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Thermomechanics of curves in space

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THERMOMECHANICS OF CURVES IN SPACE

by

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ABSTRACT

Several biological molecules are known to form helices and coiled structures, such as DNA, collagen, bacterial flagella, and proteins. The backbones of such molecules may be modeled as a curve in three dimensions. A variational problem for the functional of the total free energy required to perturb moving curves in space is considered. The total energy of a curve in three dimensions is minimized by with a general intensive energy, which is a function of position, and the invariants, curvature and torsion. Three types of moduli are identified: stretching, bending and torsional moduli. As a result, three independent force balances are obtained which serve as the equilibrium conditions. Three cases are considered, the case of constant curvature and torsion (forming a helix), the case of no work done in bending the curve, and the case of no work done in twisting the curve. Stability analysis is performed leading to an unstable helix for the case of constant torsion and curvature. The other two cases are not analyzed due to the complexity of the results. It has been assumed that the moduli do not vary with position. However, a model has been provided for the case where the moduli vary slightly and can be used in the results obtained in order to obtain shapes of curves, where the curve will tend to bend to a natural curvature and torsion.

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NOMENCLATURE

Symbol	Description
$\mathbf{R}$	Position vector
s	Arc length
$\mathbf{t}$	Tangent vector
$\mathbf{p}$	Principle normal
$\mathbf{b}$	Binormal
κ	Curvature
τ	Torsion
ξ	Displacement
ε	Total free energy
M_s	Stretching modulus
M_b	Bending modulus
M_t	Torsional modulus
$\mathbf{a}$	Radius of helix
p	Pitch of helix

1. INTRODUCTION

1.1. CURVED STRUCTURES AND BEAM THEORY

Studies on the x-ray diffraction patterns of silk fibers by Astbury suggested that the molecules had a helical structure when the fibers were "unstretched" [1]. The x-ray patterns were interpreted by Pauling and Corey as the present day α- helix. Pauling and Corey reported two helical configurations, the α- helix and the γ- helix, in which the stereochemical requirements for certain polypeptide chains of proteins were satisfied [2]. Ramachandran [3] explained the structure of the collagen molecule as an arrangement of three non-coaxial helical chains linked to one another by hydrogen bonds. The triple coiled structure consists of three helices with the requirement that the structure should necessarily have one-third of the total residues as glycine. The α- helix is shown schematically in Figures 1.1 and 1.2 and the structure of collagen in shown in Figure 1.3.

In their seminal work, Watson and Crick proposed a structure for DNA consisting of two helical chains each coiled around the same axis. The two chains are held together by purine and pyrimidine bases. Further, they found that only specific pairs of bases (adenine, A, with thymine, T, and guanine, G, with cytosine, C) bonded together [4] as shown schematically in Figure 1.4.

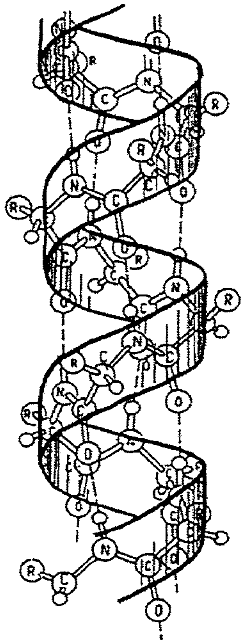

Figure 1.1 The α- helix

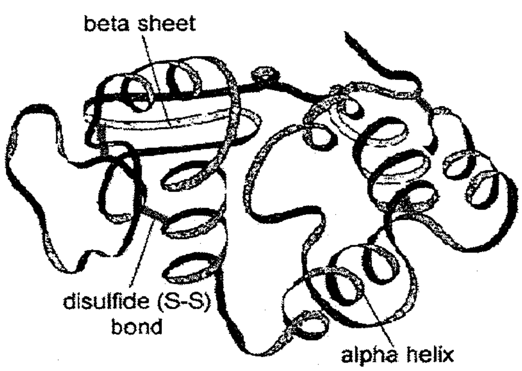

Figure 1.2 The structure of a protein molecule containing an α-helix chain

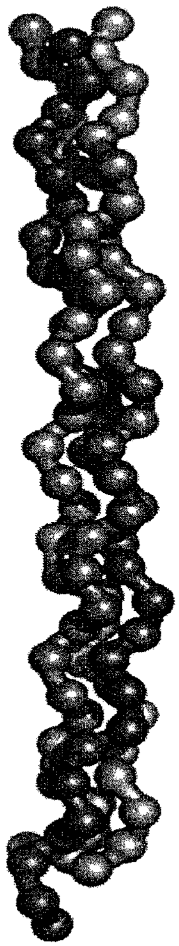

Figure 1.3 The tropocollagen triple helix

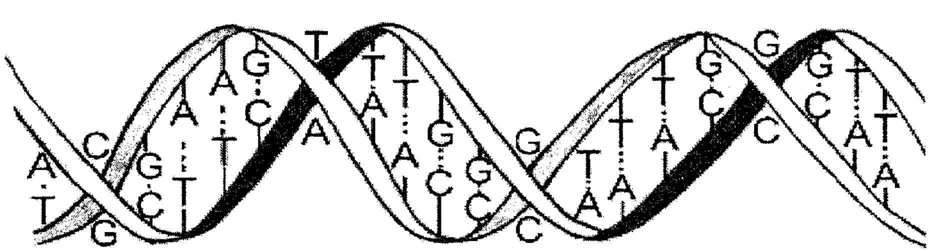

Figure 1.4: The DNA double helix

The DNA are stacked in a cell by supercoiling. The twisting of DNA into supercoils can be described by the following terms [5]:

Linking Number, L: The linking number is the number of times one DNA strand wraps around the other. It is an integer for a closed loop and constant for a closed topological domain.

Twist, T: The twist is the total number of turns in the double stranded DNA helix. This will normally tend to approach the number of turns that a topologically open double stranded helix makes free in solution. The unstressed β-DNA makes one turn about every 10.5 base pairs.

Writhe, W: Writhe is the number of turns of the double stranded DNA helix around the superhelical axis.

The linking number, twist and writhe are related as follows:

$$L = T + W \tag{1.1}$$

$$\Delta L = \Delta T + \Delta W \tag{1.2}$$

An overall view of supercoiling and a detailed view of a specific case are shown in Figures 1.5 and 1.6.

The work done in coiling or supercoiling has an important contribution to the total energy. Geometric structures with one dimension much larger than the other two dimensions can be treated by beam theory [6]. Biological structures such as flagella, microtubules, and DNA can be approximated as beams. The bending energy associated with bending a beam into a circular arc of length L with radius of curvature R may be shown to be

$$E_{bend} = \frac{EIL}{2R^2} \tag{1.3}$$

where E is Young's modulus and I is the moment of inertial of the cross section of the beam. For the case where the local curvature differs at different points, the bending energy can be shown to be

$$E_{bend} = \frac{K_{eff}}{2}\int_0^L \left|\frac{d\mathbf{t}}{ds}\right|^2 ds \tag{1.4}$$

where K_{eff} is the flexural rigidity and $K_{eff} = EI$ and **t** is the tangent vector which will be defined in the next section.

The force-extension diagram of a DNA molecule can be described by a worm-like chain (WLC) model [6]. According to this model, the energy of a stretched DNA molecule is given by a line integral of two terms: one term accounts for the resistance of the chain to bending, and the other term accounts for the stretching energy resulting from applying a force F to the end of the molecular chain, along the axis.

$$E_{WLC} = \int\left(\frac{A}{2}\left|\frac{dt(s)}{ds}\right|^2 - F\cos\theta(s)\right)ds \tag{1.5}$$

where A is a constant, s is the arc length (defined in the next chapter) and θ is the angle between the axis and the local tangent to the curve. In the absence of an external force, the integrant is a minimum when the curve is a straight line, a somewhat puzzling result. The work and the extension are averaged over the ensemble to get F versus extension. The elastic behavior of DNA has been investigated using a variety of forces such as hydrodynamic drag, magnetic beads, glass needles, and optical traps [7].

