Geometry of the toroidal $N$-helix: optimal-packing and zero-twist

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Abstract. Two important geometrical properties of $N$-helix structures are influenced by bending. One is maximizing the volume fraction, which is called optimal-packing, and the other is having a vanishing strain-twist coupling, which is called zero-twist. Zero-twist helices rotate neither in one nor in the other direction under pull. The packing problem for tubular $N$-helices is extended to bent helices where the strands are coiled on toruses. We analyze the geometry of open circular helices and develop criteria for the strands to be in contact. The analysis is applied to a single, a double and a triple helix. General $N$-helices are discussed, as well as zero-twist helices for $N > 1$. The derived geometrical restrictions are gradually modified by changing the aspect ratio of the torus.
1. Introduction

The effect of bending on the geometry and characteristics of helices of tubes with nonzero thickness is described. In particular, we explore optimization of the volume fraction, called optimal-packing in analogy to the terminology used for sphere packings, and we explore structures with zero strain–twist coupling as for ideal ropes. Our aim is to understand better the geometrical constraints on, and the behavior of, helical molecules such as biomolecules, carbon nanotubes and polymer nanofibers.

Helical biomolecules can sometimes, but not always, be described as a straight helix. For example, DNA is often bent when present in a molecular complex, e.g. with proteins and in chromatin. Therefore, it is important to understand the bending of an $N$-stranded helix from a geometrical point of view. The amount of bending in an $N$-helix is described mathematically by coiling the helix on a torus with aspect ratio $a/R \leq 1$, where the helix radius is $a$ and the torus radius is $R$. For small aspect ratio the $N$-helix is only slightly bent; for larger ratios, significant bending is present. Certain generic properties depend on the amount of bending: optimal-packing (or best packing, defined as a structure that maximizes a volume fraction), zero-twist (a structure that behaves under pull as a non-chiral structure; it rotates neither in one nor in the other way) and winding (a structure that rotates counter to unwinding under a pull).

Theoretical work on bent biomolecules, like the bending of the double helix of DNA, has largely gone in one direction. It has been assumed that deformation phenomena regarding DNA operate on a scale at which the internal double-helix structure is mostly irrelevant, and a large body of literature deals with mathematical and mechanical aspects of bent, coiled and supercoiled DNA, where the double helix of DNA is represented as a single flexible tube. An early elastic model of supercoiling in DNA was suggested by Benham [1]. Jülicher [2] has investigated configurations of closed infinitely thin rods with self-contact to describe a phase
diagram of supercoiling. For rods of nonzero diameter, Stump et al [3] used an approximate method for calculating the configurations where lines of contact are present. The influence of end-conditions on self-contact in DNA loops has been studied by Tobias et al [4] and Coleman et al [5]. The statistical mechanics of supercoils has been studied by Marko and Siggia [6]. The stability of plasmids has been studied by Tobias et al [7] and Coleman et al [8]. For a detailed description of such single-tube models, see also Coleman and Swigon [9] and Travers and Thompson [10]. Further, in Thompson et al [11], the mechanics of ply formation in DNA supercoils has been studied. For a review of DNA mechanics, see Benham and Mielke [12]. Recently, Zheng et al [13] have argued that the elastic rod model of DNA is insufficient for longer segments of DNA. A double-strand elastic theory of DNA has been given by Moakher and Maddocks [14]. Equilibrium shapes for flat knots of simple polymers have been investigated from the viewpoint of scaling by Metzler et al [15].

In the literature, elastic rod models have been used to calculate the dependence of DNA configurations on the linking number, $Lk$. This is not a trivial task, mainly because the rods have nonzero diameter. It follows from the theorem related to the linking, see Călugăreanu [16], Pohl [17], White [18] and Fuller [19], that the topological constant $Lk$ obeys the relation

$$Lk = Tw + Wr,$$

(1)

in which $Tw$ and $Wr$ are the twist and writhe of the (closed) curve. Although $Lk$ is a topological invariant integer, $Wr$ and $Tw$ are not and depend on geometry. The configurations of interest for computing $Lk$ are supercoiled configurations where the DNA makes contact with itself.

Tubular models with one or more strands have been used, for example, to describe motifs of biological chain molecules, and thick knots that are of mathematical interest. Aspects of the geometry of straight tubular helices have been studied by Przybył and Pierański [20], Neukirch and van der Heijden [21], Gonzalez and Maddocks [22], Maritan et al [23] and Stasiak and Maddocks [24]. The importance of entropy for helix formation has been examined by Snir and Kamien [25]. For various applications of tube models to biomolecules, see Banavar and Maritan [26] and Banavar et al [27], and for applications to knot theory, see Przybył and Pierański [28]. According to Gonzales and Maddocks, the thickness of a knot can also be defined in terms of a global radius of curvature [29]. Knots made with as little ‘rope’ as possible have been designated ideal knots [38]. In an earlier work, we looked at the tubular single and double helices [30]. Optimization of the volume fraction was shown to be consistent with many of the common motifs of the molecular structures, e.g. in $\alpha$-helices and DNA. In addition, a new possible motif for collagen was suggested on the basis of packing and twisting properties of a unique triple helix [31]. The study of optimal volume packing for a double helix was recently revisited by O’Hara [32] and is in agreement with earlier results for single and double helices [30].

