Ideal trefoil knot

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A set of self-contact points of the most tight, parametrically tied trefoil knot is determined. The knot is subjected to further tightening procedure based on the shrink-on-no-overlaps algorithm. Changes in the structure of the set of the self-contact points are monitored and the final form of the set is determined.

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I. INTRODUCTION

Finding the best way of packing a tube within a box seems to be rather a gardening problem than a scientific one. However, the optimal single helix, discovered in a computer simulation study of this problem, [1] and [2], proves to be ubiquitous in many proteins as their α-helical parts. As suggested in [3], it also seems that the closely packed double helix appearing in the process of twisting two ropes together [4] have been already discovered and applied by nature. Laboratory experiments allow one to observe in the real time how the optimal helices are formed in various systems, e.g. the bacterial flagellas [5] or phospholipid membranes [6].

Both processes, of packing the ropes and twisting them together, occur simultaneously when a knot tied on a rope becomes tightened. The problem of finding the most tight, least rope consuming conformations of knots was independently posed and indicated as essential by different authors; for references see [7]. Knots in such optimal, most tight conformations are often called *ideal*, a term proposed by Simon [8], and introduced into the literature by Stasiak and coworkers [9]. Ideal conformations minimize the value of the size-invariant variable $\Lambda = L/D$, where L and D are, respectively, the length and the diameter of the *perfect rope* (defined below) on which the knot is tied. The only knot whose ideal conformation is known at present is the trivial knot (unknot). See Fig. 1. Its length in the ideal, circular conformation equals πD, thus $\Lambda = \pi$. Finding the ideal conformation of a nontrivial knot is a nontrivial task. Initiated a few years ago search for the ideal conformations of nontrivial knots continues.

One of the algorithms used in the search is SONO (shrink-on-no-overlaps) [10]. SONO simulates a process in which the rope, on which a knot is tied, slowly shrinks. The rope is allowed to shrink only when no overlaps of the rope with itself are detected within the knot. When such overlaps occur, SONO modifies the knot conformation to remove them. If this is no more possible, the process ends. Unfortunately, ending of the tightening process does not mean that the ideal conformation of a given knot was found. The tightening process could have stopped also because a local minimum of the thickness energy was entered. The possibility that there exists a different, less rope consuming conformation, cannot be excluded.

SONO has been used in the search of ideal conformations of both prime and composite knots. Parameters of the least rope consuming conformations found by the algorithm were listed in [11] and [12]. In a few cases, SONO managed to find better conformations than the simulated annealing procedure [9]. However, for the most simple knots, in particular, the trefoil knot, the simulated annealing and SONO provided identical results; the Λ values are identical within experimental errors. This strongly suggests that no better conformations of the knot exist. We feel obliged to emphasize, however, that it is only an intuitively obvious conclusion — no formal proofs have been provided so far. As indicated in [3], we are in a situation similar to that, which lasted in the problem of the best packing of spheres for 400 years. That the face centered cubic and hexagonal close packed lattices were among the structures that minimize the volume occupied by closely packed hard spheres seemed to be obvious since the times of Kepler, however the formal proof of the conjecture was provided but a few years ago [13]. Waiting for the formal proofs that what we have observed in the knot tightening numerical experiments is the ideal conformation of the trefoil, seems to be a too cautious attitude. Thus, after a few years of experimenting, we decided to present the best, least rope consuming conformation of the trefoil knot we managed to find. We compare it with the most tight conformation of the knot that can be found within the analytically defined family of torus knots. In particular, we describe the qualitative change in the set of self-contacts that takes place within the trefoil knot during the tightening process. We believe that some of the features of the self-contact set we have found may be present also in ideal conformations of other knot types.

