Mathematical Mechanical Biology

Module 1: Bio-Filaments

Lecture Notes for C5.9
Notes extensively based on those by Alain Goriely, Oxford, 2015

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HEALTH WARNING:

The following lecture notes are meant as a rough guide to the lectures. They are not meant to replace the lectures. You should expect that some material in these notes will not be covered in class and that extra material will be covered during the lectures (especially longer proofs, examples, and applications). Nevertheless, I will try to follow the notation and the overall structure of the notes as much as possible.

1 Chain models

Overview

We consider the statistical mechanics of different chains of increasing complexity to describe the geometry and physical response of chains in a thermal bath. Past the entropic regime, many bio-filaments behave as elastic material and we will then use classical rod mechanics to characterise their behaviour.

1.1 FJC: Freely jointed chain models

1.1.1 Without external force

This model is also known as Random Flight Model (as we will see it is closely related to the problem of diffusion/Brownian motion). We consider a chain of links that are free to rotate with respect to one another. We have the following assumptions.

1) The chain has N links

2) Each link has a fixed length b (b for bond length)

3) The orientation of the tangent $\mathbf{t}_i$ at node $(i-1)$ is independent from the orientation of the other tangents.

4) There is no excluded volume effects.

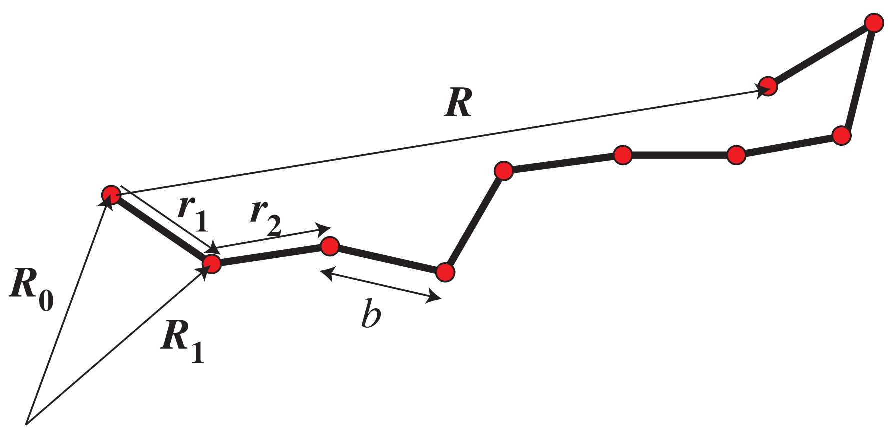

Figure 1: The freely jointed chain. Each segment has constant length with independent orientation.

The nodes have position $\mathbf{R}_i \in \mathbb{R}^3$ for $i = 0, \ldots, N$ and the vector from node $i-1$ to i is denoted by $\mathbf{r}_i = b\mathbf{t}_i$. We define the average $< . >$ of a quantity $\mathbf{a}$ as

$$< \mathbf{a} >= \int_{(\mathbb{R}^3)^N} \mathbf{a}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) p(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) dV, \tag{1}$$

where dV is the volume element of $(\mathbb{R}^3)^N$ and $p(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ is the probability distribution for the configuration vector $(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$. In our case $p = \prod_{i=1}^{N} \psi(\mathbf{r}_i)$ with

$$\psi(\mathbf{r}) = \frac{1}{4\pi b^2}\delta(|\mathbf{r}| - b). \tag{2}$$

We define the end-to-end vector as

$$\mathbf{R} \equiv \mathbf{R}_N - \mathbf{R}_0, \tag{3}$$

and compute its average

$< \mathbf{R} >= 0$

Therefore, we introduce $< \mathbf{R}^2 >$ to find a characteristic length.

$< \mathbf{R}^2 >= Nb^2$

We define the typical *end-to-end distance* as

$$\bar{R} = \sqrt{< \mathbf{R}^2 >} = \sqrt{N} b. \tag{4}$$

1.1.2 Gyration radius

The gyration radius is closely related to the *end-to-end distance*. It is defined as the root-mean-square distance of a collection of points with respects to their centre of gravity. Defining $\mathbf{s}_i$ the vector from the centre of gravity to the node at position $\mathbf{R}_i$, the *gyration radius* is

$$s^2 = \frac{1}{N+1} \sum_{i=0}^{N} \mathbf{s_i} \cdot \mathbf{s_i}. \tag{5}$$

By a theorem due to Lagrange, we also have

$$s^2 = \frac{1}{(N+1)^2} \sum_{0 \le i < j \le N} r_{ij}^2, \tag{6}$$

where $r_{ij} = \mathbf{R}_j - \mathbf{R}_i$, the vector from node i to node j.

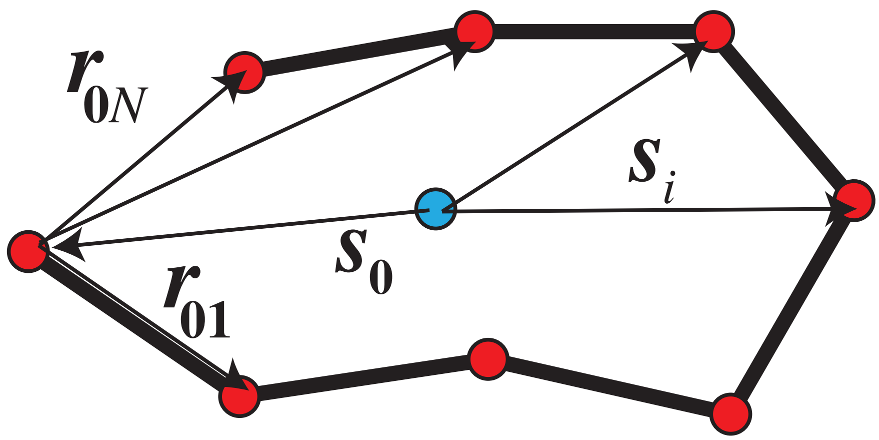

Figure 2: The gyration radius is an average distance with respect to the centre of mass of the system.

We can now compute the gyration radius for the freely jointed chain.

gyration radius for FJC

and we conclude that

$$< s^2 >= \frac{b^2}{6} N \frac{N+2}{N+1}. \tag{7}$$

For $N \to \infty$, we find (Debye, 1946)

$$< R^2 >= 6 < s^2 > . \tag{8}$$

The radius of gyration is an important notion as it can be measured by light scattering or sedimentation experiments.

1.1.3 With external force: force-extension behaviour

Next, we fix one end of the chain and apply a constant force $\mathbf{F} = F_z \mathbf{e}_z$ at the other end. We have the following assumptions

1) The chain is a FJC (with fixed bond length).
2) It is fixed at one end and under a constant force at the other end.
3) The chain is in an infinite heat bath.

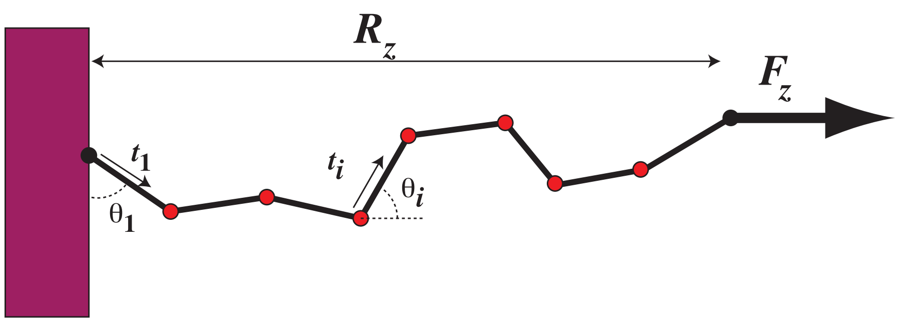

Figure 3: The freely jointed chain with external force. One end is fixed, the other one is pulled (both with free joints) with a constant force. The problem is now to find the distance along the force direction as a function of the force.