2. The circular helix

A helical helix is described by

$$x(t) = (R + a \cos(\omega t)) \cos t,$$

$$y(t) = (R + a \cos(\omega t)) \sin t,$$

$$z(t) = bt + a \sin(\omega t)$$

(2)

for $t \in \mathbb{R}$ and $a, b, \omega, R$ are positive constants. If $a \neq 0$ and $b = 0$, as we assume in the following, then equations (2) describe a helix wrapped around a torus. We call this wrapping a
The circular helix: a helical line (of radius $a$) coiling around a torus (of radius $R$) in the $x$–$z$ plane. In this plot, the circular helix has the aspect ratio $a/R = 0.1$.

circular helix; later we will discuss the case of circular $N$-helices, where $N$ is the number of strands. The torus has inner radius $R - a$ and outer radius $R + a$; its aspect ratio is $a/R$. For the center line, the radius of curvature is $R$, see figure 1. For packed tubular helices, the straight helix (a helix coiling on a straight cylinder) should intuitively be obtained in the limit $a/R = 0$.

One can define a torus pitch, $H$, as the length of repetition along the center line; for an arc of radius $R$, it must be $H = 2\pi R/\omega$. The corresponding reduced pitch is $h = H/2\pi = R/\omega$. Note that when $\omega$ is an integer the helix makes a closed loop, and $\omega$ becomes the number of times the helix coils around the torus.

To make the comparison with the straight helix ($a/R = 0$) transparent, we use an alternative parameterization of the circular helix. We redefine $t \to t^* = \omega t$, and set $\omega = R/h$. The following parameter equation gives a straight helix of radius $a$ and reduced pitch $h$ in the $z$-direction in the limit $h/R \to 0$:

$$
\begin{align*}
  x(t) &= (R - a \cos t) \cos(ht/R) - R, \\
  y(t) &= a \sin t, \\
  z(t) &= (R - a \cos t) \sin(ht/R).
\end{align*}
$$

For the straight helix, the helix line makes a constant angle, called the pitch angle $\nu_\perp$, with the horizontal plane. This is not the case with a circular helix, where

$$
\begin{align*}
  \frac{dx}{dt} &= a \sin t \cos(ht/R) - \frac{h}{R}(R - a \cos t) \sin(ht/R), \\
  \frac{dy}{dt} &= a \cos t, \\
  \frac{dz}{dt} &= a \sin t \sin(ht/R) + \frac{h}{R}(R - a \cos t) \cos(ht/R)
\end{align*}
$$

and the derivative squared is

$$
|\frac{dr}{dt}|^2 = a^2 + h^2 + a^2 \frac{h^2}{R^2} \cos^2 t - 2 a h^2 \frac{a h^2}{R} \cos t.
$$
Figure 2. The tubular circular helix: a helical tube of diameter $D$ coils around a torus in the $x$–$z$ plane.

The tangent of the circular helix makes an angle, $v$, with the center line of the torus. It follows from (5) that this angle is determined by

$$\cos^2 v = \frac{(h - \frac{ah}{R} \cos t)^2}{a^2 + (h - \frac{ah}{R} \cos t)^2}.$$  \hfill (6)

The angle $v$ is therefore not constant in $t$; it has a single minimum in the interval $[0, 2\pi]$ and becomes approximately constant in the limit of small bending. It approaches the constant value $90^\circ - v_\perp$, where $v_\perp$ is the pitch angle for a straight helix. Two important parameters for the following discussion are the relative pitch, $h/a$, measuring the repetition length of the circular helix and the aspect ratio, $a/R$, which measures the amount of bending of the helix.

We now investigate self-contacts in a tubular circular helix. For self-contacts in the straight helix, this packing problem is solved by a continuous trace of points. For the circular helix given by equations (2) there is only a discrete set of points with self-contact, as can be seen in figure 2. We assume that the tube helix has hard walls around the helix line. The cross-sections of the tubes are circular and the diameter is $D$. For packing to make sense, there are two conditions, one local and the other global in nature, that must be satisfied by the tube structure. The global condition is that the tubes are in contact at the most restrictive geometry, i.e. on the plane of the torus pointing inwards. The local condition is that the backbone tube volume should be preserved along the center line of the tubes. The backbone tube volume is preserved if $D \leq 2/\kappa$, where $\kappa$ is the local curvature of the helix line. The local condition is that the radius of the tube is smaller than or equal to the radius of curvature. When this Poisson criterion is obeyed, the volume of a tubular helix is $\pi D^2 L/4$, where $L$ is the curve length of the helix.

