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MAS A consistent treatment of link and writhe for open rods, and their relation to end rotation

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ABSTRACT

We combine and extend the work of Alexander & Antman [3] and Fuller [11, 12] to give a framework within which precise definitions can be given of topological and geometrical quantities characterising the contortion of open rods undergoing large deformations under end loading. We use these definitions to examine the extension of known results for closed rods to open rods. In particular, we formulate the analogue of the celebrated formula $Lk=Tw+Wr$ (link equals twist plus writhe) for open rods and propose an end rotation, through which the applied end moment does work, in the form of an integral over the length of the rod. The results serve to promote the variational analysis of boundary-value problems for rods undergoing large deformations.

A CONSISTENT TREATMENT OF LINK AND WRITHE FOR OPEN RODS, AND THEIR RELATION TO END ROTATION

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Abstract. We combine and extend the work of Alexander & Antman [3] and Fuller [11, 12] to give a framework within which precise definitions can be given of topological and geometrical quantities characterising the contortion of open rods undergoing large deformations under end loading. We use these definitions to examine the extension of known results for closed rods to open rods. In particular, we formulate the analogue of the celebrated formula $Lk = Tw + Wr$ (link equals twist plus writhe) for open rods and propose an end rotation, through which the applied end moment does work, in the form of an integral over the length of the rod. The results serve to promote the variational analysis of boundary-value problems for rods undergoing large deformations.

1. Introduction

In a variational analysis of an elastic structure that is acted upon by end forces and moments one needs to consider the work done by the applied loads. The work done by the applied force does not usually present any problems. One requires the distance travelled by the force, which is usually easy to obtain. More problems occur in determining the work done by the applied moment. Here one requires the end rotation as 'seen' by the moment, which may lead to complications if large deformations are allowed. This paper discusses the ambiguities associated with this end rotation and shows how a consistent treatment can be obtained.

If the structure is very long it may be modelled by an infinitely long rod. This has the advantage that powerful techniques from dynamical systems (viewing arclength along the rod as time) [8, 14] and variational analysis [23] can be used. The natural class of solutions to consider in this case are localised solutions, which decay sufficiently rapidly towards the ends (other solutions would have infinite strain energy and would therefore be non-physical). The boundary conditions to be imposed on such solutions are simple: end tangents are aligned and the ends of the rod do not interfere with the *localised* deformation. The work done by the torsional load is then simply the product of applied end twisting moment M and relative end rotation R (the angle that has gone into one end of the rod in order to produce the deformation, starting from a straight and untwisted reference configuration and keeping the other end fixed).

However, any real-world problem (be it a drill string, a marine pipeline or a DNA supercoil) deals with a finite-length rod. For such a rod more complicated boundary conditions may be encountered. For instance, the end tangents need not be aligned, so that an end rotation that could be used in an energy discussion is not straightforward to define. But even in the case of aligned end tangents
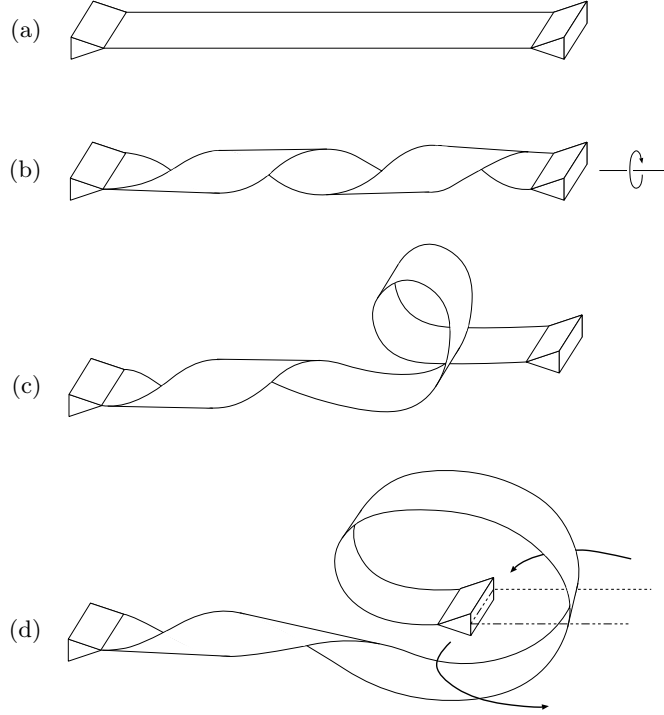
FIGURE 1. Four rod configurations that are not distinguished by a prescribed process (homotopy) of boundary conditions from a fixed reference configuration: one can go from (a) to (b) either through an end rotation or through 'looping'. (After [3]).

complications arise if large deformations are allowed. These complications are the subject of this paper.

Let us demonstrate the issue with an example. If we rotate the right end of the rod in Fig. 1(a) through an angle of -4π we obtain the configuration shown in (b). If we now move the right end of the rod to the left, the rod pops into a looped configuration as shown in (c). If we move the right end further and make the loop pass around the right clamp, as in (d), and then pull the ends out again, we return to configuration (a) without having rotated the ends. (Note that the process illustrated in Fig. 1(d) requires that whatever supports the right clamp must be released to allow the passage of the rod behind it.) We conclude that we can go from configuration (a) to configuration (b) either by end rotation or by 'looping'. What, then, is the 'real' end rotation of the deformation (a) $\rightarrow$ (b) 'seen' by the applied moment and therefore pertinent to an energy analysis?

It is apparent from this ambiguity that it is not sufficient, *a priori*, to consider only the initial and final configurations of a deformation process to decide on the end rotation. We need to be told *how* the rod was deformed from the one into the other, i.e., we need to know the deformation *history*, not just locally of the ends but globally of the entire rod. (This path dependence suggests a relation with a geometric phase; details on this are found in [13, 18, 28].)

Alexander & Antman [3] address the end rotation ambiguity for fixed boundary conditions by imagining the open rod to be part of a closed rod. A natural restriction to a class of open rod deformations is then obtained by demanding that the closed continuation should not undergo self-intersections. Applied to Fig. 1 this would mean that throwing the rod around the clamp as in (d) is excluded because

it requires an intersection with the closure (indicated by the dotted lines). In the restricted class of deformations the configurations (b) and (c) can then be assigned a unique end rotation of $R = -4\pi$ relative to (a). The ambiguity in the end rotation is thus resolved.

To distinguish between different classes of deformations Alexander & Antman use the *link* of the closed rod, i.e., the topological linking number of two lines drawn on opposite sides of the unstressed rod. Since two unknotted closed rods with equal linking number may be deformed into each other without undergoing self-intersections, there is a one-to-one correspondence between the classes of admissible deformations with unique R and the values of the link. The link is thus seen to be related to the end rotation. (Note that the -4π versus 0 ambiguity in the end rotation illustrated in Fig. 1 is reflected in the jump in link by -2 as the closed rod intersects itself.)

