Problem Sheet 1: Suggested Answers and Hints

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TO BE HANDED IN BY FRIDAY OF WEEK 3: questions 1, 2, 4, 5, 6 from Module I.

A note on how to use these notes

This hand-out is intended to be a guide for when you find yourself stuck on one of the prescribed problems. It is not intended to be a replacement that you hand in to your TA. This sheet will provide a starting point and hints for how to obtain the answer; however, it will be up to you to flesh out and fill in the gaps where necessary.

Some of the problems are not required to be handed in; these optional problems are meant to provide additional practice and/or push your understanding and encourage you to think more deeply about the biological and mathematical aspects of the problems.

To ultimately obtain the best understanding of the lecture material, give a strong attempt on the problem set before consulting these notes.

A note on how to use the note on how to use these notes

Read it.

Module I

Question 1 - Lagrange's Theorem

We are asked to prove that:

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

There are a number of ways that you can show this, and you are encouraged to find a way that makes sense to you, however we will prove it as follows:

We begin by noting that the radius of gyration was the root mean square distance from all units in our chain to the chain's center of mass. Mathematically, we can write this as:

$$s^2 = \frac{1}{N+1} \sum_{i=0}^{N} \left(\boldsymbol{R}_i - \boldsymbol{R}_{COM}\right)^2, \tag{2}$$

where $\boldsymbol{R}_{COM}$ is defined as the position of the chain's center of mass, which is:

$$\boldsymbol{R}_{COM} = \frac{1}{N+1} \sum_{j=0}^{N} \boldsymbol{R}_j. \tag{3}$$

Expanding equation (2) leads to

$$s^2 = \frac{1}{N+1}\sum_{i=0}^{N}\left(\boldsymbol{R}_i^2\right) - 2\boldsymbol{R}_{COM}\cdot\sum_{i=0}^{N}\left(\frac{1}{N+1}\boldsymbol{R}_i\right) + \frac{(N+1)}{(N+1)}\boldsymbol{R}_{COM}^2. \tag{4}$$

However, our second summation sign is the definition of $\boldsymbol{R}_{COM}$, so we have:

$$s^2 = -\boldsymbol{R}_{COM}^2 + \frac{1}{N+1}\sum_{i=0}^{N}\left(\boldsymbol{R}_i^2\right). \tag{5}$$

Now substitute the definition of $\boldsymbol{R}_{COM}$ back in, taking care of the fact that it is squared...

Question 2 - The Freely Rotating Chain

From the question, we know that the projection of $\boldsymbol{r}_{i+1}$ on $\boldsymbol{r}_i$ is $b\cos\theta$, where b and θ are both constants, and we are asked to show $<\boldsymbol{r}_i \cdot \boldsymbol{r}_{i+n}>= b^2\cos^{(i+n-i)}\theta$.

To show the required result, we use the hint from the question; considering the projections of the tangent vectors onto preceding tangent vectors. So, if we project $\boldsymbol{r}_{i+n}$ onto $\boldsymbol{r}_{i+n-1}$ and then this vector onto $\boldsymbol{r}_{i+n-2}$ and so forth until we arrive at $\boldsymbol{r}_i$, we can evaluate each of these terms to obtain the total answer.

Remember that the vector projection, that we will call $\boldsymbol{v}$ in this case, of $\boldsymbol{r}_{i+1}$ onto $\boldsymbol{r}_i$, was given by:

$$\boldsymbol{v} = (\boldsymbol{r}_{i+1} \cdot \hat{\boldsymbol{r}}_i)\,\hat{\boldsymbol{r}}_i = b\cos\theta\hat{\boldsymbol{r}}_i, \tag{6}$$

where $(\hat{\ })$ defines the unit vector.

