CHAPTER 26

ON THE WRITHING NUMBER OF A NON-CLOSED CURVE

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The paper deals with the definition and computation of the writhing number of an arbitrary fragment of a space curve. The approach is based on closing the tangent indicatrix with a geodesic. A relationship connecting the writhe with the Gauß integral over the open curve is studied. Single and double helical shapes are presented as examples.

1. Introduction

The term writhing number (or simply writhe) was first proposed by Fuller[1] for a quantity $\mathcal{W}r$ that arises as a difference between the linking number $\mathcal{L}k$ and the twist (or twisting number) $\mathcal{T}w$ of a closed ribbon in the Călugăreanu-White-Fuller formula[1,2,3]

$$\mathcal{W}r = \mathcal{L}k - \mathcal{T}w.$$

The sense of this very simple-looking and very famous relationship is that the right-hand side, though defined for a ribbon, depends only on its central curve.

Since $\mathcal{W}r$ is a characteristic of geometric complexity of a spatial curve, it makes this quantity worthy of consideration when examining long physical objects.[4] In particular, values of $\mathcal{W}r$ have been computed in a number of works for various models of large-scale structure of DNA (e.g., Refs. 5, 6, 7, 8) as well as for experimental data on these molecules.[9] RNA tertiary structures and protein folding are other neighbouring areas for an application of the geometrical and topological tools developed in DNA studies.[10,11,12] However, in the strict sense, application of writhe is confined to smoothly closed shapes, though quite a lot of interesting objects have their ends not joined (or joined non-smoothly), e.g., studies based on the recently developed experimental techniques of manipulation with single DNA molecules.[13] In such problems, the model curves require an appropriately defined measure to characterize their arrangement in space. Therefore, it seems to be helpful to extend the notion of writhe to non-closed curves and their fragments. Indeed, such attempts (explicit and implicit) have been made.[9,12,14,15,16,17,18,19,20,21] It happens that the definitions of the writhe suggested by different authors are not consistent. One of the first works where it was proposed how to compute the writhing number for an open (and non-smooth) curve, is Ref. 22.

The aim of this paper is to give a consistent and natural generalization of the notion of writhe to an arbitrary fragment of a curve and to present explicit formulas for its computation as function of arc length. The basic idea consists in a construction of the closure of the fragment under consideration in such a way that it would correspond to the closure of the tangent indicatrix by an arc of a great circle, as has been proposed by Maggs.[19,20] This approach is fully consistent with the recipe, given by Le Bret[23], on how to close the tangent indicatrix of a polygonal line.

2. Notation and preliminaries

We start our consideration with a smooth non-self-intersecting curve $A = \{\mathbf{r}(s) : [0, L] \to \mathbb{R}^3\}$ of class C^2, s being the arc length. We assume that the segment has a natural orientation in the direction the arc coordinate increases. The concatenation of two segments A and B having, respectively, a common ending and starting point will be written as $A + B$.

A continuous vector function $\mathbf{u}(s) : [0, L] \to \mathbf{S}^2 \equiv \{z \in \mathbb{R}^3; \|z\| = 1\}$ may be chosen such that $\mathbf{u}(s) \cdot \mathbf{r}'(s) = 0, \forall s$; here $'$ denotes the derivative with respect to s. Let $\epsilon > 0$ be small enough so that the ribbon $R_\epsilon = \{\mathbf{r} + \mu\mathbf{u}, -\epsilon \le \mu \le \epsilon\}$ does not cross itself.

2.1. *Twist, writhe and linking number*

The *twisting number* of the ribbon (i.e., of the pair $(\mathbf{r}, \mathbf{u})$) is defined by

$$\mathcal{T}w(\mathbf{r}, \mathbf{u}) = \frac{1}{2\pi} \int\limits_A \mathbf{r}' \times \mathbf{u} \cdot d\mathbf{u}.$$

If $\mathbf{r}$ is of class C^3 and $\mathbf{r}'' \neq \mathbf{0}$, then the twist of a ribbon may be decomposed into the twist of the Frenet frame plus the twist of the ribbon relative to the Frenet frame:[24]

$$\mathcal{T}w(\mathbf{r},\mathbf{u}) = \mathcal{T}w_F(\mathbf{r}) + \frac{1}{2\pi}\int\limits_0^L d\phi.$$

The angle $\phi = \phi(s)$ is an angle between $\mathbf{u}$ and the principal normal. By the Frenet ribbon is meant a special one formed by the principal normal vector to the curve. The Frenet ribbon is defined by the space curve $\mathbf{r}(s)$, if $\mathbf{r}'' \neq 0$. The twist of the Frenet ribbon is

$$\mathcal{T}w_F(\mathbf{r}) = \frac{1}{2\pi}\int\limits_0^L \tau(s)ds, \tag{1}$$

where $\tau(s)$ is the torsion of the curve $\mathbf{r}(s)$. Clearly, for planar curves, $\mathcal{T}w_F = 0$.

Now let the curve be smoothly closed: $\mathbf{r}(0) = \mathbf{r}(L), \mathbf{r}'(0) = \mathbf{r}'(L)$. For two closed curves A and B, $A \cap B = \emptyset$, the Gauß linking integral gives an integer-valued topological invariant

$$\mathcal{L}k(A,B) = \frac{1}{4\pi}\int\limits_B\int\limits_A \frac{(\mathbf{r}_A(s_1) - \mathbf{r}_B(s_2))\cdot(\mathbf{t}_A(s_1)\times\mathbf{t}_B(s_2))}{\|\mathbf{r}_A(s_1) - \mathbf{r}_B(s_2)\|^3} ds_1 ds_2,$$

called *linking number*.

The quantity called *writhe* may be expressed as the double integral

$$\mathcal{W}r_A = \frac{1}{4\pi}\int\limits_0^L\int\limits_0^L \frac{(\mathbf{r}(s_1) - \mathbf{r}(s_2))\cdot(\mathbf{t}(s_1)\times\mathbf{t}(s_2))}{\|\mathbf{r}(s_1) - \mathbf{r}(s_2)\|^3} ds_1 ds_2, \tag{2}$$

where $\mathbf{t} = \mathbf{r}'(s)$ is the tangent vector and s_1, s_2 are arc lengths. The right-hand side of Eq. (2) is the Gauß linking integral in the singular case of being over all distinct pairs of points on one curve. The writhe depends only on the shape of the curve.

2.2. *Basic relations*

The following theorem is due to Fuller[25,26] (we shall call it Fuller's first theorem).