The connection between link for closed rods and end rotation for open rods has been discussed by many authors. The level of detail varies, but one usually argues from the link of a closed rod to the link of an open rod, which is then identified with the end rotation. Often this involves the introduction of a closure and the use of the celebrated formula [6, 11, 32]

$$Lk = Tw + Wr, \tag{1}$$

which expresses the link Lk (of a closed rod) in terms of the twist Tw (a local property, in the sense that it can be found by integrating a density along the length of the rod) and the writhe Wr. This writhe, which is only a function of the centerline of the rod, is not a local property but several expressions exist for the calculation of the writhe of an arbitrary closed curve [2]. Some of these expressions make sense for open curves as well and therefore suggest an extension of writhe from closed to open curves [29]. The final result, then, is a formula for the open link which in terms of a suitable Euler-angle representation takes the simple form

$$\text{open link} = \frac{1}{2\pi} \int [\dot{\phi} + \dot{\psi}]. \tag{2}$$

This formula cannot be expected to hold true in general since it would make link a local property, which it is not. Indeed, the generalisation of writhe from closed to open curves used in obtaining (2) is subject to a geometrical condition (see Section 2). Certainly general validity of (2) is prevented by the polar singularity inevitably associated with Euler angles. In Section 3 formula (2) will be derived within a limited class of deformations.

The present paper improves on previous results in the following ways.

(1) The closure introduced by Alexander & Antman is effective in the definition of admissible deformations if the supports are fixed in both angle and position. This is adequate for a large class of experimental situations. If, however, the supports are allowed to move, then it is not possible to use one and the same closure for all deformations: different deformations require different closures. Thus the desired distinction between classes of deformations is lost (one can always move the closure along, so that it does not 'get in the way' during the deformation). We resolve the issue by limiting the class of admissible closures in such a way that the separation into different classes of deformations, characterised by the link, is preserved under arbitrary movement of the supports.

(2) We define a precise class of deformations within which link, twist, and writhe are well-defined. We carefully examine the restrictions imposed on the deformations and show in which sense they are necessary. As mentioned above, for a consistent definition of link and writhe it is necessary to work

within a class of *homotopies of rods*, which connect a given open rod to a reference configuration. Despite the requirement of such a connection, the newly introduced writhe and link themselves are independent of the choice of connection: within the class the writhe and link only depend on the given open rod and the reference configuration.

(3) We show that the link, twist and writhe defined for open rods satisfy the classical equality (1). Furthermore, within the class of admissible deformations the link is given by (2). In the special case that the end tangents of the open rod are aligned the link coincides with the end rotation. Our results thus formalise current practice in the literature based on (2). However, while most applications of formula (2) can be shown to fall into our class of deformations, recent experiments in molecular biology do not always do so and care is required in energy discussions (we discuss this in Section 4). Indeed, we would claim that usage of (2) presupposes the framework that we here discuss, and consequently is subject to the limitations that we describe.

The organisation of the paper is as follows. In Section 2 we first define our class of open rods. For the elements of this class we define link, twist and writhe and derive the extension of (1) to open rods. In Section 3 we independently define the end rotation and show it to be equal to the open link. We also derive (2). In Section 4 we critically review the defining conditions of the class of rods considered, illustrating their relevance with counterexamples. Section 5 discusses our work in the light of previous work in the literature.

2. Results: Link, Twist and Writhe

For our purposes a rod is a member of the set

$$\mathcal{A}^0 = \big\{\, (r, d_1) \in C^2([0, L]; \mathbb{R}^3 \times S^2) \text{ such that } |\dot{r}| \neq 0,\ \dot{r} \cdot d_1 = 0,$$
$$\text{and } r \text{ is non-self-intersecting} \,\big\}.$$

Here and in the following an overdot denotes differentiation with respect to the spatial variable s. The curve r is thought of as the centerline of a physical rod (of length L) and $d_1(s)$ as a material vector in the section at s. As alternatives to 'rod' the terms 'ribbon' [12, 2] and 'strip' [3] are also used. A closed rod is an element of $\mathcal{A}^0$ for which begin and end connect smoothly.

To each point on the centerline of the rod we can attach an orthonormal right-handed frame $(d_1(s), d_2(s), d_3(s))$ of directors by setting

$$d_3(s) = \dot{r}(s)/|\dot{r}(s)| \qquad \text{and} \qquad d_2(s) = d_3(s) \times d_1(s). \tag{3}$$

These directors track the varying orientation of the cross-section of the rod along the length of the rod. The twist of a closed rod (r, d_1) is now defined by

$$Tw(r, d_1) := \frac{1}{2\pi} \oint_r \dot{d}_1(s) \cdot d_2(s)\, ds. \tag{4}$$

It measures the number of times d_1 revolves around d_3 in the direction of d_2 as we go around the rod.

Let r_1 and r_2 be two non-intersecting curves. Then the link of r_1 and r_2 is defined by

$$Lk(r_1, r_2) := \frac{1}{4\pi} \oint_{r_1} \oint_{r_2} \frac{[\dot{r}_1(s) \times \dot{r}_2(t)] \cdot [r_1(s) - r_2(t)]}{|r_1(s) - r_2(t)|^3}\, ds dt. \tag{5}$$

The writhe of a closed curve r is

$$Wr(r) := \frac{1}{4\pi} \oint_r \oint_r \frac{[\dot{r}(s) \times \dot{r}(t)] \cdot [r(s) - r(t)]}{|r(s) - r(t)|^3}\, ds dt. \tag{6}$$
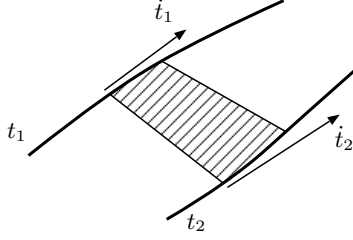
FIGURE 2. The argument of the integral in (9) is the area swept out by the geodesic connecting the curves t_1 and t_2 on S^2.

The argument of this integral is the pullback of the area form on S^2 under the Gauss map $\mathbb{R}^2 \longrightarrow S^2$,

$$G : (r(s), r(t)) \longmapsto \frac{r(s) - r(t)}{|r(s) - r(t)|},$$

so that the writhe may be interpreted as the signed area on S^2 that is covered by this map. For each direction $p \in S^2$ the signed multiplicity of the Gauss map (i.e., the number of points (s, t) for which $G(s, t) = p$, weighted by the sign of $p \cdot [G_s \times G_t]$) equals the *directional writhing number*, the number of signed crossings of the projection of r onto a plane orthogonal to the vector p [11, 2]. In other words, the writhe of a closed curve is equal to the directional writhing number averaged over all directions of S^2.