The global condition of contact between tubes is found out in two steps: firstly, by considering the set of connecting points on the helical line for which the line through the two points is perpendicular to the helical line; secondly, the distance between these two points should be equal to the tube diameter. Now, take two arbitrary points on the circular helix:

$$\vec{r}_1 = ((R - a \cos t_1) \cos(h(t_1 - \pi)/R) - R, a \sin t_1, (R - a \cos t_1) \sin(h(t_1 - \pi)/R))$$  \hfill (7)

and

$$\vec{r}_2 = ((R - a \cos t_2) \cos(h(t_2 - \pi)/R) - R, a \sin t_2, (R - a \cos t_2) \sin(h(t_2 - \pi)/R)).$$  \hfill (8)
The square of the distance between the two points is

\[ D_1^2 \equiv |\vec{r}_2 - \vec{r}_1|^2 = (R - a \cos t_2)^2 + (R - a \cos t_1)^2 + a^2(\sin t_2 - \sin t_1)^2 - 2(R - a \cos t_2)(R - a \cos t_1) \cos(h(t_2 - t_1)/R). \]  

With the chosen parameterization, the contact point for the most restrictive solution is \((x, 0, 0)\), where \(x\) is negative. The two points in contact with each other of the circular helix are in a symmetric relation to each other around \(\pi\), i.e. as the parameter along the helix we use \(t \equiv t_1 - \pi = -(t_2 - \pi)\). Then equation (9) becomes

\[ D_1^2 = 4a^2 \sin^2 t + 4(R + a \cos t)^2 \sin^2(ht/R). \]  

The derivative of the distance squared reads

\[
\frac{d}{dt} D_1^2 = 8a^2 \sin t \cos t - 8a(R + a \cos t) \sin t \sin^2(ht/R) \\
+ 8 \frac{h}{R} (R + a \cos t)^2 \sin(ht/R) \cos(ht/R).
\]  

2.1. Optimal-packing in a circular helix

The optimally packed circular helix is defined as the one with the highest volume fraction for the space occupied by the tubular structure, under the condition that the bending is constant, i.e. that the torus aspect ratio is constant. For the straight helix \((a/R = 0)\) the optimally packed helix is also called the close-packed helix [30].

For a configuration of a tube with no self-contact, there will always be a more densely packed structure with self-contacts. We therefore consider circular helix confirmations with self-contact in the following. What is the condition for self-contact at the most restrictive configuration? Given an aspect ratio \(a/R\), we find the extremums for \(D_1^2\), the interpoint distance squared along the helical line, where \(D_1 = D\), i.e. for

\[ D_1^2 = 4a^2 \sin^2 t + 4(R + a \cos t)^2 \sin^2(ht/R). \]  

The condition \(\frac{d}{dt} D_1^2 = 0\) for the extremum at \(t\) can be written as

\[
0 = \frac{a^2}{R^2} \sin(2t) - 2 \frac{a}{R} \left(1 + \frac{a}{R} \cos t\right) \sin t \sin^2(ht/R) + \frac{h}{R} \frac{a}{R} \left(1 + \frac{a}{R} \cos t\right)^2 \sin(2ht/R).
\]  

The solutions, i.e. the map of perpendicular points, of this transcendental equation are found numerically for various values of the aspect ratio, \(a/R\), and are found to be well behaved in the limit of small bending.

The map of perpendicular points, equation (13), are shown in figure 3; obviously, solutions are symmetric under reflection symmetry \(t \rightarrow -t\). For zero bending, \(a/R = 0\), the map of perpendicular points is shown in figure 3(a). On the right-hand side of the first hairpin \((t > 0)\) are the solutions with self-contact. The maximal value of the relative pitch for self-contact is \(h/a = 0.466\). For the second hairpin, the two perpendicular points are further separated from each other by an additional length of the helix and so on for consecutive hairpins. When
Figure 3. The solution of equation (13) for aspect ratios $a/R = 0.0, 0.10$ (upper row), $0.20$ and $0.30$ (bottom row) for a circular helix. Here the relative pitch, $h/a$, is plotted as a function of $t$; the curves describe points along the circular helix which are perpendicular to each other. The branch at $t = 0$ corresponds to the trivial solution; solutions are symmetric under reflection symmetry, $t \to -t$. Note the growth of the first hairpin with bending.

bending is introduced, new solutions extending to infinity appear; see left- and right-hand sides of figure 3(b). These solutions result from the merging of an upwards- and downwards-pointing hairpin. The branch at $t = 0$ is the trivial solution where the two connecting points coincide.

