C5.9 - Mathematical Mechanical Biology

Sheet 1 — MT

Section A- For practice

1. **Estimates for bio-filaments.**
   (a) Using the radius of DNA, actin filaments and microtubules given in Table 1 in the Lecture Notes, 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?

Solution: We begin by calculating the areal 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:

$$
\begin{aligned}
I_{DNA} &= \frac{\pi}{4}r^4 = \frac{\pi}{4}(1\text{nm})^4 \approx 7.85 \times 10^{-37} m^4 &(1)\\
I_{Actin} &= \frac{\pi}{4}r^4 = \frac{\pi}{4}(3.5\text{nm})^4 \approx 1.17 \times 10^{-34} m^4 &(2)\\
I_{MT} &= \frac{\pi}{4}(r_{out}^4 - r_{in}^4) = \frac{\pi}{4}((12.5nm)^4 - (10.5nm)^4) \approx 9.63 \times 10^{-33} m^4. &(3)
\end{aligned}
$$

To think about: Where do these equations for the areal moment of inertia come from?

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

$$E = \frac{\sigma}{\varepsilon}, \tag{4}$$

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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:

$$\sigma = E\varepsilon = \left(2 \times 10^9 Pa\right)(0.01) = 2 \times 10^7 Pa. \tag{5}$$

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:

$$\begin{aligned} F_{DNA} &= \left(2 \times 10^7\right)\left(\pi \times (1nm)^2\right) \approx 0.0628pN \quad (6) \\ F_{Actin} &= \left(2 \times 10^7\right)\left(\pi \times (3.5nm)^2\right) \approx 0.770pN \quad (7) \\ F_{MT} &= \left(2 \times 10^7\right)\left(\pi \times (12.5nm)^2\right) \approx 9.82pN. \quad (8) \end{aligned}$$

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

$$\xi_P = \frac{B}{k_B T}, \tag{9}$$

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.

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

$$\begin{aligned} \xi_{DNA} &= \frac{2 \times 10^7 \times 7.85 \times 10^{-37}}{1.38 \times 10^{-23} \times 310} \approx 3.7nm \quad (10) \\ \xi_{Actin} &= \frac{2 \times 10^7 \times 1.17 \times 10^{-34}}{1.38 \times 10^{-23} \times 310} \approx 0.547\mu m \quad (11) \\ \xi_{MT} &= \frac{2 \times 10^7 \times 9.63 \times 10^{-33}}{1.38 \times 10^{-23} \times 310} \approx 0.0450mm. \quad (12) \end{aligned}$$

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:

$$\eta = \frac{|\xi_{exact} - \xi_{approx}|}{\xi_{exact}}. \tag{13}$$

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2. **Lagrange's theorem.** Prove Lagrange's theorem on the gyration radius

$$s^2 = \frac{1}{(N+1)^2} \sum_{0\le i\le j\le N} \mathbf{r}_{ij}^2. \tag{14}$$

Solution: We are asked to prove that:

$$s^2 = \frac{1}{(N+1)^2} \sum_{0\le i<j\le N} \boldsymbol{r}_{ij}^2. \tag{15}$$

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:

$$s^2 = \frac{1}{N+1} \sum_{i=0}^{N} \left(\boldsymbol{R}_i - \boldsymbol{R}_{COM}\right)^2, \tag{16}$$

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

$$\boldsymbol{R}_{COM} = \frac{1}{N+1} \sum_{j=0}^{N} \boldsymbol{R}_j. \tag{17}$$

Expanding equation (16), we find:

$$s^2 = \frac{1}{N+1} \sum_{i=0}^{N} \left(\boldsymbol{R}_i^2 - 2\boldsymbol{R}_i \cdot \boldsymbol{R}_{COM} + \boldsymbol{R}_{COM}^2\right), \tag{18}$$

and we note that because $\boldsymbol{R}_{COM}$ depends on an independent summation index (i.e. one that does not explicitly include i), we can pull it out of the summation sign as such:

$$s^2 = \frac{1}{N+1} \sum_{i=0}^{N} \left(\boldsymbol{R}_i^2\right) - 2\boldsymbol{R}_{COM} \cdot \sum_{i=0}^{N} \left(\frac{1}{N+1}\boldsymbol{R}_i\right) + \frac{(N+1)}{(N+1)}\boldsymbol{R}_{COM}^2. \tag{19}$$