The link, twist and writhe of a closed rod are related by the well-known Călugăreanu-White-Fuller Theorem [6, 32, 11]:

Theorem 2.1. *Let $(r, d_1) \in \mathcal{A}^0$ be a closed rod as defined above. Then*

$$Lk(r, d_1) = Tw(r, d_1) + Wr(r). \tag{7}$$

We review two classical theorems by Fuller which are of interest to us. Note that at each point $r(s)$, the unit tangent $t(s) = \dot{r}(s)/|\dot{r}(s)|$ traces out a closed curve on S^2, called the tantrix. Fuller's first theorem relates the writhe of the curve to the area A enclosed by the tantrix on S^2:

$$Wr(r) = \frac{A}{2\pi} - 1 \ (\text{modd } 2). \tag{8}$$

Note that the equality modulo two is necessary since the area enclosed by a curve on S^2 is only defined modulo 4π.

The second theorem, stated in detail as Theorem 2.6 below, gives under certain conditions a formula for the difference in writhe between two closed curves r_1 and r_2 that can be continuously deformed into each another (see Figure 2):

$$Wr(r_1) - Wr(r_2) = \frac{1}{2\pi} \int \frac{t_2 \times t_1}{1 + t_1 \cdot t_2} \cdot (\dot{t}_1 + \dot{t}_2). \tag{9}$$

We now proceed with the introduction of the set for which the open link, twist and writhe will be defined. For the definition of this set we choose a closed planar reference curve $r_0 \in C^2([0, M]; \mathbb{R}^3)$ for some $M > L$.

Definition 2.2.

$$\mathcal{A}^1_{r_0} = \Big\{ \quad (r, d_1) \in \mathcal{A}^0 \ \text{such that} \ \exists (\bar{r}, \bar{d}_1) \in C^2([0, M] \times [0, 1]; \mathbb{R}^3 \times S^2) :$$

1. *for each* λ, $\bar{r}(\cdot, \lambda)$ *is an unknotted, non-self-intersecting closed curve,*

2. $\dot{\bar{r}}(s, \lambda) \cdot \bar{d}_1(s, \lambda) = 0$ *for* $s \in [0, M]$, $\lambda \in \{0, 1\}$,

3. $(\bar{r}, \bar{d}_1)(s, 1) = (r, d_1)(s)$ *for* $s \in [0, L]$,

4. $\bar{r}(s, 0) = r_0(s)$ *for* $s \in [0, L]$,

5. $\dot{\bar{r}}(s, 0) \cdot \dot{\bar{r}}(s, \lambda) > -1$ *for* $s \in [0, M]$, $\lambda \in [0, 1]$,

6. $\{\bar{r}(s, \lambda) \colon s \in [L, M]\}$ *is a planar curve for* $\lambda = 0$ *and* $\lambda = 1$,

    and these two planes are parallel $\Big\}$.

$\mathcal{A}^1_{r_0}$ can be thought of as a class of open rods (r, d_1) that can be connected by a homotopy—satisfying certain requirements—to the reference curve r_0. The part of the closed rod parametrised by $s \in [L, M]$ is called the closure.

Some of the conditions above are more straightforward than others. Parts 1 and 2 state that $(\bar{r}, \bar{d}_1)$ is a homotopy of well-behaved closed rods, and by parts 3 and 4 the homotopy contains the original open rod (r, d_1) at $\lambda = 1$, and the reference curve at $\lambda = 0$. Parts 5 and 6 contain the essential elements of this definition. Part 5 is the same non-opposition condition that appears in the statement of Fuller's theorem (Theorem 2.6) and is required for the conversion of the writhe to a single-integral expression. Part 6, which states that the closure should be planar at the beginning and the end of the homotopy, is central in the construction. These last two conditions are discussed more fully in Section 4.

Note that curves r_0 exist for which $\mathcal{A}^1_{r_0}$ is empty: if the three vectors $\dot{r}_0(0)$, $\dot{r}_0(L)$, and $r_0(L) - r_0(0)$ are independent, then the open curve r_0 can not be closed by a planar closure, so that the set of homotopies with planar closures that connect to r_0 is empty.

We are now in a position to define the new functionals open link, open twist and open writhe for open rods.

Definition 2.3. *Let* (r, d_1) *be a rod in* $\mathcal{A}^1_{r_0}$. *Then the open twist of* (r, d_1) *is*

$$Tw^o(r, d_1) := \frac{1}{2\pi} \int_0^L \dot{d}_1 \cdot (\dot{r} \times d_1) \, ds,$$

the open writhe of r *is*

$$Wr^o(r) := Wr(\bar{r}(\cdot, 1)) = \frac{1}{4\pi} \int_0^M \int_0^M \frac{[\bar{r}(s, 1) - \bar{r}(t, 1)] \cdot [\dot{\bar{r}}(s, 1) \times \dot{\bar{r}}(t, 1)]}{|\bar{r}(s, 1) - \bar{r}(t, 1)|^3} \, ds dt,$$

and the open link of (r, d_1) *is*

$$Lk^o(r, d_1) := Lk(\bar{r}(\cdot, 1), \bar{d}_1(\cdot, 1)) - \frac{1}{2\pi} \int_L^M \dot{\bar{d}}_1(s, 1) \cdot (\dot{\bar{r}}(s, 1) \times \dot{\bar{d}}_1(s, 1)) \, ds.$$

Note that in the last definition we subtract any twist the closure might have. It follows directly from the construction that the new concepts also satisfy the classical relationship:

Corollary 2.4. *Let $(r, d_1) \in \mathcal{A}_{r_0}^1$ be an open rod. Then*

$$Lk^o(r, d_1) = Tw^o(r, d_1) + Wr^o(r).$$

Theorem 2.5. *For any open rod $(r, d_1) \in \mathcal{A}_{r_0}^1$, the open twist, writhe, and link are well-defined.*

For writhe and link this is non-trivial, as different homotopy closures $(\bar{r}, \bar{d}_1)$ might be expected to give rise to different values.

Proof. We first state Fuller's second theorem in a more precise form.

Theorem 2.6. *Let r_λ $(0 \leq \lambda \leq 1)$ be a homotopy of closed non-self-intersecting curves, regularly parametrized with a common parameter $s \in [0, L]$. Let t_λ be the tantrix of r_λ. If $t_0(s) \cdot t_\lambda(s) > -1$ for all $s \in [0, L], \lambda \in [0, 1]$, then*

$$Wr(r_1) - Wr(r_0) = \frac{1}{2\pi} \int_0^L \frac{t_0 \times t_1}{1 + t_0 \cdot t_1} \cdot \left(\dot{t}_0 + \dot{t}_1 \right) ds. \tag{10}$$

To our knowledge, a rigorous proof was first given by Aldinger *et al.* [2].