Theorem *Let $B = \{\mathbf{r}(s)\}$ be a closed oriented space curve of class C^3 with its tangent $\mathbf{r}'(s)$, s the arc length. The tangent traces out a* closed *curve $\tilde{B}(s)$ on the unit sphere which is piecewise of class C^2. The curve $\tilde{B}(s)$ is divided into a finite family of non-self-intersecting closed piecewise C^2*

space curves. Each curve of this family then encloses a domain Ω_i defined so that the geodesic normal points into its interior. Let S_B be the sum of the areas of these domains (the components are counted with multiplicity determined by how many times the corresponding domains are encircled by the curve). Then

$$\mathcal{W}r(\mathbf{r}) = \frac{S_B}{2\pi} - 1 \qquad \bmod\ 2.$$

Let the ribbon $(\mathbf{r}, \mathbf{u})$ also be closed: $\mathbf{u}(0) = \mathbf{u}(L)$. Denote by $\mathcal{L}k(\mathbf{r} - \epsilon\mathbf{u}, \mathbf{r} + \epsilon\mathbf{u}) \equiv \mathcal{L}k(\mathbf{r}, \mathbf{u})$ the linking number of the two boundary curves $\mathbf{r} - \epsilon\mathbf{u}$ and $\mathbf{r} + \epsilon\mathbf{u}$. For ϵ small enough, $\mathcal{L}k(\mathbf{r}, \mathbf{u})$ does not depend on ϵ. This justifies omitting ϵ in the following. In other words, we shall be dealing with arbitrarily narrow ribbons.

The famous Călugăreanu-White-Fuller theorem[1,2,3] claims that the difference of the linking and twisting numbers is the writhe:

$$\mathcal{L}k(\mathbf{r}, \mathbf{u}) - \mathcal{T}w(\mathbf{r}, \mathbf{u}) = \mathcal{W}r(\mathbf{r}).$$

3. Writhe of an arbitrary open segment

Consider a spatial curve segment $A = \{\mathbf{r}_A(s), s \in [0, L_A]\}$, with the non-vanishing tangent vector. The tangent indicatrix $\tilde{A}$ need not be closed. Let $\mathbf{t}_{A0}$ and $\mathbf{t}_{A1}$ be the tangent vectors at the beginning and end points of A, respectively.

Following Maggs,[19,20] we choose to close the tangent indicatrix $\tilde{A}$ with a geodesic $\tilde{G}$ in order to get a measure for the writhe of A (Fig. 1). This choice is natural and is supported by treatment of analogous problems in optics and quantum mechanics.[27] (In the generic case $\mathbf{t}_{A0} \neq \pm\mathbf{t}_{A1}$, there are two possible geodesics, we take either of them; the cases $\mathbf{t}_{A0} = \pm\mathbf{t}_{A1}$ will be discussed later.) Let the tangent vectors at the ends of the geodesic be denoted by $\mathbf{n}_{G0}$ and $\mathbf{n}_{G1}$.

It is only possible to define and compute the fractional part of the writhe because the choice of closing geodesic is arbitrary. Then, the writhe of an open segment A may be determined by the following relation:

$$\mathcal{W}r_A = \frac{S_{A+G}}{2\pi} \qquad \bmod\ 1, \tag{3}$$

where S_{A+G} is the spherical area enclosed by $\tilde{A}$ and $\tilde{G}$ (in the same sense as in Fuller's first theorem). We are able to specify the area only modulo 2π.

It may be shown that the curve A can be closed with a curve having continuous tangent and such that its tangent indicatrix is $\tilde{G}$ plus possibly

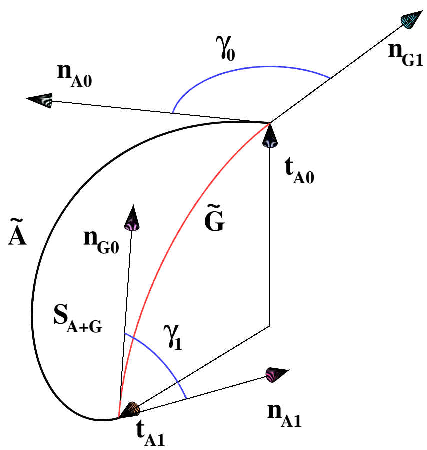

Fig. 1. The tangent indicatrix $\tilde{A}$ of the segment A closed with a geodesic $\tilde{G}$.

some pieces of great circles that do not change the enclosed spherical area modulo 2π.

Now construct a ribbon R_A for the segment A in the same manner as is done in the proof of Fuller's first theorem.[26] Generally, the ribbon R_A is determined by the unit principal normal vector $\mathbf{n}_A(s)$. Therefore, for pieces between possible inflection points of A with discontinuous normals, the twist is computed as that of the Frenet ribbon by Eq. (1). In the vicinities of the inflection points the ribbon R_A is to be arbitrary modified to make it continuous with a new modified generating vector $\mathbf{u}_A$. For the sake of simplicity, we further assume that $\mathbf{u}_{A0} = \mathbf{n}_A(0)$ and $\mathbf{u}_{A1} = \mathbf{n}_A(L_A)$. The twist $\mathcal{T}w_A$ is well-defined for the non-closed ribbon R_A, which can be closed with a ribbon R_G based on the curve G. The ribbon R_G may be constructed such that its twist equals $\mathcal{T}w_G = \frac{1}{2\pi}(\gamma_1 + \gamma_0)$, where γ_0 is an angle from the normal $\mathbf{n}_{G1}$ to $\mathbf{u}_{A0}(= \mathbf{n}_{A0})$ and γ_1 from the normal $\mathbf{u}_{A1}(= \mathbf{n}_{A1})$ to $\mathbf{n}_{G0}$.

Applying the Gauß-Bonnet theorem[28], we have

$$S_{A+G} + 2\pi\mathcal{T}w_A + \gamma_1 + \gamma_0 = 0. \tag{4}$$

Elimination of the area term from Eq. (3) and Eq. (4) results in an expression for the writhe

$$\mathcal{W}r_A = -\mathcal{T}w_A - \frac{\gamma_1 + \gamma_0}{2\pi} \quad \mod 1. \tag{5}$$

The angles γ_1 and γ_0 are determined by the equations

$$\cos\gamma_1 = \mathbf{n}_{A1}\cdot\mathbf{n}_{G0}, \quad \sin\gamma_1 = (\mathbf{n}_{A1}\times\mathbf{n}_{G0})\cdot\mathbf{t}_{A1},$$

$$\cos\gamma_0 = \mathbf{n}_{A0}\cdot\mathbf{n}_{G1}, \quad \sin\gamma_0 = (\mathbf{n}_{G1}\times\mathbf{n}_{A0})\cdot\mathbf{t}_{A0}.$$

The vectors $\mathbf{n}_{G0}$ and $\mathbf{n}_{G1}$ may be easily expressed as functions of the initial and terminal tangents of A. Indeed, the vector $\mathbf{n}_{G0}$ lies in the plane spanned by the vectors $\mathbf{t}_{A0}$ and $\mathbf{t}_{A1}$. Besides, $\mathbf{n}_{G0}\cdot\mathbf{t}_{A1} = 0$ and we may write

$$\mathbf{n}_{G0} = \pm\frac{\mathbf{t}_{A0} - (\mathbf{t}_{A0}\cdot\mathbf{t}_{A1})\mathbf{t}_{A1}}{\sqrt{1-(\mathbf{t}_{A0}\cdot\mathbf{t}_{A1})^2}}.$$

Similarly, the vector $\mathbf{n}_{G1}$ lies in the same plane and $\mathbf{n}_{G1}\cdot\mathbf{t}_{A0} = 0$. Therefore,

$$\mathbf{n}_{G1} = \mp\frac{\mathbf{t}_{A1} - (\mathbf{t}_{A0}\cdot\mathbf{t}_{A1})\mathbf{t}_{A0}}{\sqrt{1-(\mathbf{t}_{A0}\cdot\mathbf{t}_{A1})^2}}$$

(the signs depend on the choice of the geodesic).