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

$$s^2 = -\boldsymbol{R}_{COM}^2 + \frac{1}{N+1} \sum_{i=0}^{N} \left(\boldsymbol{R}_i^2\right). \tag{20}$$

Let us now substitute the definition of $\boldsymbol{R}_{COM}$ back in, taking care of the fact that it is squared:

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$$
\begin{aligned}
s^2 &= -\frac{1}{(N+1)^2}\sum_{j=0}^{N}(\boldsymbol{R}_j)\sum_{i=0}^{N}(\boldsymbol{R}_i) + \frac{1}{N+1}\sum_{i=0}^{N}\left(\boldsymbol{R}_i^2\right) \\
&= -\frac{1}{(N+1)^2}\sum_{j=0}^{N}\sum_{i=0}^{N}(\boldsymbol{R}_j \cdot \boldsymbol{R}_i) + \frac{1}{N+1}\sum_{i=0}^{N}\left(\boldsymbol{R}_i^2\right), \qquad (21)
\end{aligned}
$$

and let us use the identity $(\boldsymbol{R}_i - \boldsymbol{R}_j)^2 = \boldsymbol{r}_{ij}^2 = \boldsymbol{R}_i^2 - 2\boldsymbol{R}_i \cdot \boldsymbol{R}_j + \boldsymbol{R}_j^2$ for the double sum:

$$
s^2 = \frac{1}{2(N+1)^2}\sum_{j=0}^{N}\sum_{i=0}^{N}\left(\boldsymbol{r}_{ij}^2\right) - \frac{1}{2(N+1)^2}\sum_{j=0}^{N}\sum_{i=0}^{N}\left(\boldsymbol{R}_i^2\right) - \frac{1}{2(N+1)^2}\sum_{j=0}^{N}\sum_{i=0}^{N}\left(\boldsymbol{R}_j^2\right) + \frac{1}{N+1}\sum_{i=0}^{N}\left(\boldsymbol{R}_i^2\right). \qquad (22)
$$

However, by the same reasoning that allowed us to obtain equation (19), we can further simplify:

$$
s^2 = \frac{1}{2(N+1)^2}\sum_{j=0}^{N}\sum_{i=0}^{N}\left(\boldsymbol{r}_{ij}^2\right) - \frac{(N+1)}{2(N+1)^2}\sum_{i=0}^{N}\left(\boldsymbol{R}_i^2\right) - \frac{(N+1)}{2(N+1)^2}\sum_{j=0}^{N}\left(\boldsymbol{R}_j^2\right) + \frac{1}{N+1}\sum_{i=0}^{N}\left(\boldsymbol{R}_i^2\right). \qquad (23)
$$

Lastly, we realize that the second and third terms can be subtracted by a reordering of the indices. As such, we obtain:

$$
s^2 = \frac{1}{2(N+1)^2}\sum_{j=0}^{N}\sum_{i=0}^{N}\left(\boldsymbol{r}_{ij}^2\right), \qquad (24)
$$

or, alternatively, taking into account the terms that are counted twice, we rewrite equation (24) as equation (15) to obtain the required result.

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Section B - Regular problems

3. **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 $b\cos\theta$.

   (a) Show that $<\mathbf{r}_i \cdot \mathbf{r}_{i+n}>= b^2\cos^n\theta$.

   Hint: There are different ways to do this, but a nice way to proceed is to consider first $<\mathbf{r}_i \cdot \mathbf{r}_{i+2}>$. We can define an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{t}_{i+1}\}$, where $\mathbf{r}_{i+1} = b\mathbf{t}_{i+1}$, and $\mathbf{e}_1, \mathbf{e}_2$ are orthogonal to $\mathbf{r}_{i+1}$. In this basis

   $$\mathbf{r}_{i+2} = b\cos\theta\mathbf{t}_{i+1} + b\sin\theta\left(\cos\phi_{i+1}\mathbf{e}_1 + \sin\phi_{i+1}\mathbf{e}_2\right),$$

   for some angle ϕ_{i+1}.

