A principle for ideal torus knots

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Abstract – Using bent-helix embeddings, we investigate simple and knotted torus windings that are made of tubes of finite thickness. Knots which have the shortest rope length are often denoted as ideal structures. Conventionally, the ideal structures are found by rope shortening routines. It is shown that alternatively they can be directly determined as maximally twisted structures. In many cases these structures are also structures with zero strain-twist coupling, i.e. structures that neither rotate one or the other way under strain. We use this principle to implement rapid numerical calculations of the ideal structures and subsequently quantify them by their aspect ratio. The results are compared with the aspect ratios of biological torus molecules.

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Introduction. – Knots which are made with as little amount of rope as possible have been denoted as ideal knots [1–3]. Physical knots are made of circular tubes of finite thickness. Therefore, they are of interest in modeling real physical systems with this constriction, e.g., polymers and biopolymers [4–7]. In the mathematics literature, the rope length $L(K)$ has a precise meaning [8–10]. It is the length of the curve defining the knot divided by its thickness. In general, the minimal rope length and the corresponding knot geometry is not known. The problem has only been solved for the trivial knot, which has rope length $2\pi$. For any other knot a lower bound has been found for the rope length, $L(K) \geq 15.66$ [11], but the knots have been optimized on a case-by-case basis using different algorithms.

In many minimalization problems one does not have a way of determining if an optimum state has been reached. Examples are common algorithms for NP complete problems. This is also the case for the relatively simple problem of shortening a thick knot for which successful algorithms [12,13] and energy minimalizations [7,14,15] have been proposed. For knots, we present a twist neutrality analysis that can reveal if they are absolutely shortened or not. Further, in many cases a corresponding algorithm can be used to compute an optimal knot within a given class of embeddings [15].

In this letter, a small step towards finding a general principle for characterizing ideal knots is taken. A method for the determination of minimal torus knots for knots restricted to having a bent-helix embedding, is suggested using our principle of maximally twisted structures introduced for ropes [16,17]. For other discussions of rope-like structures, see [18–20]. Although tube models have been compared to the folding patterns of proteins [21,22], the interest in knots of toroidal geometry have traditionally been mostly mathematical.

The conditions based on which tubes can be closed to form a torus knot are straightforward. Specifically, a $(p, q)$ torus knot denoted $T(p, q)$ is obtained by looping a tube on a torus $p$ times with $q$ revolutions before joining its ends. A torus knot is topologically trivial, i.e. a unknotted loop, when either $p$ or $q$ is equal to 1. The simplest non-trivial example is the $T(3, 2)$ knot, which topologically is a trefoil knot. We consider embeddings with the following parametric description of the $T(p, q)$ knot, i.e. the bent-helix embeddings,

$$x = (R + a \cos(pt)) \cos(qt),$$
$$y = (R + a \cos(pt)) \sin(qt),$$
$$z = a \sin(pt)$$

for $0 \leq t < 2\pi$. In this letter, the torus knots are wrapped on a torus, where $a$ is the helix radius and $R$ the torus radius; $D$ will denote the thickness of the knot, see fig. 1.

The literature on the study of ideal knots is well established [2]. Yet the problem of how to minimize the length of knots, and other questions have not been answered. E.g., what is the length, $L(3, 2)$, of the simplest non-trivial
links and $(2m + 1, 2)$ torus knots from joining the ends of a circular double helix. The geometry of the typical circular double helix has been investigated in [17]. The double helix that makes a closed loop after one revolution becomes the $(2m, 2)$ torus link. The period, $T$, of the parametrization must obey $T = 2m\pi$, where $R/h = m \in \mathbb{N}$; here $R$ is the torus radius and $h$ is the reduced helical pitch, $h = H/2\pi$; the helical pitch is denoted by $H$. For the double helix, where the strands make a closed loop after two revolutions the period obeys $T = (2m+1)\pi$, and $R/h = m + 1/2, m \in \mathbb{N}$. The knot is a $(p,2) = (2m + 1, 2)$ torus knot. For the double helix, this completes the set of possible torus knots and links. For simplicity, we only discuss how to find ideal torus knots.