To prove Theorem 2.5 for the open writhe, let $(\bar{r}, \bar{d}_1)$ be a homotopy associated to (r, d_1). By definition, $\bar{r}(\cdot, 0)$ and $\bar{r}(\cdot, 1)$ are planar for $s \in [L, M]$. Let us denote the planes by V_0 and V_1; these are parallel by Definition 2.2.6. Let V be the plane through the origin parallel to both.

We have defined the class of open rods $\mathcal{A}_{r_0}^1$ such that Theorem 2.6 can be applied. Denote the tantrices of $\bar{r}(\cdot, 0)$ and $\bar{r}(\cdot, 1)$ by t_0 and t_1 respectively. Then

$$Wr(\bar{r}(\cdot, 1)) - Wr(\bar{r}(\cdot, 0)) = \frac{1}{2\pi} \int_0^M \frac{t_0(s) \times t_1(s)}{1 + t_0(s) \cdot t_1(s)} \cdot (\dot{t}_0(s) + \dot{t}_1(s)) \, ds. \tag{11}$$

The argument of the integral vanishes for $s \in [L, M]$: since $t_0(s), t_1(s) \in V$ for $s \in [L, M]$ we have $t_0(s) \times t_1(s) \perp V$ and $\dot{t}_0(s) + \dot{t}_1(s) \in V$ for $s \in [L, M]$. Hence

$$[t_0(s) \times t_1(s)] \cdot [\dot{t}_0(s) + \dot{t}_1(s)] = 0.$$

Moreover, since $\bar{r}(\cdot, 0)$ is planar, $Wr(\bar{r}(\cdot, 0)) = 0$. We conclude

$$Wr(\bar{r}(\cdot, 1)) = \frac{1}{2\pi} \int_0^L \frac{t_0(s) \times t_1(s)}{1 + t_0(s) \cdot t_1(s)} \cdot (\dot{t}_0(s) + \dot{t}_1(s)) \, ds. \tag{12}$$

Since this integral only depends on the reference curve and the open rod itself, and is otherwise independent of the choice of closure and homotopy, this proves the claim for the writhe.

For the link, let $(\bar{r}, \bar{d}_1)$ be a homotopy associated to (r, d_1) by Definition 2.2. Denote the closed curves $\bar{r}(\cdot, 1)$ and $\bar{d}_1(\cdot, 1)$ by $\hat{r}$ and $\hat{d}_1$ respectively. We denote the open twist evaluated over an interval $s \in [a, b]$ by $Tw_{[a,b]}^o$. Then

$$\begin{aligned} Tw_{[L,M]}^o(\hat{r}, \hat{d}_1) &= Tw_{[0,M]}^o(\hat{r}, \hat{d}_1) - Tw_{[0,L]}^o(\hat{r}, \hat{d}_1) \\ &= Tw_{[0,M]}^o(\hat{r}, \hat{d}_1) - Tw^o(r, d_1). \end{aligned}$$

Hence

$$\begin{aligned} Lk^o(r, d_1) &= Lk(\hat{r}, \hat{d}_1) - Tw_{[L,M]}^o(\hat{r}, \hat{d}_1) \\ &= Lk(\hat{r}, \hat{d}_1) - Tw(\hat{r}, \hat{d}_1) + Tw^o(r, d_1) \\ &= Wr(\hat{r}) + Tw^o(r, d_1) \\ &= Wr^o(r) + Tw^o(r, d_1). \end{aligned} \tag{13}$$

It follows that $Lk^o(r, d_1)$ is independent of the chosen closure $(\bar{r}, \bar{d}_1)$. $\qquad \square$

Equation (12) is an important motivation of this work, since it expresses the writhe in terms of a single rather than a double integral. For the purpose of variational analysis this is an obvious advantage. It is especially useful when the link, and therefore indirectly the writhe, can be identified with the rotation of the ends; this requires that the end tangents remain equal throughout the deformation, and this case is treated in the next section.

Remark 2.7. For simplicity we have chosen to introduce one class $\mathcal{A}_{r_0}^1$ as the basis for the definitions of open link, twist and writhe. For each of the three definitions separately, however, not all of Definition 2.2 is required. Open twist can be defined directly in terms of (r, d_1), without the need for an extension; open link requires a closure, but no homotopy; and open writhe requires a homotopy, but the director d_1 can be disposed of.

Remark 2.8. A natural question to ask is whether the open link, twist and writhe reduce to their classical counterparts when an open rod is transformed into a closed rod by lining up and connecting the ends. This is not the case, as we demonstrate in Section 4.

3. Results: End-rotation and Euler angles

It is common in applications to assume that the end tangents of the buckled rod are kept constant and equal during the deformation process. For comparison with an end rotation we introduce this additional condition. Throughout this section we also assume that $r_0|_{[0,L]}$ is straight; without loss of generality we assume that $\dot{r}_0$ is a constant unit vector v on $[0, L]$. Finally, again without loss of generality we choose the director d_1 constant on the reference curve $r_0|_{[0,L]}$:

Definition 3.1.
$$\mathcal{A}_{r_0}^2 = \big\{ (r, d_1) \in \mathcal{A}_{r_0}^1 : \ \dot{r}_0(s) = v \in S^2 \ \text{for all } s \in [0, L],$$
$$\dot{r}(0, \lambda) = \dot{r}(L, \lambda) = \dot{r}(M, \lambda) = v \ \text{for all } \lambda \in [0, 1],$$
$$\bar{d}_1(s, 0) = \bar{d}_1(0, 0) \ \text{for all } s \in [0, L] \ \big\}.$$

The following formula is a direct consequence of Theorem 2.6:

Corollary 3.2. *Let $(r, d_1) \in \mathcal{A}_{r_0}^2$ and let t be the tantrix of r. Then*

$$Wr^o(r) = \frac{1}{2\pi} \int_0^L \frac{v \times t(s)}{1 + v \cdot t(s)} \cdot \dot{t}(s) \, ds. \tag{14}$$

In the present case of a straight $r_0|_{[0,L]}$ the dependence on r_0 of the open writhe of a given open rod takes a particularly simple form:

Theorem 3.3. *Under the conditions of Corollary 3.2, let $\Omega = S^2 \setminus \{-t(s) : s \in [0, L]\}$. Then the function*

$$v \in S^2 \longmapsto \frac{1}{2\pi} \int_0^L \frac{v \times t(s)}{1 + v \cdot t(s)} \cdot \dot{t}(s) \, ds$$

is constant on connected components of Ω.