An alternative method of searching for the most tight conformations of knots consists in inflating the rope on which the knot has been tied In such a process the length of the rope is kept fixed. The maximum radius to which the rope in a given conformation of a knot can be inflated is closely

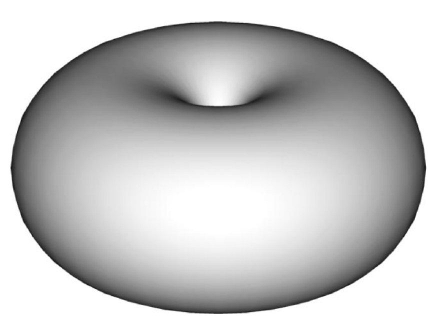

FIG. 1. Ideal unknot.

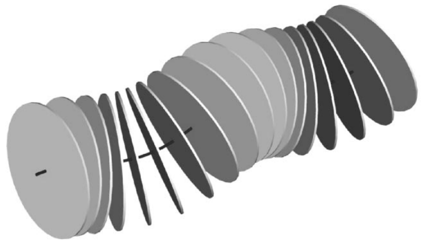

FIG. 2. Schematic construction of the perfect rope. Its perpendicular sections are always circular. None of the sections are allowed to overlap.

related with the injectivity radius considered in detail by Rawdon [14].

II. THE PERFECT ROPE

It is the aim of the computer simulations we perform to simulate the tightening process of knots tied on the *perfect rope*: perfectly flexible, but at the same time perfectly hard in its circular cross section. The surface of the perfect rope can be seen as the union of all circles centered on and perpendicular to the knot axis C. See Fig. 2.

We assume that C is smooth and simple, i.e., self-avoiding, what guaranties that at each of its points $\mathbf{r}$ the tangent vectors $\tau(\mathbf{r})$, and thus the circular cross section, are well defined. The surface remains smooth as long as: (a) the *local curvature radius* r_κ of the knot axis is nowhere smaller than $D/2$, (b) the *minimum distance of closest approach* d_* is nowhere smaller then $D/2$.

The *minimum distance of the closest approach* d_*, known also as the *doubly critical self-distance*, see [8], is defined in [15,16], as the smallest distance between all pairs of points $(\mathbf{r}_1,\mathbf{r}_2)$ on the knot axis, having the property, that the vector $(\mathbf{r}_2-\mathbf{r}_1)$ joining them is orthogonal to the tangent vectors $\tau(\mathbf{r}_1),\tau(\mathbf{r}_2)$ located at the points:

$$d_*(C)=\min_{\mathbf{r}_1,\mathbf{r}_2\in C}\{|\mathbf{r}_2-\mathbf{r}_1|:\tau(\mathbf{r}_1)\perp(\mathbf{r}_2-\mathbf{r}_1),\tau(\mathbf{r}_2)\perp(\mathbf{r}_2-\mathbf{r}_1)\}. \tag{1}$$

As shown by Gonzalez and Maddocks [16], the two conditions can be replaced by a single condition providing that the notion of the *global curvature radius* ρ_G is introduced:

$$\rho_G(\mathbf{r}_1)=\min_{\substack{\mathbf{r}_2,\mathbf{r}_3\in C\\ \mathbf{r}_1\neq\mathbf{r}_2\neq\mathbf{r}_3\neq\mathbf{r}_1}}\rho(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3), \tag{2}$$

where, $\rho(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ is the radius of the unique circle (the circumcircle) that passes through all of the three points: $\mathbf{r}_1$,$\mathbf{r}_2$ and $\mathbf{r}_3$. Using the notion of the global curvature, the condition that guaranties smoothness of the knot surface can be reformulated as: (c) the global curvature radius ρ_G of the knot axis is nowhere smaller than $D/2$.

Analysis of the conformations produced by the SONO algorithm proves that conditions (a) and (b), [and (c)] are fulfilled.

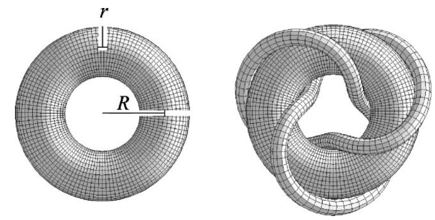

FIG. 3. The trefoil knot is a torus knot. It can be conveniently tied on the surface of a torus.

