# The effect of thermal fluctuations on elastic instabilities of biopolymers

Emanuel, M.D.

**Author**: Emanuel, Marc David
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Chapter 4

# The Writhe of a Curve

When an elastic rod is put under torsional stress, it responds by increasing the twist. To define twist we need more than just the tangent of the rod as it was done in the WLC model from the last chapter. There are two equivalent ways for describing a rod under torsional stress. One is to describe the rod as a ribbon: two space curves close to each other, for example one describing the mid-line of a semiflexible chain, the other along the outer surface of the chain. The other option is a framed curve: a space curve plus a smooth choice of a $3d$ orthonormal basis at each point of the space curve, one the tangent $\mathbf{t}$, the other two an orthonormal basis of the normal plane at that point. With a smooth choice we mean that the rotation of the basis when going along the chain is smooth, in mathematical terms a smooth section of the orthonormal frame bundle of $\mathbb{R}^3$. We get the connection between the two definitions when we choose one of the vectors in the normal plane, $\mathbf{u}$, to point to the partner curve of the ribbon. The twist can now be defined as the integral over the differential rotation of the frame.

It is clear from the definition that the choice of the ribbon is arbitrary. From a physical point of view it is practical to choose the curves to be parallel when they are fully relaxed [1]. But this last sentence makes only sense when the center curve is straight, or at most planar. This fact is a sign of the problems lying ahead.

When we keep one end of the rod fixed and start to rotate the other, twist will build up in the chain and the energy will go up, assuming linear elastic response, as:

$$\mathcal{E}_{tw} = \frac{\mathrm{P_c}}{2} \int_0^{\mathrm{L_c}} (\Delta\psi(s))^2 \mathrm{d}s \tag{4.1}$$

The reduced modulus $P_c$ is called the torsional persistence length for obvious reasons. $\Delta\psi := (\mathbf{t} \wedge \mathbf{u}) \cdot \dot{\mathbf{u}}$ is the differential change in the angle of the frames, the local twist angle. The twist is defined as the number of turns the frame rotates around the tangent

[1] Most semiflexible polymers have a helical structure and it is a common choice to include the helical twist in the definition of the chain's twist, but we choose not to do so.

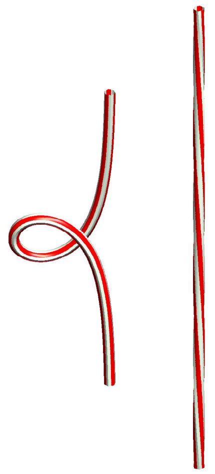

**Figure 4.1:** Applying one full turn to one chain end of a straight relaxed chain, while keeping the other end fixed, results in a loop but no twist on the left whereas the right hand side has all of the linking in the form of twist

direction integrated over the chain:

$$\mathrm{Tw} = \frac{1}{2\pi}\int_{-\mathrm{L_c}/2}^{\mathrm{L_c}/2} \mathrm{d}s\Delta\psi(s) \tag{4.2}$$

To start from $\psi$ as an angle is not so useful since its value at some point along the curve can only be calculated relative to the value at another point by integration. There is no local way to measure it. That is why this notation was chosen. Next to twisting, the rod has also another option to respond to torsional stress: it can curve out of the plane, as shown in Figure 4.1. When following the local frame along the contour in the twisted chain, it is rotating gradually around the tangent vector. In the left hand configuration no such rotation occurs, nonetheless the two ribbon lines are in the same way entangled. The problem of how to know how much the lines of a closed ribbon are entangled was to a large extend solved by Călugăreanu [130, 131, 132], later refined by Pohl [133] and White [134]. The starting point was Gauss formula for the linking number of 2 links, or loops.

$$\mathrm{Lk} = \frac{1}{4\pi}\oint_{C_1}\oint_{C_2} \frac{\mathrm{d}\mathbf{r}_1 \wedge \mathrm{d}\mathbf{r}_2 \cdot (\mathbf{r}_1 - \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|^3} \tag{4.3}$$