The question is then to find the force-displacement relationship that is $< R_z >$ as a function of F_z.

When the chain is pulled, the number of possible configurations decreases (to one when the chain is fully extended). Therefore, the entropy decreases and it takes energy to do so. The resistance of the chain to extend is an entropic response, hence the name of **entropic spring** for such structures that owe their mechanical response to entropy.

The work to extend the chain is $W = \mathbf{F} \cdot \mathbf{R}$ and therefore, which gives the total internal energy

$$E = -W = -\mathbf{F} \cdot \mathbf{R} = -F_z b \sum_{i=1}^{N} \cos\theta_i \tag{9}$$

where θ_i is the angle between $\mathbf{e}_z$ and $\mathbf{t}_i$.

The probability of finding the chain in a given orientation $\Theta = \{\theta_1, \theta_2, \ldots, \theta_N\}$ is given by the Boltzmann distribution for the canonical ensemble.

$$p(\Theta) = \frac{1}{\mathcal{Z}} e^{-\beta E(\Theta)} \tag{10}$$

where $\beta = (k_b T)^{-1}$, with k_b denoting Boltzmann's constant, and $\mathcal{Z}$ is the partition function

$$\mathcal{Z} = \int_{(S^2)^N} e^{-\beta E(\Theta)} dS := \int_{(S^2)^N} d\Omega_1 \ldots d\Omega_N \; e^{-\beta E(\Theta)} \tag{11}$$

where $(S^2)^N$ is the direct product of N spheres and $d\Omega_i = d\theta_i d\phi_i \sin\theta_i$ is the solid angle increment for the i^{th} sphere. Note that we integrate each θ from 0 to π and each angle φ from 0 to 2π.

The partition function: $\mathcal{Z} = z^N$

and we conclude that

$$\mathcal{Z} = z^N \quad \text{with} \quad z = 4\pi\frac{\sinh\alpha}{\alpha}. \tag{12}$$

where $\alpha = \beta b F_z$.

Now, we compute the average distance

$$< R_z >= \int_{(S^2)^N} p(\Theta) R_z dS. \tag{13}$$

The average distance

Finally, we have

$$< R_z >= bN \left[\coth(\alpha) - \frac{1}{\alpha} \right] \equiv bN\mathcal{L}(\alpha).$$

In the last expression, we have introduced the *Langevin function* $\mathcal{L}(\cdot)$. Note also that bN is the *contour length*, that is the maximal length of the chain.

For small forces

1.2 WLC: Worm-like chain models

The freely-jointed chain does not take into account that for short lengths, polymers are stiff. Therefore, we need to include the bending stiffness of the chain in order to penalise bending. We first consider the discrete model of Kratky and Porod (1949).

1.2.1 Without external force

We first consider the problem in the absence of an external force. We have the following assumptions.

1) The chain has $N+1$ links.

2) Each link has a fixed length b (b for bond length).

3) The internal energy to bend two links is proportional to the scalar product between their tangents.

4) There is no excluded volume effects.

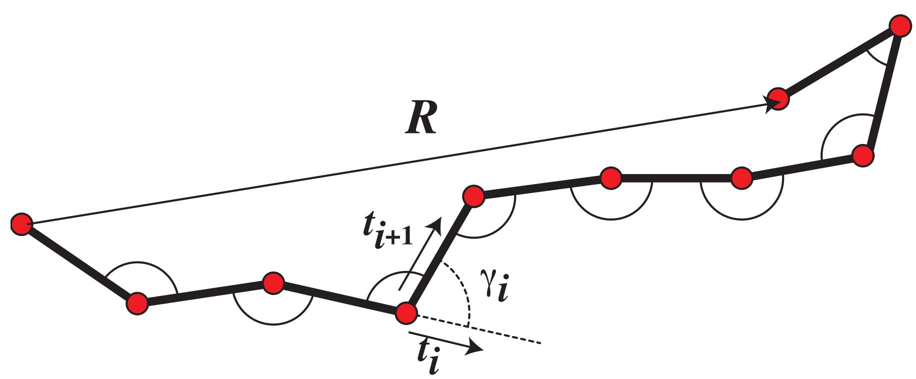

Figure 4: The worm-like chain model. We assume that the chain has a bending stiffness represented by a spring

That is, the internal energy is now

$$Q = -K \sum_{i=1}^{N} \mathbf{t}_i \cdot \mathbf{t}_{i+1} = -K \sum_{i=1}^{N} \cos \gamma_i \tag{14}$$

Note the similarity between this form of the internal energy and the the internal energy for the FJC with external force. Accordingly, following the same steps we have

$$\mathcal{Z} = z^N \quad \text{with} \quad z = 4\pi \frac{\sinh \lambda}{\lambda} \tag{15}$$

where $\lambda = \beta K$.

1.2.2 Persistence length

Next, we would like to compute the distance

$$< \mathbf{R}^2 >= b^2 < (\sum \mathbf{t}_i)^2 >= b^2 < \sum_{i,j} \mathbf{t}_i \cdot \mathbf{t}_j > . \tag{16}$$

We define the correlation between neighbours separated by n nodes as

$$\omega_n =< \mathbf{t}_i \cdot \mathbf{t}_{i+n} > . \tag{17}$$

We first evaluate the nearest neighbour correlation

Nearest neighbour correlation: $\omega =< \mathbf{t}_i \cdot \mathbf{t}_{i+1}) >$

and we conclude that

$$\omega_1 = \mathcal{L}(\lambda) \tag{18}$$

Second, we show that for stiff polymers, $\lambda \gg 1$

$\omega_n = \omega\omega_{n-1}$

$$\omega_n = \omega^{|n|} = [\mathcal{L}(\lambda)]^{|n|} . \tag{19}$$

Next, we consider the limit for stiff polymers.

For stiff polymers, $\lambda \gg 1$:

and we conclude

$$< \mathbf{t}_i \cdot \mathbf{t}_{i+n} > \sim \exp(-|n|\frac{b}{\xi_P}) \tag{20}$$

In the last expression we have defined a fundamental quantity for the mechanics of chains, the *persistence length*

$$\xi_P = \beta b K. \tag{21}$$

The persistence length is the characteristic length for which tangent-tangent correlations decay. If L is the contour length, we have the following possibilities

- $\xi_P \gg L$: The chain is very stiff.
- $\xi_P \ll L$: The chain is very flexible (low bending stiffness or high temperature, well captured by the FJC model).
- $\xi_P \approx L$: The chain is semi-flexible.

Examples from cellular filaments are given in Table 1.

Table 1: Persistence lengths and other parameters of various biopolymers (Howard 2001; Gittes *et al.* 1993).

Type	Approximate diameter	Persistence length	Contour length
DNA	2 nm	50 nm	$\lesssim$ 1 m
F-actin	7 nm	17 μm	$\lesssim$ 50 μm
Microtubule	25 nm	$\sim$ 1-5 mm	10s of μm

We can now return to the computation of the mean square end-to-end distance, $< \mathbf{R}^2 >$, given the polymer is sufficiently stiff, $\lambda \gg 1$.

Mean square of the end-to-end distance, $\lambda \gg 1$

and conclude that for large N, we have

$$< \mathbf{R}^2 > \approx b^2 \frac{1+\omega_1}{1-\omega_1} N \tag{22}$$

1.2.3 Continuous limit

We would like to relate the discrete problem to a continuous formulation of the curve and the energy. We know from classical elasticity that the elastic energy of an unshearable, inextensible beam is

$$\mathcal{E}_{el} = \frac{EI}{2} \int_0^L \kappa^2(s) ds \tag{23}$$

where κ is the *curvature*, s the *arc length* of the curve, E the *Young modulus* and I the *second moment of area* (for a circular cross-section of radius r it is given by $I = \pi r^4/4$). The product $B = EI$ is the *bending stiffness*, that is it takes a moment $M = B\kappa$ to bend a beam to a section of a ring of curvature κ. Note also that

$$|\kappa| = \left| \frac{\partial \mathbf{t}}{\partial s} \right| . \tag{24}$$

In comparing the elastic energy $\mathcal{E}_{el}$ of the continuous curve with the internal energy E of the worm-like chain we notice that the minimum of the discrete chain is at $E = -K$ whereas the minimum energy of the curve is at 0. Therefore, we shift the potential of the discrete chain so that the two minimum values of the energy coincide. That is, we define

$$U = E + E_0 = -K \sum_{i=1}^{N} (\mathbf{t}_i \cdot \mathbf{t}_{i+1} - 1)\,. \tag{25}$$

Next, we take the limit $N \to \infty$, $b \to 0$ while keeping the contour length Nb constant.