The angles γ_1 and γ_0 can be found from their trigonometrical functions

$$\cos\gamma_1 = \pm\frac{\mathbf{n}_{A1}\cdot\mathbf{t}_{A0}}{\sqrt{1-(\mathbf{t}_{A0}\cdot\mathbf{t}_{A1})^2}}, \quad \sin\gamma_1 = \pm\frac{\mathbf{b}_{A1}\cdot\mathbf{t}_{A0}}{\sqrt{1-(\mathbf{t}_{A0}\cdot\mathbf{t}_{A1})^2}}, \tag{6}$$

$$\cos\gamma_0 = \mp\frac{\mathbf{n}_{A0}\cdot\mathbf{t}_{A1}}{\sqrt{1-(\mathbf{t}_{A0}\cdot\mathbf{t}_{A1})^2}}, \quad \sin\gamma_0 = \pm\frac{\mathbf{b}_{A0}\cdot\mathbf{t}_{A1}}{\sqrt{1-(\mathbf{t}_{A0}\cdot\mathbf{t}_{A1})^2}}, \tag{7}$$

where $\mathbf{b}_A(s) = \mathbf{t}_A(s)\times\mathbf{n}_A(s)$ is the binormal vector and $\mathbf{b}_{A0}\equiv\mathbf{b}_A(0)$, $\mathbf{b}_{A1}\equiv\mathbf{b}_A(L_A)$.

We can conclude that Eq. (5), together with Eqs. (6), (7), provides a means to compute the fractional part of the writhe for an (almost) arbitrary curve with open ends.

It may happen that the tangent vector at the beginning is the same as one at the ending point: $\mathbf{t}_{A0} = \mathbf{t}_{A1}$. Then the tangent indicatrix is closed and it sweeps the spherical area S_A (Fig. 2). Equation (3) transforms to

$$\mathcal{W}r_A = \frac{S_A}{2\pi} \qquad \mathrm{mod}\ \ 1$$

and Eq. (5) to

$$\mathcal{W}r_A = -\mathcal{T}w_A - \frac{\gamma}{2\pi} \qquad \mathrm{mod}\ \ 1, \tag{8}$$

where γ is the angle from $\mathbf{u}_{A1}$ to $\mathbf{u}_{A0}$ (actually, from $\mathbf{n}_{A1}$ to $\mathbf{n}_{A0}$).

An analogue to Eq. (8) was used in the analysis of the elongation of a supercoiled DNA molecule carried out by Bouchiat and Mézard[17,18] (though their angle χ is measured in the opposite direction to γ).

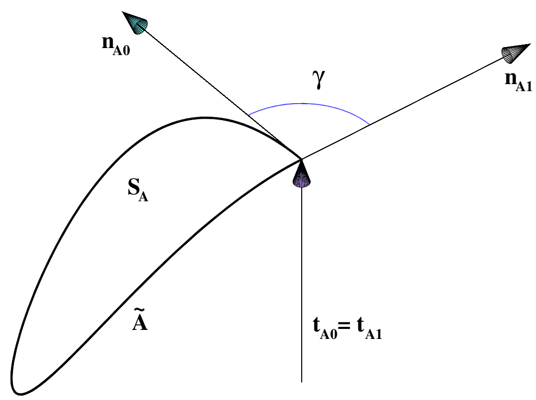

Fig. 2. The closed tangent indicatrix $\tilde{A}$ of the segment A.

Remark 1. It follows from the above that the writhe of a curve segment (closed or open) whose tangent indicatrix is geodesic and such that $\mathbf{t}_{A0} + \mathbf{t}_{A1} \neq 0$, is an integer. In other words, the writhe of any planar curve is always an integer.

Consider now the case $\mathbf{t}_{A0} = -\mathbf{t}_{A1}$. The plane of the closing geodesic G is then not determined. If we examine the behaviour of the tangent indicatrix in the vicinities $s = 0$ and $s = L_A$ (also paying attention to the neighbouring curves on $\mathbf{S}^2$ close to the critical one), then we see that the plane of the closing geodesics may rotate through $\sim \pi$ as the length of the segment changes so that the critical point $\mathbf{t}_{A0} = -\mathbf{t}_{A1}$ is passed. In mechanics terms, this phenomenon may be called flipping of the closing segment. It is the critical point where the choice of one geodesic based on a continuity argument is no longer valid.

Speaking more strictly, the value of the writhe for a segment with oppositely directed ends is not determined. It may be ascribed a value which is the average of the two limits taken as the length of the segment is precritical and post-critical. This means that the great circle plane for the closing geodesics in the critical point has to be taken orthogonal to the limiting positions of both of the great circle planes chosen for the growing segment $[\epsilon, L_A - \epsilon]$ and the decreasing one $[-\epsilon, L_A + \epsilon]$ as $\epsilon \to 0$. (We assume that the definition segment for the curve A may be infinitesimally extended in both directions.) Formally, this choice is a plane spanned by $\mathbf{t}_{A0}, \mathbf{n}_{A0} + \mathbf{n}_{A1}$. For such a closure, $\gamma_1 + \gamma_0 = \pi$ and Eq. (5) becomes

$$\mathcal{W}r_A = -\mathcal{T}w_A - \frac{1}{2} \quad \mod 1,$$

while Eq. (3) does not change (as usual, S_{A+G} means the area swept out by the closed curve $A+G$ defined as above). If, in addition, $\mathbf{n}_{A0}+\mathbf{n}_{A1} = 0$, then a plane spanned by $\mathbf{t}_{A0}$ and $\mathbf{b}_{A0}$ has to be chosen.

Remark 2. In the above consideration we have used the ribbon based on the principal normal (cf. Ref. 26), though any other continuous ribbon may be taken to obtain essentially the same formula for writhe (of course, the specific expressions for the angles γ_1 and γ_0 should be appropriately modified).

