9 Link, Twist, Writhe, and the Writhe frame

In this chapter, we shall consider some topological and geometrical properties associated with the double-helical structure of DNA. In particular the two back bones of a DNA molecule provide two curves in space which do not intersect each other. And in a mini-circle the two backbone curves are each closed. The central theorem to be discussed in this chapter will the Calugareanu-White-Fuller equation Lk=Tw+Wr, which is an equation that relates the link Lk of two closed curves, to the twist Tw of a ribbon constructed from the two curves, and the writhe Wr of one of the curves. As we shall see below Lk of any two closed non-intersecting curves in three-space is always an integer-valued topological invariant (i.e. it is constant under deformations that do not allow intersections of the two curves). In contrast twist is a real-valued non-invariant number associated with the geometry of a framed curve, while writhe is a real-valued non-invariant number associated with the geometry of a single curve. Thus the Calugareanu-White-Fuller formula states that when the two curves are closed, and an appropriate interpretation of the framed curve is made, the sum of two non-invariant, real valued quantities is an integer invariant quantity.

9.1 The Link Integral

Let us first denote by $\boldsymbol{C_1} = \boldsymbol{x(s)}$ and $\boldsymbol{C_2} = \boldsymbol{y(\sigma)}$ two non-intersecting curves, which we assume to be as smooth as necessary and in particular twice differentiable, i.e. $\boldsymbol{C^2}$ curves in $\Re^3$. Although it is not crucial for our purposes, we remark that for the definition of Lk it is not necessary that $\boldsymbol{x(s)}$ be a non self-intersecting curve, and similarly for $\boldsymbol{y(s)}$. However it is crucial that $\boldsymbol{x(s)}$ not intersect $\boldsymbol{y(s)}$.

We define the Gauss Linking integral of the two curves to be:

$$Lk(C_1,C_2) = \frac{1}{4\pi}\int_{C_1}\int_{C_2}\frac{(y(\sigma)-x(s))\cdot(y'(\sigma)\times x'(s))}{|y(\sigma)-x(s)|^3}d\sigma\, ds.$$

This double integral is invariant under re-parameterizations of the curves, so $\boldsymbol{\sigma}$ and $\boldsymbol{s}$ can be any parameterizations. If $\boldsymbol{\sigma}$ and $\boldsymbol{s}$ are arc-length parameterizations, then $\boldsymbol{y'(\sigma)}$ and $\boldsymbol{x'(s)}$ will be unit vectors. As will be seen later (actually in the exercise session) the choice of normalization factor $\frac{1}{4\pi}$

will make Lk integer valued in the case that both curves $\boldsymbol{x(s)}$ and $\boldsymbol{y(s)}$ are closed.

It will also be convenient to denote the integrand in the Link double-integral by:

$$\boldsymbol{I_{Lk}(\sigma, s) = \frac{(y(\sigma) - x(s)) \cdot (y'(\sigma) \times x'(s))}{|y(\sigma) - x(s)|^3}}$$

In the case where $\boldsymbol{x(s)}$ and $\boldsymbol{y(s)}$ are closed $\boldsymbol{I_{Lk}(\sigma, s)}$ is a doubly periodic function defined on a rectangle (or square). For simplicity we may then rewrite Lk as:

$$\boldsymbol{Lk(C_1,C_2) = \frac{1}{4\pi} \int_{C_1} \int_{C_2} I_{Lk}(\sigma, s)\, d\sigma\, ds}$$

Later, we will also need the intermediate single, integrand obtained after one integration in the Link double integral, i.e.:

$$\boldsymbol{\widehat{I_{Lk}}(s) = \int_{C_2} \frac{(y(\sigma) - x(s)) \cdot (y'(\sigma) \times x'(s))}{|y(\sigma) - x(s)|^3} d\sigma.}$$

Historically, the Link integral was first introduced by Gauss, who in his duties as an astronomer studied the interlacings of two closed or infinite curves representing the orbit of an asteroid (or a comet) and the orbit of earth (or the orbits of any two other objects). This question is important to understand what regions in the sky (or the celestial sphere) must be examined to see a given asteroid from the earth over a period of time–the possible regions that the asteroid (or other body) can appear is called the zodiacus of that body (with respect to the earth's celestial sphere). In the case where the orbits of the asteroid and the earth are linked together, which means that the asteroid trajectory intersects the interior of the ellipse in the plane defined by the earth's orbit, then it can be shown, using the Link integral, that the zodiacus is the whole of the celestial sphere (and that some parts of the zodiacus are multiply covered). (For more details of this history see the very nice article by Moritz Epple, "Orbits of Asteroids, a Braid, and the First Link Invariant", The Mathematical Intelligencer, vol. 20, number 1, 1998).