The integral is an integer counting the number of times one link crosses the other when projected in a general direction, counting with sign which link passes on top. There are several ways to prove this. A physical way is to use standard vector identities [135] to write it as the integral over the surface spanned by one loop over a signed delta function that counts the passing over the other link through it [136]. The expression closely resembles the Biot-Savart law of magneto-statics and one can think of the links as representing magnetic flux [137]. An astronomer would perhaps think of the measurement of the solid angle a planet orbit describes as seen from earth [138] as follows:

Imagine you are watching the motion of a distant comet in its orbit around the sun. Assume for the moment that your planet has a fixed position. In that case follows the unit vector pointing in the comets direction a closed path enclosing some area on the unit sphere. Now your planet is moving in its own orbit. The area that you measure from another point along your orbit changes. To be able to know how big a map is needed to draw the movement of the comet, it is worthwhile to keep track of the differential change in orbit area. Since also your orbit is closed, it seems to be that the integral should add up to zero when going around your orbit. But when the orbit of the comet at some point goes over your head, the area swept out growing over $2\pi$, there are two possibilities: either at another point it shrinks again below $2\pi$, or it keeps on growing reaching the complement of the original area when returning to the start position. That last case happens when the orbits are linked.

A more modern way to understand this is by way of the degree of an orientation preserving map $f$ from an oriented closed surface $M$ to the unit-sphere:

$$f : M -> S^2 \qquad deg_f = \frac{1}{4\pi}\int_M f^*\omega, \tag{4.4}$$

with $\omega$ being the volume 2-form on $S^2$, $f^*$ the pullback to $M$. The degree of a map is an important concept with many useful applications in physics. In case $M$ is a regular surface embedded in three dimensional Euclidean space and $f$ the Gauss map, mapping each point of $M$ to the outward surface normal, the integral is the Gaussian curvature integrated over the surface. The degree of this map tells us that this integrated Gaussian curvature integrated over the closed surface is quantized. This is the Gauss-Bonnet theorem [139]. It has important consequences for the physics of membranes and shells for it makes it possible to drop the Gaussian curvature elasticity contributions from the Hamiltonian from one component liquid membranes to crystalline virus shells.

To make the connection with the linking number we refer to the astronomer observing another orbit from its own. $M$ is in this case the Cartesian product of the two orbits and $f$ maps to the unit vector on the direction sphere pointing from one orbit to the other:

$$f : C_1 \times C_2 \to S^2 \qquad f(\mathbf{r}_1(s), \mathbf{r}_2(t)) = \mathbf{e}_{12}(s,t) = \frac{\mathbf{r}_1(s) - \mathbf{r}_2(t)}{|r_1(s) - r_2(t)|}. \tag{4.5}$$

The infinitesimal change of $\mathbf{e}(s,t)$ is in the tangent plane of the direction sphere, since $\mathbf{e}_{12}$ is a unit-vector. The infinitesimal area is the norm of the cross product of the two independent directions, or zero. But the crossproduct is directed along the outward normal and so we find

**Table 4.1:** Properties of the 3 parts of White's equation

| | Linking | Twist | Writhe |
|---|---|---|---|
| topological invariant | yes | no | no |
| locally defined | no | yes | no |
| needs a frame | yes | yes | no |
| (gauge invariant | no | no | yes) |

for the degree:

$$\mathrm{Lk} = \frac{1}{4\pi} \oint_{C_1} \mathrm{d}s \oint_{C_2} \mathrm{d}t \left( \frac{\partial \mathbf{e}_{12}(s,t)}{\partial s} \wedge \frac{\partial \mathbf{e}_{12}(s,t)}{\partial t} \right) \cdot \mathbf{e}_{12}(s,t) \tag{4.6}$$

It is not hard to convince yourself that this is exactly the Gauss integral. Since all maps are continuous, all continuous deformations that keep the surface regular, meaning non-intersecting deformations, do not change this number. It must be a topological invariant.