III. PARAMETRICALLY TIED TREFOIL KNOT

The trefoil knot can be tied on the surface of a torus. See Fig. 3. Consider the set of three periodic functions:

$$x=[R+r\cos(2\ \nu_2\ \pi\ t)]\sin(2\nu_1\pi t) \tag{3}$$

$$y=[R+r\ \cos(2\ \nu_2\pi t)]\cos(2\nu_1\pi t), \tag{4}$$

$$z=r\ \sin(2\ \nu_2\ \pi\ t). \tag{5}$$

The trajectory determined by Eqs. (3)–(5) becomes closed as t spans a unit interval. For the sake of simplicity we shall consider the [0,1) interval. For all relatively prime integer values of ν_1, ν_2 Eqs. (3)–(5) define self-avoiding closed curves located on the surface of a torus. R denotes here the radius of the circle determining the central axis of the torus while r denotes the radius of its circular cross-sections. For the trefoil knot, frequencies ν_1, ν_2 equal 2 and 3, respectively. In what follows we consider knots tied on a rope; trajectories defined by Eqs. (3)–(5) determine position of its axis.

The (ν_1,ν_2) and the (ν_2,ν_1) torus knots are ambient isotopic, i.e., they can be transformed one into another without cutting the rope on which they are tied [17]. As shown previously, the (2,3) version of the trefoil is less rope consuming [12]. Thus, the (3,2) version will not be discussed below.

Assume that the trefoil knot whose axis is defined by Eqs. (3)–(5) is tied on a rope of diameter $D=1$. In what follows we shall refer to it as the *parametrically tied trefoil* (PTT) *knot*. In such a case, the radius r of the torus on which the axis of knot is located, cannot be smaller than 1/2; below this value overlaps of the rope with itself will certainly appear; at $r=1/2$ the rope remains in a continuous self-contact along the torus axis. To keep the self-contacts we assume in what follows that $r=1/2$. To check, if the knot is free of overlaps in other regions, one can analyze the map of its internal distances. Let t_1 and t_2 be two values of the parameter t, both located in the [0,1) interval. Let (x_1,y_1,z_1) and (x_2,y_2,z_2) be the coordinates of two points indicated within the knot axis by t_1 and t_2, respectively. Let $d(t_1,t_2)$ be the Euclidean distance between the points:

$$d(t_1,t_2)=\sqrt{(x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2}. \tag{6}$$

The map of the function, see Fig. 4, displays a mirror symmetry induced by the equality $d(t_1,t_2)=d(t_2,t_1)$.

Looking for possible overlaps within the knot one looks for regions within the internal distances landscape, where $d(t_1,t_2)<1$. The most visible depression within the land-

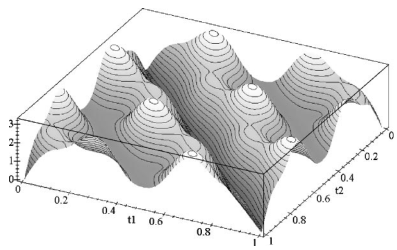

FIG. 4. The map of the intraknot distances of the most tight PTT knot.

scape of the interknot distances is located around the diagonal where $t_1 = t_2$. As easy to see, $d(t_1,t_2)=0$ along the line, but for obvious reasons this does not imply any overlaps within the knot.

Another valley within which $d(t_1,t_2)$ may go down to the critical 1 value is localized in the vicinity of lines defined by equality $|t_2 - t_1| = 1/2$. To see, if in the vicinity of the lines the height really drops to or even below 1, we plotted the map of the $d(t_1,t_2)$ function in such a manner, that regions lying below the arbitrarily chosen 1.005 level were cut off. As seen in Fig. 5 there are four such regions within the PTT knot: one in the shape of a sinusoidal band and three in shapes of almost circular patches.