   Now consider that since the bond angle θ is fixed, a configuration is completely defined by the angles ϕ_i, which are each uniformly distributed over 0 to 2π. Use this fact to show that

   $$<\mathbf{r}_i \cdot \mathbf{r}_{i+2}>= b^2\cos^2\theta,$$

   and then generalise the argument...

   (b) Compute the average end-to-end distance $< R^2 >_N$ and show that in the limit $N \to \infty$ one obtains

   $$< R^2 >_\infty = N b_{\text{eff}}^2 \tag{25}$$

   with an *effective bond length* $b_{\text{eff}}^2 = b^2 \frac{1+\cos\theta}{1-\cos\theta}$.

4. **Momentum balance.** 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.

   Hint: The handwritten notes on the next page get you started (by first deriving force balance, which you need not do, but might be helpful for your understanding and is included for completeness of the theory).

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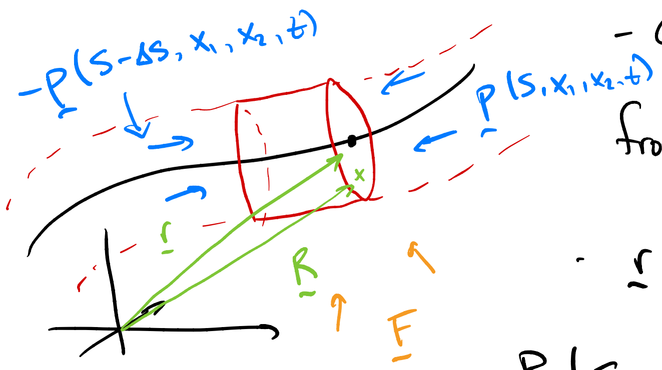
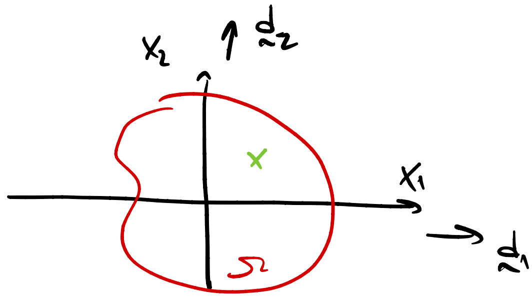


- consider a section of rod from $S-\Delta S$ to S

- $\underline{r}(S,t)$ points to the centreline, $\underline{R}(S, x_1, x_2, t)$ points to a pt in the cross-section Ω



So $\underline{R} = \underline{r} + x_1 \underline{d}_1 + x_2 \underline{d}_2$

and place $\underline{r}$ at centroid of Ω

$$\Rightarrow \int_\Omega x_1 \, dA = \int_\Omega x_2 \, dA = 0$$

- Can choose $\underline{d}_1, \underline{d}_2$ st $\int_\Omega x_1 x_2 \, dA = 0$ {principle axes of inertia}

Let $\underline{p}(S, x_1, x_2, t)$ be the contact force applied on the cross-section at S due to portion of rod from $[S, L]$

Balance of Lin. Momium:

$$\int_\Omega \underline{p}(S, x_1, x_2, t) \, dA - \int_\Omega \underline{p}(S-\Delta S, x_1, x_2, t) \, dA + \int_\Omega \int_{S-\Delta S}^{S} \underline{F} \, dS \, dA = \iint_{\Omega \, S-\Delta S}^{S} \rho \, \ddot{\underline{R}} \, dS \, dA \qquad \text{(LM)}$$

Now define $\underset{\sim}{n} = \int_\Omega \underset{\sim}{p}\, dx_1 dx_2$, $\underset{\sim}{f} = \int_\Omega \underset{\sim}{F}\, dx_1 dx_2$

