Mathematical Properties of DNA Structure in 3-Dimensional Space

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Abstract

In this paper we study the mathematical and mechanical properties of the double- helix structure of DNA in 3-dimensional space. Many of the mechanical quantities in the DNA can be described explicitly, which is not the case for the latter models, and the model is computationally efficient in that the super-coiling parameters can be computed from simultaneously solving algebraic equations.

Keywords: 3D Space, Vector-Valued Function, Special Vectors, Double-Helix, Super-Coils, Balanced Ply

1   Introduction

The Deoxyribo Nuclic Acid (DNA) is a double stranded molecule, with hundred of genes and thousands of bases. Also the double stranded of DNA is presented as in a helical form which is called "Double-Helix of DNA". DNA with its Genes sequences are nano micrones meter in size and often length in our cells. Spatial deformations of the DNA molecule are central to its biological functions. To transcribe the Genetic code, DNA must screw "through" an RNA Polymerase. This involves a rotation at about 10 turns per second which can induce large twisting stresses in the DNA. The double-helix of most DNA Molecule is right-handed, and if this internal twist is increased by stress the molecule is said to be "Overwound*", conversely, it is "underwound". The DNA molecule adopts a complex 3-dimensional shape known as a "super-Coil" in order to relieve the resulting internal stresses. If DNA becomes excessively twisted , it is unable to function, and to overcome (or relief) this stress, the DNA is affected by several

Enzymes such as " Topoisomerease and "Gyrase" that in some manners remove or add of turns of twist relative to the number of underlying helical turns in the relaxed DNA molecule. After the removal of some twist turns, the strand in 3-dimensional shape is known as an "Interwound Super-Coil". The formation of super-Coils of DNA has very important for several reasons: First: Super-Coils are a means of gathering and condensing the large volume of DNA in small cell nucleus. Second: Super-Coils ply a role in the process of coping Genes to mRNA which is called the " Transcription" and converting this mRNA to Protein in the of translation in the process of "Translation". Third: Super-Coils are one step in the process of DNA Catenation (or Knotting).

The Diagram below shows elastic (rubber) rod forming a left - hand variable balanced ply with one free end loop, and the pitch angle varies a long the ply.
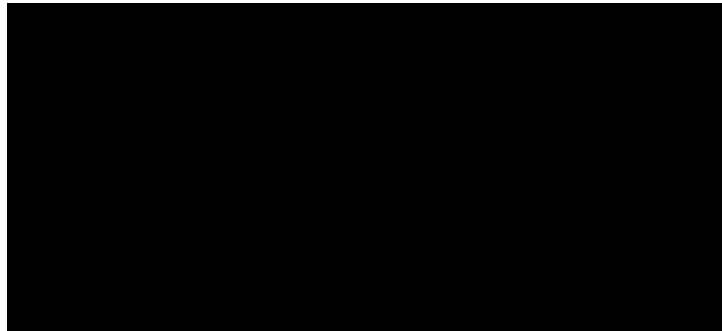

The interwound configuration of this rubber rod is said to form a "Ply". The simplest way to observe a ply physically is to twist a long rubber rod of circular cross-section. If, after imposing the twist, the ends are brought together, the rod will buckle locally and jump into this familiar ply-plus-loop form. A straight central region forms a ply, closed by two free end loops. Under such conditions the ply is described as *balanced.* Conversely, if the loops carry forces or moments, we call it *loaded.* A molecule of DNA often forms a closed loop, called a "Plasmid". A basic configuration of a twisted plasmid is shown in the figure below:
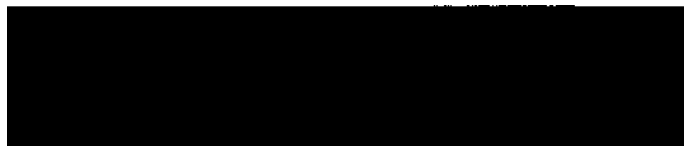
2   Mathematical Properties of DNA