Important Remarks: As already observed,

- The Link integral Lk is invariant under reparameterization.
- The integrand has no singularity, as long as $\boldsymbol{y}(\sigma) \bigcap \boldsymbol{x}(s) = \{\emptyset\}, \forall s, \sigma$. The Link integral can have different limits, as the intersection case is approached, so it is not possible to simply extend the definition of Lk to cover the intersecting case.
- In contrast, self-intersection of $\boldsymbol{y}(\sigma)$ with itself, or $\boldsymbol{x}(s)$ with itself raises no difficulty. In fact it can be shown that one can consider deformation of one curve, say $\boldsymbol{x}(s)$, in which self-intersections are generated, and even the connectivity of $\boldsymbol{x}(s)$ is changed without any singularities arising.

Theorem 1

If $\boldsymbol{y}(\sigma)$ and $\boldsymbol{x}(s)$ are (smooth) closed curves, then:

1. Lk is an integer.
2. Lk is invariant under smooth deformations of $\boldsymbol{y}(\sigma)$ and $\boldsymbol{x}(s)$ which preserve the non-intersection property $\boldsymbol{y}(\sigma) \bigcap \boldsymbol{x}(s) = \{\emptyset\}, \forall s, \sigma$.

Note that there exist similar results for curves in which closure is replaced by certain asymptotic conditions at infinity, including $|\boldsymbol{x}|, |\boldsymbol{y}| \to \infty$, as $|\sigma|, |s| \to \infty$. See Arnol'd and Khesin.

For general non-closed curves, both conclusions of the Theorem are false.

Proof

The most general, and in some ways most basic, proof of Part 1 relies on the notion of degree of a mapping. For two non-self intersecting curves, the vector field $\boldsymbol{e}(\boldsymbol{\sigma}, \boldsymbol{s})$ associated with the chord linking pairs of points, one on each curve, that is defined by

$$\boldsymbol{e}(\boldsymbol{\sigma}, \boldsymbol{s}) = \frac{\boldsymbol{y}(\boldsymbol{\sigma}) - \boldsymbol{x}(\boldsymbol{s})}{|\boldsymbol{y}(\boldsymbol{\sigma}) - \boldsymbol{x}(\boldsymbol{s})|}$$

is a smooth, singularity free, unit vector field (provided that $\boldsymbol{y}(\boldsymbol{\sigma}) \bigcap \boldsymbol{x}(\boldsymbol{s}) = \{\emptyset\}, \forall \boldsymbol{s}, \boldsymbol{\sigma}$). Moreover for two *closed* curves, the vector field $\boldsymbol{e}(\boldsymbol{\sigma}, \boldsymbol{s})$ is doubly periodic. Such mappings have an integer valued degree, that is invariant under topological deformations. It can further be shown that the link expressed in its double integral form is one representation of this integer degree. Unfortunately, such arguments are completely un-illuminating unless the reader has mastered the quite considerable machinery of degree theory. See for example Dubrovin et al. "Modern differential geometry". Fortunately, it is in fact possible to construct an elementary proof, i.e. a sequence of elementary computations which demonstrate the result, although there is little indication of 'why' the result is true. See exercise set 3 (of the Summer semester) for an outline of this elementary proof. This elementary argument uses the invariance properties that are the subject of part 2 of this Theorem.

Proof of the second part of Theorem 1.

We now show that the link integral can be rewritten in terms of the unit vector field $\boldsymbol{e}(\boldsymbol{\sigma}, \boldsymbol{s})$ as:

$$\frac{1}{4\pi} \int_{C_1} \int_{C_2} [e, \boldsymbol{e}_s, \boldsymbol{e}_\sigma] \, d\sigma \, ds$$

where $\boldsymbol{e}_\sigma$ and $\boldsymbol{e}_s$ are partial derivatives of $\boldsymbol{e}(\boldsymbol{\sigma}, \boldsymbol{s})$ with respect to $\boldsymbol{\sigma}$ and $\boldsymbol{s}$ (but for fixed curves $\boldsymbol{y}$ and $\boldsymbol{x}$), and the triple bracket $[\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}]$ denotes the scalar triple product

$$[\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}] = \boldsymbol{a} \cdot (\boldsymbol{b} \times \boldsymbol{c})$$

Of course we have all the cyclic and anti-cyclic permutation properties of the triple product, $[\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}] = [\boldsymbol{b}, \boldsymbol{c}, \boldsymbol{a}]$ etc. And in particular, $[\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{b}] = \boldsymbol{0}$

Substitution of the formula

$$\boldsymbol{e}_s = -\frac{\boldsymbol{x}'(\boldsymbol{s})}{|\boldsymbol{y}(\boldsymbol{\sigma}) - \boldsymbol{x}(\boldsymbol{s})|} + (\boldsymbol{y}(\boldsymbol{\sigma}) - \boldsymbol{x}(\boldsymbol{s}))\boldsymbol{\partial}_s \left[\frac{1}{|\boldsymbol{y}(\boldsymbol{\sigma}) - \boldsymbol{x}(\boldsymbol{s})|}\right]$$

and similarly for e_σ into the triple scalar product yields after simplification using the properties of the triple product, that

$$[e, e_s, e_\sigma] = \frac{y(\sigma) - x(s)}{|y(\sigma) - x(s)|} \cdot \frac{(y'(\sigma) \times x'(x))}{|y(\sigma) - x(s)|^2} = I_{Lk}$$

We remark in passing that this identity reveals that the link integral is the signed area on the unit sphere swept out by the vector $e(\sigma, s)$.