Here, we describe two different ways of optimizing such torus structures. First, with respect to incremental twist, $f_0$, and then with respect to volume fraction $f_V$. Mathematically, a minimal knot is one with a minimal rope length under the embedding that it is confined to a torus and has a trigonometrical parametrization equivalent to eq. (1). Imagine that the radius of the torus is very large, in this case the knot is tied on what is essentially a straight cylinder. The knot is therefore locally a two-stranded rope. The geometrical structure with zero strain-twist coupling of a rope has the property that it is maximally twisted, and this secures that the rope length of the strands is minimized [16]. Non-maximally twisted structures can reduce their rope length, per 2$\pi$ progression of the rope, upon further twisting. Similarly, the ideal torus knots are the maximally twisted double helices with closed circular geometry. Therefore, in our notation the ideal torus knot of length $L$ is the knot that maximizes $f_0 = D\Theta/L$, where $\Theta$ is the twist angle. The function $f_0$ is called the incremental twist in ref. [17], and its maxima are helices that neither rotate one or the other way under strain. The incremental twist, $f_0$, for a toroidal helix reads

$$f_0 = \frac{D}{a} \left(\frac{1}{2\pi} \int_0^{2\pi} \sqrt{1 + \frac{H}{2a} \left(1 - \frac{a}{R} \cos\phi\right)^2} \, d\phi\right),$$

where $\phi$ is an integration parameter over one pitch of the bent helix. A way to find ideal knots is the following. Take as special case the $T(p,2)$ knot, where we have $R = (p/2)h$. Calculate the incremental twist $f_0(D/R,H/D)$. Then we have

$$\frac{df_0(R/D,H/D)}{d(H/D)} = \frac{\partial f_0}{\partial(R/D)} \frac{\partial(R/D)}{\partial(H/D)} + \frac{\partial f_0}{\partial(H/D)}.$$  

The condition for an ideal knot (with extrema) is

$$\frac{\partial f_0}{\partial(R/D)} \frac{p}{4\pi} + \frac{\partial f_0}{\partial(H/D)} = 0.$$  

Here we have calculated along the line $R/D = (p/2)h/D = (p/4\pi)H/D$, since this is the condition for the strand to
make a closed loop. Under the condition that a structure with proper strand contacts exists at this extrema, the ideal knot criterion becomes the same as the twist neutrality criterion, where the twist neutrality criterion is defined to be characterized by a vanishing strain-twist coupling.

As the ideal torus knots maximize $f_\Theta$, they can be found in the following simple way. Figure 2 shows a plot of $f_\Theta$ as a function of the dimensionless pitch, $H/D$, for two examples of knot classes: The “isoknot” lines in fig. 2 correspond to the family of $T(17, 2)$ and $T(19, 2)$ torus knots with inter-strand contact. Among these knots we find the one which maximizes $f_\Theta$ at the apex of the isoknot line.

Another way of optimizing the torus structures is by maximizing the volume fraction, i.e. finding close-packed structures. The volume fraction, $f_V$, is here defined as the local volume of the two tube compared to the volume of an enclosing bent cylinder. For a toroidal double helix,

$$f_V = \left( \frac{2a}{D} + 1 \right)^{-2} \times \frac{1}{\pi} \int_0^{2\pi} \sqrt{\left( \frac{2\pi a}{H} \right)^2 + \left( 1 - \frac{a}{R} \cos \phi \right)^2} \, d\phi. \quad (5)$$

Having discussed $T(p, 2)$ knots, we will mention the simpler case of taking $q = 1$, i.e. the $T(p, 1)$ “knot”. As said, this is actually an unknotted geometry that is topologically trivial but geometrically it is a slinky which makes $p$ loops around the torus. This circular helix has been studied in [17], where the conditions for the tube to be in contact were solved. The $T(p, 1)$ geometry can be used to model biological molecules with toroidal geometry and $p$-fold symmetry.

**Results.** Detailed results for the knots and trivial knots can be found in tables 1 and 2. Results for $T(p, 2)$ knots are listed in table 1. The estimate for the rope length of the ideal torus trefoil is $L(3, 2) = 17.088$. In table 2 the characteristics of the $T(p, 1)$ optimized torus
knots are given. The ideal $T(p,q)$ (with $q \geq 3$) torus knots can be found from the closed circular triple helix by a simple generalization of the methods used in the previous section. These results are straightforwardly generalized to links. Knots correspond to $(2m + 1,q)$ embeddings while links correspond to $(2m,q)$ embeddings.

Figure 3 is a plot of the aspect ratio $A$ (outer diameter to width) of torus geometries with increasing number of loops, $p$. A fat torus has aspect ratio equal to two. The upper curve gives the aspect ratios for the $T_{\text{ZT}}(p,2)$ knots that are optimized with respect to twist. The curve below gives the aspect ratios for the $T_{\text{CP}}(p,2)$ knots that are optimized by volume fraction. The bottom curve gives the aspect ratios for the $T_{\text{CP}}(p,1)$ “knots” that are optimized with respect to volume fraction. It is seen that within these optimizations, the theoretical aspect ratio is almost a linear function of the number of loops, $p$.