In particular, the fractional part of writhe equals the twist of a special ribbon such that its generating normal vectors at the ends have the property that they could be transformed to each other by a parallel transport along the closing geodesics (i.e., $\gamma_1 + \gamma_0 = 0 \mod 2\pi$).

3.1. *Broken curve*

The above approach may be naturally extended to a sequence of disjoint segments. Let $A = \sum_{i=1}^{n} A^{(i)}$ be a set of n continuous fragments. Each $A^{(i)}$ is oriented so that $A_0^{(i)}$ and $A_1^{(i)}$ are its initial and terminal points, respectively. Based on $A^{(i)}$, a ribbon $R_A^{(i)}$ may be built as was done for a single piece of curve. We also construct n additional pieces that tie the end point of the i-th fragment to the initial point of the subsequent one. We identify formally the point $A_0^{(n+1)}$ with $A_0^{(1)}$ to make the entire curve closed. The connecting parts are built in exactly the same way as the closure of a single segment in the previous subsection. Thus, we can repeat our arguments to obtain

$$\mathcal{W}r_A = -\sum_{i=1}^{n} \mathcal{T}w_i - \frac{1}{2\pi}\sum_{i=1}^{n}(\gamma_1^{(i)} + \gamma_0^{(i)}) \quad \mod 1, \tag{9}$$

where $\mathcal{T}w_i$ is the twist of the ribbon $R_A^{(i)}$, the angles $\gamma_1^{(i)}$ and $\gamma_0^{(i)}$ are determined by their trigonometric functions

$$\cos\gamma_1^{(i)} = \pm\frac{\mathbf{n}_{A1}^{(i)} \cdot \mathbf{t}_{A0}^{(j)}}{\sqrt{1 - \left(\mathbf{t}_{A0}^{(j)} \cdot \mathbf{t}_{A1}^{(i)}\right)^2}}, \quad \sin\gamma_1^{(i)} = \pm\frac{\mathbf{b}_{A1}^{(i)} \cdot \mathbf{t}_{A0}^{(j)}}{\sqrt{1 - \left(\mathbf{t}_{A0}^{(j)} \cdot \mathbf{t}_{A1}^{(i)}\right)^2}},$$

$$\cos\gamma_0^{(i)} = \mp\frac{\mathbf{n}_{A0}^{(j)}\cdot\mathbf{t}_{A1}^{(i)}}{\sqrt{1-\left(\mathbf{t}_{A0}^{(j)}\cdot\mathbf{t}_{A1}^{(i)}\right)^2}}, \quad \sin\gamma_0^{(i)} = \pm\frac{\mathbf{b}_{A0}^{(j)}\cdot\mathbf{t}_{A1}^{(i)}}{\sqrt{1-\left(\mathbf{t}_{A0}^{(j)}\cdot\mathbf{t}_{A1}^{(i)}\right)^2}},$$

and $\mathbf{t}_{Av}^{(i)}, \mathbf{n}_{Av}^{(i)}, \mathbf{b}_{Av}^{(i)}$ are the Frenet frames at the beginning $(v = 0)$ and at the end $(v = 1)$ of the i-th segment $(i = 1, 2, \ldots, n, \quad j = 1 + (i \mod n))$.

Note that the value of writhe generally depends on both the order of fragments and the orientations along them.

3.2. *Non-smoothly closed loop*

A special case arises when the segment A forms a non-smoothly closed shape. This means a discontinuity of the tangent vector at the initial point and the tangent indicatrix is not closed. The whole procedure described above may be applied to such a loop although one complication appears: the resulting closed curve to which the basic Călugăreanu-White-Fuller formula is to be applied has a self-intersection point at the beginning of the loop considered. Generally, the writhe is not defined for such shapes. However, on the one hand, it can be shown that the Gauß integral exists unless the tangent at the loop starting point is exactly opposite to the end tangent. On the other hand, under the same limitation, we can restrict ourselves to consideration of two limiting curves approaching the self-intersection shape from two different sides. As is well known, the writhe jumps by 2 as a curve crosses itself.[25] Thus, the fractional part of the writhe is not affected by self-intersection and may be computed by Eq. (3) or Eq. (5) in the same way as for the open segment.

4. Writhe and the Gauß integral

The writhe of the smooth closed curve may be expressed as the double integral Eq. (2). It is evident that the writhe for an open segment of length L as defined above can no longer be computed as the Gauß integral over this segment though, in most cases, the double integral itself is also well-defined for smooth non-closed curves.

Our aim here is to obtain a formula connecting both values: on the one hand, the writhe that relates the difference between the linking number and the twisting for the ribbon built with the geodesic closure and, on the other hand, simply the double integral taken over the open segment.

4.1. *Open curve and its closure*

Consider an open smooth non-self-intersecting curve $A = \{\mathbf{r}(s) : [0, L] \rightarrow \mathbb{R}^3\}$ (Fig. 3). We assume here that the tangent vectors $\mathbf{t}(s) = \mathbf{r}'(s)$ are neither parallel nor antiparallel at the ends: $\mathbf{t}(0) \neq \pm\mathbf{t}(L)$ (we will examine these cases later). We extend the curve A with two straight line segments: $B = \{\mathbf{r}_B(s_1) = \mathbf{r}(L) + s_1\mathbf{t}(L), s_1 \in [0, l]\}$ and $C = \{\mathbf{r}_C(s_2) = \mathbf{r}(0) + s_2\mathbf{t}(0), s_2 \in [-l, 0]\}$. Note that both segments have the same length l. Now connect the end points of B and C with the straight line segment $D_l = \{\mathbf{r}_D(\xi) = (1-\xi)\mathbf{r}_B(l) + \xi\mathbf{r}_C(-l) = (1-\xi)(\mathbf{r}(L) + l\mathbf{t}(L)) + \xi(\mathbf{r}(0) - l\mathbf{t}(0))\}$. The direction of D_l is determined by its tangent

$$\mathbf{t}_D(l) = \frac{\frac{d\mathbf{r}_D(\xi)}{d\xi}}{\left\|\frac{d\mathbf{r}_D(\xi)}{d\xi}\right\|} = \frac{\mathbf{r}_C(-l) - \mathbf{r}_B(l)}{\|\mathbf{r}_C(-l) - \mathbf{r}_B(l)\|}.$$

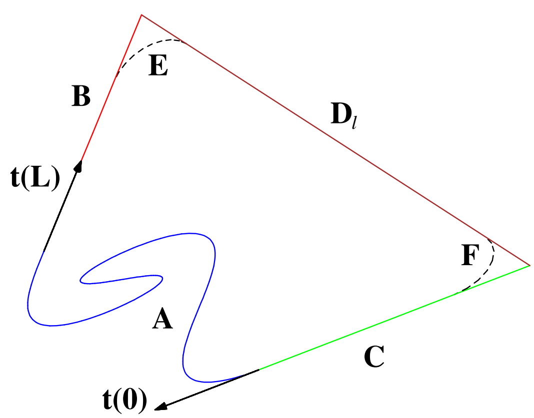

Fig. 3. The curve A is extended with the straight line segments B and C and closed with D_l.

