Torus Knots with Polygonal Faces

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Abstract

We review several methods of constructing models of torus knots with non-planar polygonal faces, with the majority of hexagons and some non-hexagons. These methods were developed by the authors throughout recent years, albeit mostly in the context of chemical research on carbon nanostructures. The resulting hypothetical molecular structures are predicted to be chemically stable if care is taken in arranging non-hexagons in the midst of hexagons. Among them, a general scheme that is applicable to arbitrary torus knots (p, q) with $p < q$ is presented. For the simplest nontrivial case, a trefoil knot, two additional routes can be drawn. Noteworthily, one of them is inspired by Escher's artwork *Knots*. These models are realized physically with the technique of mathematical beading.

Introduction

Torus knots are ones that lie on the surface of a torus in 3D. They constitute a good part of recreational mathematics among other geometric figures such as polyhedra. A torus knot can be uniquely and topologically defined by two coprime integers (p, q), where p is the number of windings the knot has around the central axis and q is that of around the center circle of the torus. A more canonical parametrization of a torus knot can be written as follows,

$$\begin{aligned} x &= (R + r\cos(q\phi))\cos(p\phi) \\ y &= (R + r\cos(q\phi))\sin(p\phi) \\ z &= r\sin(q\phi), \end{aligned} \tag{1}$$

where $R > r$ are the two characteristic radii of the torus in this representation, and ϕ ranges from 0 to 2π. In this paper we will discuss only the case where $p < q$, since in our point of view its geometric implication is simpler than otherwise. The simplest nontrivial torus knot, the trefoil knot, is given by $(p, q) = (2, 3)$.

Our goal is to construct torus knots with polygonal faces (not necessarily planar) and trivalent nodes. This is motivated by our previous studies on complex graphitic structures and on the beaded representations of them, in chemical and educational literatures as well as in Bridges. These structures are composed of trivalent carbon atoms and possess nontrivial geometries and topologies. In this context, one of the building blocks is carbon nanotubes (CNT), which refer to straight tubules obtained by rolling up a hexagonal honeycomb. We ask the question of building nanotube structures where the center line of the tube (approximately) follows Eq.1. We remind the readers of Euler's formula $\chi = V - E + F$ of a general polyhedron, where χ is the Euler characteristic of the closed surface which the polyhedron corresponds to, and V, E, and F are the number of vertices, edges, and faces of the polyhedron, respectively. In the context of graphitic carbon structures, where each node (atom) is connected with three nearest neighbors (trivalent graphs), this can be translated into the following expression:

$$\sum_{m>2}(6 - m)N_m = 6\chi, \tag{2}$$

where m runs over positive integers starting from 3 and N_k represents the number of k-member ring. As an example, for a sphere ($\chi = 2$) covered with graphitic carbon and restricting ourselves to only pentagons and hexagons, we find $N_5 = 12$ from Eq.2. A specific and perhaps iconic example of this is the C_{60} buckyball, which has the soccer ball pattern and can be approximated by the truncated icosahedron, one of the Archimedean solids.

Since for an arbitrary closed loop of tubules one has $\chi = 0$ (eg. a torus), the trivial solution to constructing torus knot CNTs would be simply bending the straight tubes according to the model torus knot space curve. This, however, greatly challenges the sense of art and chemistry of the authors, as we consider ourselves both chemists and enthusiastic Bridges practitioners. We attempt to find torus knot CNTs that are not only reasonably stable in a chemical sense but also artistically satisfying. The chemical instability can be roughly equated to the deviations from the angle and the side length constraints and the planarity of the constituent polygons. Also, from the authors' own experience without rigorous scientific verification, the stability in the molecular world can be somehow translated to that of the corresponding macroscopic model[4]. This refers to the beaded molecules that the authors have been advocating in the past few Bridges[3, 5]. Our goal is to create such models of torus knots with minimal strain energies which allow their beaded models to be realized. An example of beaded trefoil, a different version of those shown in Fig.4 will appear in the art exhibit this year in Seoul.

This paper summarizes numerous ways of achieving this goal throughout the past few years developed by the authors. We present firstly a general approach to (p, q) torus knot with $p < q$, which requires prior knowledge about constructing carbon nanotori and helical tubules. Due to the special properties of the trefoil knot, demonstrated by our beloved Escher in one of his paintings, there are other ways of approaching trefoil knot CNTs. We remark that this is a purely theoretical work in the context of chemical research while we find it rewarding from an artistic point of view.

