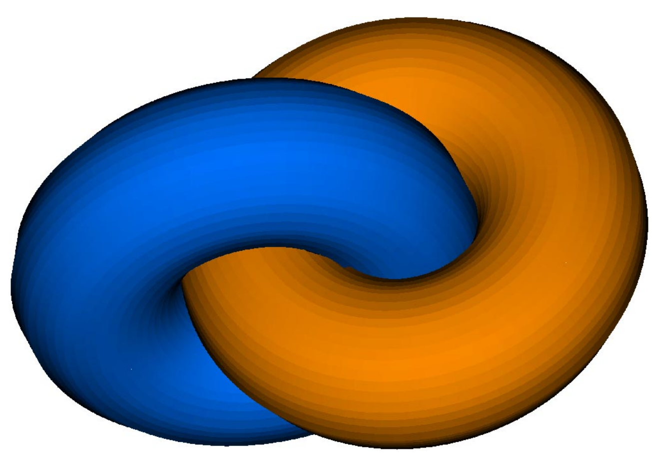

FIG. 1. A tight Hopf link can be tied with a rope of flexibility $f = 0.50$.

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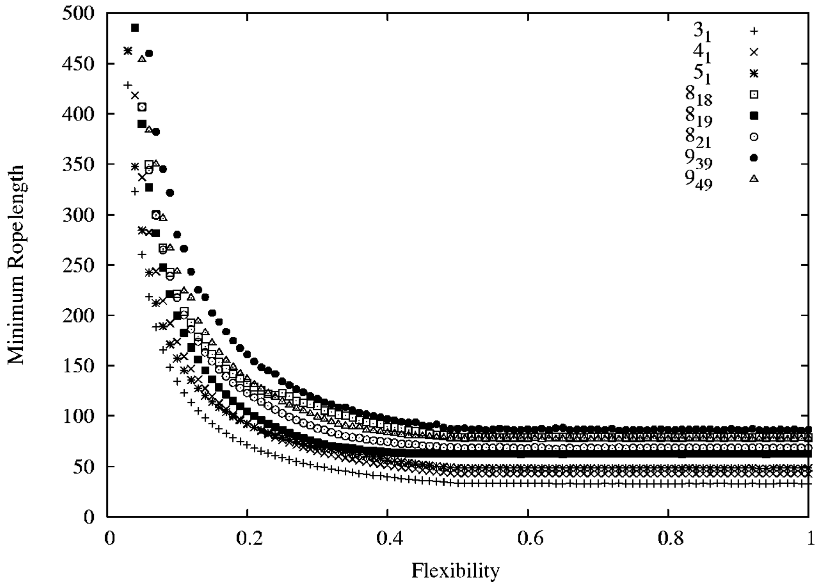

FIG. 2. Minimum L_f values for flexibilities between 0.01 and 1.00.

quired to construct the tight Hopf link shown in Fig. 1.

The concept of "thick" smooth knots was first defined in Ref. [9] by analyzing the maximal radius of a non-self-intersecting tube placed about the knot. Given a fixed length of perfectly flexible tubing with a perfectly hard shell, two behaviors limit the available conformations [3]: the minimal radius of curvature, denoted here as "M," and the distance between pairs of distinct points whose connecting chord is perpendicular to the tangents at both of the points, the so-called "doubly critical self-distance" (D). In particular, it was shown that for a fixed knot conformation K, the maximal radius of a non self-intersecting tube, the thickness radius denoted $R(K)$, is given by $R(K)=\min\{M(K),D(K)/2\}$. To eliminate the effect of scale, the length-to-radius ratio, known as the ropelength, $L(K)=\text{arclength}(K)/R(K)$, is defined. The concepts of M, D, and L are extended rigorously to polygons in Refs. [1,2]. There is some debate over whether the ropelength should be the ratio of the length to the diameter or the radius and the literature contains examples of both. For the sake of this paper, we use the length-to-radius ratio.

One can generalize [10] the definition of ropelength to model knots with restrictions on how quickly the knot can bend. We do this by defining $R_f(K)=\min\{fM(K),D(K)/2\}$, and $L_f(K)=\text{arclength}(K)/R_f(K)$ for $0<f\leqslant 1.00$. The original definition of $R(K)$ is simply the case $f=1.00$. We are interested in minimizing L_f over different knot types to see how flexibility affects the minimizing conformations. If we fix the radius of the tube about the knot to be exactly one, this is equivalent to restricting the minimization to knots whose curvature is $\leqslant f$. The existence of minimizing smooth knots at different flexibility values has been shown in Ref. [11].