The volume fraction for the tubular helix is defined as the ratio of the tubular volume to a reference volume,

$$f_V = \frac{V_S}{V_E}. \quad (14)$$

We take the reference volume $V_E$ to be the volume of a piece of a smallest enclosing torus. We have $V_E = \pi (a + D/2)^2 H$. The corresponding volume of the tubular helix is

$$V_S = \pi (D/2)^2 \int_0^{2\pi} \left[ a^2 + \left( h - \frac{ah}{R} \cos t \right)^2 \right]^{1/2} \, dt. \quad (15)$$
The volume fraction $f_V$ as a function of the relative pitch $h/a$ for a circular helix. The function $f_V$ is plotted for three values of the aspect ratio, $a/R$. Starting from above the values are $a/R = 0.0$ (solid line) and $a/R = 0.10, 0.20$, respectively (dashed lines). For zero bending, i.e. $a/R = 0$, the maximum of $f_V$ is at $h/a = 0.328$, where $f_V^* = 0.784$. Note that with increased bending, the function $f_V$ becomes nearly flat around its maximum.

The helical volume fraction can be written as a function of $h/a$ and $a/R$:

$$f_V = \frac{(D/2)^2 \int_0^{2\pi} \sqrt{a^2 + (h - \frac{ah}{R} \cos t)^2} \, dt}{2\pi h(a + D/2)^2}$$

$$= \frac{1}{2\pi} \left( \frac{2a}{D} + 1 \right)^{-2} \cdot \int_0^{2\pi} \sqrt{\left( \frac{a}{h} \right)^2 + \left( 1 - \frac{a}{R} \cos t \right)^2} \, dt. \quad (16)$$

The volume fraction, $f_V$, is plotted as a function of $h/a$ for three different aspect ratios in figure 4. For zero bending, i.e. $a/R = 0$, the maximum of $f_V$ is at $h/a = 0.328$, where the volume fraction is $f_V^* = 0.784$. It is the close-packed single helix in [30]. The maximal volume fraction decreases on further bending. For example, when $a/R = 0.1$ we find that $f_V^* = 0.717$. Furthermore, the optimal relative pitch, $h/a$, where $f_V$ is maximal (CP structure) and the single helix is optimally packed, is an increasing function of the aspect ratio; figure 5 shows how the optimal relative pitch, $h/a$, depends on the aspect ratio $a/R$.

### 2.2. Twisting-behavior of the circular helix

In this section, we discuss how a circular helix with inter-tubular contacts behaves under strain. Let us look at a strand of the circular helix of length $2\pi$ in the parameter $t$; the bending of the helix implies that this strand wraps a circle of radius $R$. Then the total twist, $\Theta$, is observed.
Figure 5. The optimal relative pitch $h/a$ as a function of the aspect ratio $a/R$ for a circular helix. The red solid curve is for the optimally packed circular helix. At zero bending, $a/R = 0$, the optimal relative pitch is 0.328 (CP). The curve is plotted in the interval $a/R \leq 0.235$. For higher aspect ratio (at approximately $a/R > 0.24$), there is no optimal relative pitch with the usual restrictive contact, the $h/a$ value corresponds to a point not located on the first hairpin in figure 3.

The twist angle $\Theta$ is measured between a vector pointing from the circular center line of the torus to the helix line, and the plane of the torus. The angle $v_\perp = 90^\circ - v$ is determined by equation (6). The curve length of this strand is

$$L = \int_0^{2\pi} ds = \int_0^{2\pi} \left[ a^2 + \left( h - \frac{ah}{R} \cos t \right)^2 \right]^{1/2} dt. \tag{18}$$

To measure how the helix behaves under strain, the following function is introduced. The incremental twist, $f_\theta$, is the dimensionless ratio of twist to length multiplied by the diameter of the tube, $D$, i.e.

$$f_\theta = \frac{D\Theta}{L}. \tag{19}$$

Figure 6 is a plot of the incremental twist, $f_\theta$, as a function of $h/a$ for three values of the bending, $a/R$. It is seen that there is an increase in incremental twist with $h/a$, i.e. $df_\theta/d(h/a) > 0$. The single packed helix will twist opposite of unwinding under strain, i.e. it will wind further. This is sometimes referred to as overwinding or winding-up. For the presented curves in figure 6 the most bent sections violate the Poisson criterion for bending.
of the individual strands and are as such unphysical [30]. In the next section, dealing with the circular double helix, we will encounter the zero-twist structures at the termination of winding.