The same procedure can be repeated when the two links, the maps $\mathbf{r}_{1,2}$, coincide, resulting in an intrinsic linking number of a link, called the writhe. The argumentation is the same except that $f$ can only be defined on the product space without the diagonal, the set of points in $S^1 \times S^1$ of the form $(s, s)$, the direction from a point of the link to another, being undefined when the points coincide. In fact the direction becomes the tangent when approaching the diagonal, but flips direction from one side of the diagonal to the other side. The torus without diagonal is homeomorphic to a cylinder or a disk with a hole cut out in the center. The resulting integral exists though but is not integer valued and varies continuously upon deformation. The big breakthrough that started with Călugăreanu's papers was the discovery of what is now usually called White's theorem relating the Gauss integral of a link with itself, or the writhe, with the linking number and twist of the framed link:

$$\mathrm{Lk} = \mathrm{Tw} + \mathrm{Wr} \tag{4.7}$$

Here the linking number is the conventional linking number, as defined by the Gauss integral (4.5), for the two ribbon curves, and the twist the integrated differential rotation of the frame around the tangent. It is more remarkable than it looks since the linking number is an integer and a topological invariant, whereas the other quantities are continuous real valued functions. The twist as a local rotation of the ribbon curves around each other is also not preserved under smooth deformations. A local inhabitant, wanting to make a tour around the world could put a stick at the start of the tour pointing in some well defined direction normal to the curve, could carefully keep track of the direction he chose by not rotating around the tube and still ending in a different direction, making on the way theories about mysterious forces. Table 4.1 gives an overview of the different properties.

So White's theorem tells us that the two quantities twist and writhe when added form a topological invariant. That it is the linking number can be seen by flattening the link on a plane in a continuous way without breaking it anywhere . For our use it is enough to assume the link is a trivial knot, so we can flatten it to a circle, otherwise there are standard moves to unknot a knot keeping track of the change in linking number. The writhe is clearly zero so the linking number must be equal to the twist.

It is also possible to give an intrinsic unified way to calculate linking number, writhe and twist [140]. One starts assigning a direction to the ribbon. Next one counts the number of times one line of the ribbon crosses the other as seen from a projection and averages over all directions. When the lines cross at the same spot of the ribbon it is contributing to the twist, else to the writhe. Both contribute to the linking number. Some care has to be taken about the multiplicity of the counting.

One way to proof White's theorem is to regularize the singular points by choosing a canonical ribbon. One common choice is the direction of curvature, defining the principal normal of the Frenet frame, or alternatively the remaining, bi-normal. The disadvantage is that this presumes a non vanishing curvature. A more elegant choice is the writhe frame, adjusting the frame and thereby the twist, at a point $s$ along the link as follows [140]: The chords starting from $s$, the chord fan, define a, possibly complicated, path on the direction sphere from $\mathbf{t}(s)$ to $-\mathbf{t}(s)$. Choose the frame normal $\mathbf{u}$, connecting $s$ with its ribbon point, such that the semicircle from $-\mathbf{t}(s)$ to $\mathbf{t}(s)$ via this normal, closes the path to a loop on $S^2$ with an enclosed area of zero (mod $4\pi$). The claim is that this zero is the linking number of the resulting ribbon.

$$\begin{aligned} 0 := \frac{1}{4\pi}\oint(\text{full loop at s}) &= \frac{1}{4\pi}\int_0^{L_c} \mathrm{d}t \left(\frac{\partial \mathbf{e}(s,s+t)}{\partial s} \wedge \frac{\partial \mathbf{e}(s,s+t)}{\partial t}\right)\cdot \mathbf{e}(s,s+t) \\ &\quad + \frac{1}{4\pi}\int_0^{\pi} \mathrm{d}\phi \left(\frac{\partial \mathbf{v}(s,\phi)}{\partial s} \wedge \frac{\partial \mathbf{v}(s,\phi)}{\partial \phi}\right)\cdot \mathbf{v}(s,\phi), \end{aligned} \tag{4.8}$$

with the unit vector $\mathbf{v} = -\mathbf{t}(s)\cos(\phi) + \mathbf{u}(s)\sin(\phi)$ following the geodesic set by $\mathbf{u}(s)$, chosen to have an enclosed area of zero (mod $4\pi$). With $\mathbf{u}(s)$ as ribbon normal, the second term equals:

$$\begin{aligned} &\frac{1}{4\pi}\int_0^{\pi} \mathrm{d}\phi \left(\frac{\partial \mathbf{v}(s,\phi)}{\partial \phi} \wedge \mathbf{v}(s,\phi)\right)\cdot \frac{\partial \mathbf{v}(s,\phi)}{\partial s}, \\ &= \frac{1}{4\pi}\int_0^{\pi} \mathrm{d}\phi\, (\mathbf{t}(s)\wedge \mathbf{u}(s))\cdot\left(-\dot{\mathbf{t}}(s)\cos(\phi) + \dot{\mathbf{u}}(s)\sin(\phi)\right) \\ &= \frac{1}{2\pi}(\mathbf{t}(s)\wedge \mathbf{u}(s))\cdot \dot{\mathbf{u}}(s) \end{aligned} \tag{4.9}$$

which is the local twist. We still have to show that equation (4.8) is indeed the inner loop integral of the linking number. The second ribbon curve is defined as $\mathbf{r}_2(s) = \mathbf{r}(s) + \epsilon\mathbf{u}(s)$ with $\epsilon$ small enough to prevent intersections. The linking number is a topological invariant so we are free to take the limit $\epsilon \downarrow 0$ in the end without changing its value. When we integrate equation (4.6) over $t$, keeping $s$ fixed, we can distinguish two different regimes.

1. When $\mathbf{r}(t)$ is far away from $\mathbf{r}(s)$, compared to the distance of the two ribbon curves, the integrand can be approximated by that of the writhe part of equation (4.8).

2. When the distance between the points is much smaller than the ribbon width the integrand lies approximately on the arc of the twist part, its position on the arc describing half a turn.

Although the intervals for the second regime shrink with decreasing $\epsilon$, the contribution to the full integral approaches that of the twist part. When $\epsilon$ goes to zero the two loop integrals are the same. This proofs White's relation since this limiting procedure does not change Lk. Note that nowhere we needed to have 0 on the left hand side of equation (4.8). In a way the writhe term can be seen as the writhe at $s$, but it depends on the rest of the link.

As a final remark: all 3 of the quantities measure areas on the unit sphere . With the total area swept out by the ribbon cross chords given (Lk) it can be divided in a local (Tw) and a nonlocal (Wr) part. Another way to think about it is as follows: given a space curve there is a gauge freedom of choosing a smooth section in the frame bundle. As seen from the space curve it is the writhe that is the gauge invariant quantity. These concepts show a strong resemblance to other geometric phases like Berry's phase and the Aharanov-Bohm effect.

The writhe being nonlocal complicates perturbation calculations enormously. Under certain conditions it is nonetheless possible to turn the writhe into a local quantity. We will call two links writhe-homotopic if: (i) they are homotopic as non-intersecting space curves and (ii) the tangent along the homotopy is nowhere anti-parallel to one of the end curves. Fuller showed [141, 142] how to relate the writhe of 2 writhe-homotopic links, with writhes $\mathrm{Wr}_{1,2}$, in a local way. When discussing Whites relation we noted that the linking number measures the area swept out by the chords. The writhe is a measure of the area swept out by the tangent, $A_t$, when traversing the curve. Fuller showed [141]:

$$\mathrm{Wr} = \frac{1}{2\pi} A_t + 1 \bmod 2 \tag{4.10}$$

from that observation he gave arguments for a local expression of the writhe difference. We will sketch the derivation along the lines of Aldinger et al. [142] and refer for the details to that paper.

The homotopy we write as $\mathbf{r}_t(s)$ with end-links $\mathbf{r}_1(s) = \mathbf{r}(s, 0)$ and $\mathbf{r}_2(s) = \mathbf{r}(s, 1)$. The main idea is that this homotopy, when framed continuously, can not change its topologically invariant linking number, and so the *nonlocal* calculation of the writhe difference can be replaced by a *local* calculation of the twist difference. They are in that case equal with opposite sign. We are free to choose the framing along the homotopy as long as the framing itself also changes continuously in $t$. We first construct a framing for the start and end link by choosing frame normals common to both links:

$$\mathbf{u}_0(s) = \mathbf{u}_1(s) := \frac{\mathbf{t}_0(s) \wedge \mathbf{t}_1(s)}{|\mathbf{t}_0(s) \wedge \mathbf{t}_1(s)|} \tag{4.11}$$