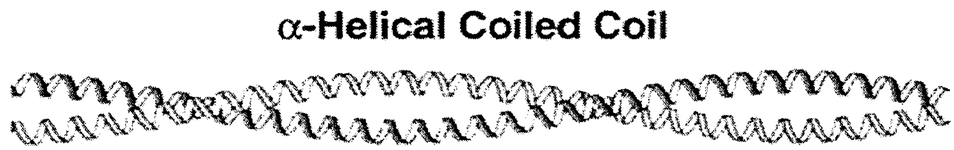

Figure 1.5: The α- helical coiled coil

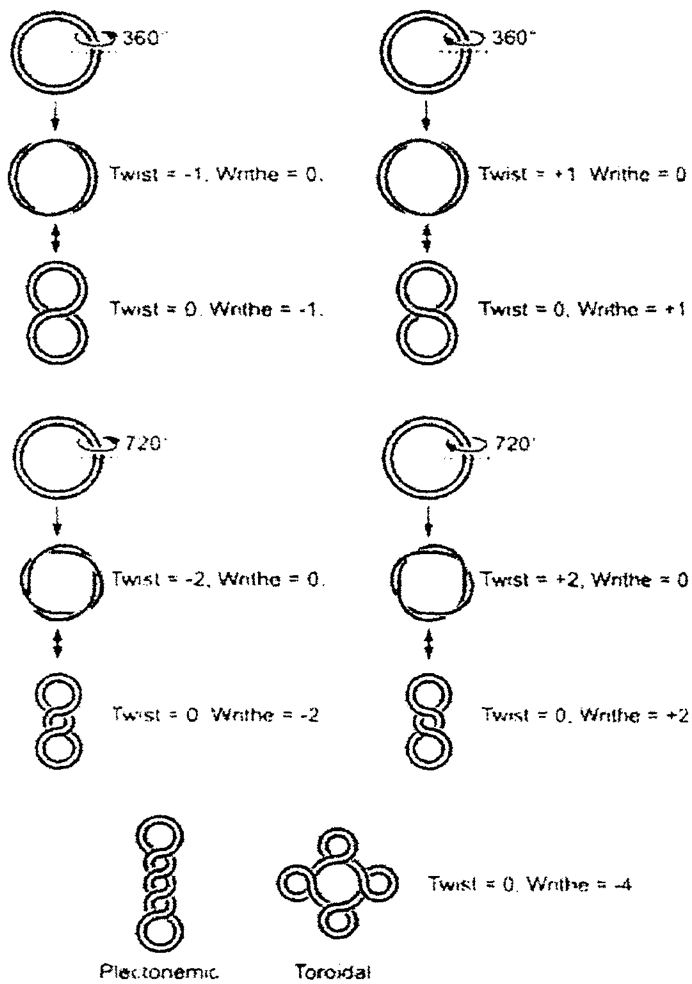

Figure 1.6: Supercoiled structure of circular DNA molecules

1.2 METHODOLOGY

The total energy ε for a smooth curve in three dimensions is minimized with a general intensive energy e. In a very general model, e is a function of position s, and the two invariants, curvature and torsion. Sarostin and van der Heijden [8] have included as invariants the derivatives of curvature and torsion, although it is not clear if they are invariants. The derivatives of e with respect to curvature and torsion were taken to be the moments which are set to zeros. Minimizing the energy, independent force balances are obtained which are the equilibrium conditions.

The process of minimizing free energy can be used to define the elastic moduli: stretching, bending and torsion. An equation of state is introduced at the very end, which includes natural curvature and torsion, emphasizing that the curve tends to bend to a natural curvature and torsion. Three cases are important here. In the first, curvature and torsion are constant, giving rise to a regular helix. In the second case, no work is done in bending the curve, and it is expected to give rise to an unstable system. The structureless random coil seen in synthetic polymers is probably an unstable system. In the third case, no work is done in twisting the curve.

This thesis addresses the determination of conditions under which a linear polymer can coil on its own. However, many researchers are of the opinion that molecules do not coil on their own. The only way that individual amino acids can be packed in a very confined region is by the formation of the α- helix structure [9]. The supercoiling is attributed to the effect of packing a large molecule into a small space. In globular proteins, helices are stabilized by the interactions of the polar groups (on the outer face) with the solvent, and by packing of apolar groups in the interior of the protein, hydrogen bonds, and interaction of their partially charged ends with oppositely charged side chains [10]. When separated from the remainder of the protein, only few peptides corresponding to stable helices in proteins form stable isolated helices in solution, but it is not known whether individual amino acids have an inherent tendency to form helices [10]. It is suspected that supercoiling of DNA has a role in biological processes [11]. Intermolecular forces can be responsible for ternary coils in collagen. There are some indications that molecules can tend to coil on their own.

2. FOUNDATION OF GEOMETRY OF CURVES IN SPACE

2.1 INTRODUCTION

For the case of curves in three-dimensional space, consider a set of points M (x, y, z) whose coordinates x, y, and z may be defined as

$x = x(t)$, $y = y(t)$, $z = z(t)$, $a \le t \le b$, or in vector form,

$$\mathbf{R} = \mathbf{R}(t) = x(t)\mathbf{i} + y(t)\mathbf{j} + z(t)\mathbf{k}, a \le t \le b \tag{2.1}$$

where **i**, **j**, and **k** are unit vectors and x(t), y(t), and z(t) are functions which are continuous on a segment [a, b], and correspond to a parameter value t, which may not be time always. Thus, the coordinates of points M may be calculated by the above formulae.

For a curve defined by the vector form, $\mathbf{R} = \mathbf{R}(t)$, $a \le t \le b$, consider the points that exist in the segment between a and b. Let these points be defined as c, d, e, f… z. If there is a bound on set of lengths of broken lines which join the subsequent points, such as ac, cd, de ….. zb, then such a curve is said to be rectifiable. The least upper bound of this length set is defined as the arc length of the curve, or simply the length of the curve, denoted by s.

The arc length may be evaluated by the following formula

$$s = \int_a^b \sqrt{|\mathbf{R}'(t)|}dt = \int_a^b \sqrt{\left[(x'(t))^2 + (y'(t))^2 + (z'(t))^2\right]}dt \tag{2. 2}$$

where the primes denote differentiation with respect to t.

2.2 FRENET - SERRET FORMULAE

The vector $\mathbf{R}'(t)$ is tangent to the space curve $\mathbf{R} = \mathbf{R}(t)$ and the length of this vector is

$$\frac{ds}{dt} = |\mathbf{R}'| = \sqrt{\left[(x'(t))^2 + (y'(t))^2 + (z'(t))^2\right]} \tag{2.3}$$

For the case $t = s, \frac{ds}{dt} = 1$, and $\mathbf{R} = \mathbf{R}(s)$, the tangent vector, of unit length, may be defined as

$$\mathbf{t} = \frac{d\mathbf{R}}{ds} \tag{2.4}$$

Using the expression $\mathbf{t}.\mathbf{t} = 1$, $\frac{d\mathbf{t}}{ds}$ can be shown to be perpendicular to **t**. Another unit vector, **p**, called the principal normal, perpendicular to **t**, may be defined as

$$\frac{d\mathbf{t}}{ds} = \kappa\mathbf{p} \tag{2.5}$$

The convention adopted is assigning **p** the same direction as $\frac{d\mathbf{t}}{ds}$

Here κ is a scalar multiplier, called the curvature. For a straight line, $\kappa = 0$. The unit vectors **t** and **p** form a plane called the osculating plane.

A right – handed set of orthogonal unit vectors may be formed by the introduction of another unit vector, the binormal **b**, which is defined as

$$\mathbf{b} = \mathbf{t} \times \mathbf{p} \tag{2.6}$$

t, b, and **p** form a figure, called the trihedral, which gives a reference point at each point in the curve. These are shown schematically in Figure 2.1.

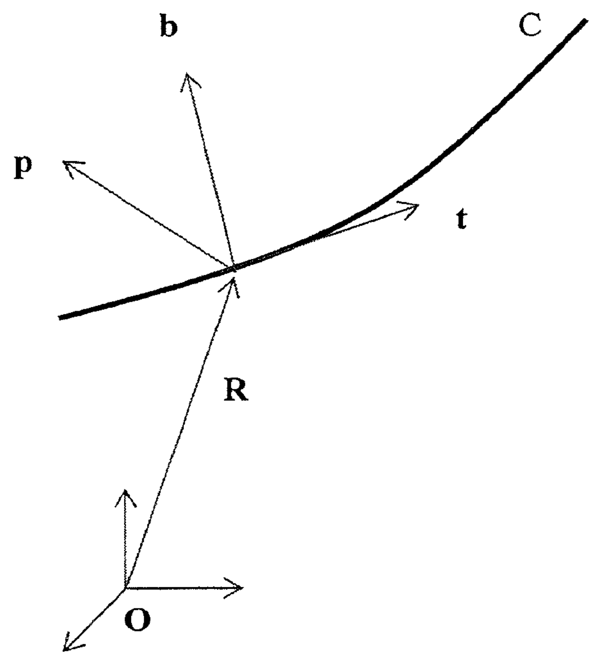

Figure 2.1 The trihedral associated with a curve C.