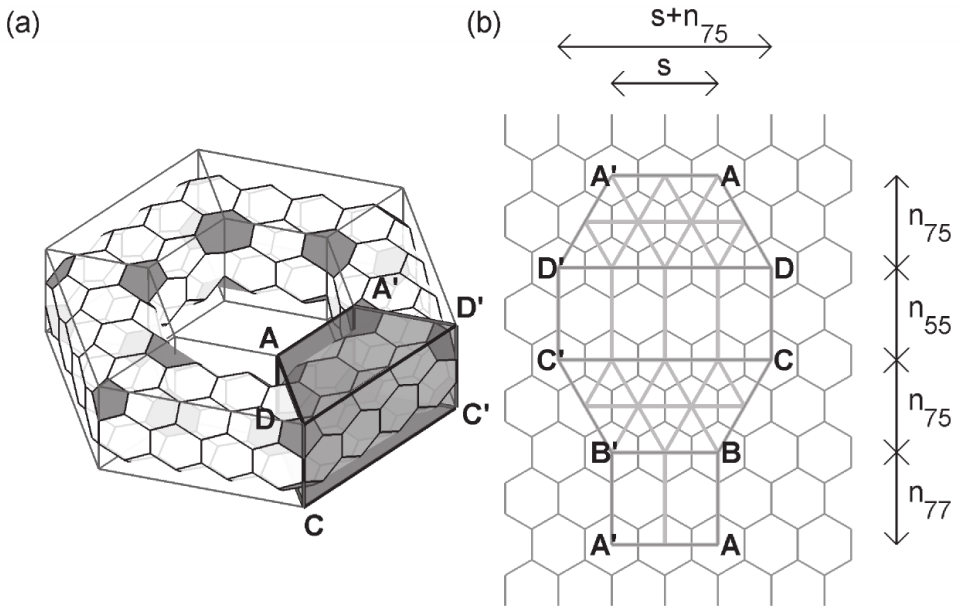

Figure 1 : *A D_{6h} toroidal CNT. Shaded polygons are ones that are not hexagonal. Adopted with permission from Ref.[1].*

Tori and Helices

Here we will briefly summarize a general approach to constructing carbon nanotori and helically coiled tubes. Readers who intend to know more are referred to a series of papers on the classification of these nanostructures[1, 2].

A toroidal CNT can be most simply cast by tiling the surface of a hexagonal prism with a hexagonal hole in the middle, as shown in Fig.1. The numerous integral parameters denote the graphical distances between the non-hexagons (shaded). For example, n_{75} defines the distance between a heptagon and its nearest-neighboring pentagon, and s denotes that of between nearest heptagons. Rather complicated combination rules exist among these parameters for one to obtain highly symmetric (D_{nh}- or D_{nd}-symmetric, where n is the rotational symmetry number) toroidal CNTs through this approach[1]. They are, however, not essential in the present context.

Our next step is to apply the so-called shifting operations to these highly symmetric toroidal CNTs, as illustrated in Fig.2. It can be understood in the following way. Firstly, the intersections between a torus and the horizontal plane in which it is residing are two concentric circles, referred to as the outer and the inner equators. We then cut through the outer equator of the toroidal CNT, shown in the central column of Fig.2(a), and reconnect the broken bonds to the atoms next to their original neighbors. The corresponding helical CNT is obtained by a final cut at any meridian and applying periodic boundary conditions. Note that the same can be applied to the inner equator of the parent toroidal CNT. This is called the horizontal shifting operation since the direction of our manipulations is always parallel with the torus's latitudes.

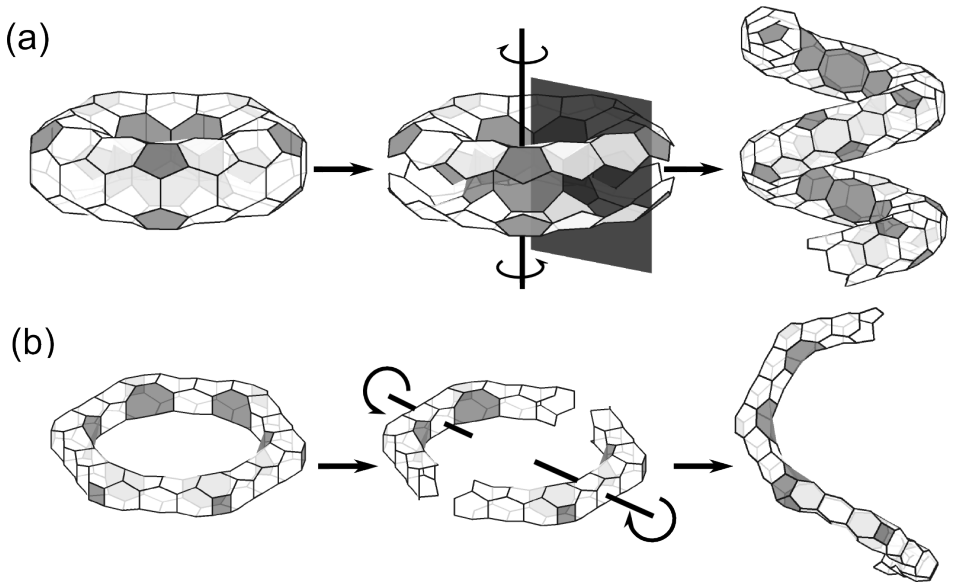

Figure 2: *Creation of helical CNTs from toroidal ones. (a) Above: application of horizontal shifting. (b) Below: application of vertical shifting.*