The proof is given in the appendix. The interpretation of this theorem is as follows: when the end tangents are aligned, the tantrix given by the rod (without closure) forms a closed curve on S^2. The integral above represents 'area enclosed by the curve' for a given 'choice of area' (*cf.* (8)). When the vector v crosses the set $\{-t(s) : s \in [0, L]\}$ the geodesic connections between v and $t(s)$ change direction, causing the integral to represent a different choice of area, and therefore causing the integral to jump by 4π.

With fixed end tangents we can introduce a fourth quantity, the end rotation. We denote $\partial(\cdot)/\partial\lambda$ by $\partial_\lambda(\cdot)$.

Definition 3.4. *Let $(r, d_1) \in \mathcal{A}_{r_0}^2$, and let $\bar{d}_3(\cdot, \cdot) = \dot{\bar{r}}(\cdot, \cdot)/|\dot{\bar{r}}(\cdot, \cdot)|$, $\bar{d}_2 = \bar{d}_3 \times \bar{d}_1$. We define the end rotation by*

$$R(r, d_1) := \int_0^1 \partial_\lambda \bar{d}_1(L, \lambda) \cdot \bar{d}_2(L, \lambda) \, d\lambda - \int_0^1 \partial_\lambda \bar{d}_1(0, \lambda) \cdot \bar{d}_2(0, \lambda) \, d\lambda.$$

To study the relationship between end rotation and open link, twist and writhe we introduce a particular choice of Euler angles for an open rod (r, d_1). Recall that for every $s \in [0, L]$ there is an orthonormal director frame $(d_1(s), d_2(s), d_3(s))$. We express this frame in terms of angles θ, ψ, ϕ with respect to a fixed basis (e_1, e_2, e_3) as follows

$$\begin{aligned}
d_1 &= (-\sin\psi\sin\phi + \cos\psi\cos\phi\cos\theta)\, e_1 + \\
&\quad (\cos\psi\sin\phi + \sin\psi\cos\phi\cos\theta)\, e_2 - \cos\phi\sin\theta\, e_3, \\
d_2 &= (-\sin\psi\sin\phi - \cos\psi\sin\phi\cos\theta)\, e_1 + \\
&\quad (\cos\psi\cos\phi + \sin\psi\sin\phi\cos\theta)\, e_2 - \sin\phi\sin\theta\, e_3, \\
d_3 &= \cos\psi\sin\theta\, e_1 + \sin\psi\sin\theta\, e_2 + \cos\theta\, e_3.
\end{aligned} \tag{15}$$

This choice of Euler angles follows Love [17, art. 253]. For rods in the class $\mathcal{A}_{r_0}^2$ we choose e_3 parallel to v; note that by this choice the non-opposition condition 5 in Definition 2.2 coincides with avoidance of the Euler-angle singularity at $\theta = \pi$. Therefore the smoothness assumptions on $(\bar{r}, \bar{d}_1)$ in $\mathcal{A}_{r_0}^2$ imply C^1-regularity for ϕ, ψ, and θ.

Lemma 3.5. *Let $(r, d_1) \in \mathcal{A}_{r_0}^2$ be an open rod with an associated homotopy $(\bar{r}, \bar{d}_1)$, and let $\bar{d}_2$ and $\bar{d}_3$ be constructed from $\bar{r}$ and $\bar{d}_1$ according to (3). Let $\phi, \psi, \theta : [0, M] \times [0, 1] \to \mathbb{R}$ be the Euler-angle representation of $(\bar{d}_1, \bar{d}_2, \bar{d}_3)$. Then*

$$R(r, d_1) = \int_0^L [\dot{\phi}(s, 1) + \dot{\psi}(s, 1)] \, ds.$$

From this Lemma we conclude

Corollary 3.6. *For open rods $(r, d_1) \in \mathcal{A}_{r_0}^2$, $R(r, d_1)$ is independent of the choice of extension $(\bar{r}, \bar{d}_1)$.*

Proof of Lemma 3.5. Using the definitions of the Euler angles, we find

$$\partial_\lambda \bar{d}_1(s, \lambda) \cdot \bar{d}_2(s, \lambda) = \partial_\lambda \phi(s, \lambda) + \partial_\lambda \psi(s, \lambda) \cos\theta(s, \lambda).$$

For $s = 0, L$ and $\lambda \in [0, 1]$ we have set $\bar{d}_3(s, \lambda) = e_3$, and hence $\theta(s, \lambda) = 0$ for $s = 0, L$; therefore $\partial_\lambda \bar{d}_1(s, \lambda) \cdot \bar{d}_2(s, \lambda) = \partial_\lambda \phi(s, \lambda) + \partial_\lambda \psi(s, \lambda)$ for $s = 0, L$.

Since $\phi + \psi$ is a continuously differentiable function on $V := [0, L] \times [0, 1]$, the integral of the tangential derivative of $\phi + \psi$ along ∂V vanishes:

$$\oint_{\partial V} \frac{\partial}{\partial \tau}(\phi + \psi) = 0,$$

where τ is the clockwise-pointing unit vector tangential to ∂V.

Hence

$$\int_0^L [\partial_s\phi(s,1) + \partial_s\psi(s,1)]\, ds - \int_0^L [\partial_s\phi(s,0) + \partial_s\psi(s,0)]\, ds =$$

$$= \int_0^1 [\partial_\lambda\phi(L,\lambda) + \partial_\lambda\psi(L,\lambda)]\, d\lambda - \int_0^1 [\partial_\lambda\phi(0,\lambda) + \partial_\lambda\psi(0,\lambda)]\, d\lambda$$

$$= \int_0^1 [\partial_\lambda\phi(s,\lambda) + \partial_\lambda\psi(s,\lambda)]\, d\lambda \Big|_{s=0}^{s=L}$$

$$= \int_0^1 \partial_\lambda \bar{d}_1(s,\lambda) \cdot \bar{d}_2(s,\lambda)\, d\lambda \Big|_{s=0}^{s=L} = R(r,d_1).$$

□

Within this framework Euler-angle formulae for open link, twist and writhe are obtained:

Lemma 3.7. *Let* (r,d_1) *be an open rod in* $\mathcal{A}_{r_0}^2$. *Then*

$$Wr^o(r) = \frac{1}{2\pi}\int_0^L \dot\psi(s)(1 - \cos\theta(s))\, ds, \tag{16}$$

and

$$Tw^o(r,d_1) = \frac{1}{2\pi}\int_0^L [\dot\phi(s) + \dot\psi(s)\cos\theta(s)]\, ds. \tag{17}$$

Proof. The formula for twist is easily found by using (15) in the definition of twist, as in the proof of Lemma 3.5. For the writhe we apply Corollary 3.2 and use the fact that $v = e_3$. □

The main result of this section states that for rods in $\mathcal{A}_{r_0}^2$ end rotation is equal to the open link:

Theorem 3.8. *Let* (r,d_1) *be an open rod in* $\mathcal{A}_{r_0}^2$. *Then*

$$R(r,d_1) = 2\pi Lk^o(r,d_1) = \int_0^L [\dot\phi(s) + \dot\psi(s)]\, ds = \phi(L) + \psi(L) - \phi(0) - \psi(0). \tag{18}$$

Proof. By Corollary 2.4 and Lemma 3.7 we obtain

$$Lk^o(r,d_1) = Wr^o(r) + Tw^o(r,d_1) = \frac{1}{2\pi}\int_0^L [\dot\phi(s) + \dot\psi(s)]\, ds.$$

Since $\int_0^L [\dot\phi(s) + \dot\psi(s)]\, ds = R$ by Lemma 3.5 we have the desired result. □

4. Critique of the approach

The example of Fig. 1 shows that end rotation can only be defined for a deformation history. For the purpose of analysis of elastic structures this dependence on deformation history is undesirable. The approach in this paper, which is shared by many others (see the next section), is therefore to construct a class of deformation histories (homotopies) within which the end rotation *can* be expressed in terms of the initial and final states only. In this section we critically review the essential ingredients of this approach.

The closure. We obtain a separation into deformation classes by the introduction of a closure. The classes are characterised by the link of the closed rod-closure combination. The price we pay with this construction is the dependence on the choice of closure, which at first sight might seem to be a defect of the formulation. As Alexander & Antman [3] point out, however, this dependence is entirely natural: the precise form of the closure can be regarded as describing the way the

rod is supported. Different systems of supports necessarily allow different classes of deformations.

Although in most applications throwing the rod around the clamp as illustrated in Fig. 1(d) is physically prevented, there do exist exceptions to this rule. In some recent experiments DNA molecules are manipulated with the help of a magnetic bead attached to the end of the molecule and held in a magnetic trap which allows the simultaneous application of a force and a moment [30]. In this case no rigid mechanical support is present and the molecule is free to loop around the beaded end. If this happens repeatedly, then the end can rotate over an arbitrarily large angle under the applied moment without a concomitant change in configuration (*cf.* Fig. 1: after a rotation of the end by -4π the rod returns to its original shape). Thus one might estimate the wrong energy, by $\pm 4\pi M$ for each 'looping', if a deformation would go outside the class, i.e., if link was not conserved. However, Rossetto & Maggs [25] in a recent paper show that for micron-sized beads the applied tension in many experiments is large enough (on the order of femtonewtons) to make these link violations rare, and they proceed to introduce a closure to study configurations of constant link.

Incidentally, the fact that a rotation of $\pm 4\pi$, and not one of $\pm 2\pi$, brings one back to where one started has its origin in the topological nature of $\mathrm{SO}(3)$, the group of rotations in $\mathbb{R}^3$. Specifically, $\mathrm{SO}(3)$ is not simply connected: for every rotation $R \in \mathrm{SO}(3)$ there are two homotopy classes of paths from the identity of the group to R. This means that for a given rod orientation there are two distinct classes of configurations for the rod which cannot be deformed into each other while keeping the ends fixed. Rods with any even number of end turns (including zero) lie in one class; rods with any odd number of turns lie in the other. The same topological property forms the basis of the famous Dirac Belt Trick [15], which in classrooms is often illustrated by rotating a cup, held in the palm of one's hand, twice around a vertical axis by a suitable motion of the arm to bring both cup (with contents) and arm back to their initial positions (see [10] for a demonstration).

The reference curve. The class $\mathcal{A}^1_{r_0}$ is defined for a fixed closed reference curve r_0 (which may or may not include the unstressed centerline of the rod). The open writhe Wr^o will, in general, depend on the choice of this curve; on the one hand, by the fact that the reference curve restricts the class of admissible homotopies via the non-opposition condition, and on the other hand, by the explicit dependence on t_0 in (12). Similarly, the end rotation R will depend on r_0, as is to be expected since R is defined (in Definition 3.4) as the end rotation incurred in deforming $(r_0, \bar{d}_1(\cdot, 0))|_{[0,L]}$ into (r, d_1).

For certain cases, however, the dependence can be described more precisely, as in Theorem 3.3 for straight reference curves. Though beyond the scope of this paper, it is also possible to prove a similar result under rotation of more general reference curves. For instance, one could extend Definition 3.4, Lemma 3.5 and Corollary 3.6 to a larger class than $A^2_{r_0}$ by requiring of $r_0|_{[0,L]}$ only that its end tangents be equal. A complication would arise, however, in that violation of the non-opposition condition would no longer coincide with the Euler-angle singularity. Consequently, the non-opposition condition would no longer assure us of C^1-regularity of ϕ, ψ, and θ.

The non-opposition condition cannot be dropped. The non-opposition condition listed in the definition of $\mathcal{A}^1_{r_0}$ (condition 5) is imposed by the application of Theorem 2.6. This might seem to be merely a technical restriction: after all, the open writhe is defined in terms of the writhe of the closed curve (Definition 2.3) and the latter is well-defined even if, somewhere along the homotopy, the non-opposition

condition is violated. Therefore it might be expected that the statement of well-posedness holds true without condition 6 (even though our proof evidently does not), and that only non-self-intersection of the closed structure is required.

In fact the situation is not that simple. Figure 3 shows homotopy paths connecting the reference configuration (a) with the deformed rod-closure combinations (b), (c) and (d), where the rod itself (represented by the thick line) is the same in each of the three deformed states. We can imagine the deformed rod to be nearly planar, with the two strands crossing at a short distance from each other. Then the rod and its closure in case (b) have writhe close to -1.[1] In case (c) one adds or subtracts 1 to the writhe of the rod-closure combination for each full turn of the end. The writhe of the combination can therefore be made arbitrarily large. In case (d), finally, the writhe is close to -2.
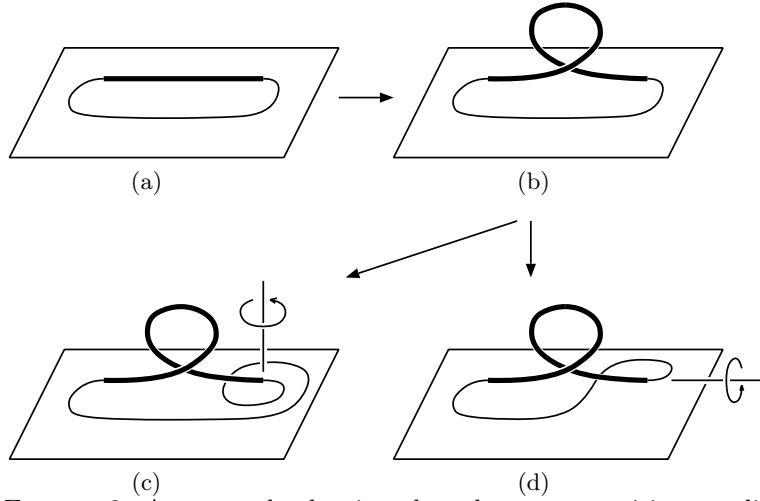

FIGURE 3. An example showing that the non-opposition condition 5 in Definition 2.2 cannot be disposed of. The three final states (b), (c) and (d), with identical shapes for the open rod, have different values of writhe. In going from (b) to either (c) or (d) the non-opposition condition is violated.