Since these form a set of orthogonal unit vectors, in addition to the definition of the binormal, other relations may be obtained by the cross products:

$$\mathbf{p} \times \mathbf{b} = \mathbf{t} \tag{2.7}$$

$$\mathbf{b} \times \mathbf{t} = \mathbf{p} \tag{2.8}$$

Another relation of importance is

$$\frac{d\mathbf{b}}{ds} = -\tau \mathbf{p} \tag{2.9}$$

where τ is a scalar multiplier called the torsion. Torsion measures the rate at which the curve twists out of its osculating plane.

It is also possible to show that

$$\mathbf{p}' = \frac{d\mathbf{p}}{ds} = -\kappa\mathbf{t} - \tau\mathbf{b} \tag{2.10}$$

Thus, at any point in space, an orthonormal basis is formed by **t, p,** and **b.** Moving along the curve, the orientation of these vectors relative to each other is maintained, although as one moves along the curve, **t, p,** and **b** rotate in space as a unit. This rotation is described by the equation:

$$\frac{d}{ds}\begin{bmatrix}\mathbf{t}\\ \mathbf{p}\\ \mathbf{b}\end{bmatrix} = \begin{bmatrix}0 & \kappa & 0\\ -\kappa & 0 & \tau\\ 0 & -\tau & 0\end{bmatrix}\begin{bmatrix}\mathbf{t}\\ \mathbf{p}\\ \mathbf{b}\end{bmatrix} \tag{2.11}$$

The anti-symmetric square matrix is an indication of rigid rotation in space. More details on the geometry of curves can be found in Kreyszig [12].

2.3 PERTURBATIONS

Consider now what happens on perturbing the position of a curve from **R** to **R** + ξ where ξ is small. Most of the results below are taken from Scriven (1969) who has expressed his results in a somewhat different form. To translate his results, note that the variation $\delta\,\mathbf{R} = \xi$ and note that Scriven's velocity

$$\mathbf{v} = \frac{d\xi}{dt} \tag{2.12}$$

In general, in his results in form of time derivatives can be written as

$$\frac{d\mathbf{q}}{dt}\Delta t = \delta\mathbf{q} \tag{2.13}$$

Thus $\mathbf{v}\ \Delta t = \delta\,\mathbf{R} = \xi$. Here, his main results, altered by above considerations are

$$\delta\begin{bmatrix}\mathbf{t}\\ \mathbf{p}\\ \mathbf{b}\end{bmatrix}=\begin{bmatrix}0 & \xi_{p,s} & \xi_{b,s}\\ -\xi_{p,s} & 0 & \xi_{b,ss}/\kappa\\ -\xi_{b,s} & -\xi_{b,ss}/\kappa & 0\end{bmatrix}\begin{bmatrix}\mathbf{t}\\ \mathbf{p}\\ \mathbf{b}\end{bmatrix} \tag{2.14}$$

where

$$\xi_{p,s}=\frac{\partial\xi_p}{\partial s}+\kappa\xi_t-\tau\xi_b \tag{2.15}$$

$$\xi_{b,s}=\frac{\partial\xi_b}{\partial s}+\tau\xi_p \tag{2.16}$$

$$\xi_{b,ss}=\frac{\partial^2\xi_b}{\partial s^2}+\xi_p\frac{\partial\tau}{\partial s}+2\tau\frac{\partial\xi_p}{\partial s}+\kappa\tau\xi_t-\tau^2\xi_b \tag{2.17}$$

where the subscript s denotes a differentiation with s where there is a single s involved. Again the matrix is anti-symmetric rotating the tangent vectors. Other relations are

$$\delta\kappa=\xi_{p,ss}-2\kappa\xi_{t,s} \tag{2.18}$$

$$\delta\tau=-\tau\xi_{t,s}+\kappa\xi_{b,s}+\frac{d}{ds}\left(\frac{\xi_{b,ss}}{\kappa}\right) \tag{2.19}$$

where

$$\xi_{t,s}=\frac{\partial\xi_t}{\partial s}-\kappa\xi_p \tag{2.20}$$

$$\xi_{p,ss}=\frac{\partial^2\xi_p}{\partial s^2}+2\kappa\frac{\partial\xi_t}{\partial s}-2\tau\frac{\partial\xi_b}{\partial s}+\frac{\partial\kappa}{\partial s}\xi_t-\frac{\partial\tau}{\partial s}\xi_b-\left(\kappa^2+\tau^2\right)\xi_p \tag{2.21}$$

For a moving curve, that is, a curve whose position changes with time, the velocity of a point on such a curve is defined by

$$\mathbf{v} = \left(\frac{\partial \mathbf{R}(x,t)}{\partial t} \right)_x \tag{2.22}$$

where x is the co-ordinate value of a point on the curve in some parameterization measured along the curve at a particular time instant.

The time derivative of the unit tangent may be obtained as follows.

$$\left(\frac{\partial \mathbf{t}}{\partial t}\right)_x = \left[\frac{\partial}{\partial t}\left(\frac{\partial \mathbf{R}}{\partial s}\right)_t\right]_x = \left[\frac{\partial}{\partial t}\left(\left(\frac{\partial \mathbf{R}}{\partial x}\right)_t \left(\frac{\partial x}{\partial s}\right)_t\right)\right]_x = \left(\frac{\partial x}{\partial s}\frac{\partial \mathbf{v}}{\partial x}\right)_t + \left(\frac{\partial \mathbf{R}}{\partial x}\right)_t \left(\frac{\partial}{\partial t}\left(\frac{1}{\left(\frac{\partial s}{\partial x}\right)_t}\right)\right)_x$$

$$= \left(\frac{\partial}{\partial s}\mathbf{v}\right)_t - \mathbf{t}\left(\frac{\partial x}{\partial s}\right)_t \left(\frac{\partial}{\partial t}\left(\frac{\partial s}{\partial x}\right)_t\right)_x = \left(\frac{\partial}{\partial s}\left(v_t \mathbf{t} + v_b \mathbf{b} + v_p \mathbf{p}\right)\right)_t - \mathbf{t}\left(\frac{\partial x}{\partial s}\right)_t \left(\frac{\partial}{\partial t}\left(\frac{\partial s}{\partial x}\right)_t\right)_x$$

(2.23)

On differentiating the expression $\mathbf{t}.\mathbf{t} = 1$, the right hand side becomes zero. Hence, what is seen on the left hand side is that $\mathbf{t}$ is perpendicular to $\left(\frac{\partial \mathbf{t}}{\partial t}\right)_x$. Thus the derivative has no tangential component. Thus, differentiating out $\boldsymbol{v}$ with respect to s, and equating all the coefficients of $\mathbf{t}$ to zero, one has

$$v_{t,s} - v_p \kappa = \frac{\partial x}{\partial s}\left(\frac{\partial}{\partial t}\left(\frac{\partial s}{\partial x}\right)_t\right)_x \tag{2.24}$$

Similarly, it possible to show that

$$\frac{\partial}{\partial t}\dot{\kappa} = \frac{d}{ds}\frac{\partial}{\partial t}\kappa - \frac{\dot{\kappa}}{\left(\frac{\partial s}{\partial x}\right)}\left\{\frac{\partial}{\partial t}\left[\frac{\partial s}{\partial x}\right]_t\right\}_x \tag{2.25}$$

where the dot is being used to show a differentiation with respect to s. Multiplying with Δt and using Eq. (2.3.14)

$$\delta\dot{\kappa} = \frac{d}{ds}\delta\kappa - \dot{\kappa}(\xi_{t,s} - \kappa\xi_p) \tag{2.26}$$

Thus, it is straightforward now to calculate all the other higher order variations.