Now let the lengths of B and C increase to infinity and compute the limiting orientation of the tangent $\mathbf{t}_D$:

$$\mathbf{t}_{D_\infty} = \lim_{l\rightarrow\infty} \mathbf{t}_D(l) = -\frac{\mathbf{t}(L) + \mathbf{t}(0)}{\|\mathbf{t}(L) + \mathbf{t}(0)\|}. \quad (10)$$

Thus, we see that in the limit $l \rightarrow \infty$, D_∞ lies in the plane defined by the initial and end tangents of the segment A.

In the case when $\mathbf{t}(0) = \pm\mathbf{t}(L)$, we can also attach two straight line segments. If $\mathbf{t}(0) = -\mathbf{t}(L)$, then all straight lines connecting these segments belong to the same plane defined by $\mathbf{t}(0)$ and $\mathbf{r}(L) - \mathbf{r}(0)$. The case $\mathbf{t}(0) = \mathbf{t}(L)$ requires a special consideration.

What we have now is a closed circuit $A + B + D_l + C$. It is smooth except for two points at the beginning and at the end of D_l. We modify B and D_l in the small vicinity of where they join themselves by introducing a planar curvilinear segment E with the tangent varying from $\mathbf{t}(L)$ to $\mathbf{t}_D$. All three segments involved belong to the same plane spanned by $\mathbf{t}(L)$ and $\mathbf{t}_D$. We can assume that the length of E does not depend on l. The length of the shortened segment B_* is decreased to be l_*.

A similar procedure may be carried out to smooth the join of the segments D_l and C. The new planar curvilinear segment F belongs to the plane spanned by $\mathbf{t}(0)$ and $\mathbf{t}_D$. The length of F is the same for every l; without loss of generality, we assume that the length of the shortened segment C_* equals l_*, as well.

We have come to the smooth closed curve $A+B_*+E+D_*+F+C_*$. We are interested in the limiting case when $l_* \to \infty$. The tangent indicatrix of the initial curve A is then closed by a geodesic corresponding to the limiting curve $E_\infty+D_\infty+F_\infty$. This follows from the construction of the curves and from Eq. (10). The limiting curve $B_\infty+E_\infty+D_\infty+F_\infty$ may be considered as an implementation of the first part G of the closure suggested in Sec. 3. Thus, the writhe of the open segment A may be computed as the writhe of the limiting closed curve $A+B_\infty+E_\infty+D_\infty+F_\infty+C_\infty$ and its fractional part satisfies Eq. (3) and Eq. (5).

However, for the smooth closed curve $A+B_\infty+E_\infty+D_\infty+F_\infty+C_\infty$, the writhe may be obtained independently by the double integral formula. Since the circuit consists of 6 parts, we have to consider all pairs involved in the double integration. For brevity, we will denote an integral over a pair of curves P and Q by (P, Q). Clearly, (P, Q) equals (Q, P).

Before proceeding, we obtain some simple estimate for the value of the double integral

$$I_2 = \int_0^{\mathcal{L}_2}\int_0^{\mathcal{L}_1} I_{\mathcal{W}r}(\sigma_1, \sigma_2)\; d\sigma_1\; d\sigma_2,$$

where

$$I_{\mathcal{W}r}(\sigma_1, \sigma_2) = \frac{(\mathbf{r}_1(\sigma_1) - \mathbf{r}_2(\sigma_2)) \cdot (\mathbf{t}_1(\sigma_1) \times \mathbf{t}_2(\sigma_2))}{\|\mathbf{r}_1(\sigma_1) - \mathbf{r}_2(\sigma_2)\|^3}.$$

The integral I_2 is taken over two smooth curves $\mathbf{r}_1(\sigma_1), \sigma_1 \in [0, \mathcal{L}_1]$ and $\mathbf{r}_2(\sigma_2), \sigma_2 \in [0, \mathcal{L}_2]$. Let $\Delta \equiv \min_{\sigma_1,\sigma_2} \|\mathbf{r}_1(\sigma_1) - \mathbf{r}_2(\sigma_2)\| > 0$. Then

$$|I_2| \leq \int_0^{\mathcal{L}_2}\int_0^{\mathcal{L}_1} |I_{\mathcal{W}r}(\sigma_1, \sigma_2)|\ d\sigma_1\ d\sigma_2 \leq \int_0^{\mathcal{L}_2}\int_0^{\mathcal{L}_1} \frac{d\sigma_1\ d\sigma_2}{\|\mathbf{r}_1(\sigma_1) - \mathbf{r}_2(\sigma_2)\|^2} \leq \frac{\mathcal{L}_1\mathcal{L}_2}{\Delta^2}. \tag{11}$$

Eq. (11) implies that $\lim_{\Delta\to\infty} I_2 = 0$ for any two curves of finite length. If one of the curves has its length of order Δ or less, i.e., $\mathcal{L}_i = \mathcal{O}(\Delta), i = 1, 2$, and the other has finite length $\mathcal{L}_{3-i}$, then the integral I_2 vanishes as $\Delta \to \infty$.

We now return to the integral over pairs of curves. The integrals (B_*, B_*), (B_*, E), (B_*, D_*), (E, E), (E, D_*), (D_*, D_*), (D_*, F), (D_*, C_*), (F, F), (F, C_*), (C_*, C_*) equal zero because the integrand vanishes for coplanar curves. If $\mathbf{t}(0) = -\mathbf{t}(L)$, then the whole closure is planar and the integrals (B_*, F), (E, F), (E, C_*) also vanish for every l_*. If $\mathbf{t}(0) \neq \pm\mathbf{t}(L)$, then the length of D_* is of order l_* for large l_*. Therefore, by applying Eq. (11), we conclude that the integrals (B_*, F), (E, F), (E, C_*) as well as (A, E), (A, D_*), (A, F) all approach zero as $l_* \to \infty$. We denote the remaining possibly non-zero integrals as follows:

$$\mathcal{W}y = \frac{1}{4\pi}\int_A\int_A I_{\mathcal{W}r}(s, \tilde{s})\ ds\ d\tilde{s},$$

$$\mathcal{S}w_1 = \frac{1}{2\pi}\int_A\int_{B_\infty} I_{\mathcal{W}r}(s, s_1)\ ds_1\ ds, \quad \mathcal{S}w_2 = \frac{1}{2\pi}\int_A\int_{C_\infty} I_{\mathcal{W}r}(s, s_2)\ ds_2\ ds,$$

$$\mathcal{S}q = \frac{1}{2\pi}\int_{C_\infty}\int_{B_\infty} I_{\mathcal{W}r}(s_1, s_2)\ ds_1\ ds_2.$$

We call them the wry, the swirl and the squint, respectively.