It is not difficult to see that one may construct a homotopy between (a) and (b) without violating the non-opposition condition, provided the loop has been twisted through an angle strictly less than π. Since the continuation homotopies to (c) and (d) satisfy all conditions of Definition 2.2 other than the non-opposition condition, it follows from Theorem 2.5 that these homotopies cannot be constructed without violating the non-opposition condition. This may also be verified by inspection.

This example shows that simply removing condition 5 from Definition 2.2 leads to ambiguities in the definition of writhe (and therefore of link). The example also suggests that if a well-defined writhe is to be constructed without the inclusion of the non-opposition condition, then additional restrictions must be imposed on the closure. In homotopy (c) the closure remains planar throughout the homotopy, but the end tangents vary; in homotopy (d) the end tangents are constant, but the closure is only planar at the beginning and the end of the homotopy. To rule out homotopies (c) and (d) (necessary for a well-defined writhe) we can require the end

---

[1]This may be verified by using the characterisation of writhe as the average of the directional writhing number, as explained in Section 2. This number is determined by counting signed crossings in a projection of the curve onto a plane.

tangents to be fixed and the closure to be planar throughout the homotopy. It is possible that for a well-defined writhe further conditions must be imposed.

Euler-angle singularity *vs.* the non-opposition condition. When the reference configuration is straight and end tangents remain constant during the homotopy, the non-opposition condition is equivalent to avoidance of the Euler-angle singularity at $\theta = \pi$. Although this is partly a coincidence, the two issues both stem from the topological properties of S^2.

The Euler-angle singularity results from the fact that S^2 is not homeomorphic to (any part of) $\mathbb{R}^2$. Any parametrization of S^2 by a single cartesian coordinate system will therefore have at least one singular point. On the other hand, the non-opposition condition is necessary—in this article—for the single-integral representation of writhe of Theorem 2.6. In this representation the ambiguity of area 'enclosed' by a curve on S^2 is resolved by taking a perturbation approach. The non-opposition condition is the realization of the unavoidable limits of this approach, and therefore again stems from the topology of S^2.

As mentioned above, however, the non-opposition condition remains an unsatisfactory element in the definition of open writhe. Perhaps a concept of open writhe is possible that bypasses this condition.

Open writhe is not rotation invariant. The definition of $\mathcal{A}^1_{r_0}$ depends on the choice of the reference configuration. For a given reference configuration, an open rod in $\mathcal{A}^1_{r_0}$ may not be freely rotated without leaving $\mathcal{A}^1_{r_0}$. This is readily demonstrated by rotating the reference configuration itself: after a rotation of π about an axis perpendicular to the plane of the reference curve the non-opposition condition is violated at every point on the curve.

This may lead to surprising results. In Figure 4 two homotopies are shown. The first is a variation on homotopy (b) of Figure 3, while in the second we lengthen the open-rod part and shorten the closure part. In addition, we construct the homotopies such that the final configurations are close, up to a rotation (emphasized by the mark at one end of the open rod). In (a) the open writhe is close to 1, while in (b) it is close to 0.
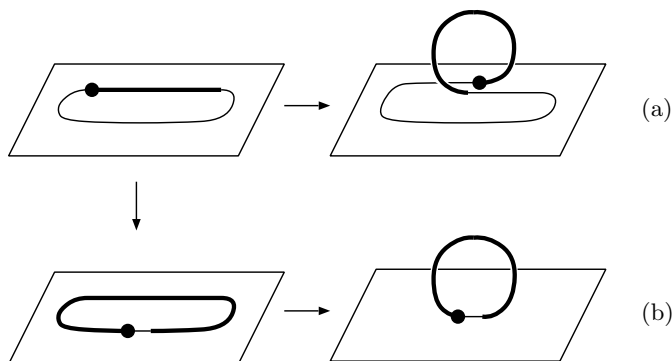

FIGURE 4. Two elements of $\mathcal{A}^1_{r_0}$ that differ only by a rotation, but for which the writhe is different. The dot emphasizes the difference in orientation.

This remark also resolves an issue raised in Remark 2.8: does the open writhe change continuously into the classical writhe for closed rods, when an open rod is transformed into a closed rod by lining up and connecting the ends? The answer is no—for the resulting closed writhe would be rotation-invariant, contradicting the remark above.

5. Discussion

The topological issues associated with large deformation discussed in this paper are not of great concern in more traditional engineering applications. As long as deformations are such that the integral in (2) remains well-defined for a suitable choice of Euler angles (i.e., as long as the angles stay away from the polar singularity) open link and end rotation are given by (2). However, in more modern applications of structural mechanics, such as in molecular biology, large deformations occur more routinely and more care is required. Indeed, Fuller's 1971 paper [11] was inspired by supercoiling DNA molecules. In this paper the author also already introduces a (planar) closing curve in order to compute the writhe of a simple (infinitely long) helix. Following the pioneering work of Fuller an extensive literature has emerged on the application of elastic rod theory to DNA supercoiling (*cf.* the survey article by Schlick [26]).

Open rods have become popular models for DNA molecules since by the early 1990s single-molecule experiments have become possible. First this involved an applied force only [27]; later, once the molecule could be prevented from swivelling at its (magnetically) loaded end, this involved both an applied force and an applied moment [30]. Analytical studies have addressed DNA in isolation [4, 9] as well as in dilute solution using a statistical mechanics approach [19, 31, 20, 5].

Benham [4] appears to have been be the first one to write down an isoperimetric variational problem based on (2) in order to find equilibrium configurations subject to constant link. He first uses Fuller's result (9) with r_2 taken to be a suitable closed planar curve. Then $Wr(r_2) = 0$, and one obtains a single-integral formula for the writhe of the curve in question r_1. When combined with the single integral for the twist (4), this leads, via (1), to a single-integral expression for the link, which in a suitable Euler-angle representation is given by (2). Benham then observes that "the integral expressions for Lk, Tw and Wr may be constructed regardless of whether the structure is closed". Many workers have since followed Benham's example to write link and writhe of an open rod as single integrals.

The implicit assumption in this approach is that there exists a continuous deformation from r_1 to the planar curve r_2 which avoids opposition of corresponding tangents. This may not be obvious, since the non-opposition condition must be applied to the closed combination of rod and suitable closure. In Section 4 we have given examples of what can go wrong if the condition is not satisfied. In addition, the example of Figure 4 shows that even within the limits of the non-opposition condition the writhe is not invariant under rotation, implying that this approach may lead to counterintuitive results.