3. PERTURBATIONS

3.1 MINIMUM FREE ENERGY REQUIRED TO PERTURB THE CURVE

ε is the total free energy(in Joules) required to perturb the curve, which is expressed over the entire length of the curve as the integral :

$$\varepsilon = \int e ds \tag{3.1}$$

where e is the free energy per unit length, in Newton (N). e is a function of the length of the curve s, curvature κ, and torsion τ, and $\ell = \int ds$. For a moving curve (Scriven, 1966),

$$\frac{\partial \ln(ds)}{\partial t} = v_{t,s} \tag{3.2}$$

Multiplying with Δt on the right hand side of (3.2), and expressing $\delta \ln(ds)$ as $\frac{1}{ds}\delta ds$, the following expression is obtained,

$$\left(\frac{\delta ds}{ds}\right) = \xi_{t,s} = \dot{\xi}_t - \kappa\xi_p \tag{3.3}$$

where the dot denotes differentiation with respect to s. The total variation in ε between two ends 0 and ℓ is then calculated by:

$$\delta\varepsilon = \int_0^\ell \left[\frac{\partial e}{\partial s}\xi_t + \frac{\partial e}{\partial \kappa}\delta\kappa + \frac{\partial e}{\partial \tau}\delta\tau + \frac{\delta(\partial s)}{\partial s}\right] ds \tag{3.4}$$

$\frac{\delta(\partial s)}{\partial s}$ may be set to zero, assuming that the length of the curve is constant.

Stretching modulus, M_s (N/m) is defined as:

$$M_s = \left(\frac{\partial e}{\partial s}\right)_{\kappa,\tau} \tag{3.5}$$

The bending modulus, M_b (N.m) is defined as :

$$M_b = \left(\frac{\partial e}{\partial \kappa}\right)_{s,\tau} \tag{3.6}$$

and the torsional modulus, M_t (N.m) is defined as:

$$M_t = \left(\frac{\partial e}{\partial \tau}\right)_{\kappa,s} \tag{3.7}$$

Therefore,

$$\delta\varepsilon = \int \left(M_s \xi_t + M_b \delta\kappa + M_t \delta\tau\right) ds \tag{3.8}$$

It is known that

$$\delta\kappa = \xi_{p,ss} - 2\kappa\xi_{t,s} = \ddot{\xi}_p + 2\kappa\dot{\xi}_t - 2\tau\dot{\xi}_b + \dot{\kappa}\xi_t - \dot{\tau}\xi_b - (\kappa^2 + \tau^2)\xi_p - 2\kappa\left(\dot{\xi}_t - \kappa\xi_p\right) \tag{3.9}$$

and

$$\delta\tau = \kappa(\dot{\xi}_b + \tau\xi_p) + \frac{\partial}{\partial s}\left(\frac{\ddot{\xi}_b + 2\tau\dot{\xi}_p + \dot{\tau}\xi_p + \kappa\tau\xi_t - \tau^2\xi_b}{\kappa}\right) \tag{3.10}$$

Substituting (3.10) and (3.9) in (3.8),

$$\delta\varepsilon = \int_0^{\ell} \left[\begin{aligned} &M_s\xi_t + M_b\left(\ddot{\xi}_p + 2\kappa\dot{\xi}_t - 2\tau\dot{\xi}_b + \dot{\kappa}\xi_t - \dot{\tau}\xi_b - (\kappa^2 + \tau^2)\xi_p - 2\kappa\dot{\xi}_t + 2\kappa^2\xi_p\right) \\ &+ M_t\left(-\tau\dot{\xi}_t + \tau\kappa\xi_p + \kappa\dot{\xi}_b + \kappa\tau\xi_p + \frac{\partial}{\partial s}\left(\frac{\ddot{\xi}_b + 2\tau\dot{\xi}_p + \dot{\tau}\xi_p + \kappa\tau\xi_t - \tau^2\xi_b}{\kappa}\right)\right)\end{aligned}\right] ds \tag{3.11}$$

or

$$\delta\varepsilon=\int_0^{\ell}\begin{bmatrix}\xi_t\left(M_s+M_b\dot{\kappa}+M_t\dot{\tau}\right)+\xi_b\left(-M_b\dot{\tau}+M_t\dfrac{\dot{\kappa}\tau^2}{\kappa^2}-2M_t\dfrac{\tau\dot{\tau}}{\kappa}\right)\\ +\dot{\xi}_b\left(-2M_b\tau+M_t\kappa-M_t\dfrac{\tau^2}{\kappa}\right)+\ddot{\xi}_b\left(-\dfrac{M_t\dot{\kappa}}{\kappa^2}\right)+\dddot{\xi}_b\left(\dfrac{M_t}{\kappa}\right)\\ +\xi_p\left(-\left(\kappa^2-\tau^2\right)M_b+2M_b\kappa^2+2M_t\tau\kappa+M_t\dfrac{\ddot{\tau}}{\kappa}-M_t\dfrac{\dot{\tau}\dot{\kappa}}{\kappa^2}\right)\\ +\dot{\xi}_p\left(3M_t\dfrac{\dot{\tau}}{\kappa}-2M_t\dfrac{\tau\dot{\kappa}}{\kappa^2}\right)+\ddot{\xi}_p\left(M_b+2M_t\dfrac{\tau}{\kappa}\right)\end{bmatrix}ds \tag{3.12}$$

Now, steps are taken to eliminate the derivatives of ξ inside the integral in the above equation. This is done by transforming the integrals into other integrals by integration by parts. M_b and M_t are assumed to be constant with respect to s. The results are for these integrals that

$$\begin{aligned}\int_0^{\ell}\dot{\xi}_b\left(-2M_b\tau+M_t\kappa-M_t\frac{\tau^2}{\kappa}\right)ds&=\xi_b\left(-2M_b\tau+M_t\kappa-M_t\frac{\tau^2}{\kappa}\right)\Bigg|_0^{\ell}\\ &-\int_0^{\ell}\xi_b\left(-2M_b\dot{\tau}+M_t\dot{\kappa}-M_t\left(\frac{2\tau\dot{\tau}}{\kappa}-\frac{\dot{\kappa}\tau^2}{\kappa^2}\right)\right)ds\end{aligned} \tag{3.13}$$

$$\int_0^{\ell}\ddot{\xi}_b\left(-\frac{M_t\dot{\kappa}}{\kappa^2}\right)ds=\dot{\xi}_b\left(\frac{-M_t\dot{\kappa}}{\kappa^2}\right)\Bigg|_0^{\ell}+\xi_bM_t\left(\frac{\ddot{\kappa}}{\kappa^2}-\frac{2\dot{\kappa}^2}{\kappa^3}\right)\Bigg|_0^{\ell}+\int_0^{\ell}\xi_bM_t\left(\frac{6\dot{\kappa}\ddot{\kappa}}{\kappa^3}-\frac{6\dot{\kappa}^3}{\kappa^4}-\frac{\dddot{\kappa}}{\kappa^2}\right)ds \tag{3.14}$$

$$\int_0^{\ell} \dddot{\xi}_b\left(\frac{M_t}{\kappa}\right)ds=\left(\ddot{\xi}_b\left(\frac{M_t}{\kappa}\right)+\dot{\xi}_b\left(\frac{M_t\dot{\kappa}}{\kappa^2}\right)+\xi_b M_t\left(\frac{2\dot{\kappa}^2}{\kappa^3}-\frac{\ddot{\kappa}}{\kappa^2}\right)\right)\Bigg|_0^{\ell}$$
$$-\int_0^{\ell}\xi_b M_t\left(\frac{6\dot{\kappa}\ddot{\kappa}}{\kappa^3}-\frac{6\dot{\kappa}^3}{\kappa^4}-\frac{\dddot{\kappa}}{\kappa^2}\right)ds \tag{3.15}$$

$$\int_0^{\ell}\dot{\xi}_p\left(3M_t\frac{\dot{\tau}}{\kappa}-2M_t\frac{\tau\dot{\kappa}}{\kappa^2}\right)ds=\xi_p\left(3M_t\frac{\dot{\tau}}{\kappa}-2M_t\frac{\tau\dot{\kappa}}{\kappa^2}\right)\Bigg|_0^{\ell}-\int_0^{\ell}\xi_p M_t\left(\frac{3\ddot{\tau}}{\kappa}-\frac{3\dot{\tau}\dot{\kappa}}{\kappa^2}-\frac{2\tau\ddot{\kappa}}{\kappa^2}-\frac{2\dot{\tau}\dot{\kappa}}{\kappa^2}+\frac{4\tau\dot{\kappa}^2}{\kappa^3}\right)ds \tag{3.16}$$

$$\int_0^{\ell}\ddot{\xi}_p\left(M_b+2M_t\frac{\tau}{\kappa}\right)ds=\left(\dot{\xi}_p\left(M_b+2M_t\frac{\tau}{\kappa}\right)-2M_t\xi_p\left(\frac{\dot{\tau}}{\kappa}-\frac{\tau\dot{\kappa}}{\kappa^2}\right)\right)\Bigg|_0^{\ell}$$
$$+\int_0^{\ell}2M_t\xi_p\left(\frac{\ddot{\tau}}{\kappa}-\frac{2\dot{\tau}\dot{\kappa}}{\kappa^2}-\frac{\tau\ddot{\kappa}}{\kappa^2}+\frac{2\tau\dot{\kappa}^2}{\kappa^3}\right)ds \tag{3.17}$$