In Fig. 3 the aspect ratios for ten different biological torus molecules (viruses, chaperones and protein complexes) derived using all-atom van der Waals models are plotted, for a summary see Table 3. These molecules do not consist of a single long-chain molecule, but of $p$ shorter chains. A typical number for $p$ is seven. Whether, or not, they can be directly compared to the ideal torus structures is therefore subject to confirmation. To a first approximation the aspect ratio of our measured torus molecules follows the linear trend.

Discussion. – It is unknown which principles are effective in shortening of knots. And if such principles can lead to a unique solution. The presented analysis of maximally twisted structures gives an idea of how to proceed. For the limited case of torus knots, the suggested principle is a direct way of absolute shortening. The study of closed circular-helix structures that are maximally twisted turns out to provide a simple analysis of the lower bounds on rope lengths. Data on $T(p,1)$ and $T(p,2)$ knots is included, and it could straightforwardly be extended to larger classes of torus knots. Further, the computation of the rope length of the $T(3,2)$ torus knot gives a value which agrees with previous results in the literature.

By looking at the experimentally determined aspect ratios of torus molecules, one can even speculate that the principle of maximal twist might play a role in determining

Table 2: $T(p,1)$ torus slinky found by optimizing volume fraction. The first column is the knot type, the following columns are geometric quantities that characterize the knot: $a/R$ and $H/D$. The fourth column is the rope length, $L(p,1)$, of the knot computed using the criterion of maximal $f_V$. The last column is the aspect ratio, $A$, of the knot.

| Type | $a/R$ | $H/D$ | $L(p,1)$ | $A_{\text{CP}}$ |
|------|-------|-------|----------|---------------|
| $(9, 1)$ | 0.16968 | 1.35594 | 22.3099 | 3.3413 |
| $(11, 1)$ | 0.14972 | 1.31317 | 27.8621 | 3.72327 |
| $(13, 1)$ | 0.13481 | 1.28131 | 33.6390 | 4.09197 |
| $(15, 1)$ | 0.12301 | 1.25664 | 39.5856 | 4.45214 |
| $(17, 1)$ | 0.11330 | 1.23694 | 45.6612 | 4.80656 |
| $(19, 1)$ | 0.10512 | 1.22084 | 51.8356 | 5.15696 |
| $(21, 1)$ | 0.09811 | 1.20741 | 58.0886 | 5.50436 |
| $(23, 1)$ | 0.09200 | 1.19604 | 64.4035 | 5.84955 |
| $(25, 1)$ | 0.08664 | 1.18628 | 70.7694 | 6.19298 |
| $(27, 1)$ | 0.08188 | 1.17780 | 77.1777 | 6.53499 |
| $(29, 1)$ | 0.07763 | 1.17036 | 83.6217 | 6.87585 |

Fig. 3: (Colour on-line) Plot of the aspect ratio $A = D_e/W$ as a function of the number of loops, $p$, for torus knots $T(p,2)$ that are maximally twisted (top curve) and close-packed (middle curve). The three depicted knots are from left to right, $T_{\text{ZT}}(7,2)$, $T_{\text{ZT}}(11,2)$ and $T_{\text{ZT}}(21,2)$ corresponding to the yellow point (top curve) below the arrow. The bottom curve is the aspect ratio for the torus slinky $T(p,1)$ which is close-packed. The three symbols, □, ○, and △, identify ten torus molecules where the aspect ratio has been calculated from molecular structures (table 3). Here, the symbol □ is used for viruses, ○ for protein complexes and △ for chaperones.

Table 3: Biological torus molecules: listed are PDB ID, bibliographical reference, type and the $(p,f)$-fold) symmetry. The last column is the measured aspect ratio, $A$, of the torus molecule using all-atom van der Waals models.

| PDB ID | Ref. | Type | $p$ | $A$ |
|--------|------|------|-----|-----|
| 4H5P   | [36] | virus | 4   | 2.60 |
| 4H5O   | [36] | virus | 5   | 3.28 |
| 4H5Q   | [36] | virus | 6   | 2.96 |
| 1RXM   | [37] | complex | 6   | 2.71 |
| 1I5L   | [38] | complex | 7   | 2.41 |
| 2C7D   | [39] | chaperone | 7   | 2.33 |
| 3KFE   | [40] | chaperone | 8   | 3.60 |
| 1C9S   | [41] | complex | 11  | 4.24 |
| 1H5W   | [42] | virus | 12  | 4.24 |
| 3KML   | [43] | virus | 17  | 3.63 |
what the geometry is of biological torus molecules that are formed naturally on the nano-meter scale. In any case, it is remarkable how symmetric Nature’s torus molecules can be.

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