Our knot population consists of eight different knot types. Using the classical notation, the knots are 3_1, 4_1, 5_1, 8_{18}, 8_{19}, 8_{21}, 9_{39}, and 9_{49}. These knots were chosen to give a variety of small and larger crossing knots that are alternating and nonalternating. We also analyzed the rest of the prime knots

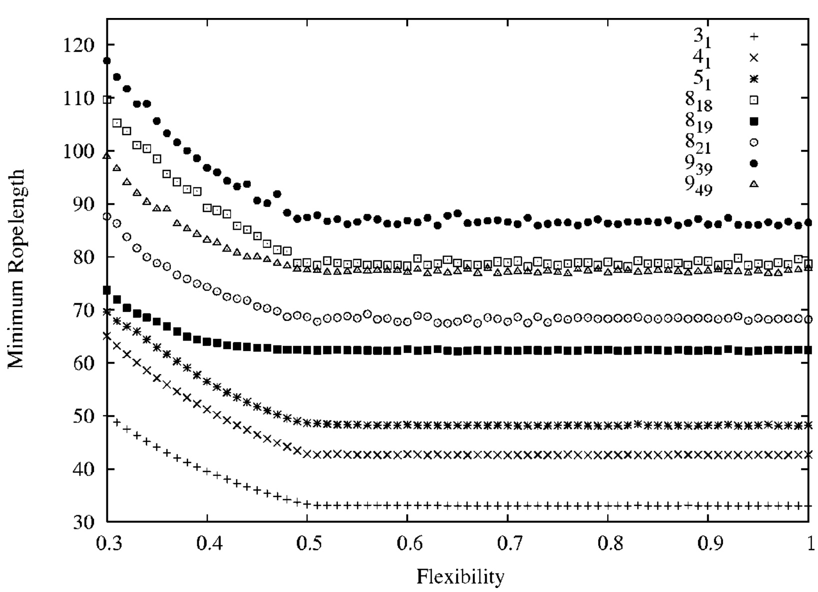

FIG. 3. Minimum L_f values for flexibilities between 0.30 and 1.00. Notice the phase change at 0.50.

TABLE I. For f values between 0.01 and 0.50, we fit a function of the form $a+b/x$ to the data. The table contains the values of a, b, $L_{1.00}$, and $L_{0.50}$ values for the eight knots.

	Fit $a+b/x$		Min L_f	
	a	b	1.00	0.50
3_1	8.06	12.62	33.08	33.29
4_1	10.62	16.31	42.69	42.82
5_1	15.71	14.65	48.26	48.82
8_{18}	37.40	19.25	78.69	78.95
8_{19}	13.46	18.94	62.44	62.46
8_{21}	26.59	19.06	68.22	68.67
9_{39}	47.03	22.63	86.48	87.47
9_{49}	32.30	20.98	77.90	77.53

through 9 crossings (an additional 76 knots) for f values of 1, 3/4, 1/2, 1/4, 1/8, and 1/16. Similar behaviors were observed for the larger knot population; however, we report the the specifics for the eight knots mentioned above. We restricted our attention to equilateral conformations of the different knot types with 64 edges.

We use a modified Metropolis Monte Carlo procedure [12] for flowing the knots to minimizing conformations. Our algorithm begins by choosing two random vertices. We then compute an upper bound $\theta_{\max}$ for the maximum size of a crankshaft rotation that yields the same knot type. A random angle θ is chosen so that $-\theta_{\max} < \theta < \theta_{\max}$ and the crankshaft rotation is completed. If the new knot has a smaller value for L_f, the new knot is accepted. Otherwise, the new knot is accepted with probability $\exp[(-\Delta L_f)/k]$, where $k>0$ decreases to 0 through the computations.