We now need to show that for all doubly-periodic unit vector fields e, the first variation of the Link integral is identically zero. In the proof we will integrate by parts (in s on the δe_s term and in σ on the δe_σ term), using the appropriate 'product rule' for the derivative of a scalar product, namely

$$[a, b, c]' = [a', b, c] + [a, b', c] + [a, b, c'].$$

We compute the first variation of Lk when the vector field is subject to a first order variation:

$$\delta Lk = \frac{1}{4\pi} \int \int \delta[e, e_s, e_\sigma]\, ds\, d\sigma$$

$$= \frac{1}{4\pi} \int \int ([\delta e, e_s, e_\sigma] + [e, \delta e_s, e_\sigma] + [e, e_s, \delta e_\sigma])\, ds\, d\sigma$$

We then integrate by parts on δe_σ and δe_s, leading to boundary terms BT and new integrals

$$\delta Lk = BT + \frac{1}{4\pi} \int \int ([\delta e, e_s, e_\sigma] - [e_s, \delta e, e_\sigma]$$

$$-[e, \delta e, e_{\sigma s}] - [e_\sigma, e_s, \delta e] - [e, e_{s\sigma}, \delta e])ds\, d\sigma.$$

Now because of the identity $e_{s\sigma} = e_{\sigma s}$, and the skew-symmetry of the triple product:

$$\delta Lk = BT + \frac{1}{4\pi} \int ([\delta e, e_s, e_\sigma] - [e_s, \delta e, e_\sigma] - [e_\sigma, e_s, \delta e])ds\, d\sigma$$

$$= BT + \frac{3}{4\pi} \int \int [\delta e, e_s, e_\sigma] ds\, d\sigma$$

But $e(\sigma, s)$ is a unit vector field, so

$$e \cdot e_s = e \cdot e_\sigma = e \cdot \delta e = 0,$$

or in other words e_s, e_σ and δe are co-planar, all three being perpendicular to the vector field e. Consequently,

$$[e_s, e_\sigma, \delta e] = 0, \quad \forall s, \sigma.$$

Accordingly, we may conclude that $\delta Lk = BT$, where the boundary terms take the explicit form

$$BT = \left[\int [e, \delta e, e_\sigma] d\sigma \right]_{s=0}^{s=L} + \left[\int [e, e_s, \delta e] ds \right]_{\sigma=0}^{\sigma=L}.$$

Thus far, all the computations are valid for arbitrary curves, but now we use the hypothesis that x and y are closed curves, and we furthermore assume that the variations preserve closedness so that $x + \delta x$ and $y + \delta y$ are also periodic. This implies that:

$$\delta e(\sigma, L) = \delta e(\sigma, 0) \quad \forall \sigma,$$

and

$$\delta e(0, s) = \delta e(L, s) \quad \forall s.$$

Therefore we have that

$$BT = 0 \Rightarrow \delta Lk = 0,$$

which is the conclusion necessary to complete the proof of the Theorem.

9.2 The Writhe Integral

We now move to consider the writhe double integral, which, contrary to link, is a property of a single non-self-intersecting curve in space, and is defined by integrating twice over one curve $C_1 = x(s)$ that is non self-intersecting, i.e. $x(s) = x(t) \Rightarrow s = t$. We define writhe by:

$$Wr(C_1) = \frac{1}{4\pi} \int_{C_1} \int_{C_1} \frac{(x(\sigma) - x(s)) \cdot (x'(\sigma) \times x'(s))}{|x(\sigma) - x(s)|^3} d\sigma \, ds.$$

We also denote the integrand of the writhe double integral by I_{Wr}:

$$I_{Wr}(\sigma, s) = \frac{(x(\sigma) - x(s)) \cdot (x'(\sigma) \times x'(s))}{|x(\sigma) - x(s)|^3}$$

and the intermediate single-integral integrand:

$$\widehat{I_{Wr}}(s) = \int_{C_1} \frac{(x(\sigma) - x(s)) \cdot (x'(\sigma) \times x'(s))}{|x(\sigma) - x(s)|^3} d\sigma$$

These writhe integrands are directly analogous to the formulas arising in the link case but for two parameterizations of the same curve, rather than parameterizations of two different curves.