Then LM becomes

$$\int_{S-\Delta S}^{S} \frac{\partial \underset{\sim}{n}}{\partial S} + \underset{\sim}{f}\, dS = \int_{S-\Delta S}^{S} \rho A \ddot{\underset{\sim}{r}}\, dS$$

area of Ω

from which we get

$$\boxed{\frac{\partial \underset{\sim}{n}}{\partial S} + \underset{\sim}{f} = \rho A \ddot{\underset{\sim}{r}}}$$

The Balance of Angular Momentum reads

$$\int_\Omega \underset{\sim}{R} \wedge \underset{\sim}{p}\,\Big|_S \, dA - \int_\Omega \underset{\sim}{R} \wedge \underset{\sim}{p}\,\Big|_{S-\Delta S} \, dA + \int_{S-\Delta S}^{S}\int_\Omega \underset{\sim}{R} \wedge \underset{\sim}{F}\, dA\, dS$$

$$= \frac{d}{dt} \underbrace{\int_{S-\Delta S}^{S}\int_\Omega \underset{\sim}{R} \wedge (\rho \dot{\underset{\sim}{R}})\, dA\, dS}_{\text{angular momium for the section}} \qquad \text{(AM)}$$

Now define $\underset{\sim}{m} = \int_\Omega (x_1 \underset{\sim}{d}_1 + x_2 \underset{\sim}{d}_2) \wedge \underset{\sim}{p}\, dA$,

and $\underset{\sim}{l} = \int_\Omega (x_1 \underset{\sim}{d}_1 + x_2 \underset{\sim}{d}_2) \wedge \underset{\sim}{F}\, dA$

now simplify ...

5. **Kirchhoff in the local basis.** Write the static (i.e. time independent) Kirchhoff equations (Equations (51)-(52) in the typed notes) in the local basis in the absence of intrinsic curvature and twist (so that $\widehat{u}_1,\ \widehat{u}_2,\ \widehat{u}_3$ are zero). That is, obtain a compact set of equations for the components $\mathsf{n}_1, \mathsf{n}_2, \mathsf{n}_3$ of $\mathbf{n} = \mathsf{n}_1\mathbf{d}_1 + \mathsf{n}_2\mathbf{d}_2 + \mathsf{n}_3\mathbf{d}_3$ and $\mathsf{m}_1, \mathsf{m}_2, \mathsf{m}_3$ of $\mathbf{m} = \mathsf{m}_1\mathbf{d}_1 + \mathsf{m}_2\mathbf{d}_2 + \mathsf{m}_3\mathbf{d}_3$.

   Hint: To get started, calculate the spatial derivatives of each of the basis vectors. This is done by expressing the strain vector $\mathbf{u}(s)$ in the local basis with components $(\mathsf{u}_1(s), \mathsf{u}_2(s), \mathsf{u}_3(s))$ that depend on the arc length parameter s and expanding the relationships $\mathbf{d}_i'(s) = \mathbf{u} \times \mathbf{d}_i$:

$$\frac{d\boldsymbol{d}_1}{ds} = \mathsf{u}_3\boldsymbol{d}_2 - \mathsf{u}_2\boldsymbol{d}_3 \tag{26}$$

$$\frac{d\boldsymbol{d}_2}{ds} = \mathsf{u}_1\boldsymbol{d}_3 - \mathsf{u}_3\boldsymbol{d}_1. \tag{27}$$

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

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Section C - Tougher problems, optional

6. **The freely rotating chain revisited**. Consider again a chain with N links with constant bond length b and bond angle θ. Compute the gyration radius and show that for large N one recovers the result of Debye given in Eq. (7) in the typed notes.

   Solution: We wish to find the gyration radius of the freely rotating chain model:

$$< s^2 >= \frac{1}{(N+1)^2} \sum_{0 \le i < j \le N} < \boldsymbol{r}_{ij}^2 > . \tag{29}$$

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 noting that (from the earlier problem), we can write:

$$< \boldsymbol{R}^2 >_N = b^2 \left(\frac{(1+\alpha)N}{1-\alpha} - \frac{2\alpha}{1-\alpha} \left(\frac{1-\alpha^N}{1-\alpha} \right) \right). \tag{30}$$