For each of these knots, the minimization algorithm was run for f values between 0.01 and 1.00 by increments of

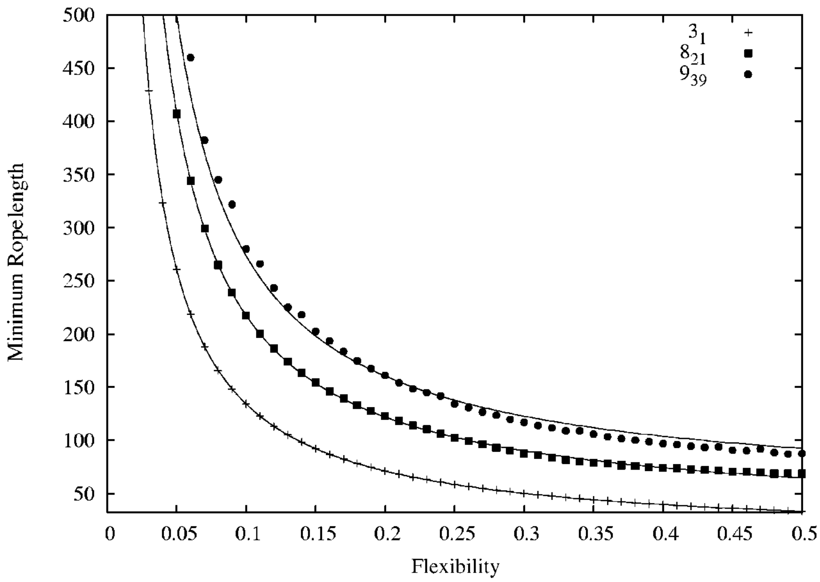

FIG. 4. The graphs of three of the knots with their fitting curves.

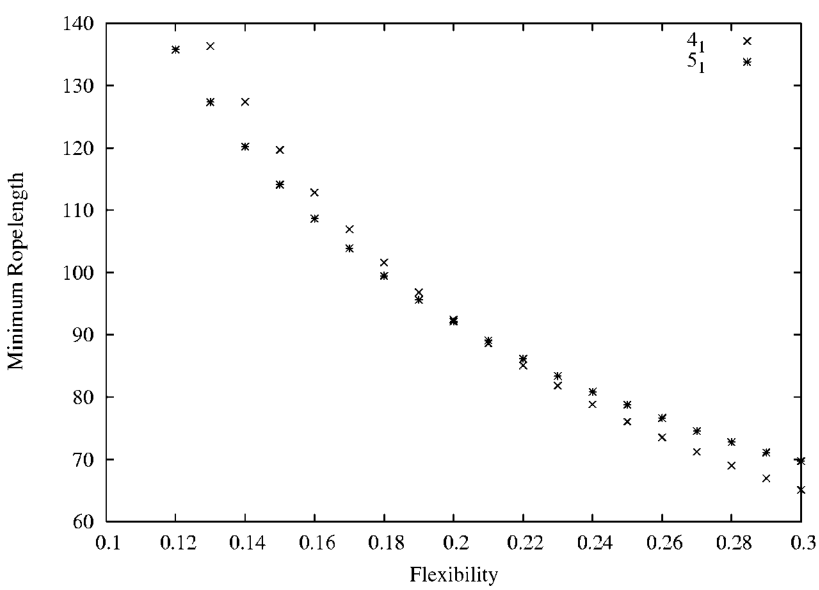

FIG. 5. The graphs of the 4_1 and 5_1 knots cross near $f=0.20$.

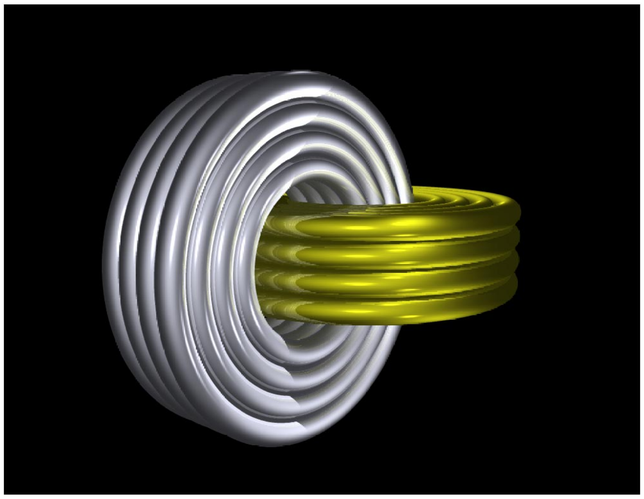

FIG. 6. The packed Hopf links exhibit a family of links for which arbitrarily little flexibility is sufficient to tie a ropelength-minimized conformation.