Continuous limit of the chain

So that we can identify $B = Kb$ and the persistence length is

$$\xi_P = B\beta = B/(k_b T), \tag{26}$$

The last expression can be used to define a bending stiffness for a semi-flexible filament as $B = \xi_P/\beta$.

For the continuous problem, we can write the Hamiltonian

$$H = \frac{B}{2} \int_0^L \left(\frac{\partial \mathbf{t}}{\partial s}\right)^2 ds, \tag{27}$$

for which we can write the (formal) partition function in terms of the functional integral

$$\mathcal{Z} = \int \mathcal{D}[\mathbf{t}(s)] e^{-\beta H[\mathbf{t}(s)]} \delta(|\mathbf{t}(s)| - 1). \tag{28}$$

A proper definition of this integral is out of the scope of these lectures. The interesting aspect of a continuous formulation is that we can compute the tangent-tangent correlation given by

$$< \mathbf{t}(s) \cdot \mathbf{t}(s') > \propto e^{-|s-s'|/\xi_P} \tag{29}$$

As an example, we compute in this context the end-to-end distance

End-to-end distance

and conclude that

$$< \mathbf{R}^2 >= L^2 f_D(L/\xi_P) \tag{30}$$

where $f_D(x) = 2x^{-2}(x - 1 + e^{-x})$ is the Debye function.

1.2.4 With external force: force-extension behaviour

Next, we can consider the WLC with external force. In the continuous case, this is described by the Hamiltonian

$$H = \frac{B}{2}\int_0^L \left(\frac{\partial \mathbf{t}}{\partial s}\right)^2 ds - \mathbf{F}\cdot\mathbf{R}. \tag{31}$$

Let $\mathbf{F} = F\mathbf{e}_z$, then we can write $R_z = \int_0^L \frac{\partial \mathbf{R}}{\partial s}\cdot\mathbf{e}_z$ so that we have

$$H = \int_0^L ds\left[\frac{B}{2}\left(\frac{\partial \mathbf{t}}{\partial s}\right)^2 - F\frac{\partial \mathbf{R}}{\partial s}\cdot\mathbf{e}_z\right]. \tag{32}$$

Assuming again a heat bath at constant temperature and fixing one end in space with a free hinge, the probability of finding the rod in a configuration with curve $\mathbf{R}(s)$ is given by the Boltzmann distribution

$$p[\mathbf{R}(s)] = \frac{1}{\mathcal{Z}}e^{-\beta H[\mathbf{R}(s)]}, \tag{33}$$

with partition function

$$\mathcal{Z} = \int \mathcal{D}[\mathbf{R}(s)]e^{-\beta H[\mathbf{R}(s)]}. \tag{34}$$

And, as before,

$$< R_z >= \beta^{-1}\frac{\partial \log \mathcal{Z}}{\partial F}. \tag{35}$$

However, this cannot be solved analytically in general.

The WLC approximate fit for the force-displacement curve is

$$F = \frac{k_b T}{\xi_P}\left[\frac{1}{4}\left(1 - \frac{< R_z >}{L}\right)^{-2} - \frac{1}{4} + \frac{< R_z >}{L}\right] \tag{36}$$

Note that beyond the entropic regime, DNA and other bio-filaments do not respond as a WLC (in the case of DNA, this behaviour is found for $F_z \lesssim 6$pN, from 6pN to about 7pN, DNA responds as an elastic filament (see next Section) and past 70pN, it enters into a rupture/melting of some of its internal structure and can change its configuration (from B-DNA to S-DNA).

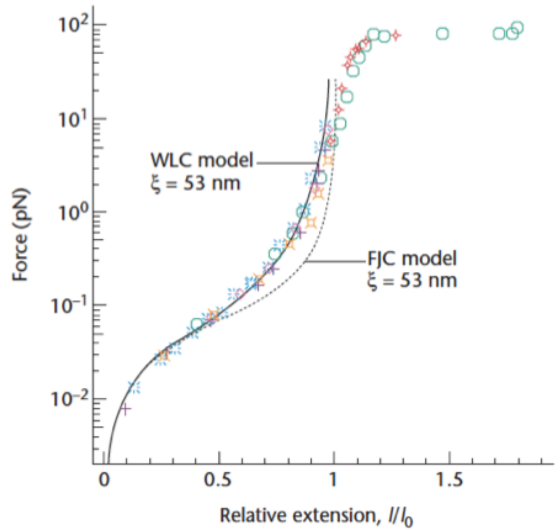

Figure 5: Comparison between experiments on DNA and the WLC/FJC models (from Strick et al. 1996 (doi: 10.1038/npg.els.00029), reproduced without permission)..

1.3 Continuous filaments

When stochastic motion can be ignored, that is when the elastic energy of the rod is much larger than the typical energy provided by the thermal bath $k_b T$ (low temperature, high bending stiffness, or large forces), a theory of elastic rods can be used to model many different behaviours of bio-filaments (coiling, super-coiling, twisting, buckling,....).

Here we develop a general theory of shearable, extensible, hyperelastic rods. Then, we consider the appropriate reductions that lead to reduced theories (inextensible rods, planar elastica, beam theory).

1.3.1 Frenet frame

We define a dynamical *space curve* $\mathbf{r}(S, T)$ as a smooth function of a material parameter S and the time T, *i.e.* $\mathbf{r} : \mathbb{R}^2 \to \mathbb{R}^3$. At any time t the arc length s is defined as

$$s = \int_0^S d\sigma \left| \frac{\partial \mathbf{r}(\sigma, T)}{\partial \sigma} \right|. \tag{37}$$

The unit tangent vector $\boldsymbol{\tau}$ to the space curve, $\mathbf{r}$, is

$$\boldsymbol{\tau} = \frac{\partial \mathbf{r}}{\partial s}, \tag{38}$$

and we can construct the standard *Frenet frame* (or *Frenet-Serret frame*) of tangent, $\boldsymbol{\tau}$, normal, $\boldsymbol{\nu}$, and binormal, $\boldsymbol{\beta}$, vectors which form a right-handed orthonormal basis on $\mathbf{r}$. Along the curve, this triad moves as a function of arc length according to the *Frenet equations*:

$$\frac{\partial \boldsymbol{\tau}}{\partial s} = \kappa\, \boldsymbol{\nu}, \tag{39}$$

$$\frac{\partial \boldsymbol{\nu}}{\partial s} = \tau\, \boldsymbol{\beta} - \kappa\, \boldsymbol{\tau}, \tag{40}$$

$$\frac{\partial \boldsymbol{\beta}}{\partial s} = -\tau\, \boldsymbol{\nu}. \tag{41}$$

where the *curvature*

$$\kappa = \left| \frac{\partial \boldsymbol{\tau}}{\partial s} \right|, \tag{42}$$

measures the turning rate of the tangent along the curve and is geometrically given by the inverse of the radius of the best fitting circle at a given point. The *torsion* τ measures the rotation of the Frenet triad around the tangent , $\boldsymbol{\tau}$ as a function of arc length and is related to the non-planarity of the curve. If the curvature and torsion are known for all s, the triad $(\boldsymbol{\nu}, \boldsymbol{\beta}, \boldsymbol{\tau})$ can be obtained as the unique solution of the Frenet-Serret equations up to a translation and rotation of the curve. The space curve $\mathbf{r}$ is obtained by integrating the tangent vector $\mathbf{t}$, using (38).