The DNA molecule can be regarded as an elastic rod with circular cross-section of radius *r*. This rod can usually be treated as homogeneous, in extensional and linearly elastic. The problem under consideration is shown in Figures below: In Fig. (a) below: A loop of arc length s is bent into a circle has n- left-handed turns of twist inserted to the closure of the loop. In Fig. (b) below: A writhed loop showing a single balanced ply region of length D , and super-helix angle β, where the strands are in contact with each other and two end loops of half-length L,
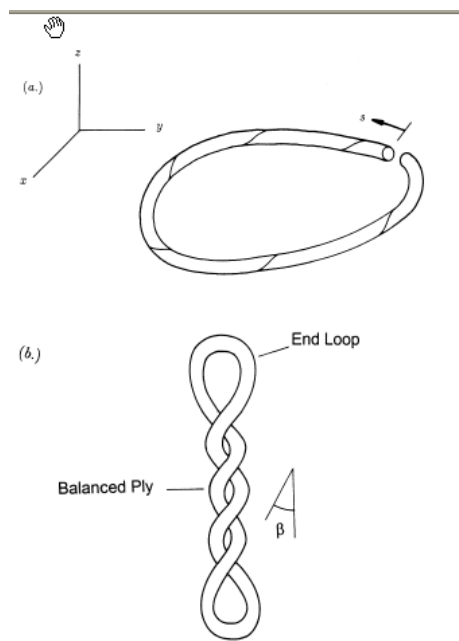
The details of the description of the end loops may be found in Stump et al.[1998]. They described that the shape depends on just the helix angle β and the standoff distance d . Furthermore, the dimensionless half-length of the end loop L is given approximately by:

$$L = 3.1489 \ d\beta^{-\frac{31}{2}} - 0.1365 \ d\beta^{-1} - 1.041 \ d\beta^{-\frac{1}{2}} - 1.375 \ d$$

Provided, the conservation (variable) arc-length s is given by:

$$s = \frac{2D}{\cos \beta} + 2ndL$$

where *n* is the number of end loops in the super-coiled DNA.

Note that the twist (*Tw*) measures the number of rotation turning on itself of the cross –section over the length of the molecule. The writhe (*Wr*) is due to super-coils and measures the three-dimensional complexity of the path taken by the centerline of the strand.
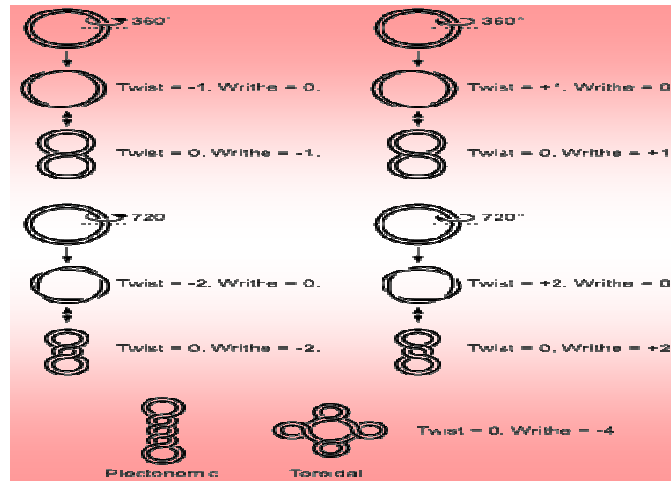
Within the balanced ply segments, the strands are assumed to have the shape of a uniform helix:
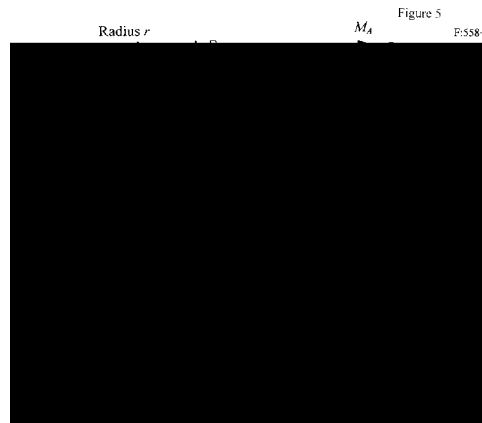
The vector position (path) of strand - helix is given by [Stump et al., 2000]:

$$R(t) = (r\cos t)\hat{i} + (r\sin t)\hat{j} + (\cot\beta)\,t\,\hat{k} = (r\cos t\,,\; r\sin t\,,\; (\cot\beta)\,t).$$

Here $x = r\cos t$ *and* $y = r\sin t$ describe a circle of radius r, but $z = (\cot\beta)\,t$ increases (or decreases) indirect to t.

The vertical distance between the "coils" equals the increase in z as t jump by 2π, and called the "Pitch", that is

$$Pitch = 2\pi\left|\cot\beta\right|.$$

Now we will present the mathematical and mechanical properties of the double-helix structure of DNA in 3-dimensional space as follow:

(i) The variable arc-length along the strand is given by:

$$s = \int_0^t \left\|R'(u)\right\| \, du = \frac{t}{\sin\beta}.$$

(ii) The reparametrization of the strand in terms of *s* is given by:

$$R(s) = \left(r\cos(s\sin\beta)\right)\hat{i} + \left(r\sin(s\sin\beta)\right)\hat{j} + \left(s\cos\beta\right)\hat{k}$$
$$= \left(r\cos(s\sin\beta),\ r\sin(s\sin\beta),\ s\cos\beta\right)$$

(iii) The curvature of the strand is a constant (not depend on *t* or s) and given by:

$$\kappa = \frac{\left\|R'(t)\times R''(t)\right\|}{\left\|R'(t)\right\|^3} = \left\|R''(s)\right\| = \frac{r}{r^2 + \cot^2\beta},$$

and the radius of curvature is given by:

$$\rho = \frac{1}{\kappa} = \frac{r^2 + \cot^2\beta}{r}.$$

(iv) The Unit Tangent Vector to the curve of Strand is given by:

$$T = \frac{R'(t)}{\left\|R'(t)\right\|} = \frac{1}{\sqrt{r^2 + \cot^2\beta}}\left\{\left(-r\sin t\right)\hat{i} + \left(r\cos t\right)\hat{j} + \left(\cot\beta\right)\hat{k}\right\}$$

$$= \frac{1}{\sqrt{r^2\sin^2\beta + \cos^2\beta}}\left\{\left(-r\sin\beta\ \sin(s\sin\beta)\right)\hat{i} + \left(-r\sin\beta\ \cos(s\sin\beta)\right)\hat{j} + \left(\cot\beta\right)\hat{k}\right\}$$

(v) The unit normal vector to the curve of strand is given by:

$$N = \frac{T'(t)}{\left\| T'(t) \right\|} = (-\cos t)\hat{i} + (-\sin t)\hat{j} + (0)\hat{k}$$

$$= \frac{T'(s)}{\left\| T'(s) \right\|} = (-\cos(s\sin\beta))\hat{i} + (-\sin(s\sin\beta))\hat{j} + (0)\hat{k}.$$

(vi) The binormal vector to the curve of strand is given by:

$$B = T \times N = \det \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ -\dfrac{r\sin t}{\sqrt{r^2 + \cot^2\beta}} & \dfrac{r\cos t}{\sqrt{r^2 + \cot^2\beta}} & \dfrac{\cot\beta}{\sqrt{r^2 + \cot^2\beta}} \\ -\cos t & -\sin t & 0 \end{bmatrix}$$

$$= \frac{\cot\beta\sin t}{\sqrt{r^2 + \cot^2\beta}}\hat{i} + \frac{-\cot\beta\cos t}{\sqrt{r^2 + \cot^2\beta}}\hat{j} + \frac{r}{\sqrt{r^2 + \cot^2\beta}}\hat{k}$$

$$= \frac{\cot\beta\sin(s\sin\beta)}{\sqrt{r^2 + \cot^2\beta}}\hat{i} + \frac{-\cot\beta\cos(s\sin\beta)}{\sqrt{r^2 + \cot^2\beta}}\hat{j} + \frac{r}{\sqrt{r^2 + \cot^2\beta}}\hat{k}.$$