0.01. We used Scharein's KNOTPLOT [13] to create a base equilateral conformation of each knot type and used this conformation as a common starting point for each of the values of f. The graph of L_f versus f should be nonincreasing since $L_{f_1}(K) \geq L_{f_2}(K)$ when $f_1 < f_2$ for any fixed conformation K. In other words, a more flexible material can always yield the same conformation realized using a less flexible material. We could smooth the data by using previously computed conformations as starting conformations. However, so as not to bias our computations, we decided to use a common starting configuration for each knot type.

The eight knots exhibited similar behavior. For values of f between 0.50 and 1.00, the minimizing conformations and L_f values were nearly identical. Figure 2 shows the entire graph of the flexibility f versus minimal L_f and Fig. 3 shows a graph for flexibility between 0.30 and 1.00. There is a clear phase change that occurs for each of the knots where the graph changes to a roughly horizontal line. For the 3_1, 4_1, 5_1, 8_{18}, 8_{21}, 9_{39}, and 9_{49} knots, the phase change is at 0.50. For the 8_{19} knot, the phase change appears to be at a value slightly less than 0.50. We concentrate on this phenomenon later in this paper. The data shows that a flexibility greater than 0.50 results in little or no improvement in the minimum ropelength. In other words, increasing the flexibility beyond 0.50 results in a small (if any) increase of entanglement possibilities. A flexibility of 0.50 is sufficient for tying the tight Hopf link seen in Fig. 1 and to wrap a circle of radius two about a straight tube of radius one. In a tight knot or link regime, we expect the most tight packing to resemble the packing of the Hopf link, and thus, a flexibility of 0.50 is sufficient for pulling the knot tight.

Pieranski *et al.* [14] determined that a flexibility of 0.90 appears to be sufficient to tie the tightest trefoil. They also considered length shortening evolutions and have observed that the appearance of self-contact changes the rate of evolution. More recent studies [15] suggest that the flexibility required to tie ropelength minima may be even higher. Thus, there may be two phase changes for each knot type with the other phase change occurring at the minimum flexibility sufficient to tie a ropelength minimum. Our computations suggest that the first phase change occurs at a flexibility value always ≤ 0.50. To date, there are no analytic solutions for ropelength minima except for the trivial case of the unknot and for a special class of links [16]. For the class of links, a flexibility of 0.50 is sufficient to tie the tightest conformations. When minimizing conformations are determined for more knots and links, we will know where, and if, the second phase change occurs, although it appears that these values will have to be determined distinctly for each knot and link. Furthermore, Cantarella *et al.* [17] have shown that the tightest clasp needs full flexibility (i.e., $f=1.00$) to obtain a critical state (which appears to be minimal) and the Borromean rings require a flexibility strictly greater than 0.50 to obtain a critical state. However, the length improvement in the tight clasp from $f=0.50$ to $f=1.00$ is approximately 0.17%. In using the full flexibility, the clasp loses some self contact points, which in the case of tying real knots may make the knot more likely to slip. In our computations, the difference

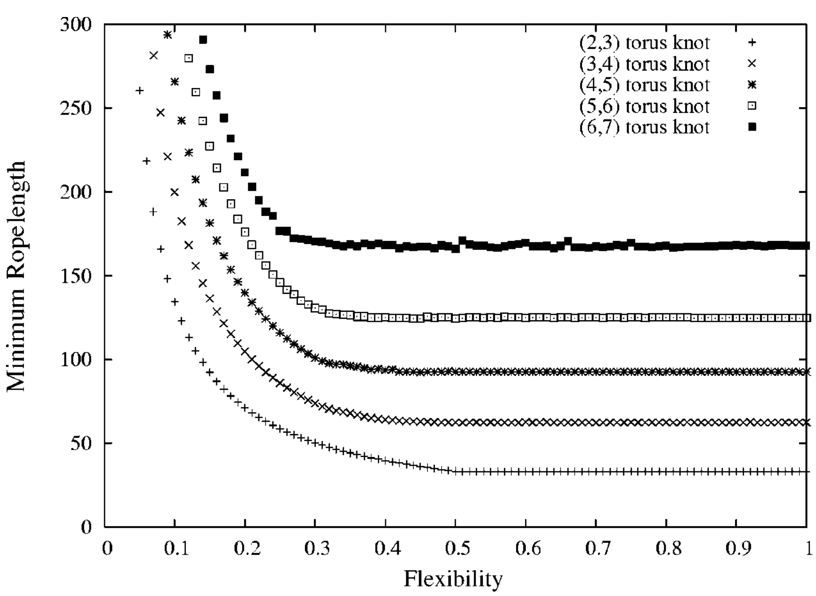

FIG. 7. The amount of flexibility needed to tie a ropelength-minimized $(n,n+1)$ torus knot decreases as n increases.