3. The circular double helix

The general circular double helix has a parametric equation

\[ \vec{r}_1 = ((R - a \cos t_1) \cos (ht_1/R) - R, a \sin t_1, (R - a \cos t_1) \sin (ht_1/R)), \]

\[ \vec{r}_2 = ((R - a \cos t_2) \cos (ht_2/R + \pi h/R) - R, a \sin t_2, (R - a \cos t_2) \sin (ht_2/R + \pi h/R)) \]

for \( t_1, t_2 \in \mathbb{R} \). We use a parameterization where the strand center lines corresponding to the two points of contact are in a symmetric relation to each other around \(-\pi/2\), that is, set \( t \equiv t_1 = -(t_2 + \pi) \). Now, the square of the distance between a point starting on one helix and ending on the next becomes

\[ D_2^2 = 4a^2 \sin^2 t + 4(R - a \cos t)^2 \sin^2(ht/R + \pi h/2R), \]

and the derivative of \( D_2^2 \) reads

\[ \frac{d}{dt} D_2^2 = 8a^2 \sin t \cos t + 8a(R - a \cos t) \sin t \sin^2(ht/R + \pi h/2R) \]

\[ + 8 \frac{h}{R} (R - a \cos t)^2 \sin(ht/R + \pi h/2R) \cos(ht/R + \pi h/2R). \]
3.1. Optimal-packing in a circular double helix

What is the condition for the two tubes touching at the most restrictive configuration? The condition for the extremum of $D^2$ is

$$
0 = \frac{a^2}{R^2} \sin(2t) + 2 \frac{a}{R} \left(1 - \frac{a}{R} \cos t\right) \sin t \sin^2(\frac{h t}{R} + \frac{\pi h}{2R})
$$

$$
+ \frac{h}{a} \frac{a}{R} \left(1 - \frac{a}{R} \cos t\right)^2 \sin(2\frac{h t}{R} + \frac{\pi h}{R})
$$

(23)

and the solutions, i.e. perpendicular points on different strands, are plotted in figure 8.

For the branch at $t = -\pi/2$, the phase difference is $\pi$ and the two points opposite to each other are in the same equatorial plane. For high pitch this becomes the minimal distance. For lower pitch the distance along this branch is not minimal. At zero bending (figure 8(a)), there is a straight line of contact when $t = 0$, moving left to the maximum at $t = -\pi/2$ and then following the straight line to infinity. In the second hairpin the two perpendicular points are further separated from each other by an additional length of the helix, and so on for consecutive hairpins. When bending is introduced, new sets of perpendicular points appear; see the downwards-pointing hairpin in figure 8(b). Upon further bending, upwards- and downwards-pointing hairpins can nest and extended solutions can cross over, as has happened in figure 8(c). This phenomenon is frequently observed in the evolution of these maps.

The volume of the two tubes becomes

$$
2V_S = 2\pi (D/2)^2 \int_0^{2\pi} \left[a^2 + \left(h - \frac{ah}{R} \cos t\right)^2\right]^{1/2} dt
$$

(24)

and the volume fraction as a function of $a/h$ and $a/R$ is

$$
f_V = \frac{2V_S}{V_E} = \frac{1}{\pi} \left( \frac{2a}{D} + 1 \right)^{-2} \cdot \int_0^{2\pi} \sqrt{\frac{a^2}{h^2} + \left(1 - \frac{a}{R} \cos t\right)^2} dt
$$

(25)

In figure 9, the volume fraction, $f_V$, is plotted as a function of $h/a$. For zero bending (solid line) the maximum of $f_V$ is at $h/a = 0.636$, where the volume fraction is $f_V^* = 0.769$. It is the close-packed double helix of [30]. The optimal packing depends on the amount of bending, i.e. on the aspect ratio $a/R$: the maximum of $f_V$ is a decreasing function of $a/R$; see the discussion below figure 9.

3.2. Zero-twist of the circular double helix

We now discuss how a circular double helix with inter-tubular contacts behaves under strain. In figure 10, the incremental twist $f_\Theta$ is plotted as a function of $h/a$ for four values of the aspect ratio $a/R$. For zero bending (solid line) the maximum of $f_\Theta$ is at $h/a = 0.636$, where $f_\Theta^* = 0.1478$. This is the zero-twist structure of a straight double helix with $df_\Theta = 0$. One sees that for small values of $h/a$ the incremental twist $f_\Theta$ is an increasing function and therefore the circular double helix will wind-up under strain (rotate counter to unwinding); at larger values
Figure 7. The circular double helix: two helical tubes coil around a torus in the $x$–$z$ plane. In this plot, the two double helices have aspect ratios $a/R = 0.1$ and 0.2, respectively. These particular depicted double helices are actually the so-called torus links as the individual strands have closed paths.

of $h/a$ it is a decreasing function and unwinds as expected. With bending, there is generally a nontrivial maximum of $f_\phi$ and therefore a zero-twist structure. The zero-twist structures for straight helices are described in [37, 39].