The band contains in its middle the above mentioned continuous line of self-contacts points; it is the axis of the torus on which the knot is tied. The circular patches contain three additional contact points; when R becomes too small, overlaps appear around the points. Numerical analysis we performed reveals that (with the five decimal digits accuracy we applied) the overlaps occurring within these regions vanish above $R=1.1158$. For $R=1.1159$ the distance between the closest points located within these regions of the knot equals 0.9999. For $R=1.1158$ the distance is equal to 1.0000. Where, within the PTT knot the self-contact points are located is shown in Fig. 6

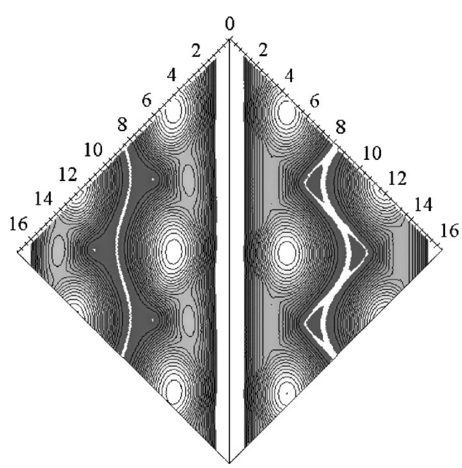

FIG. 5. Maps of the intraknot distances as seen from above. Left — the most tight PTT knot. Right — the most tight STT knot. The sets of the self-contact points are located within the white regions of the map.

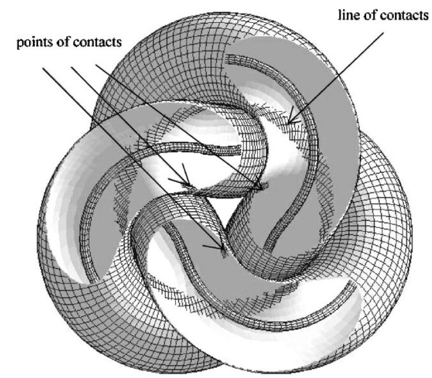

FIG. 6. Location of the self-contact points within the most tight PTT knot.

IV. SONO TIED TREFOIL KNOT

Considerations presented above indicated the value of R, at which the PTT knot reaches its most tight conformation. The length L_t of the rope engaged in this conformation of the trefoil knot equals 17.0883. Can one tie the trefoil knot using a shorter piece of the rope? Theoretical considerations indicate that this possibility cannot be excluded. As proven in [18] the piece of rope used to tie the trefoil knot cannot be shorter than $Lm=(2+\sqrt{2})\pi \approx 10.72$. This lower limit leaves a lot of place for a possible further tightening of the knot. Application of SONO reveals that the tightening is possible providing the conformation of the knot is allowed to leave the subspace of the parametrically tied torus conformations. This happens spontaneously in numerical simulations in which the most tight PTT knot is supplied to SONO as the initial conformation. SONO algorithm manages to make it shorter. In the simulations we performed, SONO reduced the length of the knot by about 4% to $L_{exp}=16.38$. The discrete representation of the knot used in the simulations contained $N=327$ nodes. Below we describe the final conformation. For the sake of simplicity we shall refer to trefoil knots processed by the SONO algorithm as the SONO tied trefoil (STT) knots.

The differences in the conformation of the most tight conformations of the PTT and STT knots is a subtle one. The essential difference lies in the structure of the sets of their self-contact points. As mentioned above, the circular line of self-contact points present in the family of the PTT knots stays intact as R is changed within the family. Tightening of a PTT knot achieved by decreasing the radius R of the torus stops when additional dscrete points of contacts appear at three locations within the knot. This happens as R becomes equal 1.1158. Further tightening of the knot within the family of PTT knots is not possible, it becomes possible within the family of the STT knots.