1.3.2 General frames

In order to study the motion of elastic filamentary structures that can sustain bending and stretching but also twisting and shearing, we need to generalise the notion of space curves to geometric rods. A *general frame* for a given curve is a frame (a set of three linearly independent vectors) defined at each point along the curve that is orthornormal.

A geometric *rod* is defined by its centerline $\mathbf{r}(S,T)$ where T is time and S is a material parameter taken to be the arc length in a stress free configuration $(0 \le S \le L)$ and two orthonormal vector fields $\mathbf{d}_1(S,T)$, $\mathbf{d}_2(S,T)$ representing the orientation of a material cross section at s. Together $\mathbf{d}_1(S,T)$, $\mathbf{d}_2(S,T)$ and the vector $\mathbf{d}_3(S,T) \equiv \mathbf{d}_1(S,T) \times \mathbf{d}_2(S,T)$ form a general frame. The

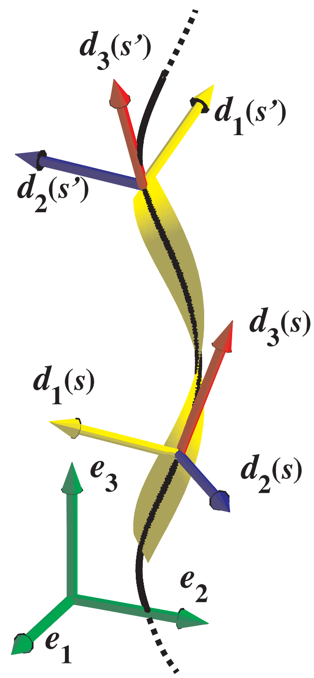

Figure 6: The director basis represents the evolution of a local basis along the rod.

components of a vector $\mathbf{a} = \mathsf{a}_1\mathbf{d_1} + \mathsf{a}_2\mathbf{d_2} + \mathsf{a}_3\mathbf{d_3}$ in the local basis are denoted by $\boldsymbol{\mathsf{a}} = (\mathsf{a}_1, \mathsf{a}_2, \mathsf{a}_3)$.[1] To understand the mathematical structure of the system, it is convenient to introduce a matrix describing the basis

$$\mathbf{D} = \begin{pmatrix} \mathbf{d}_1 & \mathbf{d}_2 & \mathbf{d}_3 \end{pmatrix}, \tag{43}$$

so that $\mathbf{a} = \mathbf{D}\boldsymbol{\mathsf{a}}$. We can now compute the derivative of the frame (w.r.t S or T)

[1]We use the $\mathsf{sans\text{-}serif\ fonts}$ to denote the components of a vector in the local basis.

Derivative of the frame

Thus there are antisymmetric matrices (the *twist matrix* $\mathbf{U}(S,T)$ and the *spin matrix* $\mathbf{W}(S,T)$) such that

$$\frac{\partial \mathbf{D}}{\partial S} \equiv \begin{pmatrix} \frac{\partial \mathbf{d}_1}{\partial S} & \frac{\partial \mathbf{d}_2}{\partial S} & \frac{\partial \mathbf{d}_3}{\partial S} \end{pmatrix} = \mathbf{DU}, \tag{44}$$

$$\frac{\partial \mathbf{D}}{\partial T} \equiv \begin{pmatrix} \frac{\partial \mathbf{d}_1}{\partial T} & \frac{\partial \mathbf{d}_2}{\partial t} & \frac{\partial \mathbf{d}_3}{\partial T} \end{pmatrix} = \mathbf{DW}. \tag{45}$$

The entries of $\mathbf{U}$ and $\mathbf{W}$ are not independent. By differentiating (44) with respect to time and (45) with respect to arc length and then equating their cross-derivatives, we obtain a compatibility relation

Compatibility relations

So that

$$\frac{\partial \mathbf{U}}{\partial T} - \frac{\partial \mathbf{W}}{\partial S} = [\mathbf{U}, \mathbf{W}]\,, \tag{46}$$

where $[\mathbf{U}, \mathbf{W}] = \mathbf{U}\mathbf{W} - \mathbf{W}\mathbf{U}$.

These matrices are associated with the axial vectors u and w respectively,

$$\mathbf{U} = \begin{pmatrix} 0 & -\mathsf{u}_3 & \mathsf{u}_2 \\ \mathsf{u}_3 & 0 & -\mathsf{u}_1 \\ -\mathsf{u}_2 & \mathsf{u}_1 & 0 \end{pmatrix}, \quad \mathbf{W} = \begin{pmatrix} 0 & -\mathsf{w}_3 & \mathsf{w}_2 \\ \mathsf{w}_3 & 0 & -\mathsf{w}_1 \\ -\mathsf{w}_2 & \mathsf{w}_1 & 0 \end{pmatrix}. \tag{47}$$

Alternative formulation

So that a complete kinematic description is given by:

$$\frac{\partial \mathbf{r}}{\partial S} = \mathbf{v}, \tag{48}$$

$$\frac{\partial \mathbf{d}_i}{\partial S} = \mathbf{u} \times \mathbf{d}_i, \qquad i = 1, 2, 3, \tag{49}$$

$$\frac{\partial \mathbf{d}_i}{\partial T} = \mathbf{w} \times \mathbf{d}_i \qquad i = 1, 2, 3, \tag{50}$$

where $\mathbf{u}$, $\mathbf{v}$ are the *strain* vectors and $\mathbf{w}$ is the *spin* vector. The orthonormal frame $(\mathbf{d_1}, \mathbf{d_2}, \mathbf{d_3})$ is different from the Frenet-Serret frame (normal,binormal,tangent)=$(\boldsymbol{\nu}, \boldsymbol{\beta}, \boldsymbol{\tau})$. We define the *stretch* by $\alpha = \frac{\partial s}{\partial S}$. The two first components $\mathsf{v}_1, \mathsf{v}_2$ of the *stretch vector* $\mathbf{v}$ represent transverse shearing of the cross-sections while $\mathsf{v}_3 > 0$ is associated with stretching and compression. Since the vectors $\mathbf{d}_i$ are normalized, the norm of $\mathbf{v}$ gives the stretch of the rod during deformation: $\alpha = |\mathbf{v}| = |\boldsymbol{\mathsf{v}}|$. The two first components of the *Darboux vector* are associated with bending while u_3 represents twisting, that is the rotation of the basis (not the curve) around the $\mathbf{d}_3$ vector. To understand the mathematical structure of the system, it is convenient to introduce a matrix describing the basis

$$\mathbf{D} = \begin{pmatrix} \mathbf{d}_1 & \mathbf{d}_2 & \mathbf{d}_3 \end{pmatrix}, \tag{51}$$

so that $\mathbf{a} = \mathbf{D}\boldsymbol{\mathsf{a}}$.