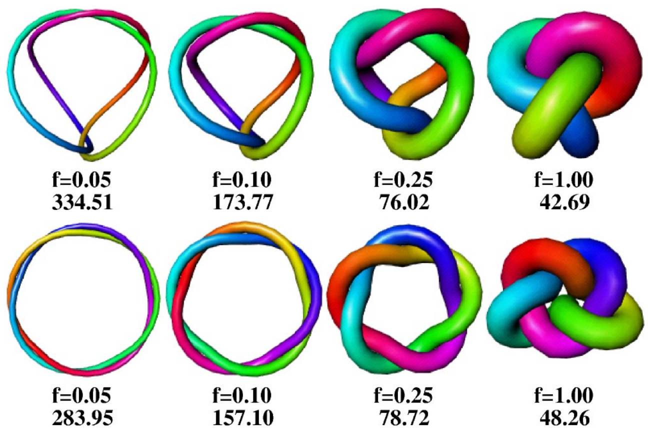

FIG. 8. Minimal conformations of the 4_1 and 5_1 knots for various values of f.

between the minimal ropelength using $f=0.50$ and $f=1.00$ was at worst 1.5%. Thus, we propose that natural materials will forego the minimal tightening gain to make the material stronger.

For f values $0<f\leqslant 0.50$, the graphs can be approximated by a function of the form $a+b/x$. One might assume that the value of a would be equal to the limiting constant value observed from $f=0.50$ to $f=1.00$. However, this is not the case. Table I shows that the value of a for each knot is much different than the limiting value from 0.50 to 1.00. In fact, there appears to be no simple relationship between these values. Figure 4 shows the fitting curves of the form $a+b/x$ for a few of the knots. The fitting curves are very close together so we chose 3_1, 8_{21}, and 9_{39} as representative knots.

Furthermore, the graphs of 4_1 and 5_1 cross near $f=0.20$ (see Fig. 5). As seen in Fig. 6, the 4_1 approaches a more three-dimensional presentation as $f\rightarrow 0$ while the 5_1 approaches a planar conformation. The 4_1 knot is a twist knot, that is, it can be constructed as a series of twists from two parallel segments with the ends clasped together. On the other hand, the 5_1 knot is a torus knot, that is, it can be constructed to lie on a torus. In our experiments, twist knots tended to more three-dimensional conformations while torus knots approached planar conformations resembling interlocked circles. In Table I, the value of b for the 4_1 is 16.31 and for the 5_1 is 14.65, which implies that the growth rate for the 5_1 is smaller as $f\rightarrow 0$.

Note that the 8_{19} knot, also a torus knot, has a nearly horizontal graph from 0.45 to 1.00. Thus, the 8_{19} knot requires even less flexibility from the knot-making material than the other knots analyzed.

This suggests a natural question: are there knots or links for which arbitrarily low flexibility is sufficient to tie a ropelength-minimized conformation? The answer is yes. Consider a family of packed Hopf links [18], an example of which is shown in Fig. 7. If we fix the radius of each strand at one and increase the number of strands in each of the packed loops, the circle formed by a single strand within a packed loop will have larger and larger radii. Thus, the curvature of each strand will approach zero as the number of strands increases.

The 8_{19} is a $(3,4)$ torus knot, meaning that the knot can be formed on a torus so that it wraps three times around the longitude and four times around the meridian. The $(n,n+1)$ torus knots are nonalternating for $n\geqslant 3$. We conjecture that as $n\rightarrow\infty$, the ropelength-minimized $(n,n+1)$ torus knots can be made with arbitrarily low flexibility. This is supported by Fig. 8. We ropelength-minimized the $(n,n+1)$ torus knots for $n=2,3,4,5,6$ for $f=0.01$ to $f=1.00$ by increments of 0.01. Notice that as n increases, the graphs are horizontal for more flexibility values.

III. DISCUSSION

Intuitively, one would imagine that additional flexibility would be advantageous in tying tight knots. To some extent this is true: a perfectly flexible material will have the broadest range of possible conformations. However, flexibility comes at the cost of tensile strength and other physical attributes. We have shown that a flexibility of 0.50 is sufficient to tie nearly minimal ropelength conformations. Thus, one gains very little additional entanglement when the material is more flexible. This is a basic design principle for tube or ropelike materials.

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