This fails at s-points where the tangents are parallel. To overcome this we can infinitesimally distort the start link at these points. We will see in the end that the final result only depends on the tangents of the start and end loop and we can remove the distortion. Along the homotopy we will rotate the frame normals with the tangent rotations [143]:

$$\mathbf{u}_t(s) = \mathbf{u}_0(s) + \sin(\phi)(\mathbf{n}_t(s) \wedge \mathbf{u}_0(s)) + 2\sin^2(\frac{\phi}{2})(\mathbf{n}_t(s) \wedge (\mathbf{n}_t(s) \wedge \mathbf{u}_0(s)) \tag{4.12}$$

with $\phi$ the angle between the tangents at $s$, and $n$ the common normal:

$$\mathbf{n}_t(s) = \frac{\mathbf{t}_0(s) \wedge \mathbf{t}_t(s)}{|\mathbf{t}_0(s) \wedge \mathbf{t}_t(s)|} \tag{4.13}$$

We have now constructed a ribbon homotopy with a writhe homotopic centerline. The twist difference is easy to calculate, using the standard vector identity [135]:

$$\mathbf{v_1} \wedge (\mathbf{v_2} \wedge \mathbf{v_3}) = (\mathbf{v_1} \cdot \mathbf{v_3})\mathbf{v_2} - (\mathbf{v_1} \cdot \mathbf{v_2})\mathbf{v_3},$$

namely:

$$\begin{aligned}
\mathrm{Wr}_2 - \mathrm{Wr}_1 &= \mathrm{Tw}_1 - \mathrm{Tw}_2 \\
&= \frac{1}{2\pi} \oint \mathrm{d}s \left[ (\mathbf{t}_1(s) - \mathbf{t}_2(s)) \wedge \left( \frac{\mathbf{t}_1(s) \wedge \mathbf{t}_2(s)}{|\mathbf{t}_1(s) \wedge \mathbf{t}_2(s)|} \right) \right] \cdot \frac{\partial}{\partial s} \left( \frac{\mathbf{t}_1(s) \wedge \mathbf{t}_2(s)}{|\mathbf{t}_1(s) \wedge \mathbf{t}_2(s)|} \right) \\
&= \frac{1}{2\pi} \oint \mathrm{d}s \left[ -(\mathbf{t}_1(s) + \mathbf{t}_2(s)) \frac{(1 + \mathbf{t}_1(s) \cdot \mathbf{t}_2(s))}{|\mathbf{t}_1(s) \wedge \mathbf{t}_2(s)|} \right] \cdot \frac{\frac{\partial}{\partial s}(\mathbf{t}_1(s) \wedge \mathbf{t}_2(s))}{|\mathbf{t}_1(s) \wedge \mathbf{t}_2(s)|}
\end{aligned}$$

Using $|\mathbf{t}_1 \wedge \mathbf{t}_2|^2 = 1 - (\mathbf{t}_1 \cdot \mathbf{t}_2)^2$ this simplifies to:

$$\mathrm{Wr}_2 - \mathrm{Wr}_1 = \frac{1}{2\pi} \oint \mathrm{d}s \frac{(\mathbf{t}_1 \wedge \mathbf{t}_2) \cdot (\dot{\mathbf{t}}_1 + \dot{\mathbf{t}}_2)}{1 + \mathbf{t}_1 \cdot \mathbf{t}_2}. \tag{4.14}$$

The 2nd condition on the homotopy makes sure that this change does not cover the full sphere. In case condition (ii) is not fulfilled, Fuller's equation gives the writhe mod 2. In principle following any non intersecting homotopy one can use Fuller's equation, using continuity to deal with the anti-parallel points, to calculate the relative writhe. This we will use in the next chapter to calculate the writhe of the plectoneme.

In our setup we do not have a loop but a chain with the end tangents aligned with the force. We first have to close this chain to a loop before using the concepts of writhe and White's relation. Starostin [144] showed that this can be done by closing the loop with a geodesic on the tangent sphere. In our case, with the two end tangents parallel we don't have to care about this closing, since the area the tangents sweep out between both ends is automatically closed. We can define the writhe of the straight chain to be zero and calculate the writhe from equation (4.14) relative to it. This approach presupposes that the chain can not loop around an endpoint. In the magnetic bead experiments we are referring to, this is not possible thanks to the diameter of the bead, 1 μm, relative to a deflection length of the order of 10 nm and even to the chain length of 700 nm for part of the experiments.