1.3.2.1 The case of inextensible, unshearable rods A particularly important class of rods is obtained by taking $\mathsf{v}_1 = \mathsf{v}_2 = 0,\ \mathsf{v}_3 = 1$. In this case there is no stretch, $s = S$ and $\alpha = 1$, and the possible deformations of rods are restricted so that the vectors spanning the cross sections remain perpendicular to the tangent axis. It will be the geometric constraint used to characterise rods which are both unshearable and inextensible (here we just call *inextensible rods* those rods that are both inextensible and unshearable). Geometrically, the vectors $(\mathbf{d_1}, \mathbf{d_2})$ lie in the normal plane to the tangent axis and are related to the normal and binormal vectors by a rotation through the *register angle* φ,

$$\mathbf{d}_1 = \boldsymbol{\nu}\cos\varphi + \boldsymbol{\beta}\sin\varphi, \tag{52}$$
$$\mathbf{d}_2 = -\boldsymbol{\nu}\sin\varphi + \boldsymbol{\beta}\cos\varphi. \tag{53}$$

This rotation implies that

$$\mathsf{u} = (\kappa\sin\varphi, \kappa\cos\varphi, \tau + \frac{\partial\varphi}{\partial S}) \tag{54}$$

where κ and τ are the usual *Frenet curvature and torsion.* These relations can also be inverted to yield φ, κ and τ as functions of the twist vector components:

$$\cot\varphi = \frac{\mathsf{u}_2}{\mathsf{u}_1}, \tag{55}$$
$$\kappa = \sqrt{\mathsf{u}_1^2 + \mathsf{u}_2^2}, \tag{56}$$
$$\tau = \mathsf{u}_3 + \frac{\mathsf{u}_2'\mathsf{u}_1 - \mathsf{u}_1'\mathsf{u}_2}{\mathsf{u}_1^2 + \mathsf{u}_2^2}. \tag{57}$$

The quantities τ, $\frac{\partial\varphi}{\partial S}$ and u_3 play related but distinct roles. The torsion τ is a property of the curve alone and is a measure of its non-planarity. Hence a curve with null torsion is a plane curve, and any two rods having the same curvature and torsion for all s and t have the same space curve $\mathbf{r}$ as axis, and can only be distinguished by the orientation of the local basis. The quantity $\frac{\partial\varphi}{\partial S}$, *the excess twist*, is a property that is independent of the centreline. It represents the rotation of the local basis with respect to the Frenet frame as the arc length increases. An untwisted rod, characterized by $\frac{\partial\varphi}{\partial S} = 0$ is therefore called a *Frenet rod.* In a Frenet rod, the angle φ between the binormal $\mathbf{b}$ and the vector field $\mathbf{d}_2$ is constant, hence the binormal is representative of the orientation of the local basis $(\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3)$. The twist density, u_3, is a property of both the space curve and the rod, measuring the total rotation (as can be seen from the third component of (54)) of the local basis around the space curve as the arc length increases.

1.3.3 The mechanics of Kirchhoff rods

The stress acting on the cross section at $\mathbf{r}(S)$ from the part of the rod with $S' > S$ gives rise to a resultant force $\mathbf{n}(S,T)$ and resultant moment $\mathbf{m}(S,T)$ attached to the central curve. By applying the balance of linear and angular momenta one obtains

$$\frac{\partial\mathbf{n}}{\partial S} + \mathbf{f} = \rho A \frac{\partial^2\mathbf{r}}{\partial T^2}, \tag{58}$$
$$\frac{\partial\mathbf{m}}{\partial S} + \frac{\partial\mathbf{r}}{\partial S} \times \mathbf{n} + \mathbf{l} = \rho\left(I_2\mathbf{d_1} \times \frac{\partial^2\mathbf{d}_1}{\partial T^2} + I_1\mathbf{d_2} \times \frac{\partial^2\mathbf{d}_2}{\partial T^2}\right), \tag{59}$$

where $\mathbf{f}(S,T)$ and $\mathbf{l}(S,T)$ are the body force and couple per unit reference length applied on the cross section at S. These body forces and couple can be used to model different effects such as short and long range interactions between different parts of the rod or can be the result of active stress, self-contact, or contact with another body. $A(S)$ is the cross-section area (in the reference frame), $\rho(S)$ the mass density (mass per unit reference volume), and $I_{1,2}(S)$ are the second moments of area of the cross section corresponding to the directions $\mathbf{d}_{1,2}$ at a material point S. Explicitly, they read

$$I_1 = \int_{\mathcal{S}} x_2^2 \; dx_1 dx_2 \;, \quad I_2 = \int_{\mathcal{S}} x_1^2 \; dx_1 dx_2. \tag{60}$$

where $\mathcal{S}$ is the section at point S and a point on this section is given by a pair $\{x_1, x_2\}$ and located at $\mathbf{r}(S) + x_1\mathbf{d}_1(S) + x_2\mathbf{d}_2(S)$.

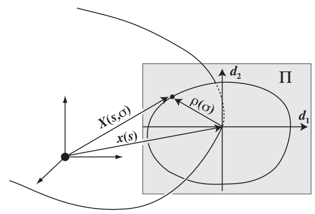

Figure 7: Cross-section of a rod and local coordinates

To close the system, we assume that the resultant stresses are related to the strains.

1.3.4 Constitutive laws

1.3.4.1 Extensible and shearable rods First, we consider the case where the rod is extensible and shearable and we assume that the rod is hyperelastic. That is, we assume that there exists a strain-energy density function $W = W(\mathsf{y}, \mathsf{z}, s)$ such that the constitutive relations for the resultant moment and force in the local basis are given by

$$\mathsf{m} = \mathsf{f}(\mathsf{u} - \hat{\mathsf{u}}, \mathsf{v} - \hat{\mathsf{v}}, S) = \partial_{\mathsf{y}} W(\mathsf{u} - \hat{\mathsf{u}}, \mathsf{v} - \hat{\mathsf{v}}, S), \tag{61}$$

$$\mathsf{n} = \mathsf{g}(\mathsf{u} - \hat{\mathsf{u}}, \mathsf{v} - \hat{\mathsf{v}}, S) = \partial_{\mathsf{z}} W(\mathsf{u} - \hat{\mathsf{u}}, \mathsf{v} - \hat{\mathsf{v}}, S), \tag{62}$$

where $\hat{\mathsf{v}}$, $\hat{\mathsf{u}}$ are the strains in the unstressed reference configuration ($\mathsf{m} = \mathsf{n} = \mathbf{0}$ when $\mathsf{u} = \hat{\mathsf{u}}$, $\mathsf{v} = \hat{\mathsf{v}}$). Without loss of generality, one can choose the general basis so that $\hat{\mathsf{v}}_1 = \hat{\mathsf{v}}_2 = 0$. Furthermore, if S is the arc length of the unstressed configuration then $\hat{\mathsf{v}}_3 = 1$. Typically, W is assumed to be continuously differentiable, convex, and coercive. The rod is *uniform* if its material properties do not change along its length (*i.e.* W has no explicit dependence on s) and the stress-free strains $\hat{\mathsf{v}}$, $\hat{\mathsf{u}}$ are independent of s.

1.3.4.2 Inextensible rods In the second case, we assume that the rod is inextensible and unshearable, that is we take $\mathbf{v} = \mathbf{d}_3$ and the material parameter $S = s$ becomes the arc length. In that case, there is no constitutive relationship for the resultant force and the strain-energy density is a function only of $(\mathsf{u} - \hat{\mathsf{u}})$, that is

$$\mathsf{m} = \partial_{\mathsf{y}} W(\mathsf{u} - \hat{\mathsf{u}}) = \mathsf{f}(\mathsf{u} - \hat{\mathsf{u}}). \tag{63}$$

For a quadratic strain energy $W = \mathsf{y}^{\mathrm{T}}\mathbf{K}\mathsf{y}$, the constitutive relations for the local basis components m are

$$\mathsf{m} = \mathbf{K}(\mathsf{u} - \hat{\mathsf{u}}), \quad \mathbf{K} = \begin{pmatrix} K_1 & K_{12} & K_{13} \\ K_{12} & K_2 & K_{23} \\ K_{13} & K_{23} & K_3 \end{pmatrix}, \; K_1 \leq K_2. \tag{64}$$

Note that, in general, due to the arbitrary phase in the definition of the general basis, one can choose the vector $\mathbf{d}_1$ so that either $K_{12} = K_{21} \equiv 0$ or $\hat{u}_1 \equiv 0$ or $\hat{u}_2 \equiv 0$. In the simplest, and most widely used, case the energy is further simplified to

$$W_1 = K_1(\mathsf{u}_1 - \hat{\mathsf{u}}_1)^2 + K_2(\mathsf{u}_2 - \hat{\mathsf{u}}_2)^2 + K_3(\mathsf{u}_3 - \hat{\mathsf{u}}_3)^2, \tag{65}$$

where $\hat{\mathbf{u}}$ is the unstressed Darboux vector that defines the shape of the rod when unloaded. At this point of our discussion, we do not have the tools that would allow us to express these coefficients in terms of other material properties of the materials (geometry, Young's modulus,...). These relations come from the analysis of bending and twisting of cylinders in the general 3D theory of linear elasticity. The resultant moment and coefficients $\{K_1, K_2, K_3\}$ are

$$\mathbf{m} = EI_1(\mathsf{u}_1 - \hat{\mathsf{u}}_1)\mathbf{d}_1 + EI_2(\mathsf{u}_2 - \hat{\mathsf{u}}_2)\mathbf{d}_2 + \mu J(\mathsf{u}_3 - \hat{\mathsf{u}}_3)\mathbf{d}_3 \tag{66}$$

where E is the Young's modulus, μ is the shear modulus, J is a parameter that depends on the cross-section shape and and I_1 and I_2 are the second moments of area given by (60).