The integrand I_{Wr} is a function of s and σ that satisfies $I_{Wr}(s, \sigma) = I_{Wr}(\sigma, s)$. We also remark that by the hypothesis of non-self-intersection of the curve $x(s)$ we have that

$$|x(s) - x(\sigma)| \to 0 \Rightarrow s \to \sigma.$$

Consequently, I_{Wr} is a smooth function away from the diagonal $s = \sigma$. However, an analysis of the limiting behaviour of the integrand close to the diagonal is necessary in order that the single and double integrals introduced above are well-defined. In fact I_{Wr} is also smooth at the diagonal, as is shown in the proof of the following lemma.

Lemma

$I_{Wr}(s, s) = 0$

Proof: Expanding $x(\sigma)$ in a finite Taylor series we see that

$$x(\sigma) = x(s) + (\sigma - s)x'(s) + \frac{1}{2}(\sigma - s)^2 \hat{x}'' \tag{9.171}$$

$$x(\sigma) = x(s) + (\sigma - s)x'(s) + \frac{1}{2}(\sigma - s)^2 x''(s) + \frac{1}{6}(\sigma - s)^3 \hat{x}''' \tag{9.172}$$

and

$$x'(\sigma) = x'(s) + (\sigma - s)x''(s) + \frac{1}{2}(\sigma - s)^2 \bar{x}''' \tag{9.173}$$

where x' denotes the derivative of the vector function x with respect to s, and $\hat{x}''$, $\hat{x}'''$ and $\bar{x}'''$ denote the vectors of the finite truncation terms,

$$\hat{x}'' = \begin{pmatrix} x_1''(\xi_1) \\ x_2''(\xi_2) \\ x_3''(\xi_3) \end{pmatrix}, \qquad \hat{x}''' = \begin{pmatrix} x_1'''(\psi_1) \\ x_2'''(\psi_2) \\ x_3'''(\psi_3) \end{pmatrix}, \qquad \bar{x}''' = \begin{pmatrix} x_1'''(\chi_1) \\ x_2'''(\chi_2) \\ x_3'''(\chi_3) \end{pmatrix}$$

with $|\xi_i - s| \leq |\sigma - s|$, $|\psi_i - s| \leq |\sigma - s|$ and $|\chi_i - s| \leq |\sigma - s|$ for all $i = 1, 2, 3$.
Now we can expand the integrand I_{Wr} (using (9.172) and (9.173) in the numerator and (9.171) in the denominater) as:

$$\frac{A \cdot ((x'(s) + (\sigma - s)x''(s) + \frac{1}{2}(\sigma - s)^2 \bar{x}''') \times x'(s))}{|\sigma - s|^3 \underbrace{|x'(s) + \frac{1}{2}(\sigma - s)\hat{x}''|^3}}$$

where A is a place holder for

$$A = (\sigma - s)x'(s) + \frac{1}{2}(\sigma - s)^2 x''(s) + \frac{1}{6}(\sigma - s)^3 \hat{x}'''.$$

In simplifying the numerator there is substantial cancellation, and the lowest power of $(\sigma - s)$ to survive is of fourth order, for example a term like

$$\frac{1}{6}(\sigma - s)^4 \hat{x}''' \cdot (x''(s) \times x'(s)).$$

On the other hand, the braced term in the denominator is positive (assuming s is a smooth parameterization so that x' is a non-zero vector, for example a unit vector if s is an arc-length parameterization so that the braced term is greater than $1/2$ for $|\sigma - s|$ sufficiently small). Then the denominator behaves as $(\sigma - s)^3$, while the numerator behaves as $(\sigma - s)^4$. Therefore $I_{Wr} \to 0$ as $\sigma \to s$.

Some properties and non-properties of Writhe:

- Wr is not invariant under general smooth deformations of x,
- Wr is invariant under translations, rotations, re-parameterizations and dilations of x,
- Wr changes sign when x is reflected in a plane. Consequently, planar non-intersecting curves have zero writhe. In fact, the writhe integrand vanishes point-wise in s and σ when the curve is planar.
- Wr changes sign when x is inverted in a sphere. This property generalizes reflections in a plane, although it is much less obvious. Consequently curves lying on a sphere must also have zero writhe, which is a property that can be shown straightforwardly using the Calugareanu-Fuller White formula (see exercises). The writhe integrand does not vanish point-wise for such spherical curves.

- Wr is not necessarily an integer, even for closed curves.
- Wr is not, and cannot be, well-defined for self-intersecting curves.
- All the cancellations in the Taylor expansion of the integrand I_{Wr} in the limit $s \to \sigma$ that a numerical evaluation of writhe on some discretization of a curve requires some special care close to the diagonal.