Frequently, the end rotation needed in an energy analysis is simply assumed to be equal to the link as given by (2) (e.g., [9, 20]). We have shown that end rotation can only be defined in a consistent way within a class of homotopies of rods. Such a class is constructed with the help of a closure. We define end rotation independent of link and show the two to be equal within a suitable class of allowed deformations. We should also remark that our closure is a rod (r, d_1) rather than just a centerline r. Most authors initially only introduce a closed centerline, which makes the writhe well-defined, and subsequently assume the closure to be twistless if a link or end rotation is required. We formalise this practice by explicitly specifying a d_1 for the entire closed structure.

Knowing the precise restrictions on allowed deformations is important in statistical mechanics studies. To obtain the correct averages one must consider ensembles of admissible configurations. In numerical computations this means that one must take care to simulate configurations (through a Monte Carlo algorithm, a 'growth' algorithm or otherwise) with the right topological constraints. Specifically, one

wants the configurations to be unknotted and to have constant link (although it is good to remember that DNA in its natural environment functions in the presence of topology-changing enzymes). This means that one must forbid self-crossings of the configuration as well as crossings of an (imaginary) closure. Mindful of this, the authors in [31] graft the ends of the molecule to an external surface and run 'sticks' out from the ends of the molecule to infinity, thereby 'virtually closing' the generated chain at infinity. A similar construction is used in [25]. In this latter work knotted configurations are not eliminated, it being argued that the molecular statistics is dominated by unknotted configurations.

In order to avoid the awkward non-opposition condition in Fuller's second theorem there have been direct approaches via the double integral (6) instead. In [29, 21] simple shapes are considered with planar closures for which the integral can be evaluated explicitly. It is then shown that the closure gives a relative contribution to the writhe which tends to zero as the length of the rod tends to infinity. The double integral is also used in the numerical study in [31], where it is shown that the contribution to Wr from the interaction of the closure with the basic chain is of the order of 1%. Various numerical schemes for the computation of the writhe double integral for a discretised curve are discussed and compared in [16]. Useful rigorous error bounds on numerically computed values of Wr based on polygonal (i.e., piece-wise linear) approximation are given in [7].

Our approach to a consistent definition of link, writhe and end rotation is firmly based on the introduction of a closure. There have been various formulations of writhe for open curves without the use of a closure. One approach, especially taken in knot theory and in studies of self-avoiding chains, is based on the characterisation of writhe as the average over all planar projections of the sum of signed crossings [11] (e.g., [22, 1]). This approach does not require a closure and can be applied to curves with arbitrary end tangents. It could form the basis of an alternative extension of (1) to open rods. (Here we can remark that link also has an interpretation in terms of crossing numbers, namely: the linking number of two curves is equal to the number of all signed crossings of the curves in a regular planar projection, i.e., one satisfying a transversality condition; see [24].) The precise relation between the writhe of an open curve obtained via these planar projections and the open writhe obtained by using the tantrix area on S^2, or the double integral (6), is still an open problem.

If an exact writhe is not required and the fractional part modulo 2 is sufficient then formula (8) in terms of the area enclosed by the tantrix on the unit sphere can be used. Rossetto & Maggs [25] point out that this approach can also be used to generalise the writhe to curves whose end tangents are not aligned and therefore have open tantrices. By exploiting the connection between writhe and a geometric phase they show that the canonical way to close the curve is by means of a geodesic (great circle). This geodesic is unique as long as the two end points are not antipodal. The fractional writhe is then again given by the enclosed area. This prescription is used by Starostin [29] to derive results for the writhe of smooth as well as polygonal curves. Cantarella [7] generalises Fuller's second theorem, and with it the spherical area formula (8), to polygonal curves.

Appendix A. Proof of Theorem 3.3

Let $f : S^2 \to \mathbb{R}$ be the function mentioned in the assertion. Pick $v_0 \in \Omega$ and let Ω_0 be the connected component of Ω containing v_0. Define the set

$$A = \{v \in \Omega_0 : f(v) = f(v_0)\}.$$

The function f is continuous on Ω_0, implying that the set A is relatively closed in Ω_0. We will show below that f is constant on all open balls $B \subset \Omega_0$, implying that A is also open. Since A is non-empty it follows that $A = \Omega_0$ and the Lemma is proved.

For a given vector $\omega \in S^2$, let R_ϕ denote the rotation around ω through an angle ϕ. We fix the direction of rotation in the following way: with respect to an orthonormal basis $(\omega, w, \omega \times w)$ for a suitable $w \in S^2$, write R_ϕ as

$$R_\phi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix}.$$

With this choice,

$$\frac{d}{d\phi} R_\phi v|_{\phi=0} = \omega \times v \qquad \text{for any } v \in S^2. \tag{19}$$

Set $v_\phi = R_\phi v$. Using equation (19), we have

$$\frac{d}{d\phi} \frac{v_\phi \times t}{1 + v_\phi \cdot t} \cdot \dot{t} = \frac{[(1 + v_\phi \cdot t)((\omega \times v_\phi) \times t) - (v_\phi \times t)((\omega \times v_\phi) \cdot t)]}{(1 + v_\phi \cdot t)^2} \cdot \dot{t}. \tag{20}$$

Setting $\gamma = |\omega \times v_\phi|$ we introduce an orthonormal coordinate system

$$e_1 = v_\phi, \quad e_2 = \gamma^{-1} \omega \times v_\phi, \quad e_3 = \gamma^{-1} v_\phi \times (\omega \times v_\phi),$$

and we write t_1, t_2, t_3 for the coordinates of t with respect to this basis; these are functions of the curve parameter s. The right-hand side of (20) becomes

$$\gamma \frac{(1 + t_1)(t_3 \dot{t}_1 - t_1 \dot{t}_3) - t_2(t_2 \dot{t}_3 - t_3 \dot{t}_2)}{(1 + t_1)^2}.$$

Using the equalities $t_1^2 + t_2^2 + t_3^2 = 1$ and $t_1 \dot{t}_1 + t_2 \dot{t}_2 + t_3 \dot{t}_3 = 0$ this is seen to be equal to

$$-\gamma \frac{d}{ds} \frac{t_3}{1 + t_1}.$$

Therefore

$$\frac{d}{d\phi} \int \frac{v_\phi \times t}{1 + v_\phi \cdot t} \cdot \dot{t}\, ds = -\gamma \int \frac{d}{ds} \frac{t_3}{1 + t_1}\, ds = 0.$$

The last equality results from the assumption of aligned end tangents. This proves the Theorem.

Acknowledgments

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