We can use this result in equation (29), provided that we replace N with $k = i - j$. The point is that the $\mathbf{r}_{ij}$ are like partial displacement vectors, i.e. vectors pointing from the ith to the jth node, while $\mathbf{R}$ is just the vector from the first to the last node. But the above computation for $< \boldsymbol{R}^2 >_N$ is valid for any length chain, and so we can replace $< \mathbf{r}_{ij}^2 >$ by $< \boldsymbol{R}^2 >_{j-i}$. As such, expanding the single sum sign into a double sum, we have:

$$< s^2 >= \frac{1}{(N+1)^2} \sum_{j=1}^{N} \sum_{k=0}^{j} < \boldsymbol{R}^2 >_k = \frac{b^2}{(N+1)^2(1-\alpha)} \sum_{j=1}^{N} \sum_{k=0}^{j} \left((1+\alpha)k - 2\alpha \left(\frac{1-\alpha^k}{1-\alpha} \right) \right). \tag{31}$$

Let us take each of the terms and evaluate the sums carefully. Considering the first term:

$$\begin{aligned}
\sum_{j=1}^{N} \sum_{k=0}^{j} (1+\alpha)k = (1+\alpha) \sum_{j=1}^{N} \frac{j(j+1)}{2} &= \frac{(1+\alpha)}{2} \sum_{j=1}^{N} j^2 + j \\
&= \frac{(1+\alpha)}{2} \left[\frac{N(N+1)(2N+1)}{6} + \frac{N(N+1)}{2} \right] \\
&= \frac{(1+\alpha)N(N+1)(N+2)}{6},
\end{aligned} \tag{32}$$

where we have used some standard summation identities.

Taking the second term now:

$$
\begin{aligned}
\sum_{j=1}^{N}\sum_{k=0}^{j} 2\alpha\left(\frac{1-\alpha^k}{1-\alpha}\right) &= \frac{2\alpha}{1-\alpha}\sum_{j=1}^{N}\sum_{k=0}^{j}\left(1-\alpha^k\right) \\
&= \frac{2\alpha}{1-\alpha}\sum_{j=1}^{N}\left(j+1-\frac{1-\alpha^{j+1}}{1-\alpha}\right) \\
&= \frac{2\alpha}{1-\alpha}\left[\frac{N(N+1)}{2}+N-\frac{1}{1-\alpha}\left(N-\alpha\left\{\frac{\alpha-\alpha^{N+1}}{1-\alpha}\right\}\right)\right] \\
&= \frac{\alpha N(N+1)}{(1-\alpha)}-\frac{2\alpha^2 N}{(1-\alpha)^2}+\frac{2\alpha^3}{(1-\alpha)^3}\left(1-\alpha^N\right), \qquad (33)
\end{aligned}
$$

where we have used some more standard summation identities and have evaluated two geometric series.

We now combine equations (32) and (33) substitute these results back into equation (31):

$$
< s^2 >= \frac{b^2(1+\alpha)N(N+2)}{6(N+1)(1-\alpha)} - \frac{\alpha N b^2}{(1-\alpha)^2(N+1)} + \frac{2\alpha^2 b^2 N}{(1-\alpha)^3(N+1)^2} - \frac{2\alpha^3 b^2\left(1-\alpha^N\right)}{(1-\alpha)^4(N+1)^2}. \qquad (34)
$$

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:

$$
< s^2 >\sim \frac{b^2 N(1+\cos\theta)N}{6N(1-\cos\theta)} = \frac{N b_{\text{eff}}^2}{6}, \qquad (35)
$$

which is the Debye limit required.

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7. **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

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

Solution: Solutions are in the following handwritten pages.

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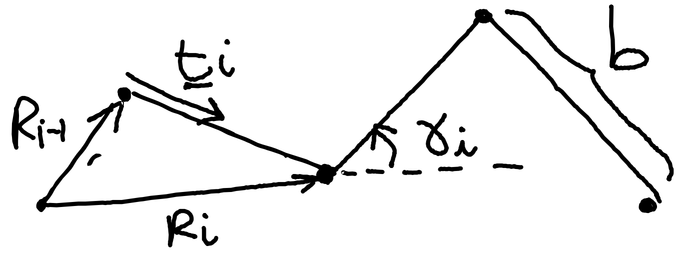
QUESTION 4 PS1

NOTE: Given two random vectors $\underline{v}_1$ & $\underline{v}_2$

$\langle \underline{v}_1 \cdot \underline{v}_2 \rangle = 0 \not\Rightarrow \underline{v}_1 \cdot \underline{v}_2 = 0$

We want to compute the gyration radius for the Worm-like model.