Substituting (3.16) to (3.20) in (3.15),

$$\delta\varepsilon=\int_0^{\ell}\begin{bmatrix}\xi_t\left(M_s+M_b\dot{\kappa}+M_t\dot{\tau}\right)+\xi_b\left(M_b\dot{\tau}-M_t\dot{\kappa}\right)+\\ \xi_p\left(M_b\left(\kappa^2-\tau^2\right)+2M_t\tau\kappa\right)\end{bmatrix}ds$$
$$+\left(\xi_b\left(-2M_b\tau+M_t\kappa-\frac{M_t\tau^2}{\kappa}\right)+\ddot{\xi}_b\left(\frac{M_t}{\kappa}\right)+\xi_p\left(\frac{M_t\dot{\tau}}{\kappa}\right)+\dot{\xi}_p\left(M_b+\frac{2M_t\tau}{\kappa}\right)\right)\Bigg|_0^{\ell} \tag{3.18}$$

Assuming that at the two ends of the curve 0 and ℓ are at the same conditions, the limit term in (3.18) may be set to zero. The expression reduces to:

$$\delta\varepsilon = \int_0^\ell \begin{bmatrix} \xi_t\left(M_s + M_b\dot{\kappa} + M_t\dot{\tau}\right) + \xi_b\left(M_b\dot{\tau} - M_t\dot{\kappa}\right) + \\ \xi_p\left(M_b\left(\kappa^2 - \tau^2\right) + 2M_t\tau\kappa\right) \end{bmatrix} ds$$

(3.19)

3.2 CONDITIONS OF EQUILIBIRIUM

Work is the product of force **F** and displacement ξ in the direction of the force, and work is performed on a body through a change in energy, $\delta\varepsilon$. Therefore,

$$\delta\varepsilon = \int_0^\ell \xi.\mathbf{F}ds \tag{3.20}$$

The necessary condition for ε to attain its extremum value is that its first variation, $\delta\varepsilon = 0$. Since the perturbation ξ is small but arbitrary, its coefficients may be set to zero, that is, $\mathbf{F} = \mathbf{0}$. Under these conditions, a force balance can be performed by equating the coefficients of force to zero.

Condition 1: $$F_s = \left(M_s + M_b\dot{\kappa} + M_t\dot{\tau}\right) = 0 \tag{3.21}$$

Condition 2: $$F_b = \left(M_b\dot{\tau} - M_t\dot{\kappa}\right) = 0 \tag{3.22}$$

Condition 3: $$F_t = \left(M_b\left(\kappa^2 - \tau^2\right) + 2M_t\tau\kappa\right) = 0 \tag{3.23}$$

For the three conditions, three special cases are considered.

Case 1: Constant curvature κ and constant torsion τ.

The derivatives of κ and τ with respect to s may be set to zero, and Equation (3.23) reduces to:

$$M_b\left(\kappa^2 - \tau^2\right) + 2M_t\tau\kappa = 0 \tag{3.24}$$

For a circular helix with the parametric equation

$$\mathbf{R} = \mathbf{i}a\cos\theta + \mathbf{j}a\sin\theta + \mathbf{k}p\theta \tag{3.25}$$

where a is the radius and p is the pitch, the curvature and torsion are constants (Sokolnikoff, 1958). It is possible to show that

$$\kappa = \frac{a}{a^2 + p^2} \tag{3.26}$$

$$\tau = \frac{-p}{a^2 + p^2} \tag{3.27}$$

Substituting these values in (3.24), we obtain,

$$M_b\left(\frac{a^2}{\left(a^2+p^2\right)^2}\right) - M_b\left(\frac{p^2}{\left(a^2+p^2\right)^2}\right) = \frac{2M_t ap}{\left(a^2+p^2\right)^2} \tag{3.28}$$

On further simplification,

$$\frac{a^2 - p^2}{ap} = \frac{2M_t}{M_b} \tag{3.29}$$

This quadratic equation may be solved for the ratio p/a and the ratio M_t/M_b. The result is:

$$\frac{p}{a} = -\frac{M_t}{M_b} \pm \sqrt{\left(\frac{M_t}{M_b}\right)^2 + 1} \tag{3.30}$$

A plot of the ratio p/a versus M_t/M_b is obtained and shown in Figure 3.1. The ratio p/a cannot be negative, hence only one root is shown.

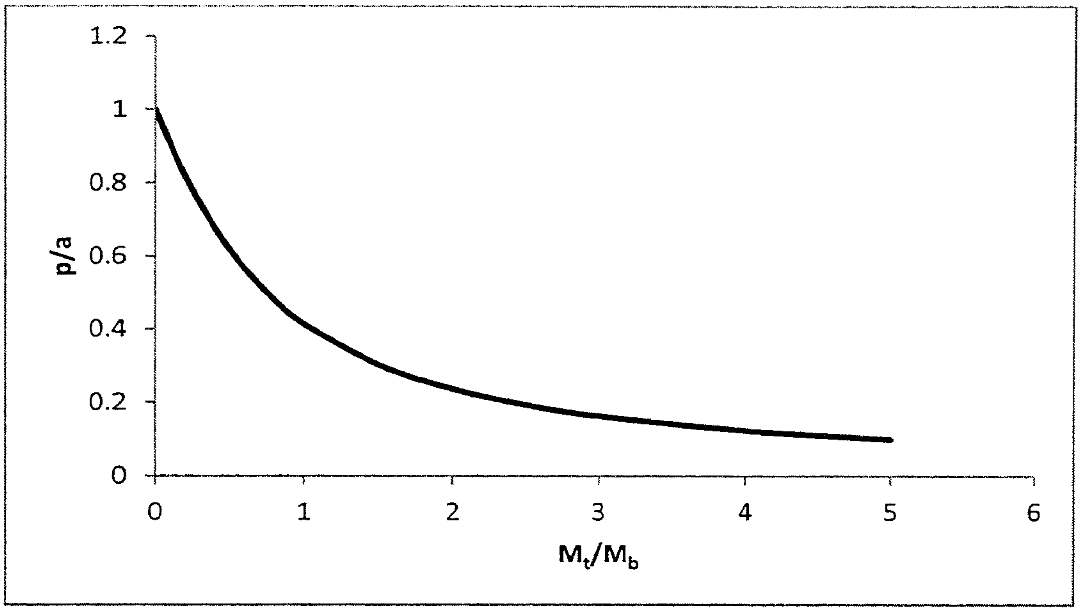

Figure 3.1. A plot of p/a versus M_t/M_b.

Case 2:

$M_b = 0$. For this case, the force balance reduces to:

$$\left(M_s + M_t\dot{\tau}\right) = 0 \tag{3.31}$$

$$\left(-M_t\dot{\kappa}\right) = 0 \tag{3.32}$$

$$\left(2M_t\tau\kappa\right) = 0 \tag{3.33}$$

The two cases are

(i) $\kappa = \text{constant} \neq 0$, and $\tau = 0$ and $M_s = 0$.

(ii) $\kappa = 0, \quad \dot{\tau} = -M_s / M_t$

where if $M_s = 0$ then τ is a constant or varies linearly with s if M_s is not zero.

Now, (i) is a special case of Case 1, but (ii) may not be.

Case 3: $M_t = 0$

For this case, the force balance reduces to:

$$\left(M_s + M_b\dot{\kappa}\right) = 0 \tag{3.34}$$

$$\left(M_b\dot{\tau}\right) = 0 \tag{3.35}$$

$$\left(M_b\left(\kappa^2 - \tau^2\right)\right) = 0 \tag{3.36}$$

According to Equation (3.35), τ is a constant and according to Equation (3.36), $\kappa = \pm\tau$, so κ is also a constant. If κ is a constant, according to (3.34), M_s becomes zero. Again this is a special case of Case 1, where τ and κ are constants but are related.