For a rod with uniform circular cross section of radius R, these parameters are:

$$I_1 = I_2 = \frac{J}{2} = \frac{\pi R^4}{4}. \tag{67}$$

The products $EI_1 \equiv K_1$ and $EI_2 \equiv K_2$ are the *principal bending stiffnesses* of the rod, and $\mu J \equiv K_3$ is the *torsional stiffness*.

1.3.5 The basic Kirchhoff rods

The most commonly used model of rod is obtained by assuming that the rod is unshearable, inextensible as detailed in Section 1.3.4.2 with a circular cross-section ($I_1 = I_2 = I$). In this case, we have the following set of equations provided by

1) Kinematics

$$\mathbf{r}' = \mathbf{d}_3 \tag{68}$$
$$\frac{\partial \mathbf{D}}{\partial s} = \mathbf{DU}, \tag{69}$$
$$\frac{\partial \mathbf{D}}{\partial t} = \mathbf{DW}. \tag{70}$$

2) Mechanics

$$\frac{\partial \mathbf{n}}{\partial s} + \mathbf{f} = \rho A \frac{\partial^2 \mathbf{r}}{\partial t^2}, \tag{71}$$
$$\frac{\partial \mathbf{m}}{\partial s} + \frac{\partial \mathbf{r}}{\partial s} \times \mathbf{n} + \mathbf{l} = \rho I \left(\mathbf{d_1} \times \frac{\partial^2 \mathbf{d}_1}{\partial t^2} + \mathbf{d_2} \times \frac{\partial^2 \mathbf{d}_2}{\partial t^2} \right), \tag{72}$$

3) Constitutive theory

$$\mathbf{m} = EI\left[\mathsf{u}_1\mathbf{d}_1 + (\mathsf{u}_2 - \hat{\mathsf{u}}_2)\mathbf{d}_2\right] + \mu J(\mathsf{u}_3 - \hat{\mathsf{u}}_3)\mathbf{d}_3, \qquad I = \frac{J}{2} = \frac{\pi R^4}{4}. \tag{73}$$

A few comments are in order

1) The material is described by its response through two bending and twisting stiffnesses EI and μJ, its density ρ and by its geometry (radius R, stress-free curvature $\hat{\mathsf{u}}_2$ and twist $\hat{\mathsf{u}}_3$, length L).

2) One can always choose the orientation of the director basis so that $\hat{\mathsf{u}}_1 \equiv 0$.

3) The system is characterised by three coordinates $\mathbf{r}$, three curvatures $\mathbf{u}$, three spins $\mathbf{w}$, three resultant forces $\mathbf{n}$, and three resultant moments $\mathbf{m}$. That is, 15 variables. The last 3 sets of equations provide 9 equations. The first one provide another 3. The second and third equations provide only three independent relationships. They are really both a set of 9 equations for the elements of $\mathbf{D}$ but written in a suitable set of coordinates, say the Euler angles, they provide only each three independent relationships. Further, these two sets are not independent as they are connected to each other by the compatibility condition (46).

4) One of the practical problems of rod theory is that the mechanical balance is easily written in terms of an external basis, whereas the constitutive law is written in the local basis.

5) In a given problem, one can usually solve the equations in components of either the local basis or an external fixed basis, then compute the curvatures, then integrate the curvatures to obtain the local basis and the shape of the rod. Doing so, one can often decouple the problem into problems of smaller dimensions.

6) The body force $\mathbf{f}$ and body couple $\mathbf{l}$ are given based on the physics of the problem (gravity, magnetic forces, electrical forces, self-contact,...). Body couples can also occur, for instance for the effect of internal molecular motors on motile filaments such as cilia and flagella.

7) The rotary inertia term (R.H.S. of (72)) is often ignored based on a discussion and analysis of typical time scales.

8) A rod is said to be *initially straight* if the unstressed curvatures vanish identically $\hat{\mathbf{u}} = \mathbf{0}$.

1.3.6 The Planar elastica: Bernoulli-Euler equations

We now consider a reduction of the three-dimensional basic rod above. We assume that the rod is planar, unshearable and inextensible, has a circular cross-section, is naturally straight and that there is no body force or couple. Therefore, it has no torsion. We further assume that it has no twist, so that

$$\mathbf{u} = (0, \kappa, 0). \tag{74}$$

A convenient representation of the rod is obtained by assuming that it lies in the $x-y$ plane and introducing the angle θ between the tangent vector and the x-axis. That is

$$\boldsymbol{\tau} = \mathbf{d}_3 = \cos\theta \mathbf{e}_x + \sin\theta \mathbf{e}_y, \tag{75}$$

Reduction

So that

$$F' = \rho A\ddot{x} \tag{76}$$
$$G' = \rho A\ddot{y} \tag{77}$$
$$EI\theta'' + G\cos\theta - F\sin\theta = \rho I\ddot{\theta} \tag{78}$$

This is now a set of three equations for three unknowns.

1.3.6.1 Static solutions We first consider the static case. Therefore $\ddot{x} = \ddot{y} = 0$ and $\ddot{\theta} = 0$ and we conclude that F and G are constant and therefore $\mathbf{n}$ is a constant vector. WLOG, we choose $\mathbf{e}_x$ to be along this constant force so that $G = 0$ and

$$EI\theta'' - F\sin\theta = 0 \tag{79}$$

or

$$\theta'' + \alpha^2\sin\theta = 0 \tag{80}$$

where $\alpha^2 = -F/EI$ is positive if $F < 0$, that is if the force is compressive. We recognise at this point the equation for the pendulum (in which $\alpha^2 = g/l$, gravity acceleration divided by length of the bob). Therefore, any solution of the pendulum in time is a solution of the elastica in space (with appropriate boundary value), a fact already known by Euler (see Fig.8).

Rather than writing the general solution for the problem (in terms of elliptic functions), we can look at appropriate limits. For instance, we can look at the simple case where the rod is compressed and pinned-pinned (see Fig.9) so that there is no curvature at either ends.

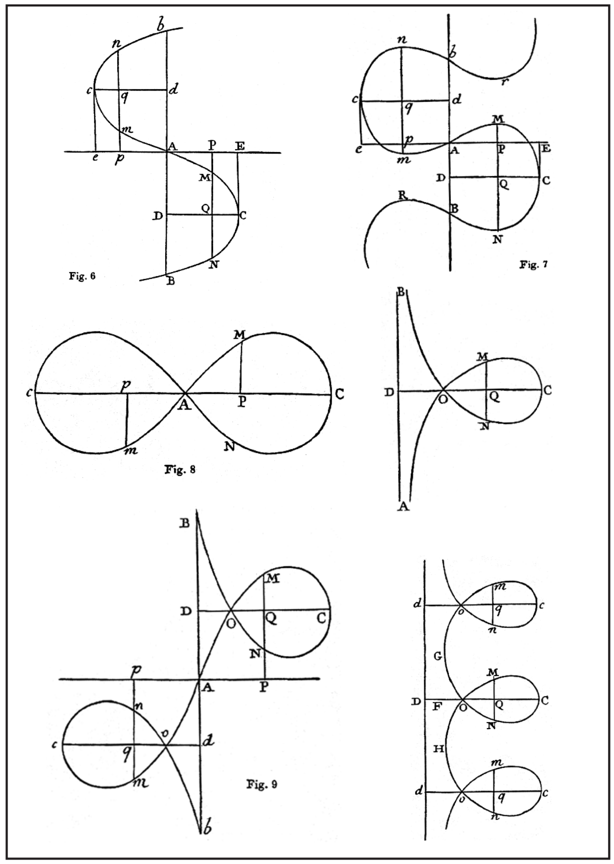

Figure 8: Euler's Drawing of spatial equilibria of the elastica.