As opposed to the above mentioned, there is also vertical shifting, as shown in Fig.2(b). We emphasize that both of these graphical operations are subject to the discrete nature of the molecular structure to whom they are implemented. For example it is obvious that the twisting angle of the vertically shifted toroidal CNT in the figure can only take values that are multiples of $\pi/2$, since the girth of the parent CNT contains four carbon atoms. The importance of this observation will become clear as we move on to the construction of torus knot.

Torus Knot from Helices

We are now in a position to tackle torus knots, which are far more complicated than a torus or helix. The central concept utilized here is the analogy between torus knots and polygrams. For a (p, q) torus knot with $p < q$, there is a uniquely defined polygram $\{q/p\}$ (up to an ambiguity of chirality). See Fig.3 for example. Here a $(2, 7)$ torus knot tube is illustrated in part (a), which is obtained simply by embedding a tube onto the central knot curve defined in Eq.1. The color convention is chosen such that segments above the plane of the paper are reddish and those below are bluish. In Fig.3(b) the knot is flattened on to the plane and clearly shows its correspondence to a $\{7/2\}$ heptagram. The nodes of the polygram represent the loci where the torus knot space curve passes through the horizontal plane.

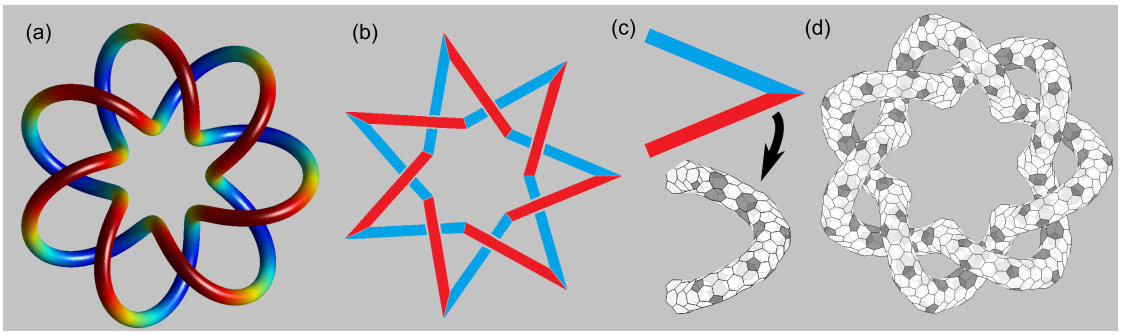

Figure 3 : *Illustration of (a) a* $(2, 7)$ *torus knot tube, and (b) the corresponding* $\{7/2\}$ *heptagram. (c) Replacement of a rotational unit cell of the heptagram with a horizontally shifted helical CNT which has a complete full turn. (d) The completed* $(2, 7)$ *torus knot CNT.*

Following this observation, one can divide the torus knot into q identical segments according to its rotational symmetry. As shown in Fig.3(c), each of the segments is composed of a red and a blue section. This can then be replaced with a slice of helical CNT as discussed in the previous section which has one complete turn. The full torus knot CNT can then be obtained by applying the rotational symmetry to it, see Fig.3(d). Note that this usage of symmetry automatically introduces the vertical shifting operation mentioned earlier. At each of the joints, the adjacent segments are rotated $2p\pi/q$ with respect to each other. After q turns of rotation, the torus knot structure is completed and one traverses p rounds around the central axis.

The essence of this approach lies upon the fact that a torus knot can be thought of as a helix wrapped around a scaffold torus and with its two ends reconnected. The minor radius (r in Eq.1) of the torus is equal to the radius of the helix, while the major radius is given by $R = h\csc(p\pi/q)$. The rather complicated geometry of torus knots calls for at least two mutually commensurable mechanisms of bending a tube, and the aforementioned two shifting operations meet this requirement. In our convention, a rotational unit cell is a horizontally shifted helical CNT, while the unit cells themselves are vertically shifted with respect to each others. We also like to emphasize that careful selections of parameters for the parental torus and helix are needed to construct stable torus knot models of this kind.

