Twisting and Writhing Numbers in Circular DNA

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1 Introduction

Since the discovery that DNA could join its two ends to form a loop [4], the topology and shape of twisted closed loops has become important to biology. The shape of a molecule drastically affects its interactions with the environment.

2 Theory

Let $\alpha(s)$ be a closed curve in R^3, parameterized by arc-length, such that all of its derivatives agree at its beginning $\alpha(0)$ and end $\alpha(L)$. This curve represents the DNA molecule [5].

Let $\beta(s) = \alpha(s) + \epsilon\, u(s)$ where $u(s)$ is an arbitrary smoothly varying unit vector that is always perpendicular to the curve α at $\alpha(s)$. In the limit as ϵ goes to zero, $\beta(s)$ becomes parameterized by arc-length. Assuming $u(0) = u(L)$, β is a smooth closed curve. This β curve represents the "second strand" of the DNA's double helix [5].

Three numbers have received much attention for describing these two curves: the linking number $Lk(\alpha, \beta)$, which tells how many times (an integer) the curves wrap around each other, the total twist number $Tw(\alpha, u)$, and the writhing number $Wr(\alpha)$ [5].

These numbers have strict mathematical definitions. Swigon et al [11] give the clearest form of the defining integral for the writhe. It is very similar to the linking number integral.

$$Lk(\alpha, \beta) = \frac{1}{4\pi} \int_0^L \int_0^L \frac{(\alpha'(s) \times \beta'(t)) \cdot (\alpha(s) - \beta(t))}{|\alpha(s) - \beta(t)|^{3/2}} \, \mathrm{d}s \, \mathrm{d}t \tag{1}$$

$$Wr(\alpha) = \frac{1}{4\pi} \int_0^L \int_0^L \frac{(\alpha'(s) \times \alpha'(t)) \cdot (\alpha(s) - \alpha(t))}{|\alpha(s) - \alpha(t)|^{3/2}} \, \mathrm{d}s \, \mathrm{d}t \tag{2}$$

To understand the twisting number, define an orthonormal basis $\{\alpha'(s), u(s), v(s)\}$, where $v(s) = \alpha'(s) \times u(s)$. This basis rotates with the coordinate s along the curve, and has an angular velocity vector $\omega(s)$ given in radians turned per unit arc-length traversed. $\omega(s) \cdot \alpha'(s)$ is the twist at the point $\alpha(s)$ on the curve, and the integral of this is the total twist.

$$Tw(\alpha, u) = \frac{1}{2\pi} \int_0^L \omega(s) \cdot \alpha'(s) \, \mathrm{d}s \tag{3}$$

For calculations, note that $\omega(s) \cdot \alpha'(s) = u'(s) \cdot v(s)$ [5].

The usefulness of Wr appears because these numbers obey the following relationship [5].

$$Lk = Wr + Tw \tag{4}$$

The linking number is a topological constant of the curves, but twist can still be removed from the DNA molecule by converting it into writhe.

3 Application to the Shape of DNA

I was hoping to find that writhe, like twist, was just an integral of a local writhe over the length of the curve. Then writhe might be directly related to curvature $\kappa = |\alpha''(s)|$ [3], and so one could see the molecule reaching a lower energy state by transferring twisting (torsional, $E_\omega = \frac{1}{2}A(\omega \cdot \alpha')^2$) energy into bending ($E_\kappa = \frac{1}{2}C\,\kappa^2$) energy.

This is only roughly what happens; writhe is not quite that simple. Fuller states that by treating the molecule as a mathematical curve without width, one can put an indefinitely large amount of writhe into the curve while keeping the total curvature limited [5], so curvature and writhe cannot be too closely related.

In both theoretical calculations and computer simulations, DNA does reduce its energy by converting twist into writhe. Gebe and Schurr [7] show that after "manually" changing the linking number beyond a certain amount, the writhe becomes nonzero and starts absorbing the energy added to the system by changing the linking number. Ramachandran and Schlick [10] discuss discontinuities in how the writhing number changes with the linking number. Quian and White [9] calculate that if a DNA molecule has an intrinsic curvature, then the writhe will absorb all of the twist, so that $Lk = Wr + 0$. Others also investigate writhe in DNA [1, 13].

4 Conclusion

Both the linking number and the total twisting number have fairly intuitive definitions. However, the writhing number still remains an enigma. It comes wrapped in several layers of abstraction whenever it appears, particularly in the mathematical journals [12]. A clearer explanation of what this physically represents is needed.

Also, to better understand how twist is converted into writhe, it would be informative to solve Fuller's briefly mentioned calculus of variations problem [5] for the shape of a bent elastic rod. This may yield the shape of the rod and perhaps shed some light on writhe.

For more details on how the numbers Lk, Wr, and Tw are related, see Klenin and Langowski's readable explanation [8].

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