9.3 The Twist of a Ribbon

By a *ribbon* we mean a curve $x(s)$ along with a (usually unit) normal vector field $d_1(s)$. Recall that when combined with the unit tangent vector $d_3(s)$ field, the externally defined normal field $d_1(s)$ induces a proper orthonormal adapted framing of the curve $x(s)$. Moreover, given the curve $x(s)$, we have seen that any orthonormal adapted framing is equivalent to an initial frame, at $s = 0$ say, plus $u_3(s)$ a scalar function of the arc-length parameter s defining the (local) twist of the orthonormal framing. The natural way of defining the twist, or total twist, Tw of a ribbon is then as the single integral:

$$Tw = \frac{1}{2\pi} \int_0^L u_3(s) ds,$$

i.e. the total twist is the integral of the local twist density $u_3(s)$ normalized by the factor 2π. (So that for a planar curve, which has writhe zero, total twist 1 corresponds to a complete turn of the normal field about the curve. Similar arguments about non-planar curves with non-zero writhe should be treated with caution.)

Alternatively, a ribbon can be regarded as being defined by two space curves $x(s)$ and $y(s)$ which make up its two edges. Notice that it must be the *same* parameter as argument for both curves, so that there is a well-defined chord vector that sweeps out the surface of the ribbon. We will actually reserve the term ribbon for the case where the second curve y can be constructed from x and a local twist u_3 via the relations:

$$y(s) = x(s) + \varepsilon d_1(s)$$

which imply after differentiation (and assuming that the parameter s represents arc-length for the curve $x(s)$)

$$y'(s) = x'(s) + \varepsilon d_1'(s) = d_3(s) + \varepsilon(u(s) \times d_1(s))$$

Note that s is assumed to be arclength for x, but will not in general be arclength for y.

9.4 The Calugareanu-White-Fuller Theorem

The Calugareanu-White-Fuller formula applies in the case that $\boldsymbol{x(s)}$ is a smoothly closed curve in $\boldsymbol{\Re^3}$, with $\boldsymbol{d_1(s)}$ a smoothly closed normal vector field. We therefore have a ribbon as defined in the previous subsection. Moreover the ribbon is completely closed in the sense that both the base curve $\boldsymbol{x(s)}$ and the normal field are periodic. For such completely closed ribbons, which do not self-intersect themselves (which is a reasonable hypothesis for $\boldsymbol{\varepsilon}$ sufficiently small), the formula states that

$$\boldsymbol{Lk = Tw + Wr}$$

where $\boldsymbol{Lk}$ is the link of the two edge curves $\boldsymbol{x(s)}$ and $\boldsymbol{y(s)}$ of the ribbon, Tw is the total twist of the ribbon frame, and Wr is the writhe of the base curve $\boldsymbol{x(s)}$.

We will outline an elementary proof of this formula. We need to start with a Lemma, essentially due to Calugareanu. Let

$$\widehat{\boldsymbol{I_{Lk}}}(\boldsymbol{s,\varepsilon})$$

denote the single link integrand for the specific two curves defining the edges of the ribbon, i.e. $\boldsymbol{x(\sigma)}$ and $\boldsymbol{y(s) = x(s)+\varepsilon d_1(s)}$ The Calugareanu Lemma states that:

$$\lim_{\varepsilon\to 0} \widehat{\boldsymbol{I_{Lk}}}(\boldsymbol{s,\varepsilon}) = \boldsymbol{2u_3(s)} + \widehat{\boldsymbol{I_{Wr}}}(\boldsymbol{s})$$

Here $\widehat{\boldsymbol{I_{Lk}}}$ and $\widehat{\boldsymbol{I_{Wr}}}$ are the single-integral integrands introduced earlier by carrying out one of the integrations in respectively the link and writhe double integrals. It is of some interest to remark that this Lemma does *not* require $\boldsymbol{x}$ or $\boldsymbol{d_1}$ to be closed. The limit can be considered as the non-uniform limit $\boldsymbol{\varepsilon \to 0}$ of the link integral when the ribbon shrinks to a single curve. The proof of this lemma is the essential core of the proof of the CFW formula, and therefore we will give a fragrance of the proof of the lemma.

We have to evaluate:

$$\lim_{\varepsilon\to 0}\int_0^L \frac{(\boldsymbol{x(\sigma) - x(s) - \varepsilon d_1(s)}) \cdot \left(\boldsymbol{x'(\sigma)} \times \left(\boldsymbol{x'(s) + \varepsilon d_1'(s)}\right)\right)}{|\boldsymbol{x(\sigma) - x(s) - \varepsilon d_1(s)}|^3} d\sigma$$

An essential part of the estimation will involve the fact that for any smooth curve $\boldsymbol{x(s)}$, s being the arclength, $\exists\, \boldsymbol{K}$ such that $|\boldsymbol{x(s) - x(\sigma)}| > \boldsymbol{K}|\boldsymbol{s - \sigma}|$ (K is called the distor constant), therefore we have:

$$\frac{1}{|\boldsymbol{x(s) - x(\sigma)}|} < \frac{1}{\boldsymbol{K}\,|\boldsymbol{s - \sigma}|}$$