Thus, the writhe of A may be represented as a sum

$$\mathcal{W}r = \mathcal{W}y + \mathcal{S}w_1 + \mathcal{S}w_2 + \mathcal{S}q. \tag{12}$$

The first summand $\mathcal{W}y$ is simply the double integral over the open segment under consideration. Therefore, Eq. (12) provides a connection between this integral and the writhe.

Let us now examine the case of parallel tangents $\mathbf{t}(0) = \mathbf{t}(L)$. The two attached segments B and C then have opposite directions and, instead of the straight line D, we connect them by a circular arc $\breve{D}$ joining B and C at the same distance l from the ends of A. The arc $\check{D}$ lies in the plane spanned by the vectors $\mathbf{r}(L) - \mathbf{r}(0)$ and $\mathbf{t}(0)$ and its length is of order l for large l. Again, the smoothing curves E and F can be constructed in a similar way as it is done in the regular case. Thus, we obtain the smooth planar closure of the curve A.

After letting the lengths of B_* and C_* go to infinity and analysing the double integral components in the expression for the writhe, we come to the same Eq. (12) with the right-hand terms defined as above.

It may occur that the ray B or C intersects the curve A. Then, generally, the writhe of the whole closed curve $A+B+E+D+F+C$ is not defined. The situation is the same as for a non-smoothly closed loop (Sec. 3.2). In the generic case, when the tangents in the point of the intersection are neither coincident nor of opposite direction, the fractional part of the writhe still can be found by examination of the two limiting positions of the curves in the vicinity of the intersection point. Since the writhe jumps by 2 as the curve goes through itself, the half-sum of the writhes for those curves may be taken as the value of the writhe. The same approach may be applied to another singular case when the rays B and C cross each other. Moreover, the constraint of non-self-intersection of the initial open fragment A may also be weakened in the similar fashion.

Next we clarify the structure of the integrals $\mathcal{S}w$ and $\mathcal{S}q$.

4.2. *Swirl*

Consider

$$\mathcal{S}w_1 = \frac{1}{2\pi}\int_0^L\int_0^\infty \frac{(\mathbf{r}(s) - \mathbf{r}(L) - s_1\mathbf{t}(L))\cdot(\mathbf{t}(s)\times\mathbf{t}(L))}{\|\mathbf{r}(s) - \mathbf{r}(L) - s_1\mathbf{t}(L)\|^3}\, ds_1\, ds = \\ = \frac{1}{2\pi}\int_0^L (\mathbf{R}(s)\cdot(\mathbf{t}(s)\times\mathbf{t}_1)\hat{I}_{\mathcal{S}w}(s)\, ds. \quad (13)$$

Here we denote

$$\hat{I}_{\mathcal{S}w}(s) = \int_0^\infty \frac{ds_1}{[(\mathbf{R} - (\mathbf{R}\cdot\mathbf{t}_1)\mathbf{t}_1)^2 + (\mathbf{R}\cdot\mathbf{t}_1 - s_1)^2]^{\frac{3}{2}}}$$

and $\mathbf{R} \equiv \mathbf{R}(s) \equiv \mathbf{r}(s) - \mathbf{r}(L)$, $\mathbf{t}_1 \equiv \mathbf{t}(L)$. We can represent $\hat{I}_{\mathcal{S}w}(s)$ as

$$\hat{I}_{\mathcal{S}w}(s) = \int_0^\infty \frac{ds_1}{[a^2 + (b - s_1)^2]^{\frac{3}{2}}}, \quad b \equiv b(s) \equiv \mathbf{R}\cdot\mathbf{t}_1, \quad a^2 \equiv a^2(s) \equiv (\mathbf{R} - b\mathbf{t}_1)^2,$$

and carry out the integration to get

$$\hat{I}_{\mathcal{S}w}(s) = \left. \frac{s_1 - b}{a^2\sqrt{a^2 + (b - s_1)^2}} \right|_0^\infty = \frac{1}{\sqrt{a^2+b^2}(\sqrt{a^2+b^2} - b)}. \tag{14}$$

Substituting $a(s), b(s)$ into Eq. (14) and the result into Eq. (13) yields

$$\mathcal{S}w_1 = \frac{1}{2\pi}\int_0^L \frac{\mathbf{R}(s)\cdot(\mathbf{t}(s)\times\mathbf{t}_1)}{\|\mathbf{R}(s)\|(\|\mathbf{R}(s)\| - \mathbf{R}(s)\cdot\mathbf{t}_1)}\, ds. \tag{15}$$

Let us introduce the spherical coordinate system with the origin at the point $\mathbf{r}(L)$ and let the z-axis be directed along the ray B (Fig. 4). Then $\mathbf{R}(s) = (\rho\cos\psi\cos\phi, \rho\cos\psi\sin\phi, \rho\sin\psi)$, $\mathbf{t}_1 = (0, 0, 1)$, and $\rho \equiv \rho(s)$, $\phi \equiv \phi(s)$, $\psi \equiv \psi(s)$ are the functions describing the curve A.

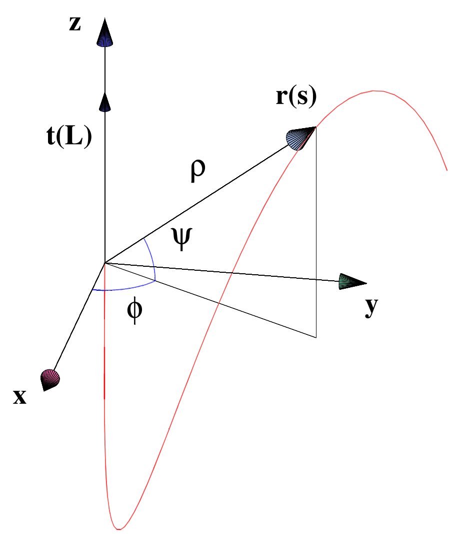

Fig. 4. The spherical coordinates ρ, ϕ, ψ. The z-axis is directed along the tangent $\mathbf{t}(L)$ at the end point of the curve $\mathbf{r}(s)$.

In these coordinates, Eq. (15) takes the form

$$\mathcal{S}w_1 = \frac{1}{2\pi}\int_0^L \phi'(1 + \sin\psi)\, ds.$$

Note that the swirl is zero if $\phi(s) = const$, i.e., if the whole curve A is planar. The swirl also vanishes when $\psi(s) = -\frac{\pi}{2}$ which means that the curve A is a straight line continuation of the ray B. It is natural that the swirl is scale-invariant: it does not depend explicitly on how far the points of the curve are from the ray. The second integral $\mathcal{S}w_2$ over the ray C_∞ has the same structure.