(vii) The torsion (twisting) of the strand will affect a rotation of the cross-sectional pattern. In fact the unit normal vector *N* turns toward the binormal vector *B* at the rate *Tw* , and the fact that *N* and B are rigidly fixed at right angles, imply that *B* turns towaed – *N* at the same rate. If this happened, the unit tangent vector *T* would be forced by rigidity into turning in the direction –*B*, but *T* turns only in the direction *N*.
Thus, the Torsion of the strand is given by (using dot product):

$$T_w = -N \cdot \frac{dB}{ds} = \pm\left\| \frac{dB}{ds} \right\| = \pm\frac{\cos\beta}{\sqrt{r^2 + \cot\beta}} \ .$$

Stump et al. [2000] showed that Twisting of the strand is:

$$T_w = -\frac{s\cos\beta\sin^3\beta}{\pi\,\delta\,d\cos 2\beta} \quad : \quad \frac{2}{3} \le \delta \le 1,$$

where *d* is the standoff distance in the balanced ply.

(viii) The writhe number (*Wr*) of the super-coil is given by Stump et al. [1998] (Using spherical image method of Fuller [1987]) as follows:

$$W_r = -\frac{D}{\pi d}\sin\beta + \frac{n}{2d}\left(F_{loop} - 1\right),$$

where d is the standoff distance in the balanced ply, D is the length of one strand in the balanced ply, n is the number of end loops in the super-coiled DNA, and the factor floop depends only on the super helix angle ß which is given approximately :

$$F_{loop} = -0.4355\beta^{\frac{1}{2}} - 10.87\beta^{\frac{3}{2}} + 56.11\beta^2 - 89.27\beta^{\frac{5}{2}} + 49.22\beta^3.$$

(ix) The linking number *(LK)* is expressed by:

$$LK = T_w + W_r.$$

(x) The total number of crossovers nodes with a wavelength µ along the ply axis is given by:

$$n_c = \frac{2D}{\mu} = \frac{D}{\pi r}\tan\beta.$$

(xi) The electrical repulsion force (E_f) acting along the strand. Since the structure is an equilibrium, then the outward force must balance the pressure due to the interwound helical shape, which lead to:

$$E_f = \frac{\sin^4\beta}{d^3\cos 2\beta} = P,$$

where P is the pressure between the strands.

Note that the electrical repulsion keeps the strands in the molecule apart.

(xii) Finally, the tangential tension force on the cross section of the rod is given by:

$$T_f = \frac{\sin^4\beta}{d^2\cos 2\beta}.$$

3   Conclusion and Open Problems

We have presented the Mathematical Model of DNA super-coils in 3-dimensional space, which leads to simple algebraic expressions for predicting the shape of the structure. The model needs as input three relatively easily measured quantities:

The total length of the DNA (s), the number of end loops (n) and predicts several geometric and mechanical properties such as: the super-helix angle (β), standoff distance (d) in the balanced ply, and the tension in the strand (T). The model has several advantages over finite element and molecular dynamic models: Many of the mechanical quantities in the DNA can be described explicitly, which is not the case for the latter models, and the model is computationally efficient in that the super-coiling parameters can be computed from simultaneously solving algebraic equations. It is natural to ask the following questions:

- How can we extend our results to the variable non-balanced ply"?
- How can we examine the solutions of the variable loaded ply?
- What is the desirable mathematics (mechanical) properties of DNA structure which can be added to this collection?

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