Buckling problem

That is, the critical buckling force is

$$F_c = EI\frac{n^2\pi^2}{L^2} \tag{81}$$

For $n = 1$, we recognise the classical Euler buckling criterion, a fundamental concept in many scientific fields.

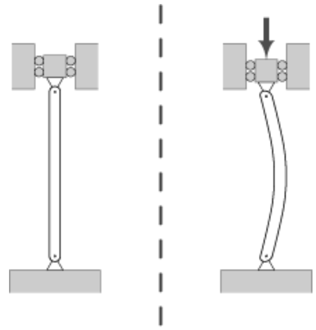

Figure 9: Buckling of a planar compressed pinned-pinned rod.

1.3.7 From elastica to beams

We consider again the elastica

$$EI\theta'' + G\cos\theta - F\sin\theta = \rho I\ddot{\theta} \tag{82}$$

and assume that θ is small so that there is only a small deflection $x \sim s$ and the curve can be written $y = w(x)$ with

$$w'(x) = \theta \tag{83}$$

so that, to first order, we have

$$EIw''' + G - Fw' = \rho I\ddot{w}' \tag{84}$$

an extra x-derivative leads to

$$EIw'''' + \rho A\ddot{w} - Fw'' = \rho I\ddot{w}'' \tag{85}$$

In the static case, we have the classical beam equation

$$EIw'''' - Fw'' = 0 \tag{86}$$

Note that the beam equation that we have derived is slightly different from the classical Timoshenko beam equation obtained under a different asymptotic limit and reads

$$EIw'''' + \rho A\ddot{w} - Fw'' + \rho g = 0 \tag{87}$$

the ρg term is just the added effect of a body force due to gravity (in the y-direction). The difference is in the extra time-derivative that depends on the rotary inertia of the cross-sections (which can be ignored in many applications).

2 Problems

Problems marked with a star* are meant to challenge you beyond the regular course. It is up to you to decide if you want to try them. You will not be marked down for not answering them or for any mistake. I suggest that you give them a try and think about these problems as a way to gain a deeper understanding of the material.

1) **Lagrange's theorem.** Prove Lagrange's theorem on the gyration radius

$$s^2 = \frac{1}{(N+1)^2} \sum_{0 \le i \le j \le N} \mathbf{r}_{ij}^2. \tag{88}$$

2) **The freely rotating chain.** Consider a chain with N links with constant bond length b and bond angle θ. Since we are considering a chain in 3D, each bond is free to rotate. This is different from the FJC as the correlations between orientations are imposed so that the projection of $\mathbf{r}_{i+1}$ on $\mathbf{r}_i$ is $b\cos\theta$. First show that $< \mathbf{r}_i \cdot \mathbf{r}_{i+n} >= b^2 \cos^n \theta$ and use this fact to compute the average end-to-end distance $< R^2 >_N$ and show that in the limit $N \to \infty$ one obtains

$$< R^2 >_\infty = N b_{\text{eff}}^2 \tag{89}$$

with an *effective bond length* $b_{\text{eff}}^2 = b^2 \frac{1+\cos\theta}{1-\cos\theta}$. Compute the gyration radius and show that for large N one recovers the result of Debye given in Eq. (8).

3) **Estimates for bio-filaments**

   (a) Using the radius of DNA, actin filaments and microtubules given in Table 1, determine the areal moment of inertia I for each of these molecules. Be careful and remember that microtubules are hollow and recompute the general form of I for a tube (take a thickness of microtubules of 2nm).

   (b) Given that the elastic modulus of actin is 2.3 GPa, take as your working hypothesis that E is universal for the macromolecules of interest here and has a value 2 GPa. In light of this choice of modulus, compute the stress needed to stretch both actin and DNA with a strain of 1%. Convert this result into a pulling force in piconewtons.

   (c) Using the results above, compute the persistence lengths of all three of these molecules and compare them with the results from Table 1. In particular given that the measured persistence length of DNA is 50 nm, how well does the estimate agree with the 2GPa rule of thumb from above?

4) **Computing average displacements.** Consider a system described by the canonical ensemble with total energy

$$Q = U - W \tag{90}$$

where U is the internal energy and the work W is given as product of work conjugate variable $W = \boldsymbol{\xi}.\mathbf{X}$, (think of $\mathbf{X}$ as a generalised force and $\boldsymbol{\xi}$ as a generalised displacement). Introduce the free energy $\mathcal{E} = -\beta^{-1}\log(\mathcal{Z})$ where $\mathcal{Z}$ is the partition function and show that the relationship

$$< R_z >= -\frac{\partial \mathcal{E}}{\partial F_z}. \tag{91}$$

can be generalised to

$$< \boldsymbol{\xi} >= -\frac{\partial \mathcal{E}}{\partial \mathbf{X}}. \tag{92}$$

5) **Radius of Gyration of the Worm-like Chain model.**

(a) Assuming large stiffness $K\beta \gg 1$ and that the number of links, N, satisfies $N \gg 1$, find the radius of gyration of the worm-like chain model, accurate to $O(1)$ in N, i.e. terms scaling like $1/N$ or smaller can be neglected.

(b) Highlight how the statistics of a Worm like chain model with link-length, b, is similar to a freely jointed chain model with a link length of

$$b\sqrt{\frac{1+\mathcal{L}(K\beta)}{1-\mathcal{L}(K\beta)}}.$$

6) Derive the momentum balance equations for constant density ρ,

$$\frac{\partial \mathbf{m}}{\partial S} + \frac{\partial \mathbf{r}}{\partial S} \times \mathbf{n} + \mathbf{l} = \rho \left(I_2 \mathbf{d_1} \times \frac{\partial^2 \mathbf{d}_1}{\partial T^2} + I_1 \mathbf{d_2} \times \frac{\partial^2 \mathbf{d}_2}{\partial T^2} \right),$$

where I_1 and I_2 should be found and any further assumptions stated.

7) Write the static (i.e. time independent) Kirchhoff equations given (71) in the local basis in the absence of stress free curtvature and twist (so that $\widehat{u}_2$, $\widehat{u}_3$ are zero in (71) et. seq.). That is, obtain a compact set of equations for the variables **n** and **m**.

8) **Axon injury.** During injury, an axon can be extended and deformed so that it buckles. The axon lies inside a tissue. As a simple model of this process, we model the axon as a beam on a foundation subject to an axial force. The equation for deflection $W = W(x)$ of a beam on a Winkler foundation (see Equations (86 with $B = EI$, $F = -P$ and an extra kW term for the foundation pulling the beam down the foundation) is given by

$$BW'''' + PW'' + kW = 0. \tag{93}$$

We will further assume that the beam is clamped at $x = \pm L$, that is $W(\pm L) = W'(\pm L) = 0$. First non-dimensionalise the equation so that it reads

$$w'''' + \lambda w'' + \beta w = 0, \tag{94}$$

and study its solution by looking at solution of the form $w = e^{i\omega x}$. Show that for clamped boundary condition, the only case of interest occurs for $\lambda^2 - 4\beta > 0$ in which case the solution reads

$$w = A\cos(\omega_+ x) + B\cos(\omega_+ x) + C\sin(\omega_- x) + D\sin(\omega_- x). \tag{95}$$

Find the conditions for which a non-trivial solution occurs and test your solution with the physiological values $B = 6 \times 10^{-19}\text{Nm}^2$, $k = 12\text{Nm}^{-2}$ and $L = 15\mu\text{m}$. Compare your solution to the profile of Fig. 2 and Fig. 3 of the paper [Min D. Tang-Schomer, Ankur R. Patel, Peter W. Baas, and Douglas H. Smith. *Mechanical breaking of microtubules in axons during dynamic stretch injury underlies delayed elasticity, microtubule disassembly, and axon degeneration.* The FASEB Journal, 24(5):1401–1410, 2010.]