4.3. *Squint*

Now consider the integral $\mathcal{S}q$ over the two rays B_∞ and C_∞. It is convenient to introduce special Cartesian coordinates with origin at the point $\mathbf{r}(0)$ and the x-axis directed along $\mathbf{r}(L)-\mathbf{r}(0)$ (Fig. 5). Let the y-axis lie in the plane of the ray B_∞ and the z-axis be chosen such that the whole coordinate system is right-handed. Denote by $\phi \in [0,\pi]$ the angle from the x-axis to the direction of $\mathbf{t}(L)$. The orientation of the ray C_∞ is defined by two angles: $\psi \in [0,\pi]$ between the x-axis and $\mathbf{t}(0)$ and $\theta \in [0,2\pi]$ between the xy-plane and the plane spanned by the x-axis and $\mathbf{t}(0)$. In this coordinate system we may represent both rays as follows:

$$\begin{aligned} \mathbf{r}_B(s_1) = (g + s_1\cos\phi, s_1\sin\phi, 0), \quad g \equiv \|\mathbf{r}(L) - \mathbf{r}(0)\|, \\ \mathbf{t}_B = (\cos\phi, \sin\phi, 0), \quad s_1 \in [0,\infty], \\ \mathbf{r}_C(s_2) = (s_2\cos\psi, s_2\sin\psi\cos\theta, s_2\sin\psi\sin\theta), \\ \mathbf{t}_C = (\cos\psi, \sin\psi\cos\theta, \sin\psi\sin\theta), \quad s_2 \in [-\infty, 0]. \end{aligned}$$

We wish to compute the integral

$$\begin{aligned} \mathcal{S}q &= \frac{1}{2\pi}\int_{-\infty}^{0}\int_{0}^{\infty} \frac{(\mathbf{r}_B(s_1) - \mathbf{r}_C(s_2))\cdot(\mathbf{t}_B(s_1)\times\mathbf{t}_C(s_2))}{\|\mathbf{r}_B(s_1) - \mathbf{r}_C(s_2)\|^3}\, ds_1\, ds_2 = \\ &= \frac{1}{2\pi}(\mathbf{t}_B\times\mathbf{t}_C)\int_{-\infty}^{0}\int_{0}^{\infty} \frac{\mathbf{r}_B(s_1) - \mathbf{r}_C(s_2)}{\|\mathbf{r}_B(s_1) - \mathbf{r}_C(s_2)\|^3}\, ds_1\, ds_2 = \\ &= \frac{g}{2\pi}\sin\psi\sin\phi\sin\theta\int_{-\infty}^{0}\int_{0}^{\infty} \frac{1}{(s_1^2 + 2ps_1 + q^2)^{\frac{3}{2}}}\, ds_1\, ds_2, \end{aligned}$$

where $p \equiv p(s_2) \equiv g\cos\phi - s_2(\cos\psi\cos\phi + \sin\psi\sin\phi\cos\theta)$, $q^2 \equiv q^2(s_2) \equiv s_2^2 - 2gs_2\cos\psi + g^2$.

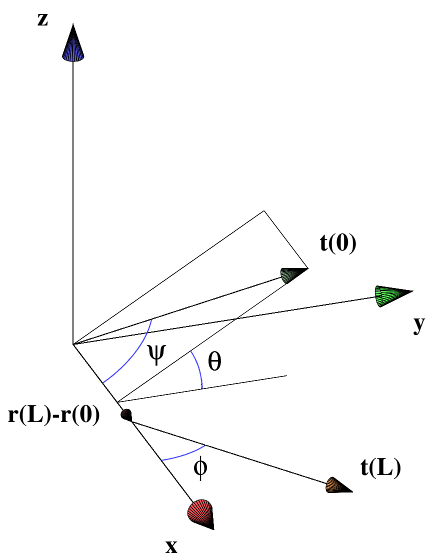

Fig. 5. The angles ϕ, θ, ψ determine the orientation of the tangents $\mathbf{t}(0)$ and $\mathbf{t}(L)$ at the ends of the curve segment.

It is easy to perform the first integration:

$$\mathcal{S}q = \frac{g}{2\pi}\sin\psi\sin\phi\sin\theta\int\limits_{-\infty}^{0}\left(\left.\frac{s_1+p}{(q^2-p^2)\sqrt{s_1^2+2ps_1+q^2}}\right|_0^\infty\right)ds_2 =$$

$$= \frac{g}{2\pi}\sin\psi\sin\phi\sin\theta\int\limits_{-\infty}^{0}\frac{ds_2}{q(p+q)} =$$

$$= \frac{g}{2\pi}\sin\psi\sin\phi\sin\theta\int\limits_{-\infty}^{0}\frac{1}{\sqrt{s_2^2-2gs_2\cos\psi+g^2}}\times$$

$$\times\frac{ds_2}{g\cos\phi - s_2(\cos\psi\cos\phi+\sin\psi\sin\phi\cos\theta)+\sqrt{s_2^2-2gs_2\cos\psi+g^2}}.$$

The last integral can also be done and the result may be presented as an algebraic formula which does not depend on g. However, the derivation of the final expression involves complicated algebra, and we instead prefer to obtain $\mathcal{S}q$ in a different way.

We can consider both rays and the straight line connecting them as an (infinite) polygonal line with three links. The writhe of this line, as defined in the previous section, is exactly equal to $\mathcal{S}q$. Then the squint is essentially proportional to the signed area of the spherical triangle formed by the geodesics that join the vertices corresponding to the vectors $\mathbf{t}(0)$, $\mathbf{r}(L) - \mathbf{r}(0)$, and $\mathbf{t}(L)$. The triangle has its two sides equal to ψ and ϕ and the angle between them θ. By the cosine rule for sides of spherical triangles, we find the third side χ from

$$\cos\chi = \cos\psi\cos\phi + \sin\psi\sin\phi\cos\theta,$$

and the signed area of the triangle can be calculated by l'Huilier's theorem[29] as

$$S = 4\nu \arctan\sqrt{\tan\frac{\Sigma}{2}\tan\frac{\Sigma-\phi}{2}\tan\frac{\Sigma-\psi}{2}\tan\frac{\Sigma-\chi}{2}},$$

where $\nu = \mathrm{sign}((\mathbf{r}(0) - \mathbf{r}(L)) \cdot (\mathbf{t}(0) \times \mathbf{t}(L))) = \mathrm{sign}(\sin\psi\sin\phi\sin\theta)$ and $\Sigma = \frac{1}{2}(\phi + \psi + \chi)$. Then the squint is $\mathcal{S}q = \frac{S}{2\pi}$.

5. Example: helical shapes of arbitrary length

Helical structures are common in DNA modelling. They are also often met in various physical and, in particular, biomechanical models. Besides, the computation of the writhe (and twist) of a helix (a helical ribbon) is a favourite example of an application of Fuller's first theorem (e.g., see Refs. 24, 25, 30) though the author is not aware of works where the writhe is computed for a piece of helix with a *non-integer* number of turns.