The proof requires different estimates close to, and away from the diagonal. Accordingly we break the integral into two parts for σ close to s and for σ far from s:

$$\int_C = \int_{C\setminus(s-\varepsilon^{\frac{1}{5}},s+\varepsilon^{\frac{1}{5}})} + \int_{(s-\varepsilon^{\frac{1}{5}},s+\varepsilon^{\frac{1}{5}})}$$

We now develop the numerator of the integrand in powers of ε:

$$\varepsilon^0 : (x(\sigma) - x(s)) \cdot (x'(\sigma) \times x'(s))$$

$$\varepsilon^1 : -d_1(s) \cdot (x'(\sigma) \times x'(s)) + (x(\sigma) - x(s)) \cdot (x'(\sigma) \times (-u_2(s) \cdot x'(s) + u_3(s) \cdot d_2(s)))$$

etc...

details to be included later ....

The above lemma can be re-written in a formal way involving the integrands of the double integrals

$$I_{Lk}(s, \varepsilon, \sigma) = 2u_3(s)\delta(s - \sigma) + I_{Wr}(s, \sigma)$$

where δ stands for a Dirac delta function, which recasts the Twist integral as a double integral over s and σ.

With the help of the above Lemma, we are in good shape to derive the CFW formula after a second integration:

Proof of the Calugareanu-White-Fuller formula.

After integration of the above identity, we conclude that

$$\lim_{\varepsilon \to 0} Lk(x(\sigma), y(s)) = Tw + Wr$$

But for a closed ribbon we know that the LHS is independent of ε, which is just the topological invariance of Lk for two closed curves. Thus we have the identity

$$Lk(x(\sigma), y(s)) = Tw + Wr$$

for all ε, which is exactly the CFW formula.

Remark: The only role played by complete closure of the ribbon is that it guarantees independence of the LHS on ε. Thus it is interesting to consider whether there are other circumstances, less restrictive than complete closure, in which the LHS can be shown to be either independent of, or have a simple dependence on ε. If so, a generalization of the CWF formula would arise. See the discussion of the writhe frame later in these notes for another generalization.

9.4.1 The self-linking of a closed curve

We now turn to consideration of various interesting, specific choices for the normal field $\boldsymbol{d}_1(s)$. First let us take

$$\boldsymbol{d}_1(s) = \boldsymbol{n}(s) = \boldsymbol{x}''(s)/|\boldsymbol{x}''(s)|,$$

i.e. $\boldsymbol{n}(s)$ is the principal normal of $\boldsymbol{x}$ (which we assume to be smooth and well defined everywhere, i.e. there are no points of vanishing curvature $|\boldsymbol{x}''(s)| = \mathbf{0}$).

Because the geometrical normal has a local, intrinsic, definition in terms of derivatives of the curve $\boldsymbol{x}$, whenever $\boldsymbol{x}$ is smoothly closed, then $\boldsymbol{n}$ will be closed too. Thus we may apply the CFW formula. For the Frenet frame $u_3(s) = \tau(s)$, i.e. the twist of the frame is just the geometric torsion of the curve $\boldsymbol{x}$. Then the CFW formula is used to define the Self-Linking of the curve $\boldsymbol{x}$

$$SLk(\boldsymbol{x}(\sigma)) = \frac{1}{2\pi}\int_0^L \tau(s)ds + Wr(\boldsymbol{x})$$

As SLk is just the particular link that arises when the ribbon is generated by the Frenet frame, it is automatically an integer valued homotopy invariant, but *only among deformations that avoid points of vanishing curvature, i.e. inflection points.* For more general deformations one has to somehow deal with the possibility that the principal normal framing could change discontinuously. We remark that for a smoothly closed curve there is no reason to believe that in general $\frac{1}{2\pi}\int \tau(s)ds$ or Wr is an integer, but if one is an integer, then by the CFW formula, so is the other.

9.4.2 The natural frame

The natural frame, whose definition is that $u_3(s) \equiv \mathbf{0}$, may or may not be closed for a general smoothly close curve. However, as we have seen, up to a rotation of the initial choice of normal, the natural frame is uniquely defined for any smooth curve, and there are no difficulties analogous to thise arising at inflection points for the Frenet frame. Is the CFW formula interesting for the natural frame? It does not immediately apply because the natural frame may not be closed. However it does lead to some interesting conclusions after some preliminary calculations.