3.3. The optimally packed double helix becomes a zero-twist structure under bending

Let us systematically investigate how the optimally packed (CP) and zero-twist (ZT) structures depend on the aspect ratio $a/R$ in a circular double helix. In a straight helix, i.e. for $a/R = 0$, the close-packed structure and zero-twist structures have $h/a$ values of 0.636 and 0.821, respectively. The two properties, being close-packed or being zero-twist, cannot be satisfied at the same time. This is not true when bending is allowed. Figure 11 depicts the values of $h/a$ for the optimally packed double helices (red dotted line) and for the zero-twisted double helices (blue solid line) as a function of bending. The pitch of the optimally packed helix increases more rapidly than that of the zero-twist helix upon increasing bending. At an aspect ratio of $a/R = 0.201$, the circular double helix is both zero-twisted and optimally packed. The closed circular double helix in figure 7(b) has $a/R = 0.20$, so it is approximately such a structure.

4. The circular triple helix

The general symmetric circular triple helix has a parametric equation

$$r_1 = ((R - a \cos t_1) \cos(ht_1/R) - R, a \sin t_1, (R - a \cos t_1) \sin(ht_1/R))$$
$$r_2 = ((R - a \cos t_2) \cos(ht_2/R + 2\pi h/3R) - R, a \sin t_2, (R - a \cos t_2) \sin(ht_2/R + 2\pi h/3R))$$
$$r_3 = ((R - a \cos t_3) \cos(ht_3/R + 4\pi h/3R) - R, a \sin t_3, (R - a \cos t_3) \sin(ht_3/R + 4\pi h/3R))$$

(26)

for $t_1, t_2, t_3 \in \mathbb{R}$. We use a parameterization where $t \equiv t_1 = -(t_2 + 2\pi/3)$. Now, the square of the distance between a point starting on one helical line and ending on the next becomes

$$D_3^2 = 4a^2 \sin^2 t + 4(R - a \cos t)^2 \sin^2(ht/R + h\pi/3R)$$

(27)
Figure 8. The circular double helix. The solution of equation (23) for aspect ratios $a/R = 0.0, 0.10$ (upper row) and $0.20, 0.30$ (bottom row), i.e. the relative pitch $h/a$ plotted against $t$ for points on the two center lines which are perpendicular to each other. The vertical line at $t = -\pi/2$ represents solutions where the phase difference is $\pi$, and the two perpendicular points are in the same equatorial plane.

and the derivative of $D_3^2$ reads

$$\frac{d}{dt}D_3^2 = 8a^2 \sin t \cos t + 8a(R - a \cos t) \sin t \sin^2(ht/R + h\pi/3R)$$

$$+ 8\frac{h}{R}(R - a \cos t)^2 \sin(ht/R + h\pi/3R) \cos(ht/R + h\pi/3R).$$

The corresponding maps of perpendicular points are shown in figure 12.

4.1. Optimal-packing and zero-twist in a circular triple helix

What is the condition for tubes touching at the most restrictive condition, that is, $D_3 = D$? The condition for the extremum at $t$ can be written as

$$0 = \frac{a^2}{R^2} \sin(2t) + 2\frac{a}{R} \left(1 - \frac{a}{R} \cos t \right) \sin t \sin^2(ht/R + \pi h/3R)$$

$$+ \frac{h}{a} \frac{a}{R} \left(1 - \frac{a}{R} \cos t \right)^2 \sin(2ht/R + 2\pi h/3R).$$

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Figure 9. The circular double helix. The volume fraction $f_V$ as a function of $h/a$. The function $f_V$ is plotted for four values of the aspect ratio, $a/R$. Starting from above the values are $a/R = 0.0$ (solid line) and $a/R = 0.10$, $0.20$ and $0.30$, respectively (dashed lines). For zero bending, i.e. $a/R = 0$, the maximum of $f_V$ is at $h/a = 0.636$, where $f_V^* = 0.769$.

Figure 10. The circular double helix. Incremental twist, $f_\theta$, as a function of $h/a$. The function $f_\theta$ is plotted for four values of the aspect ratio, $a/R$. Starting from above the values are $a/R = 0.0$ (solid line) and $a/R = 0.10$, $0.20$ and $0.30$, respectively (dashed lines). For zero bending, $a/R = 0$, the maximum of $f_\theta$ is at $h/a = 0.821$, where $f_\theta^* = 1.478$.

The volume of the helical tubes becomes

$$3V_S = 3\pi (D/2)^2 \int_0^{2\pi} \left[ a^2 + \left( h - \frac{ah}{R} \cos t \right)^2 \right]^{1/2} dt.$$  \hspace{1cm} (30)
Figure 11. The circular double helix. The relative pitch $h/a$ for the CP and the ZT helix as a function of the aspect ratio $a/R$. The dotted red curve is for the optimally packed double helix and the solid blue curve for the zero-twist double helix. At zero bending, $a/R = 0$, the relative pitch is 0.636 (CP) and 0.821 (ZT), respectively. The point where the two curves intersect is at an aspect ratio of $a/R = 0.201$.