$\underline{t}_i$: is the unit vector $i = 1, \dots, N$ for the i-th link

The resistance of the link to bending is associated to the parameter:

$$\lambda = \frac{K}{K_B T}$$

K → measure of the energy penalty associated with bending.

The larger λ, the stiffer the link.
When $\lambda \gg 1$ we have that:

$$\langle \underline{t}_i \cdot \underline{t}_{i+n} \rangle = \underbrace{\mathcal{L}(\lambda)}_{\text{Langevin function}}{}^{|n|} \triangleq \omega_1^{|n|}$$

NOTE: this is analogous to Q2 provided we exchange: $\cos\theta \longleftrightarrow \omega_1$

$$\langle s^2 \rangle \overset{\text{LAGRANGE THEOREM}}{=} \frac{1}{(N+1)^2} \sum_{0 \le i < j \le N} \langle r_{ij}^2 \rangle$$

$$r_{ij} = |R_j - R_i| = \sum_{m=i+1}^{j} b\, t_m \quad (*)$$

this is the end to end displacement for the subchain $i \mapsto j$

$$r_{ij} = R_j - R_i \overset{(j>i)}{=} R_j - \sum_{m=i+1}^{j-1} R_m + \sum_{m=i+1}^{j-1} R_m - R_i$$

$$= \underbrace{R_j - R_{j-1}}_{b\underline{t}_j} + \sum_{m=i+2}^{j-1} \underbrace{R_m - R_{m-1}}_{b\underline{t}_m} + \underbrace{R_{i+1} - R_i}_{b\underline{t}_{i+1}}$$

We will use:

$$\sum_{i=a}^{b} 1 = b-a+1$$

$$\sum_{i=1}^{N} j = \frac{N(N+1)}{2}$$

$$\sum_{i=1}^{N} j^2 = \frac{N(N+1)(2N+1)}{6}$$

We evaluate $\langle r_{ij}^2 \rangle$:

$$\langle r_{ij}^2 \rangle \overset{(*)}{=} b^2 \left\langle \left(\sum_{m=i+1}^{j} \underline{t}_m\right)\left(\sum_{k=i+1}^{j} t_k\right)\right\rangle$$

$$\underset{\text{(splitting the sum)}}{=} b^2 \left\langle \sum_{m=i+1}^{j} \underline{t}_m^2 + 2 \sum_{m=i+1}^{j-1} \sum_{k=m+1}^{j} \underline{t}_k \cdot t_m \right\rangle$$

$$= b^2 \underbrace{\sum_{m=i+1}^{j} \overbrace{\langle \underline{t}_m^2 \rangle}^{=1}}_{j-i} + \underbrace{2b^2 \sum_{m=i+1}^{j-1} \sum_{k=m+1}^{j} \langle t_k \cdot t_m \rangle}_{B}$$

B we know $\langle t_k \cdot t_m \rangle \overset{\text{as } k>m}{=} w_1^{k-m}$

$$\boxed{\begin{aligned} p &= k-m \\ p_{min} &= 1 \\ p_{max} &= j-m \end{aligned}}$$

$$\sum_{m=i+1}^{j-1} \sum_{p=1}^{j-m} w_1^p \overset{\text{GEOMETRIC SUM}}{=} \sum_{m=i+1}^{j-1} w_1 \left(\frac{1 - w_1^{j-m}}{1 - w_1} \right)$$

$j-m \to q$

$$= \left(\frac{w_1}{1-w_1}\right)\left(\underbrace{\sum_{m=i+1}^{j-1} 1}_{j-i-1} - \sum_{q=1}^{j-i-1} w_1^{q}\right)$$