Recall that for a given curve $\boldsymbol{x}$ if $\{\boldsymbol{d}_i\}$ is an adapted framing corresponding to a twist $u_3(s)$, and $\{\boldsymbol{d}_i\}$ is another adapted framing corresponding to a twist $v_3(s)$, then we can define the scalar angle function between the frames by the ODE

$$\varphi'(s) = u_3 - v_3.$$

In other words

$$\varphi|_{s=0}^{s=L} = \int_0^L (u_3 - v_3)ds.$$

Now, suppose that the curve x is smoothly closed, and that the adapted framing corresponding to the twist $u_3(s)$ is closed. When is the second adapted framing also closed? Purely from the geometry inherent to the definition of the angle φ, the second frame also closes when

$$2N\pi = \varphi|_{s=0}^{s=L}$$

for some integer N. Using the previous identity this condition is equivalent to

$$2N\pi = \int_0^L (u_3 - v_3)ds.$$

Now the Frenet frame of any smoothly closed curve is known to be closed, so we can apply the above argument to the Frenet frame (which has twist $u_3 \equiv \tau$ the geometrical torsion) to conclude that the natural frame (which has twist $v_3 \equiv 0$) is closed iff

$$\int_0^L \tau ds = 2\pi N.$$

Thus we see that a smoothly closed curve has a closed natural framing iff the integral of torsion is an integer multiple of 2π. Because the self link SLk is always an integer, we also see from the CFW formula, that Wr of a smoothly closed curve is an integer iff the natural framing is closed.

9.5 Some interesting implications for DNA

We now consider some implications of the above arguments that are pertinent to modelling DNA.

- We have already seen that when two smoothly closed curves $\boldsymbol{x}$ and $\boldsymbol{y}$ are deformed, the (integer) Link $\boldsymbol{Lk(x,y)}$ is constant unless the curves $\boldsymbol{x}$ and $\boldsymbol{y}$ cross each other. In particular if $\boldsymbol{x}$ crosses $\boldsymbol{x}$, or $\boldsymbol{y}$ crosses $\boldsymbol{y}$ the link remains constant. However when $\boldsymbol{x}$ crosses $\boldsymbol{y}$ it can be shown, for example by the methods used in one of the exercise sessions, that $\boldsymbol{Lk(x,y)}$ jumps by $\pm \mathbf{1}$ (in certain atypical cases, the jump could be a different integer, but such cases are all pathological). When a ribbon passes through itself, there are *two* intersections of the two edge curves, and consequently it can be shown that the link changes by $\pm \mathbf{2}$

- On ribbon or strand passages, where Lk is jumping by $\pm \mathbf{2}$, the total twist Tw is a continuous function. Therefore due to the Calugareanu-White-Fuller formula, the writhe has to change discontinuously by $\pm \mathbf{2}$ in exactly the same way as the Lk of the ribbon. But writhe is a property of a single curve $\boldsymbol{x}$, thus we see (either by the above argument or by a direct analysis) that when a curve is deformed in such a way that it passes through itself, its writhe jumps by $\mathbf{2}$.

- For the elastic rod models that we have considered previously, the elastic energy has the following form:

$$E = \int_0^L \sum_{i=1}^{3} \frac{1}{2} K_i (u_i - \widehat{u_i})^2$$

  For isotropic rods, where $\widehat{u_1} \equiv \widehat{u_2} \equiv 0$ and $K_1 \equiv K_2$, we can simplify this energy to

$$E = \int_0^L \frac{1}{2} K_1 \kappa^2 + \frac{1}{2} K_3 (u_3 - \widehat{u_3})^2$$

  where we have used the fact that the geometric curvature $\boldsymbol{\kappa}$ satisfies the identity $\kappa^2 = (u_1^2 + u_2^2)$.

  For this isotropic elastic energy we know that there is the integral $m_3 = K_3(u_3 - \widehat{u_3}) = const$. Assuming further that K_3 and $\widehat{u_3}$ are both independent of s, we may then conclude that u_3 is constant at an equilibrium, because

$$u_3 = \widehat{u_3} + \frac{m_3}{K_3}$$

  Remembering the Calugareanu-White-Fuller formula

$$Lk = \frac{1}{2\pi} \int_0^L u_3 ds + Wr,$$

if we further restrict attention to isotropic DNA mini-circles that are completely closed, and because we know $\boldsymbol{u_3}$ to be a constant, we could then write

$$u_3 = \frac{2\pi(Lk - Wr)}{L}$$

where the RHS depends only on an integer (the link) and the rod centerline, through the non-local double integral formula for the writhe. We may therfore re-express the Energy solely as a functional dependent on a smoothly closed centreline $\boldsymbol{x}$, with a given constraint imposed by a fixed integer Lk:

$$E = \int_{)}^{L} \frac{1}{2} K_1 (x''(s))^2 \, ds + \frac{1}{2} K_3 L \left(\frac{2\pi(Lk - Wr(x))}{L} - \widehat{u_3} \right)^2 ,$$

where it should be re-iterated that the writhe is a double integral, so that the second term is a quadratic function of a non-local energy. Despite its many restrictions, this formulation of an elastic rod model of DNA is widely used (and abused) in many numerical simulations.

9.5.1 The Writhe Frame

Finally we turn to a consideration of what can be said about the $\boldsymbol{Lk = Tw + Wr}$ formula in the case of a non-closed ribbon? In particular we will show that $\boldsymbol{Tw + Wr}$ has a simple interpretation for a ribbon in which the base curve is smoothly closed, but the adapted framing is open.