Escher's Trefoil Knot

It appears that more direct ways of implementing a trefoil CNT exist, as suggested by one of the paintings of Escher's, *Knots*, see Fig.4. It can be seen from the lower and the upper left of the painting that a set of Cartesian coordinate systems can be assigned continuously to all points of a trefoil. This allows a simpler route to construct a trefoil CNT solely from toroidal CNT, even without the complication of intervening helical tubes as in the previous section.

Figure 4: *Left: Escher's rendering of a trefoil knot. With permission from the M. C. Escher Company. Right: An enantiomeric pair of beaded molecules of the corresponding trefoil CNT.*

step	1	2	3	4	5	6	7	8	9	10	11	12
x	$+a_1$	0	0	$-a_2$	0	0	$+a_3$	0	0	$-a_2$	0	0
y	0	$+a_2$	0	0	$-a_1$	0	0	$+a_2$	0	0	$-a_3$	0
z	0	0	$+a_3$	0	0	$-a_2$	0	0	$+a_1$	0	0	$-a_2$

Table 1: *One possible recipe for making a right-angle trefoil, with* $2a_2 = a_1 + a_3$.

Upon scrutinizing the geometry of Escher's trefoil, one can find that it is composed of three arcs, each of which spans an angle of $3\pi/2$. Naively one gets $9\pi/2$ accounting for the three unit cells. This contradicts with the fact that a trefoil knot circles the central axis twice, which corresponds to an angle of 4π. What really happens here is that the arc angle *projected onto the plane of paper* would be $4\pi/3$, whose triple is 4π indeed. Due to the same reason, the relative positions of the three unit cells are made such that the local x-, y-, and z-axes of one unit cell are exactly the y-, z-, and x-axes of the next unit cell. The other circular permutation corresponds to the trefoil with the opposite handiness. An example of the such construction scheme is presented in the right side of the figure: an enantiomeric pair of beaded trefoil knots. A different version of this pair of the beaded trefoil CNTs will appear in the art exhibit as well.

Another Possibility

There is another closely related approach which makes use of the commensurability between the geometry of the trefoil and 3D Euclidean space as well. This can best be illustrated by Fig.5(a). Starting from the origin, one first makes a step of length a_1 in the x direction, followed by a step of length a_2 in the y direction, then a_3 in the z direction, *etc.*, see Table.1 for the complete recipe. Also, $a_1 \neq a_2$ and $a_3 = 2a_2 - a_1$ are required to exclude self-intersection. This approach to the construction of the trefoil has been known in recreational mathematics for a long time, though the authors could not find its original source. We remark that this is an example of 3D turtle geometry restricted to right-angle turns[6]. And the work presented by Verhoeff et al. in previous Bridges are also highly related[7], especially the Fig. 8 of [8].

We now need to find a way to assemble CNTs according to this scaffold. This was tackled by the authors last year at the Bridges[3], with the application of zome geometry. The methodology is applicable here since all the connected straight segments form right angles with each other. The straight CNTs are joined together by spherical fullerenes, e.g. C_{60} buckyballs, with holes that appropriately accommodate the CNTs. See our previous report for more discussion. One example of the trefoil CNT is shown in Fig.5(b).

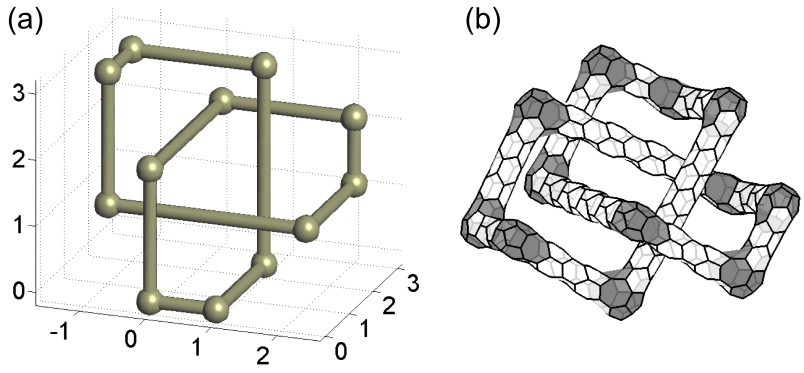

Figure 5: *(a) A lattice stick representation of the trefoil knot constructed according to Table.1 with* $(a_1, a_2) = (1, 2)$. *(b) The corresponding trefoil CNT[3].*

Conclusion

To conclude, we have reviewed three separate methods to the construction of torus knots with non-planar polygonal faces. We require the non-regularity of the polygons to be minimal such that the overall structure is stable in terms of the prediction from theoretical chemical simulations and/or the feasibility to construct its beaded representation. While the first of these proposed methods was designed for general (p, q) torus knots with $p < q$, the other two are restricted to the trefoil knot. Generalizations to include the $p > q$ case, knots other than torus knots, or general space curves are still open problems.

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