Then, we find for the volume fraction, $f_V$, as a function of $a/h$ and $a/R$:

$$f_V = 3V_S/V_E$$

$$= \frac{3}{2\pi} \left(\frac{2a}{D} + 1\right)^{-2} \cdot \int_0^{2\pi} \sqrt{\frac{a^2}{h^2} + \left(1 - \frac{a}{R} \cos t\right)^2} \, dt. \quad (31)$$

This volume fraction has been plotted in figure 13 for four values of the aspect ratio $a/R$. For zero bending (solid line) the maximum of $f_V$ is at $h/a = 0.943$, where $f_V^* = 0.744$. In figure 14, the accompanying rotation per unit length, $f_{\Theta_1}$, is plotted for the triple helix as a function of $h/a$ for four values of the aspect ratio. Now, the maximum of $f_{\Theta_1}$ is at $h/a = 0.927$, where $f_{\Theta_1}^* = 1.022$.

4.2. The optimally packed triple helix separates from the zero-twist structure with bending

Figure 15 is a plot of the optimal $h/a$ for optimally packed and zero-twist circular helices as a function of the aspect ratio $a/R$. The optimal relative pitch $h/a$ is approximately equal for $a/R = 0$, that is, a straight helix: $h/a = 0.943$ and 0.927 for optimally packed and zero-twist, respectively. Further bending makes the two lines separate; the optimally packed structure always has a larger relative pitch than the zero-twist structure. Therefore, the triple helix cannot become both optimally packed and zero-twist by additional bending, and is only approximately so at zero bending. We have suggested this to be relevant for understanding the mechanics of the triple helix of collagen [31].
Figure 12. The circular triple helix. The solution of equation (29) for aspect ratios $a/R = 0.0, 0.10$ (upper row), 0.20 and 0.30 (bottom row). Here the relative pitch, $h/a$, is plotted as a function of $t$. The branch starting at $t = 0$, and extending to infinity, represents the most restrictive solution for contact.

5. The general $N$-helix

What happens at larger $N$? In figure 16, we have plotted the optimal-packing and zero-twist curves for the case of $N = 4$. It is observed that at $a/R = 0$ the relative pitch for optimal-packing is $h/a = 1.362$. At $N \geq 5$, the location of the optimally packed structure moves to infinity. This corresponds to the pitch angle being $v_\perp = 90^\circ$, i.e. that the tubes are straight and parallel (as $\tan v_\perp = h/a$). For the straight $N$-helix, the zero-twist angle moves towards $v_\perp = 45^\circ$ ($h/a = 1$) for large $N$ and its relative pitch, $h/a$, is always less than one. Likewise, for the bent $N$-helix, the zero-twist line changes rapidly with $N$ for $N = 2, 3$ and 4. For $N > 4$, the zero-twist lines display only a little change with $N$. At large $N$, the solutions for $N$ or $N + 1$ strands become nearly identical. For the overall trend with increasing $N$ of optimal-packing and zero-twist, compare figures 11, 15 and 16.

6. Discussion and conclusion

The tubular geometry of open and closed toroidal helices is investigated using differential geometry and numerical calculations. A particular requirement is that the tubes do not intercept
Figure 13. The circular triple helix. The volume fraction $f_V$ as function of $h/a$. The function $f_V$ is plotted for four values of the aspect ratio $a/R$. Starting from above, the values are $a/R = 0.0$ (solid line) and $a/R = 0.10, 0.20$ and $0.30$, respectively (dashed lines). For zero bending, $a/R = 0$, the maximum of $f_V$ is at $h/a = 0.943$, where $f^*_V = 0.744$. It should be noted that $f_V$ is rather flat around its maximum, i.e. $f_V = 0.744$ in the interval $h/a = 0.888–1.003$.

Figure 14. The circular triple helix. Incremental twist, $f_{\theta}$, as a function of $h/a$. The function $f_{\theta}$ is plotted for four values of the aspect ratio $a/R$. Starting from above, the values are $a/R = 0.0$ (solid line) and $a/R = 0.10, 0.20$, and $0.30$, respectively (dashed lines). For zero bending, $a/R = 0$, the maximum of $f_{\theta}$ is at $h/a = 0.927$, where $f^*_{\theta} = 1.022$.

themselves and each other. For this purpose, the question of when there are tube–tube contacts present is derived, and the most restrictive conditions studied. Upon increased bending, i.e. increased aspect ratio $a/R$ of the torus, the conditions are modified and become increasingly strict.
Figure 15. The circular triple helix. The optimal relative pitch $h/a$ as a function of the aspect ratio $a/R$. The red dotted curve is for the optimally packed triple helix and the blue solid curve for the zero-twist triple helix; at zero bending, $a/R = 0$, the relative pitch is 0.943 (CP) and 0.927 (ZT), respectively.