As such, we can write:

$$<\boldsymbol{r}_i\cdot\boldsymbol{r}_{i+n}>=<\boldsymbol{r}_i\cdot\left(\frac{\boldsymbol{r}_{i+n}\cdot\hat{\boldsymbol{r}}_{i+n-1}}{b}\right)\boldsymbol{r}_{i+n-1}>=<\boldsymbol{r}_i\cdot\left(\frac{\boldsymbol{r}_{i+n}\cdot\hat{\boldsymbol{r}}_{i+n-1}}{b}\right)\dots\left(\frac{\boldsymbol{r}_{i+2}\cdot\hat{\boldsymbol{r}}_{i+1}}{b}\right)\boldsymbol{r}_{i+1}>. \tag{7}$$

Clearly $\boldsymbol{r}_{i+n} \neq \left(\frac{\boldsymbol{r}_{i+n}\cdot\hat{\boldsymbol{r}}_{i+n-1}}{b}\right)\boldsymbol{r}_{i+n-1}$, however, the above equation is true: Why is this?

Lastly, we combine equation (6) and equation (7) above to obtain the required result.

We now consider the average end-to-end distance using our previous result:

$$<\boldsymbol{R}^2>_N = \sum_{i=1}^{N}<\boldsymbol{r}_i^2>+2\sum_{i=1}^{N}\sum_{j=1}^{N-i}<\boldsymbol{r}_i\cdot\boldsymbol{r}_{i+j}>= b^2\left(N+2\sum_{i=1}^{N}\left[\sum_{j=1}^{N-i}(\cos\theta)^j\right]\right). \tag{8}$$

Using geometric series (twice) this can be simplified to

$$\begin{aligned}<\boldsymbol{R}^2>_N &= b^2\left(N+\frac{2\cos\theta}{1-\cos\theta}\left[N-\frac{\cos^N\theta}{\cos\theta}\left\{\frac{1-\frac{1}{\cos^N\theta}}{1-\frac{1}{\cos\theta}}\right\}\right]\right)\\ &= b^2\left(N+\frac{2N\cos\theta}{1-\cos\theta}-\frac{2\cos\theta}{1-\cos\theta}\left\{\frac{1-\cos^N\theta}{1-\cos\theta}\right\}\right). \end{aligned} \tag{9}$$

Lastly, we find the gyration radius of the freely rotating chain model:

$$<s^2>=\frac{1}{(N+1)^2}\sum_{0\le i<j\le N}<\boldsymbol{r}_{ij}^2>. \tag{10}$$

It should be commented that the calculation is messy. The main goal is to understand the method of calculation and to find the leading order terms when we consider the limit of $N\to\infty$.

From here on in, we define $\cos\theta = \alpha$ and we begin by cleaning up equation (9) as follows:

$$< \boldsymbol{R}^2 >_N = b^2 \left(\frac{(1+\alpha)N}{1-\alpha} - \frac{2\alpha}{1-\alpha} \left(\frac{1-\alpha^N}{1-\alpha} \right) \right). \tag{11}$$

We realize that we can use this result in equation (10), provided that we replace N with $k = i - j$. As such, expanding the single sum sign into a double sum, we have:

$$< s^2 > = \frac{1}{(N+1)^2} \sum_{j=1}^{N} \sum_{k=0}^{j} < \boldsymbol{R}^2 >_k = \frac{b^2}{(N+1)^2(1-\alpha)} \sum_{j=1}^{N} \sum_{k=0}^{j} \left((1+\alpha)k - 2\alpha \left(\frac{1-\alpha^k}{1-\alpha} \right) \right). \tag{12}$$

Now take each of the terms and evaluate the sums carefully. Using standard summation identities and evaluating geometric series this can be simplified to

$$< s^2 > = \frac{b^2(1+\alpha)N(N+2)}{6(N+1)(1-\alpha)} - \frac{\alpha N b^2}{(1-\alpha)^2(N+1)} + \frac{2\alpha^2 b^2 N}{(1-\alpha)^3(N+1)^2} - \frac{2\alpha^3 b^2 \left(1-\alpha^N\right)}{(1-\alpha)^4(N+1)^2}. \tag{13}$$

In the limit of $N \to \infty$, the first term is much larger than all the other terms. By substituting $\alpha = \cos\theta$ again, we find:

$$< s^2 > \sim \frac{b^2 N(1+\cos\theta)N}{6N(1-\cos\theta)} = \frac{N b_{\text{eff}}^2}{6}, \tag{14}$$

which is the Debye limit required.