NOTE: we absorb the -1 term in the geometric sum

$$= \frac{w_1}{1-w_1}\left(j-i + \sum_{q=0}^{j-i-1} w_1^{q}\right) \quad \frac{1-w_1^{j-i+1}}{1-w_1}$$

$$\langle r_{ij}^2\rangle = b^2\left[\frac{1+w_1}{1-w_1}(j-i) + \frac{2w_1}{(1-w_1)^2} - \frac{2w_1^{j-i+1}}{1-w_1}\right]$$

$$\langle s^2\rangle = \frac{1}{(N+1)^2}\sum_{j=1}^{N}\sum_{i=0}^{j-1}\langle r_{ij}^2\rangle = \left\{\begin{array}{l} p=j-i \\ p_{min}=1 \\ p_{max}=j \end{array}\right\}$$

CHANGE INDEX INNER SUM

$$= \frac{b^2}{(N+1)^2(1-w_1)}\sum_{j=1}^{N}\sum_{p=1}^{j}\left[\underbrace{(1+w_1)p}_{A} + \underbrace{\frac{2w_1}{(1-w_1)}}_{B} - \underbrace{\frac{2w_1^{p+1}}{(1-w_1)}}_{C}\right]$$

NOTE: we are interested in $\langle s^2\rangle$ up to $\theta(1)$. Given the factor $(N+1)^{-2}$ we only need to estimate A, B, C to a precision of $\theta(N^2)$

$$\text{A} \; \sum_{j=1}^{N} (1+w_1)\frac{(j+1)j}{2} = \frac{(1+w_1)}{2}\sum_{j=1}^{N} j^2+j$$

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

$$= \frac{1+w_1}{12} N(N+1)(2N+1+3) = \frac{(\omega+1)N(N+1)(N+2)}{6}$$

$$\Rightarrow \text{A} = \frac{1+\omega_1}{6}\left(N^3+3N^2\right) + \theta(N)$$

$$\text{B} \; \frac{2w_1}{1-w_1}\sum_{j=1}^{N} j = \frac{N(N+1)\omega_1}{1-w_1} = \frac{N^2\omega_1}{1-w_1} + \theta(N)$$

$$\text{C} \; \frac{2\omega_1}{1-\omega_1}\sum_{j=1}^{N}\sum_{p=1}^{j} w_1{}^p = \frac{2\omega_1{}^2}{(1-\omega_1)^2}\left[N - \frac{\omega_1(1-\omega_1^N)}{1-\omega_1}\right]$$

Since $\omega_1 \in (-1,1)$ $\omega_1^N \longrightarrow 0$ as $N>>1$
so that C $\sim \theta(N)$ and there is neglegible

[This is a consequence of the properties of the $\mathcal{L}(\lambda)$ function]

$$\langle s^2 \rangle = \frac{b^2}{(1+N)^2}\left[\frac{1+w_1}{1-w_1}\left(\frac{N^3+3N^2}{6}\right) + \frac{w_1}{(1-w_1)^2}N^2\right] + o(1)$$

Taylor expanding the denominator:

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

$$\langle s^2 \rangle = b^2\left[\left(\frac{1+w_1}{1-w_1}\right)\left(\frac{N-2+\overset{1}{\cancel{3}}}{6}\right) + \frac{w_1}{(1-w_1)^2}\right] + o(1)$$

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

(b)

	$\langle R^2 \rangle$	$\langle S^2 \rangle$
FJC	Nb^2	$\frac{N}{6} b^2$
WLM	$\frac{N(w_1+1)}{(1-w_1)} b^2$	$\frac{N}{6} b^2 \left(\frac{1+w_1}{1-w_1}\right)$

There is a clear analogy in the statistical properties of the two models, clear when we define the effective lenght for the WLM to be:

$$\boxed{b_{eff}^2 = b^2 \frac{1+w_1}{1-w_1}}$$

In the limit of stiff chains, i.e. $\lambda >> 1$ we have:

$$w_1 = \mathcal{L}(\lambda) \to 1 \Rightarrow b_{eff}^2 >> b^2$$