4. RESULTS AND DISCUSSION

4.1 STABILITY

The second variation of $\delta\varepsilon = \int \xi.\mathbf{F}ds$ is given by:

$$\delta^2\varepsilon = \int \left(\delta\xi\,.\,\mathbf{F} + \xi\,.\,\delta\mathbf{F}\right)ds \geq 0 \tag{4.1}$$

Noting that $\delta(ds) = 0$ for constant s and substituting $\mathbf{F} = \mathbf{0}$ at equilibrium this reduces to

$$\delta^2\varepsilon = \int \xi.\delta\mathbf{F}ds \geq 0 \tag{4.2}$$

The condition for ε to be a minimum is that $\delta^2\varepsilon \geq 0$.

Case 1

For this case, ξ_t is set to zero. Equation (4.2) is reduced to:

$$\delta^2\varepsilon = \int \left[\xi_b\delta F_b + \xi_p\delta F_t\right]ds \tag{4.3}$$

For the case of constant curvature and torsion, from the conditions of equilibrium in Equation (3.22), the component force F_b becomes zero and therefore δF_b becomes zero, and substituting the value of F_t from Equation (3.23),

$$\delta^2\varepsilon = \int \xi_p\left(2M_b\left(\kappa\delta\kappa - \tau\delta\tau\right) + 2M_t\left(\tau\delta\kappa + \kappa\delta\tau\right)\right)ds \geq 0 \tag{4.4}$$

Substituting the values of $\delta\kappa$ and $\delta\tau$ from Equation (2.18) and Equation (2.19),

$$\delta^2\varepsilon=\int \xi_p \begin{bmatrix} \ddot{\xi}_p\left(2M_b\kappa+2M_t\tau+\left(\dfrac{2\tau}{\kappa}\right)(2M_t\kappa-2M_b\tau)\right)+ \\ \dot{\xi}_p\left(\left(\dfrac{2\dot{\tau}}{\kappa}\right)(2M_t\kappa-2M_b\tau)-\left(\dfrac{2\dot{\kappa}\tau}{\kappa^2}\right)(2M_t\kappa-2M_b\tau)+\left(\dfrac{\dot{\tau}}{\kappa}\right)(2M_t\kappa-2M_b\tau)\right)+ \\ \xi_p\left((2M_b\kappa+2M_t\tau)\left(-\kappa^2-\tau^2\right)+4M_b\kappa^3+8M_t\kappa^2\tau-4M_b\kappa\tau^2+(2M_t\kappa-2M_b\tau)\left(\dfrac{\ddot{\tau}}{\kappa}-\dfrac{\dot{\kappa}\dot{\tau}}{\kappa^2}\right)\right)+ \\ \xi_b(-\dot{\tau})(2M_b\kappa+2M_t\tau)+\dot{\xi}_b\left((-2\tau)(2M_b\kappa+2M_t\tau)+2M_t\kappa^2-2\kappa\tau M_b\right)+ \\ \ddot{\xi}_b\left(\dfrac{-1}{\kappa}\right)(2M_t\kappa-2M_b\tau)+\dddot{\xi}_b\left(\dfrac{1}{\kappa}\right)(2M_t\kappa-2M_b\tau)+\xi_t(2M_b\kappa+2M_t\tau)\dot{\kappa}+ \\ \dot{\xi}_t\left[(2\kappa)(2M_b\kappa+2M_t\tau)-4M_b\kappa^2-4M_t\kappa\tau+2M_b\tau^2-2M_t\kappa\tau\right] \end{bmatrix} ds$$

(4.5)

By the method of integration by parts, the derivatives of ξ are eliminated, the terms outside the integral are set to zero, and in addition the ξ_t and $\dot{\xi}_t$ components are set to zero, and Equation (4.5) becomes:

$$\delta^2\varepsilon=\int \xi_p \begin{bmatrix} \xi_p\begin{bmatrix} (2M_b\kappa+2M_t\tau)\left(\kappa^2-\tau^2\right)+(2M_t\kappa-2M_b\tau)\left(2\tau\kappa+\dfrac{\ddot{\tau}}{\kappa}+\dfrac{\dot{\kappa}\dot{\tau}}{\kappa^2}\right)+2M_b\ddot{\kappa}+2M_t\ddot{\tau} \\ +\dfrac{2\tau}{\kappa}(2M_t\ddot{\kappa}-2M_b\ddot{\tau})+(2M_t\dot{\kappa}-2M_b\dot{\tau})\left(\dfrac{2\dot{\tau}\kappa-2\tau\dot{\kappa}}{\kappa^2}\right)+(2M_t\dot{\kappa}-2M_b\dot{\tau})\left(\dfrac{2\tau\dot{\kappa}}{\kappa^2}-\dfrac{3\dot{\tau}}{\kappa}\right) \\ +(2M_t\kappa-2M_b\tau)\left(\dfrac{2\tau\ddot{\kappa}}{\kappa^2}-\dfrac{2\dot{\kappa}}{\kappa^3}(\ddot{\kappa}\tau+\dot{\kappa}\dot{\tau})\right) \end{bmatrix} \\ +\xi_b\begin{bmatrix} (2M_b\kappa+2M_t\tau)(\dot{\tau})+(2M_t\kappa-2M_b\tau)\left(-\dot{\kappa}+\dfrac{4\dot{\kappa}\ddot{\kappa}}{\kappa^3}-\dfrac{6\dot{\kappa}^3}{\kappa^4}-\dfrac{\dddot{\kappa}}{\kappa^2}+\dfrac{2\kappa\ddot{\kappa}}{\kappa^3}\right) \\ +2\tau(2M_b\dot{\kappa}+2M_t\dot{\tau})+(2M_b\dot{\kappa}-2M_t\dot{\tau})\left(\dfrac{\tau^2}{\kappa}-\kappa-\dfrac{\ddot{\kappa}}{\kappa^2}+\dfrac{2\dot{\kappa}^2}{\kappa^3}\right) \\ -2M_b\left(\dfrac{\tau\dddot{\kappa}+3\dot{\tau}\ddot{\kappa}+2\ddot{\tau}\dot{\kappa}}{\kappa^2}-\dfrac{2\dot{\kappa}}{\kappa^3}(\ddot{\kappa}\tau+2\dot{\kappa}\dot{\tau})-2\left(\dfrac{2\dot{\kappa}\ddot{\kappa}\tau+\dot{\kappa}^2\dot{\tau}}{\kappa^3}\right)+\dfrac{6\dot{\kappa}^3\tau}{\kappa^4}-\dfrac{\ddot{\tau}}{\kappa}+\dfrac{\dddot{\tau}\kappa}{\kappa^2}\right) \end{bmatrix} \end{bmatrix} ds$$

(4.6)

Under the condition of constant curvature κ and constant torsion τ, Equation (4.5) becomes:

$$\delta^2\varepsilon = \int \xi_p^{\,2}\left[\left(2M_b\left(\kappa^3 - 3\kappa\tau^2\right) + 2M_t\left(3\kappa^2\tau - \tau^3\right)\right)\right]ds \geq 0 \tag{4.7}$$

Substituting the expressions for κ and τ from Equations (3.26) and (3.27) and substituting the value of M_b from Equation (3.29), and expressing the equation in terms of the ratio of pitch to radius (p/a), the following equation is obtained:

$$\delta^2\varepsilon = \int \xi_p^{\,2}\left[\frac{M_b a^3}{\left(a^2+p^2\right)^3}\left[-1-2\left(\frac{p}{a}\right)^2 - \left(\frac{p}{a}\right)^4\right]\right]ds \geq 0 \tag{4.8}$$

The term $\dfrac{M_b a^3}{\left(a^2+p^2\right)^3}$ is always positive in Equation (4.8), and the term

$\left[-1-2\left(\dfrac{p}{a}\right)^2 - \left(\dfrac{p}{a}\right)^4\right]$ is not positive. As a result, the helix is unstable. On setting M_b

to zero in equation (4.7), the result is

$$\delta^2\varepsilon = \int \xi_p^{\,2}\left[\frac{2M_t a^3}{\left(a^2+p^2\right)^3}\left[\left(\frac{p}{a}\right)^3 - 3\left(\frac{p}{a}\right)\right]\right]ds \geq 0 \tag{4.9}$$

Solving the cubic equation analytically, the result is that the term is positive for values of p/a that are more than $\sqrt{3}$ and values of p/a between 0 and $-\sqrt{3}$. The third root is zero and discarded. It is of importance that the condition of equilibrium Eq. (3.30) and Figure 3.1 shows that p/a cannot be more than 1.0 and further p/a cannot be negative. So the result is that the helix is unstable.