In this section we shall be dealing with a circular right-handed helix: $\mathbf{r}(s) = (\cos as, \sin as, \sqrt{1-a^2}s)$, $s \in [0, L]$, s arc length, L the length of the segment and $a \in [0, 1]$. The limiting values of the parameter a correspond to a straight line ($a = 0$) and a circle of the unit radius ($a = 1$). The curve is periodic with period $T = \frac{2\pi}{a}$. The curvature and the torsion are $\kappa = a^2$ and $\tau = a\sqrt{1-a^2}$, respectively. The tangent indicatrix of the helix is a circular arc on $\mathbf{S}^2$ of radius a.

5.1. *Writhe of a single helix*

Applying Eq. (5) to the single helix yields

$$\mathcal{W}r(L) = \frac{1}{\pi}\left[\arctan\left(\sqrt{1-a^2}\sin\frac{aL}{2}, \cos\frac{aL}{2}\right) - \frac{L}{2}a\sqrt{1-a^2}\right] + \\ +2\,\mathrm{round}\left(\frac{aL}{4\pi}\right), \quad (16)$$

where we denote by $z = \arctan(x, y)$ a function such that $\sin z = \frac{x}{\sqrt{x^2+y^2}}$, $\cos z = \frac{y}{\sqrt{x^2+y^2}}$, $-\pi < z \le \pi$ and round(x) is the function that gives an integer nearest to x; for half-integers round$(n + \frac{1}{2}) = n$ for negative $n \in \mathbb{Z}$ and round$(n+\frac{1}{2}) = n+1$ for non-negative $n \in \mathbb{Z}$. The last term in the right-hand side of Eq. (16) is added to make the writhe a continuous function of arc length L. Fig. 6 shows the writhe vs. number of periods L/T for three different values of the parameter a.

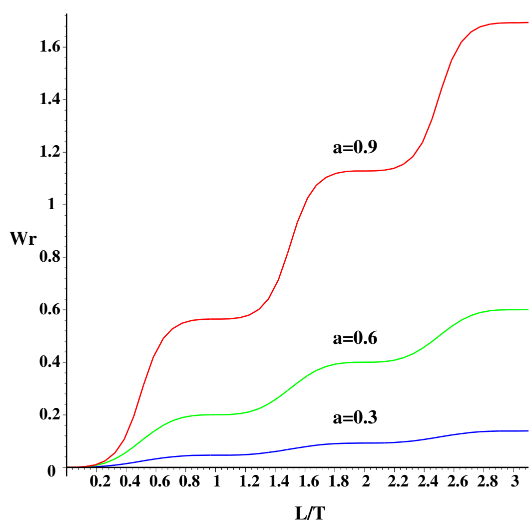

Fig. 6. The writhe $\mathcal{W}r$ of the circular helix as a function of the arc length L normalized on the period $T = 2\pi/a$, for three different values of the parameter a.

We may use Eq. (16) to compute the writhe for the particular lengths $L = \frac{\pi m}{a}$ (m is the number of half-periods):

$$\mathcal{W}r\left(\frac{mT}{2}\right) = \frac{m}{2}(1 - \sqrt{1 - a^2}). \tag{17}$$

For an integer number of periods, i.e., for even m, Eq. (17) coincides with the expressions presented in Refs. 25, 30.

In the limiting case $a \to 0$, Eq. (16) produces $\mathcal{W}r \to 0$ as it should be for a straight line. Another limiting value of the parameter is $a \to 1$, the helix approaches a circle $\mathbf{r}(s) = (\cos s, \sin s, 0)$, covered $L/2\pi$ times. Then Eq. (16) gives $\mathcal{W}r \to \text{round}\left(\frac{L}{2\pi}\right)$ and, in particular, $\mathcal{W}r \to \text{round}\left(\frac{m}{2}\right)$ for m half-periods. The latter should not be a surprise in case of even m, because the closure chosen does not shrink to a point as the ends of the helical curve approach each other in the limit after an integer number of periods.

5.2. *Writhe of a double helix*

The procedure for calculation of the writhe of a double helix is very similar to that for a single helical shape. The helix is assumed to be closed at both ends in the same manner as is described above for an arbitrary open curve. The difference is that each of the two closing curves joins two different helices. Each of the two helical curves will be called a strand. The length of each strand is the same and is denoted by L. Both strands have the same axis, otherwise they may be located arbitrarily with respect to each other (as happens in B-form DNA, for example).

We apply Eq. (9) to two disjoint strands of the double helix and obtain

$$\mathcal{W}r = -\frac{L}{\pi}a\sqrt{1 - a^2} \qquad \text{mod } 1.$$

If we think about the double helix as a continuously growing structure, then it is evident that the last equation gives not only the fractional part of $\mathcal{W}r$, but its exact value as function of one strand length. Note also the negative sign of the writhe for the right-handed ($a > 0$) double helix.

Let $h = L\sqrt{1 - a^2}$ be the length of the axis of the double helix. Then

$$\mathcal{W}r = -\frac{ha}{\pi}.$$

We see that the growing double helix delivers an example of a family of curves $A(h)$, parametrized with a continuous parameter h, such that the writhe is a linear function of length. Clearly, the writhe per unit length of the (double) helix axis is constant.

Note also that the writhe, rather unexpectedly, does not depend on the offset angle φ which controls the mutual location of the strands (in terms of DNA we may reformulate the last observation as an invariance property of writhe with respect to the widths of the minor or major grooves). The symmetric case of $2\varphi = \pi$ was considered in Ref. 30, where a formula was obtained for the limiting value of the writhe per unit length when the integer number of turns tends to infinity.

We remark that the writhe for n-strand helical shapes ($n \geq 3$) may be easily computed on the basis of the results derived for the single and double helices.

6. Conclusion

We have considered the generalization of the notion of writhing number for an arbitrary space curve and we have obtained effective formulas for its computation. The writhe of an open curve is defined here as a difference between the linking number and the twist of a ribbon based on a curve closure such that the tangent indicatrix is closed with a geodesic. The approach allows us to represent the writhe as a function of the arc coordinate measured along a curve. In some sense, we can then think about the writhe as being locally defined (cf. Ref. 31). The technique was extended to the sequences of the disjoint fragments of curves in space.

A relation was established between the writhe and the Gauß integral taken over the open fragment. It is shown, that the difference between these two quantities may be represented as three single integrals. We clarified the structure and meaning of these integrals.

Application of the formulas presented was illustrated on single and double helices of arbitrary length. In particular, the writhe as a continuous function of arc length is defined for a helix. A double helix of finite length, with "geodesic" closures at the ends, provides an example of a one-parameter family of curves that realize linear dependence of writhe on length, and the writhe is invariant with respect to the value of the offset between the strands.

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