Figure 16. The circular quadruple helix. The relative pitch $h/a$ as a function of the aspect ratio $a/R$. The red dotted curve is for the optimally packed quadruple helix and the blue solid curve for the zero-twist quadruple helix; at zero bending, $a/R = 0$, the relative pitch is 1.362 (CP) and 0.960 (ZT), respectively. With more than $N = 4$ strands, the optimal-packing line will move to infinity; the zero-twist line only moves slightly and approaches a curve starting at $h/a = 1$.

The effectiveness of the local packing is described by a volume fraction and when maximized we define these structures as being the optimally packed toroidal helices. The twisting properties of the toroidal helices are also derived and the zero-twist structures found in the case of multiple strands. For double-stranded circular helices, there exists one that is
Table 1. Optimal-packing of circular single, double and triple helices: $a/R$ is the aspect ratio of the torus that the helix coils on and measures the amount of bending, $h/a$ is the relative pitch, i.e. the ratio of reduced helix pitch to helix radius, $2a/D$ is the ratio of the helix diameter and the diameter of the helical tubes, $f_v^*$ is the volume fraction of the straight helix and $f_v/f_v^*$ is the relative volume fraction compared to that of the straight helix.

| Type      | $a/R$ | $h/a$ | $2a/D$ | $f_v$ | $f_v/f_v^*$ |
|-----------|-------|-------|--------|-------|-------------|
| Single helix | 0.00  | 0.328 | 1.022  | 0.784 | 1.000       |
|           | 0.10  | 0.401 | 0.936  | 0.717 | 0.915       |
|           | 0.20  | 0.550 | 0.786  | 0.652 | 0.832       |
| Double helix | 0.00  | 0.636 | 1.201  | 0.769 | 1.000       |
|           | 0.10  | 0.796 | 1.105  | 0.726 | 0.944       |
|           | 0.20  | 0.992 | 1.030  | 0.691 | 0.899       |
| Triple helix | 0.00  | 0.943 | 1.424  | 0.744 | 1.000       |
|           | 0.10  | 1.197 | 1.340  | 0.715 | 0.961       |
|           | 0.20  | 1.511 | 1.280  | 0.694 | 0.933       |

both optimally packed and zero-twisted with $a/R = 0.201$. Only at this value does the circular double helix satisfy the two criteria at the same time.

The straight double helix of DNA is not a zero-twist structure, but is close-packed [37]. However, it follows from the analysis of the twisting behavior that molecular bent double helices, such as DNA, might behave as zero-twist structures under certain conditions. This can be important for coiling of DNA (or RNA) when it is subject to strain, as otherwise it would twist under strain.

As the twisting and packing properties change fairly rapidly with $a/R$, such properties can become determining for the specific geometry of molecular complexes. Perhaps it will be advantageous for molecular structures, such as the chromatin fiber, to be both optimally packed and zero-twist. The usual B-form of DNA is not a symmetric double helix; therefore, for the geometry of the chromatin fiber one needs to carefully model the asymmetric double helix as was done for the straight helix in [30].

For triple helices the straight helix is a structure that is approximately optimally packed and zero-twist at the same time; with bending, the solutions that are optimally packed and zero-twisted begin to separate further. These results are likely to be relevant for understanding the coiling of chiral structures in nature, specifically the difference between the coiling of double helices (as DNA) and triple helices (such as collagen and some polysaccharides).

The effect of bending on the volume fraction on single, double and triple circular helices is summarized in table 1. It is observed that there is a significant difference in the local packing behavior of the structures, depending on the number of strands. For example, a bending of 10% ($a/R = 0.1$) of the single helix will reduce the local volume fraction by 17%, and the same amount of bending on the triple helix will only reduce the volume fraction by 7% compared to the straight helix. For molecules where molecular forces are similar, this can be expected to be revealed through differences in persistence lengths.
One of the conclusions of this paper is that the internal double-helical structure of DNA cannot be ignored when modeling complex DNA structures. The analysis given is relevant for closed circular DNA molecules, which occur in some simple biological systems, e.g. plasmids, viruses, see Vinograd and Lebowitz [33] and Clewell and Helinski [34], and is relevant for the coiling of DNA inside the chromosomes. Other examples are packing of RNA in viruses, as in the coronavirus torovirus, which has a toroidal geometry [35], and the horseshoe-shaped TLR3 molecule (toll-like receptor 3, PDB entry 2A0Z [36]) with its near-perfect toroidal helix packing. The analysis might be relevant for the coiling and twisting of carbon nanohelices, as reported in [40–42].

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