Case 2

For this case, M_b is set to zero. The components of force become:

$$
\begin{aligned}
F_s &= M_s + M_t\dot{\tau} \\
F_b &= -M_t\dot{\kappa} \\
F_t &= 2M_t\tau\kappa
\end{aligned}
\tag{4.10}
$$

The criterion for stability after setting F_s to zero becomes:

$$\delta^2\varepsilon = \int\left(\xi_b\left[\delta\left[-M_t\dot{\kappa}\right] + \xi_p\delta\left[2M_t\tau\kappa\right]\right]\right)ds \geq 0 \tag{4.11}$$

Substituting the values of $\delta\dot{\kappa}$ and $\delta\dot{\tau}$,

$$\delta^2\varepsilon = \int\left[\begin{array}{l}
\xi_b\left[\begin{array}{l}\dddot{\xi}_p(-M_t) + \dot{\xi}_p\left(M_t\left(\tau^2-\kappa^2\right)\right) + \xi_p\left(2M_t\tau\dot{\tau} - 4M_t\kappa\dot{\kappa}\right) + \ddot{\xi}_b\left(2M_t\tau\right) + \dot{\xi}_b\left(3M_t\dot{\tau}\right) \\ +\xi_b\left(M_t\ddot{\tau}\right) + \xi_t\left(-M_t\ddot{\kappa}\right)\end{array}\right] \\
+\xi_p\left[\begin{array}{l}\ddot{\xi}_p\left(6M_t\tau\right) + \dot{\xi}_p\left(\dfrac{-4M_t\dot{\kappa}\tau}{\kappa} + 6M_t\dot{\tau}\right) + \xi_p\left(-2M_t\tau\left(\tau^2+\kappa^2\right) + 8M_t\kappa^2\tau + 2M_t\ddot{\tau} - \dfrac{2M_t\dot{\kappa}\dot{\tau}}{\kappa}\right) \\ +\dddot{\xi}_b\left(2M_t\right) + \ddot{\xi}_b\left(\dfrac{-2M_t\dot{\kappa}}{\kappa}\right) + \dot{\xi}_b\left(-6M_t\tau^2 + 2M_t\kappa^2\right) + \xi_b\left(-6M_t\tau\dot{\tau} + \dfrac{2M_t\tau^2}{\kappa}\right) \\ +\xi_t\left(2M_t\dot{\kappa}\tau + 2M_t\dot{\tau}\kappa\right)\end{array}\right]
\end{array}\right]ds \tag{4.12}$$

By the method of integration by parts, the derivatives of ξ are eliminated, the terms outside the integral are set to zero, and in addition the ξ_t and $\dot{\xi}_t$ components are set to zero, and Equation (4.12) becomes:

$$\delta^2\varepsilon=\int\left[\xi_b\left[\xi_p\left(-2M_t\kappa\dot{\kappa}\right)\right]+\xi_p\left[\begin{array}{l}\xi_p\left(6M_t\kappa^2\tau+\frac{4M_t}{\kappa}\left(\ddot{\kappa}\tau+\dot{\kappa}\dot{\tau}-\frac{\dot{\kappa}^2\tau}{\kappa}\right)-2M_t\tau^3+2M_t\ddot{\tau}-\frac{2M_t\dot{\kappa}\dot{\tau}}{\kappa}\right)\\+\xi_b\left(6M_t\tau\dot{\tau}+\frac{2M_t\tau^2}{\kappa}-2M_t\left(\frac{\ddot{\kappa}}{\kappa}-\frac{3\dot{\kappa}\ddot{\kappa}}{\kappa^2}+\frac{2\dot{\kappa}^3}{\kappa^3}\right)-4M_t\kappa\dot{\kappa}\right)\end{array}\right]\right]ds$$

(4.13)

Due to the complexity of the results, further analysis has not been undertaken.

Case 3

For this case, M_t is set to zero. The components of force become:

$$\begin{aligned}F_s&=M_s+M_b\dot{\kappa}\\F_b&=M_b\dot{\tau}\\F_t&=M_b\left(\kappa^2-\tau^2\right)\end{aligned}$$

(4.14)

The criterion for stability after setting F_s to zero becomes:

$$\delta^2\varepsilon=\int\left(\xi_b\left[\delta\left[M_b\dot{\tau}\right]+\xi_p\delta\left[M_b\left(\kappa^2-\tau^2\right)\right]\right]\right)ds\geq 0 \qquad (4.15)$$

Substituting the values of $\delta\dot{\kappa}$ and $\delta\dot{\tau}$,

$$
\delta^2\varepsilon = \int \left[\begin{array}{l}
\xi_b \left[\begin{array}{l}
\dddot{\xi}_p \left(\dfrac{2M_b\tau}{\kappa} \right) + \ddot{\xi}_p \left(\dfrac{5M_b\dot{\tau}}{\kappa} - \dfrac{4M_b\tau\dot{\kappa}}{\kappa^2} \right) + \\
\dot{\xi}_p \left(2M_b\kappa\tau + \dfrac{4M_b\ddot{\tau}}{\kappa} - \dfrac{6M_b\dot{\tau}\dot{\kappa}}{\kappa^2} - \dfrac{2M_b\tau\ddot{\kappa}}{\kappa^2} + \dfrac{4M_b\dot{\kappa}^2\tau}{\kappa^3} \right) \\
+\xi_p \left(4M_b\kappa\dot{\tau} + 2M_b\dot{\kappa}\tau + \dfrac{M_b\dddot{\tau}}{\kappa} - \dfrac{2M_b\dot{\kappa}\ddot{\tau}}{\kappa^2} - \dfrac{M_b\ddot{\kappa}\dot{\tau}}{\kappa^2} + \dfrac{2M_b\dot{\kappa}^2\dot{\tau}}{\kappa^3} \right) + \\
\ddddot{\xi}_b \left(\dfrac{M_b}{\kappa} \right) + \dddot{\xi}_b \left(\dfrac{-2M_b\dot{\kappa}}{\kappa^2} \right) + \ddot{\xi}_b \left(M_b\kappa - \dfrac{M_b\tau^2}{\kappa} - \dfrac{M_b\ddot{\kappa}}{\kappa^2} + \dfrac{2M_b\dot{\kappa}^2}{\kappa^3} \right) + \\
\dot{\xi}_b \left(M_b\dot{\kappa} - \dfrac{4M_b\tau\dot{\tau}}{\kappa} + \dfrac{M_b\tau^2}{\kappa} \right) + \\
\xi_b \left(\dfrac{-2M_b\tau\ddot{\tau}}{\kappa} - \dfrac{2M_b\dot{\tau}^2}{\kappa} + \dfrac{2M_b\tau\dot{\tau}\dot{\kappa}}{\kappa^2} + \dfrac{M_b\tau^2\dot{\kappa}}{\kappa^2} + \dfrac{2M_b\tau\dot{\tau}}{\kappa} - \dfrac{M_b\tau^2\dot{\kappa}}{\kappa} \right) + \\
\dot{\xi}_t \left(M_b\dot{\tau} \right) + \xi_t \left(M_b\ddot{\tau} - M_b\dot{\tau} \right)
\end{array} \right] \\
+\xi_p \left[\begin{array}{l}
\ddot{\xi}_p \left(\dfrac{-4M_b\tau^2}{\kappa} + 2M_b\kappa \right) + \dot{\xi}_p \left(\dfrac{-6M_b\tau\dot{\tau}}{\kappa} + \dfrac{4M_b\tau^2\dot{\kappa}}{\kappa^2} \right) + \\
\xi_p \left(2M_b\kappa^3 - 6M_b\kappa\tau^2 - \dfrac{2M_b\tau\ddot{\tau}}{\kappa} + \dfrac{2M_b\tau\dot{\tau}\dot{\kappa}}{\kappa^2} \right) + \dddot{\xi}_b \left(\dfrac{-2M_b\tau}{\kappa} \right) \\
+\ddot{\xi}_b \left(\dfrac{2M_b\tau\dot{\kappa}}{\kappa^2} \right) + \dot{\xi}_b \left(-6M_b\kappa\tau + \dfrac{2M_b\tau^3}{\kappa} \right) + \xi_b \left(-2M_b\kappa\dot{\tau} + \dfrac{4M_b\tau^2\dot{\tau}}{\kappa} - \dfrac{2M_b\tau^3}{\kappa^2} \right) \\
+\xi_t \left(2M_b\kappa\dot{\kappa} - 2M_b\tau\dot{\tau} \right)
\end{array} \right]
\end{array} \right] ds
$$