Question 3 - Estimates for Bio-filaments

We begin by calculating the area moments of inertia, otherwise known as the second moments of area. For the case of DNA, Actin and microtubules, we make the assumption that their cross-sectional areas are circular, therefore:

$$\begin{aligned} I_{DNA} &= \frac{\pi}{4}r^4 = \frac{\pi}{4}(1\text{nm})^4 \approx 7.85 \times 10^{-37}m^4 && (15) \\ I_{Actin} &= \frac{\pi}{4}r^4 = \frac{\pi}{4}(3.5\text{nm})^4 \approx 1.17 \times 10^{-34}m^4 && (16) \\ I_{MT} &= \frac{\pi}{4}(r_{out}^4 - r_{in}^4) = \frac{\pi}{4}((12.5nm)^4 - (10.5nm)^4) \approx 9.63 \times 10^{-33}m^4. && (17) \end{aligned}$$

Where do these equations for the area moment of inertia come from? How can we derive them?

Using the fact that the Young's modulus, E, is $2GPa$ for our macromolecules, we use the equation:

$$E = \frac{\sigma}{\varepsilon}, \tag{18}$$

where σ is the stress and ε is the associated strain.

If we require that the strain is 1%, then we find that the required stress is given by:

$$\sigma = E\varepsilon = \left(2 \times 10^9 Pa\right)(0.01) = 2 \times 10^7 Pa. \tag{19}$$

Should this result depend on the type of material that we are working with? Why? Why not?

The associated force needed to stretch our macromolecules is then given by $\sigma = \frac{F}{A}$. Using the circular cross-sectional area assumption again, we find:

$$\begin{aligned} F_{DNA} &= \left(2 \times 10^7\right)\left(\pi \times (1nm)^2\right) \approx 0.0628pN && (20) \\ F_{Actin} &= \left(2 \times 10^7\right)\left(\pi \times (3.5nm)^2\right) \approx 0.770pN && (21) \\ F_{MT} &= \left(2 \times 10^7\right)\left(\pi \times (12.5nm)^2\right) \approx 9.82pN. && (22) \end{aligned}$$

Lastly, we find the persistence lengths. Remember that in the continuum limit, the persistence length was given by:

$$\xi_P = \frac{B}{k_B T}, \tag{23}$$

where B was the bending stiffness, given by $B = EI$, and k_B was Boltzmann's constant, given by $k_B = 1.38 \times 10^{-23} m^2 kg.s^{-2} K^{-1}$ in SI units. Are we allowed to use the continuum assumption in this instance? Why? Why not?

Assuming we are dealing with these macromolecules in the human body, $T \approx 310K$. As such, the persistence lengths can be found:

$$\xi_{DNA} = \frac{2 \times 10^7 \times 7.85 \times 10^{-37}}{1.38 \times 10^{-23} \times 310} \approx 3.7nm \tag{24}$$

$$\xi_{Actin} = \frac{2 \times 10^7 \times 1.17 \times 10^{-34}}{1.38 \times 10^{-23} \times 310} \approx 0.547\mu m \tag{25}$$

$$\xi_{MT} = \frac{2 \times 10^7 \times 9.63 \times 10^{-33}}{1.38 \times 10^{-23} \times 310} \approx 0.0450mm. \tag{26}$$

In regards to determining agreement with the theoretical values, it is best to come up with a quantitative measurement, rather than just saying "it's close". You are free to come up with your own measurement, however, a possible error metric, that we will define as η, could be:

$$\eta = \frac{|\xi_{exact} - \xi_{approx}|}{\xi_{exact}}. \tag{27}$$

What would be an acceptable error? Are your calculated values in close agreement? Why? Why not?