For any curve $\boldsymbol{x}$, define a new adapted framing with the twist

$$v_3(s) = -\frac{1}{2} \widehat{I_{Wr}}(x(s)).$$

This twist is a function of $\boldsymbol{s}$ that is defined non-locally through the single writhe integrand $\widehat{I_{Wr}}$. Nevertheless, it uniquely defines (up to the usual choice of initial condition) an adapted framing that we will call the *Writhe frame.*

Now suppose that $\boldsymbol{x}$ is smoothly closed, and that $\boldsymbol{u_3(s)}$ is any twist that defines a closed ribbon on $\boldsymbol{x}$. We may therefore apply the CFW formula. But by our definition of $\boldsymbol{v_3(s)}$ the CFW formula takes the form

$$Lk = Tw + Wr = \frac{1}{2\pi} \int_0^L (u_3 - v_3) ds.$$

And we also know that for any two adapted framings defined by twists $u_3(s)$ and $v_3(s)$, the angle $\varphi(s)$ between their normal vectors satisfies

$$\varphi|_{s=0}^{s=L} = \int_0^L (u_3 - v_3) ds.$$

By assumption $u_3(s)$ is a twist that defines a closed ribbon on x, so Lk of that ribbon is an integer. Consequently, by the above formulas we see that $\varphi|_{s=0}^{s=L}$ is an integer multiple of 2π. In other words, the writhe frame is also closed.

Once we know that the writhe frame is closed for any smoothly closed curve x, it makes sense to consider the link Lk for the writhe framing of the curve. In particular, we may take $u_3(s) \equiv v_3(s)$ and still apply the CFW formula to conclude that the link of the writhe framing is zero. Therefore, the writhe frame has the appealing interpretation of being an intrinsically defined, closed, zero link framing of any smoothly closed curve.

Knowing that the writhe framing of any smoothly closed curve is closed, leads to another application as follows. Suppose now that $u_3(s)$ is a twist defining an arbitrary adapted framing $d_1(s)$ of a given smoothly closed curve x. And denote the writhe framing by $d_1(s)$. Using the freedom for choosing initial conditions, we may assume without loss of generality that

$$d_1(0) = d_1(0),$$

i.e. the angle between the frame defined by $u_3(s)$ and the writhe frame vanishes initially, i.e. $\varphi(0) = 0$. Then

$$\int_0^L (u_3 - v_3) = \varphi(L)$$

which is the angle between the two frames at $s = L$, or more precisely between d_1 and d_1 at s=L. But the writhe frame is known to be closed so that $d_1(0) = d_1(L) = d_1(0)$ by construction, and therefore $\varphi(L)$ is th angle between $d_1(L)$ and $d_1(0)$, which is the angle by which the frame $\{d_i\}$ associated with $u_3(s)$ fails to be closed.

The above arguments can be re-phrased as a version of the CFW formula for the case of non-closed ribbons with smoothly closed base curves: The quantity

$$2\pi(Tw + Wr) \mod 2\pi$$

is the angle of discontinuity by which the ribbon fails to close. The ribbon closes precisely when $(Tw + Wr)$ is an integer, in which case the CFW formula states that that integer is the link of the ribbon.

Open Question 1: Twist and writhe and the double integral formula for Lk are all well-defined quantities for adapted framings of non-closed curves. Is there an interesting formula that relates the three quantities for a) non-closed framings of smoothly closed curves, b) framings of non-smoothly closed curves. Notice that the arguments immediately above give an appealing interpretation of the sum $(\boldsymbol{Tw} + \boldsymbol{Wr})$, but do not provide a connection to the double integral representation of Lk unless the ribbon is closed.

Open Question 2: For some framings of a given smooth curve $\boldsymbol{x}$ that are defined by specifying the twist, there are explicit solutions for the framing in terms of the curve $\boldsymbol{x}$ and its derivatives. For instance for the Serret-Frenet framing, where $\boldsymbol{v_3(s)} = \boldsymbol{\tau(s)}$ with the geometrical torsion $\boldsymbol{\tau}$ being an expression involving third derivatives of the curve $\boldsymbol{x}$, one normal framing is $\boldsymbol{d_1(s)} = \boldsymbol{n(s)} = \boldsymbol{x''(s)}/|\boldsymbol{x''(s)}|$. Is there also an explicit form for the writhe frame? Notice that because the writhe frame is defined purely in terms of a non-local function of $\boldsymbol{x(s)}$ and its derivatives, and because the writhe frame is always closed for any smoothly closed curve $\boldsymbol{x}$, it is plausible that an expression for a writhe normal does exist in terms of some non-local integral expression of $\boldsymbol{x(s)}$ and its derivatives. Such an expression would be one possible way to better understand the interplay between bending and twisting of rods whose centrelines are not closed. It could also give an alternate, and simpler proof of the CFW formula.