(4.16)

By the method of integration by parts, the derivatives of ξ are eliminated, the terms outside the integral are set to zero, and in addition the ξ_t and $\dot{\xi}_t$ components are set to zero, and Equation (4.16) becomes:

$$
\delta^2\varepsilon = \int \left[\begin{array}{l}
\xi_b \left[\begin{array}{l}
\xi_p \left(\begin{array}{l}
\frac{4M_b\ddot{\tau}}{\kappa} - \frac{4M_b\dot{\kappa}\ddot{\tau}}{\kappa^2} + \frac{8M_b\ddot{\kappa}\dot{\tau}}{\kappa^2} - \frac{20M_b\dot{\kappa}^2\dot{\tau}}{\kappa^3} + 2M_b\kappa\dot{\tau} + \frac{4M_b\tau\dddot{\kappa}}{\kappa^2} \\
- \frac{16M_b\tau\dot{\kappa}\ddot{\kappa}}{\kappa^3} - \frac{12M_b\tau\dot{\kappa}^3}{\kappa^4}
\end{array} \right) \\
+\xi_b \left(\begin{array}{l}
\frac{2M_b\tau\dot{\tau}\dot{\kappa}}{\kappa^2} + \frac{M_b\tau^2\dot{\kappa}}{\kappa^2} + \frac{2M_b\tau\dot{\tau}}{\kappa} - \frac{M_b\dot{\kappa}\tau^2}{\kappa} - \frac{2M_b\dddot{\kappa}}{\kappa^2} + \frac{12M_b\ddot{\kappa}^2}{\kappa^3} \\
- \frac{12M_b\dot{\kappa}^2\ddot{\kappa}}{\kappa^4} + \frac{96M_b\dot{\kappa}^4}{\kappa^5} + \frac{2M_b\dddot{\kappa}}{\kappa^4} - 8M_b\dot{\kappa}\dddot{\kappa} - \frac{8M_b\ddot{\kappa}^2}{\kappa^5} - \frac{8M_b\dot{\kappa}\dddot{\kappa}}{\kappa^5} + \\
\frac{40M_b\dot{\kappa}^2\ddot{\kappa}}{\kappa^6} - \frac{8M_b\ddot{\kappa}^2}{\kappa^3} - \frac{M_b\tau^2\ddot{\kappa}}{\kappa^2} + \frac{2M_b\tau^2\dot{\kappa}^2}{\kappa^3} + \frac{6M_b\dot{\kappa}\dddot{\kappa}}{\kappa^3} - \frac{2M_b\dot{\tau}}{\kappa} + \frac{M_b\tau^2\dot{\kappa}}{\kappa^2}
\end{array} \right)
\end{array} \right] \\
+\xi_p \left[\begin{array}{l}
\xi_p \left(\begin{array}{l}
2M_b\kappa^3 - 6M_b\kappa\tau^2 - \frac{16M_b\tau\ddot{\tau}}{\kappa} + \frac{4M_b\tau\dot{\kappa}\dot{\tau}}{\kappa^2} - \frac{2M_b\dot{\tau}^2}{\kappa} - \frac{8M_b\tau\dot{\tau}\dot{\kappa}}{\kappa} + \frac{4M_b\tau^2\ddot{\kappa}}{\kappa^2} \\
+ \frac{8M_b\tau\dot{\tau}\dot{\kappa}}{\kappa^2} + 2M_b\ddot{\kappa} - \frac{4M_b\tau^2\ddot{\kappa}}{\kappa}
\end{array} \right) \\
+\xi_b \left(\begin{array}{l}
4M_b\kappa\dot{\tau} + \frac{4M_b\tau^2\dot{\tau}}{\kappa} - \frac{2M_b\tau^3}{\kappa^2} - \frac{12M_b\dot{\kappa}^3\tau}{\kappa^4} - \frac{4M_b\dot{\kappa}\ddot{\tau}}{\kappa^2} - \frac{2M_b\ddot{\kappa}\dot{\tau}}{\kappa^2} + \frac{2M_b\dddot{\tau}}{\kappa} \\
+ \frac{4M_b\kappa\dot{\kappa}\dot{\tau}}{\kappa^4} - \frac{2M_b\dddot{\kappa}\tau}{\kappa^2} + \frac{2M_b\tau\dddot{\kappa}}{\kappa^2} + \frac{12M_b\dot{\kappa}^3\tau}{\kappa^4} + 6M_b\dot{\kappa}\tau - \frac{6M_b\tau^2\dot{\tau}}{\kappa} + \frac{2M_b\dot{\kappa}\tau^3}{\kappa^2}
\end{array} \right)
\end{array} \right]
\end{array} \right] ds \tag{4.17}
$$

Again, due to the complexity of the results, further analysis has not been undertaken.

4.2 DISCUSSION

It appears that Case 1, (constant curvature and torsion), the condition for equilibrium shows that a helix can form where the pitch to diameter ratio is determined by the bending and torsional moduli. It says that such helices form spontaneously, which is somewhat strange because it takes work to curve or twist into this shape. However, the stability analysis shows that they are all unstable. Both the equilibrium and the stability results are difficult to interpret for the other two cases because of the complexity of the results.

Although in deriving these results, the bending and torsional moduli have been taken to be constants, the results can still be applied where M_t and M_b vary slightly with s, κ or τ. It is possible to provide a model for these. Using the results of Helfrich, W. [19] for a surface and translating them for a curve,

$$e = k_c(\kappa - \kappa_o)^2 + k_t\tau \tag{4.18}$$

where k_c, k_t and κ_o are constants. It gives rise to

$$M_b = 2k_c\left(\kappa - \kappa_0\right) \tag{4.19}$$

$$M_t = k_t \tag{4.20}$$

According to Equation (4.1.19) when the curvature remains close to κ_o, the bending modulus M_b is close to zero. This curvature for a surface is called the natural radius of curvature. These moduli provide a set of equations for us to solve to get the equilibrium shapes.

4.3 REMARKS

There are still some important issues to settle and those have not been undertaken here. There are three conditions of equilibrium, Eq. (3.21-23) but only two unknowns, κ and τ. Since the curve has been assumed to be unstretchable, the first equation could be ignored. This needs to be ascertained. Similarly after taking the second variation of ε, the integrant contains terms in ξ_p^2 , ξ_b^2, and $\xi_p\ \xi_b$. With only the squared terms present, for ε to be a minimum, the coefficients of the squared terms have to be ≥ 0. However, when the product terms are present, the integrant in a matrix form needs to be diagonalized such that there is $(\xi_p + m\xi_b)^2$ and $(\xi_p + n\xi_b)^2$ instead, where, m and n are known constants. Their coefficients will have to be ≥ 0 for ε to be a minimum [20].

So it is observed that it has been possible to provide information of shapes at various levels, but obviously more work is needed.

5. CONCLUSIONS

It is possible to define bending and torsional moduli which provides the conditions for equilibrium. It has been assumed that the moduli are constants, and that the curve cannot be stretched. In principle, it is possible to calculate the shapes of curves if the moduli are known. The conditions of stability have been determined under the assumption that there is no perturbation in the tangential direction, and of course, the moduli remain constant.

It is possible to introduce an equation of state, whereby the moduli can be calculated and used in above results, provided that they vary only little, and obtain corresponding shapes of curves which tend to bend to a natural curvature and torsion. It has been shown that information about shapes of curves may be obtained. Future work may be directed towards obtaining information about relating the pitch and the coil to the elastic moduli. Also, it is not known if two identical solutions in the form of helices constitute a double helix when they are with a phase lag of 180°. Also in the case where curvature and torsion are each two valued, one large and one small, it is not known if these would constitute a supercoil.

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