Question 4 - Radius of Gyration of the Worm-like Chain model

Radius of Gyration WLC

$$\underline{r}_{ij} = \underline{R}_j - \underline{R}_i = \sum_{p=i}^{j} \underline{r}_p$$

$$\langle s^2 \rangle \overset{\text{Lagrange}}{=} \frac{1}{(N+1)^2} \sum_{0 \le i \le j \le N} \langle \underline{r}_{ij}^2 \rangle$$

$$= \frac{1}{(N+1)^2} \sum_{0 \le i \le j \le N} \sum_{p=i}^{j} \sum_{q=i}^{j} \langle \underline{r}_p \cdot \underline{r}_q \rangle$$

from Notes

$$= \frac{1}{(N+1)^2} \sum_{0 \le i \le j \le N} \sum_{p=i}^{j} \underbrace{\sum_{q=i}^{j} \omega_1^{|p-q|}}$$

$$\Big[\underbrace{\underbrace{\omega_1 + \dots + \omega_1^{p-i}}_{}}_{q<p} + \underbrace{\underbrace{1}_{q=p} + \underbrace{(\omega_1 + \dots + \omega_1^{j-p})}_{q>p}}_{}$$

$$\frac{\omega_1(1-\omega_1^{p-i})}{1-\omega_1} + \frac{1-\omega_1^{j-p+1}}{1-\omega_1}$$

$$= \frac{1}{(N+1)^2} \sum_{0 \le i \le j \le N} \sum_{p=i}^{j} \left(\frac{\omega_1}{1-\omega_1} + \frac{1}{1-\omega_1}\right) - \left(\frac{\omega_1^{p-i+1} + \omega^{j-p+i}}{1-\omega_1}\right)$$

$$\cancel{= \frac{1}{(N+1)^2} \sum_{0 \le i \le j \le N} (j-i)\left(\frac{1+\omega_1}{1-\omega_1}\right) - \frac{1}{1-\omega_1}\left\{\frac{1-\omega^{j-i+1}}{1-\omega_1}\right.} +$$

$$= \frac{1}{(N+1)^2} \sum_{0 \le i \le j \le N} (j-i)\left(\frac{1+w_1}{1-w_1}\right) - \frac{1}{1-w_1}\left(\frac{w_1}{1-w_1}\left(1-w_1^{j-i+1}\right) + \frac{w_1^{i}}{1-w_1}\left(1-w_1^{j-i+1}\right)\right)$$

$$= \frac{1}{(N+1)^2}\left[\left(\frac{1+w_1}{1-w_1}\right)\left(\frac{N^3}{6}+\frac{N^2}{2}+\frac{N}{3}\right) - \frac{w_1}{(1-w_1)^2}\left(\frac{N^2}{2}+\frac{3N}{2}+1\right)\right] + J$$

$$J = \frac{1}{(N+1)^2}\frac{w_1^2}{(1-w_1)^2}\Bigg(\underbrace{\sum_{0\le i\le j\le N} w_1^{j-i}}_{O(N)}\Bigg) + \frac{1}{(N+1)^2}\frac{1}{1-w_1}\sum_{0\le i\le j\le N} w_1^{i} - \frac{1}{(N+1)^2}\frac{w_1}{(1-w_1)}\underbrace{\sum_{0\le i\le j\le N} w_1^{j}}_{O(N)}$$

$$\therefore \langle S^2\rangle = \frac{1}{(N+1)^2}\left[\left(\frac{1+w_1}{1-w_1}\right)\frac{N^3}{6} + \left(\frac{1}{2}\left(\frac{1+w_1}{1-w_1}\right) - \frac{w_1}{2(1-w_1)^2}\right)N^2 + O(N)\right]$$

$$\frac{1}{N^2}\left(1-\frac{2}{N}+\cdots\right)$$

$$= \left(\frac{1+w_1}{1-w_1}\right)\frac{N}{6} \cancel{\ast} + \left(\frac{1}{6}\left(\frac{1+w_1}{1-w_1}\right) - \frac{w_1}{2(1-w_1)^2}\right) + O\left(\frac{1}{N}\right)$$

$b_{eff}^2 = \left(\frac{1+w_1}{1-w_1}\right)b^2$, WLC model resembles FJC model as leading orders for $\langle S^2\rangle$ and $\langle \underline{R}^2\rangle$ match.