During the tightening process carried out by SONO, the set of the self-contact points undergoes both qualitative and quantitative changes. First of all, the line of contacts present in the PTT knot changes its shape becoming distinctly non circular. Secondly, the three contact points give birth to pieces of new line of self-contacts. Unexpectedly, the new pieces do not connect onto a new line, wiggling around and crossing the old line, but they are mounted into the old line

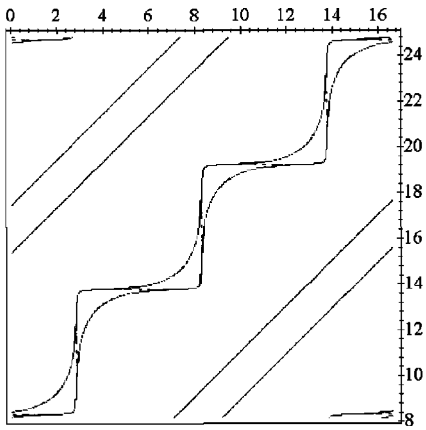

FIG. 7. The set of the self-contact points as seen within the intraknot distances map.

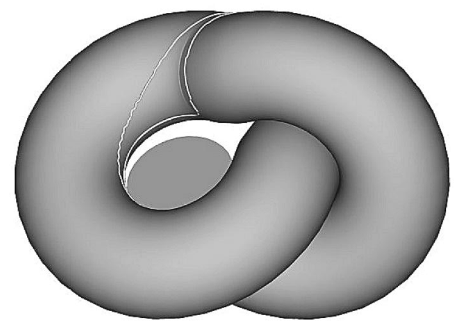

FIG. 8. Location of the line of self-contact points within the most tight STT (ideal) knot. A part of the rope was removed.

in such a manner, that a single, self-avoiding and knotted line of self-contacts is created. That this is the case was revealed by a precise analysis of the interknot distances function. A map covering the interknot distances only within the very thin [1.000 00,1.000 02] interval shows two separated lines, see Fig. 7, corresponding to a single, self-avoiding and knotted line of contact. See Fig. 8.

In addition to the line, a set of three points of self-contacts is formed. The points are located at places where the line of self-contacts becomes almost tangent to itself. The self-contact line runs twice around the knot. As a result, each of the circular cross-sections of the rope stays here in touch with another two such sections. The close packed structure formed in such a manner is much more stable than the structure of the most tight PTT knot, where single contacts were predominant. Let us note, that Fig. 1(e) presented in Ref. [16] a similar self-contact line structure can be seen. Unfortunately, inspecting the figure one cannot see, if the ''self-contact spikes'' shown there form a single, self-avoiding, knotted or a double, crossing itself line. The problem was not discussed in the text. Let us emphasize, however, that the difference between the two possibilities is confined to a zero-measure set.

V. DISCUSSION

Ideal knots are objects of which very little is known. The only knot whose ideal conformation is known rigorously is the unknot. Its ideal conformation, a circle of a radius identical with the radius of the rope on which it is tied, can be conveniently described parametrically. The set of the self-contact points is here limited to a single point: the center of the circle. All circular sections of the rope meet at this point. The maximum local curvature and the minimum double critical self-distance limiting conditions are simultaneously met.

The situation in the case of the trefoil knot, the simplest non trivial prime knot, is radically different. Here the most tight parametrically defined conformation proves to be not ideal. As demonstrated by the present authors, it can be tightened more with the use of the SONO algorithm. The set of the self-contact points becomes rebuilt during the tightening process. Its topology becomes different. In the case the PTT knot the set of the self-contact points consists of a circle and three separated points. As the numerical experiments performed by us suggest, that in the case of the STT knot, the set of the self-contact points turns unexpectedly into a single line. The structure of the set of self contact points in other prime knots remains an open question.

The choice of the parametrization, Eqs. (3)–(5), which we used to define the conformation from which SONO started its knot tightening action, was stimulated by the fact that the trefoil knot is a torus knot. Following Trautwein and Kauffman [7] one could try to construct Fourier parametrizations that would be located closer to the most tight conformation found by SONO. Preliminary calculations we performed indicated that to reproduce with a reasonable accuracy the structure of the most tight STT knot one has to take into account a large number of harmonics. One of the reasons of the slow convergence of the Fourier parametrization is that the Cartesian coordinate system is not well suited; in the case of torus knots the toroidal coordinate system is more natural. Finding a precise but concise parametric description of the most tight trefoil knot is an interesting task.

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