9) **From 3D to 2D.** Starting with the exact equation of a general rod in the plane given by

$$F' + f = \rho A\ddot{x}, \tag{96}$$
$$G' + g = \rho A\ddot{y}, \tag{97}$$
$$EI\theta'' + G\cos\theta - F\sin\theta = \rho I\ddot{\theta}. \tag{98}$$

Derive a general equation for the beam. Essentially all you need to do is to complete and generalise the argument given in Section 1.3.7 by expanding the equation for small $\theta = \epsilon\varphi$. The result is an equation of 4th order for $w = w(x)$. Could you also specify what boundary conditions should be chosen in the case of a clamped-clamped beam (where the tangent are held horizontal) and a pinned beam (where the position of rod at the end is fixed but the there is no moment applied at the boundary)?

10) **Twisting and pulling DNA.** Single-molecule tweezer experiments have revealed many fascinating behaviors, some of which have been reported as counterintuitive. For instance, two different groups (J. Gore, Z. Bryant, M. Nollmann, M. Le, N. Cozzarelli, and C. Bustamante, *DNA overwinds when stretched* Nature 442, 836 (2006) and T. Lionnet, S. Joubaud, R. Lavery, D. Bensimon, and V. Croquette, *Wringing out DNA* Phys. Rev. Lett. 96, 178102 (2006)) measured the twist response of single-molecules of DNA when pulled by optical tweezers. In these beautiful experiments a bead attached to the DNA is pulled by optical tweezers and the angular displacement is controlled via an applied torque. The experimental observations are that the DNA overwinds when pulled, and extends when overwound. Both groups describe these behaviors as surprising: "simple intuition suggests that DNA should unwind under tension" [Gore et al] and "DNA should lengthen as it is unwound" [Lionnet et al]. The goal of this problem is to show that contrarily to the authors' assertions, the experimentally observed microscopic response is not particular to DNA, and, is in fact generic for most macroscopic helical elastic filaments.

(a) First, we consider the argument used in these papers. If helical DNA is modelle by an elastic cylinder which remains cylindrical while stretched and twisted (and assumes that fluctuations can be neglected), then the simplest elastic energy associated with deformations from the unstressed reference state (i.e. only stretching and twisting along the axis are allowed) is

$$\mathrm{E} = \frac{1}{2}(A\theta^2 + 2B\theta z + Cz^2) \tag{99}$$

where $z = (L_1 - L_0)/L_0$ is the axial stretch (L_0, L_1 being the initial and observed contour lengths), and θ is the rotational displacement of the end. Show that the requirement that the energy be positive definite ($A > 0$, $C > 0$, $AC - B^2 > 0$) implies that a pure tension extends the spring and a pure axial torque twists the spring in the same direction, as expected. Show that during extension (with no moment at the end), the cylinder will rotate depending on the sign of B.

(b) Now consider a finer model of DNA represented as a static uniform helical unshearable inextensible rod with constant intrinsic curvature and constant intrinsic torsion (as detailed by the static version of the equations given in Section 1.3.5). Choose $\hat{\mathsf{u}}_1 = 0$, in which case $\hat{\mathsf{u}}_2 = \hat{\kappa}$ is the intrinsic curvature and $\hat{\mathsf{u}}_3 = \hat{\tau}$ is the intrinsic torsion. A

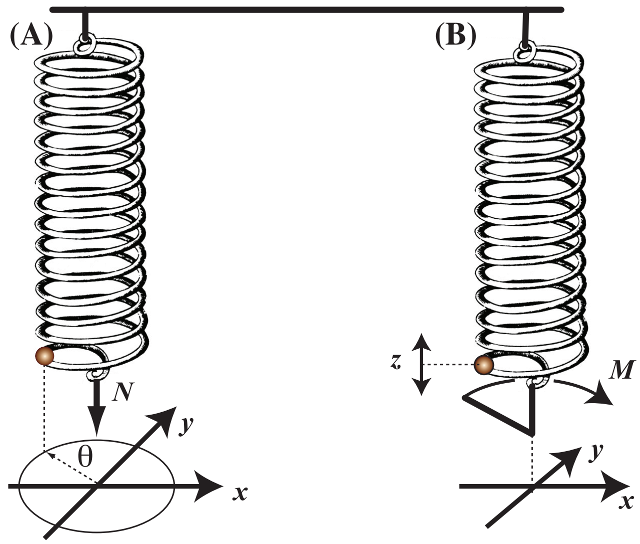

Figure 10: A wrench applied to a helical spring gives rise to another helical equilibrium. Two simple questions are to determine: (A) the sign of the increment of the rotation angle θ when an axial tension is applied with no torque, and (B) whether a spring extends or contracts as a result of a axial torque loading with no applied force. Drawings adapted from those of Robert Hooke's 1678 Lectures De Potentia Restitutiva

wrench is a prescribed axial torque and axial force both applied along the axis $\mathbf{e}_z$ of the helical spring, that is $\mathbf{m} \equiv M\mathbf{e}$ and $\mathbf{n} \equiv N\mathbf{e}$ are the only stresses acting on the rod. Show that under a constant wrench the rod remains cylindrical and

$$M = \epsilon \left[K_1\kappa(\kappa - \hat{\kappa}) + K_3\tau(\tau - \hat{\tau})\right] / \sqrt{\kappa^2 + \tau^2}, \tag{100}$$

$$N = \epsilon\sqrt{\kappa^2 + \tau^2} \left[K_3\kappa(\tau - \hat{\tau}) - K_1\tau(\kappa - \hat{\kappa})\right]/\kappa \tag{101}$$

where $\mathsf{u}_2 = \kappa$, $\mathsf{u}_3 = \tau$, and $\epsilon = \pm 1$ if the spring is right or left-handed. Find the constant K_i.

(c) The first experiment described in the aforementioned papers consists in applying a pure axial force, that is $M = 0$ Show that in such case, all equilibria lie in the curvature-torsion plane on an ellipse centered at the origin and passing by the point of intrinsic curvature

$$\kappa(\kappa - \hat{\kappa}) + \Gamma\tau(\tau - \hat{\tau}) = 0. \tag{102}$$

Based on the geometry of this ellipse consider the possible shapes of the helix.

(d) We define the *coiling angle per unit arc length* to be $\rho^2 = \kappa^2 + \tau^2$, so that in the unstressed state $\hat{\rho}^2 = \hat{\kappa}^2 + \hat{\tau}^2$. Close to the unstressed state, we can then introduce the axial stretch $z = \tau/\rho - \hat{\tau}/\hat{\rho}$ and rotation angle $\theta = \rho - \hat{\rho}$. Expand to first order z and θ as a function of N

$$z = Nz_1 + \mathrm{O}(N^2), \tag{103}$$

$$\theta = N\theta_1 + \mathrm{O}(N^2), \tag{104}$$

and use this to show that a helix will initially overwind when pulled from its minimum energy state if and only if $\Gamma < 1$. (We remark that if the filament is formed from a three-dimensional homogeneous linearly elastic material with Poisson ratio in [0,1/2], e.g.

standard metals, then $\Gamma \in [2/3, 1]$), and conclude that initial over-winding in response to positive tension always arises for simple helical springs, a slightly surprising but yet completely classic effect in contradiction with the statements in the two papers.

(e) Plot the graph of θ as a function of N and show that it has a maximum. That is, initially, the helix will overwind, then invert its rotation and unwind.

(f) Return to the first part of the problem and show that the problem with the simple model used by bio-phycisit is that B depends on N and cannot therefore be taken as a constant.