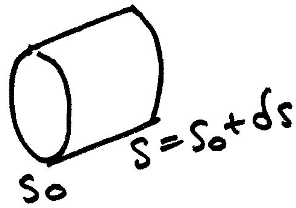
Question 5 - Derivation of momentum balance

Moment balance

Contact moment, exerted by $(s,L]$ on $[0,s]$ is

$$\underline{m}(s,T) + \underline{r}(s,T) \wedge \underline{n}(s,T)$$

As with force balance



$$(\underline{m} + \underline{r} \wedge \underline{n})\Big|_{s} - (\underline{m} + \underline{r} \wedge \underline{n})\Big|_{s_0} + \delta s \, \underbrace{\underline{L}}_{\text{body moment per unit length}} + \underbrace{\underline{r} \wedge \underline{f} \, \delta s}_{\text{moment exerted by body force}}$$

$$= \frac{d}{dT} \delta s \underbrace{\int dx_1 dx_2}_{\text{Integrate over cross section}} \underbrace{R(s,T,x_1,x_2) \wedge \rho \dot{R}(s,T,x_1,x_2)}_{\text{Angular momentum per unit volume}}$$

$\cdot \equiv d/dT$

$$= \delta s \int dx_1 dx_2 \, R \wedge \rho \ddot{R}$$

$$R(s,T,x_1,x_2) = r(s,T) + x_1 \underline{d}_1(s,T) + x_2 \underline{d}_2(s,T)$$

material coord
∴ no s,T dependence

$$= \delta s \Big[\rho A \, \underline{r} \wedge \ddot{\underline{r}} + \rho \int dx_1 dx_2 \, x_1^2 \, \underline{d}_1 \wedge \ddot{\underline{d}}_1 + \rho \int dx_1 dx_2 \, x_2^2 \, \underline{d}_2 \wedge \ddot{\underline{d}}_2 \Big] + O(\delta s^2)$$

assuming $\int_{\text{Cross Section}} dx_1 dx_2 \, x_1 = \int dx_1 dx_2 \, x_2 = 0$

eg. by symmetry

Question 6 - Static Kirchhoff Equations in the Local Basis

Before we begin to manipulate the static equivalents to equations (70) and (71) from the bio-filaments notes, let us calculate the spatial derivatives of each of the basis vectors. This is done by introducing a strain vector, $\mathsf{\mathbf{u}}(s)$, with components $(\mathsf{u}_1(s), \mathsf{u}_2(s), \mathsf{u}_3(s))$ that depend on the arc parameter, s:

$$\frac{\partial \boldsymbol{d}_1}{\partial s} = \mathsf{u}_3 \boldsymbol{d}_2 - \mathsf{u}_2 \boldsymbol{d}_3 \tag{28}$$

$$\frac{\partial \boldsymbol{d}_2}{\partial s} = \mathsf{u}_1 \boldsymbol{d}_3 - \mathsf{u}_3 \boldsymbol{d}_1. \tag{29}$$

$$\frac{\partial \boldsymbol{d}_3}{\partial s} = \mathsf{u}_2 \boldsymbol{d}_1 - \mathsf{u}_1 \boldsymbol{d}_2 \tag{30}$$

In calculating this, we have assumed something the basis vectors . What assumption did we implicitly make?

Let us now take the static version of the force balance and substitute $\boldsymbol{n} = n_1 \boldsymbol{d}_1 + n_2 \boldsymbol{d}_2 + n_3 \boldsymbol{d}_3$, where each of our components depends on s:

$$\frac{d\boldsymbol{n}}{ds} + \boldsymbol{f} = \frac{d}{ds}\left(n_1 \boldsymbol{d}_1 + n_2 \boldsymbol{d}_2 + n_3 \boldsymbol{d}_3\right) + \boldsymbol{f} = 0. \tag{31}$$

Now use equations (28)-(30) to calculate the derivative term in (31)...

Then write $\boldsymbol{f} = (f_1, f_2, f_3)$ and extract the $\boldsymbol{d}_1$, $\boldsymbol{d}_2$ and $\boldsymbol{d}_3$ components to obtain the force balance in local basis.

Apply a similar process to the static version of the moment balance... To close the system of equations, use the linear constitutive relation for the unstressed reference configuration:

$$\mathbf{m} = EI(\mathsf{u}_1 - \hat{\mathsf{u}}_1)\mathbf{d}_1 + EI(\mathsf{u}_2 - \hat{\mathsf{u}}_2)\mathbf{d}_2 + \mu J(\mathsf{u}_3 - \hat{\mathsf{u}}_3)\mathbf{d}_3 \tag{32}$$

If we were to consider the time-dependent forms of the Kirchhoff equations, we would obtain a similar set of 6 equations, but with components from the spin vector, $\mathsf{\mathbf{w}}(s,t) = (\mathsf{w}_1(s,t), \mathsf{w}_2(s,t), \mathsf{w}_3(s,t))$. This would then mean that we have 9 unknowns (i.e. for $\boldsymbol{n}$, $\mathsf{\mathbf{u}}$ and $\mathsf{\mathbf{w}}$). What other relation would we need in order to close the system of equations?

Question 7 - Beam buckling weakly nonlinear

Define θ as the angle between the tangent $\mathbf{d}_3$ and the x-axis. Letting $\mathbf{n} = n_x\mathbf{e}_x + n_y\mathbf{e}_y$ be the resultant force in the beam and $\mathbf{m} = m\mathbf{e}_z$ be the moment, the balance of linear momentum simply gives that n_x and n_y are constants, while

$$m'(s) + n_y \cos\theta - n_x \sin\theta = 0. \tag{33}$$

The compressive force $P > 0$ at the end of the beam is only in the horizontal direction, hence $n_x = -P$, while $n_y = 0$. With the linear constitutive law $m = EI\theta'(s)$, we thus obtain

$$\theta''(s) + \frac{P}{EI}\sin\theta = 0, \tag{34}$$

and the boundary conditions for a clamped beam are $\theta = 0$ at $s = 0, L$.

Linearising about small θ leads to

$$\theta = \begin{cases} A\sin(\frac{n\pi s}{L}) & \text{if } \frac{L^2P}{\pi^2 EI} = n^2, \\ 0 & \text{else} \end{cases} \tag{35}$$

Now we define $\lambda = \frac{L^2P}{\pi^2 EI}$ and rewrite θ as $\theta = \delta\Theta$, where δ is a small parameter and Θ is order 1. We also scale the length $s = L\xi$. Writing $\lambda = n^2 + \epsilon\lambda_1$ and expanding in (34) gives

$$\Theta''(\xi) + \pi^2(N^2 + \epsilon\lambda_1)(\Theta - \delta^2\frac{\Theta^3}{6} + \dots) = 0 \tag{36}$$

This system only balances if $\delta = \sqrt{\epsilon}$ – can you see why? With this choice we now expand $\Theta = \Theta_0 + \epsilon\Theta_1 + \dots$. Now equate powers of ϵ at leading and first order...

You should find

$$\Theta_0 = A_0 \sin(n\pi\xi). \tag{37}$$

with no information at leading order on amplitude A_0. The condition on amplitude comes from using Fredholm alternative Theorem for the first order problem. That is, you should get that $\Theta_{1_h} = \sin(n\pi\xi)$ is a solution of the homogeneous problem for order ϵ, i.e. there exists a zero-eigenfunction. The condition on A_0 comes from formulating the solvability condition for the Θ_1 problem...