Biofilaments Overview

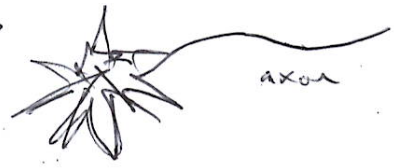
- Motivation - Filamentary structures (long and slender) w/ elastic properties are abundant in biology
  - appear across many length scales

Exs

- ▫ Subcellular DNA, ~~proteins (especially~~

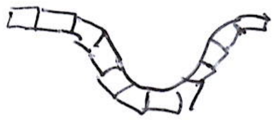
  protein filaments - eg ~~[illegible]~~ make up cytoskeleton · give structure to cells

  axon - nerve fiber



- ▫ Cellular · Mostly biomembrane (next module) but a line of cells may behave as filament

  eg crypts in intestine



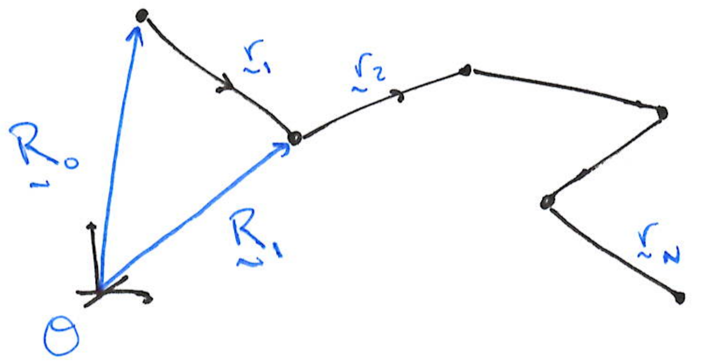
- ▫ Tissue/organ · arteries, airways, umbilical cord, muscle fibre, elephants trunk, plant branch or stem, or root

- ▫ Organism worm, snake

- The Mechanical behaviour/properties crucial to function - Natural shape, ~~res~~ stiffness · resistance to bending, stretching, twisting

BIOFILAMENTS

1.1 The freely jointed chain model (FJC)



Assume: i) N links, of fixed length b

ii) Orientation of tangent $\underset{\sim}{t}_i = \frac{\underset{\sim}{r}_i}{b}$ is <u>independent</u> of other tangents and random

iii) No excluded volume effects (not worried about overlapping)

<u>Defn</u> The average of a quantity $\underset{\sim}{a}$ is

$$\langle \underset{\sim}{a} \rangle := \int_{(\mathbb{R}^3)^N} dV \, \underset{\sim}{a}(\underset{\sim}{r}_1, \ldots, \underset{\sim}{r}_N) \, p(\underset{\sim}{r}_1, \ldots, \underset{\sim}{r}_N)$$

where $p(\underset{\sim}{r}_1, \ldots, \underset{\sim}{r}_N)$ is the prob. distrib. fn for configuration state $\underset{\sim}{r}_1, \ldots, \underset{\sim}{r}_N$

For our assumptions,

$$\varphi = \prod_{i=1}^{N} \frac{1}{4\pi b^2}\, \delta\big(|\underset{\sim}{r}_i| - b\big)$$

since length is b

since $\underset{\sim}{r}_i$ lives on sphere radius b

The end-to-end displacement $\underset{\sim}{R} := \underset{\sim}{R}_N - \underset{\sim}{R}_0$

$$= \sum_{i=1}^{N} \underset{\sim}{r}_i$$

Its mean value is

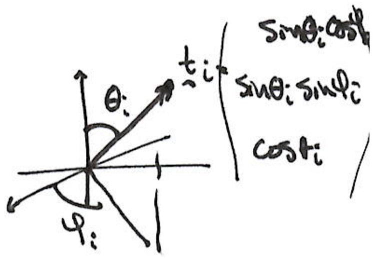
$$\langle \underset{\sim}{R} \rangle = \int_{(\mathbb{R}^3)^N} dV \left(\sum b\, \underset{\sim}{t}_i \right) \frac{1}{(4\pi b^2)^N} \underbrace{\delta\big(|\underset{\sim}{r}_1| - b\big) \cdots \delta\big(|\underset{\sim}{r}_N| - b\big)}_{\Downarrow}$$

only int. over spheres radius b

since integ. over sphere rad. b

$$= \frac{(b^2)^N}{(4\pi b^2)^N} \cdot b \int d\Omega_1\, d\Omega_2 \ldots d\Omega_N \sum \underset{\sim}{t}_i$$

$$d\Omega_i = \sin\theta_i\, d\theta_i\, d\varphi_i$$



But each integral indep, and $\int d\Omega_i\, \underset{\sim}{t}_i = \underset{\sim}{0}$

$$\therefore \langle \underset{\sim}{R} \rangle = \underset{\sim}{0}$$

However, the second moment $\langle \underset{\sim}{R}^2 \rangle \neq 0$

and its square root gives the lengthscale

of typical end-to-end distance

$$\underset{\sim}{R}^2 = \sum \underset{\sim}{r}_i \cdot \sum \underset{\sim}{r}_j = \sum \underset{\sim}{r}_i \cdot \underset{\sim}{r}_i + \sum_{i \neq j} \underset{\sim}{r}_i \cdot \underset{\sim}{r}_j$$

For $i \neq j$: $\langle \underset{\sim}{r}_i \cdot \underset{\sim}{r}_j \rangle = \langle \underset{\sim}{r}_i \rangle \cdot \langle \underset{\sim}{r}_j \rangle$ as $\underset{\sim}{r}_i, \underset{\sim}{r}_j$

uncorrelated $= \underset{\sim}{0}$ as $\langle \underset{\sim}{r}_i \rangle = \underset{\sim}{0}$ by similar

calc to above.

$$\therefore \langle \underset{\sim}{R}^2 \rangle = \langle \sum \underset{\sim}{r}_i \cdot \underset{\sim}{r}_i \rangle = \sum \langle \underset{\sim}{r}_i \cdot \underset{\sim}{r}_i \rangle = \underbrace{N \langle \underset{\sim}{r}_1 \cdot \underset{\sim}{r}_1 \rangle}_{}$$

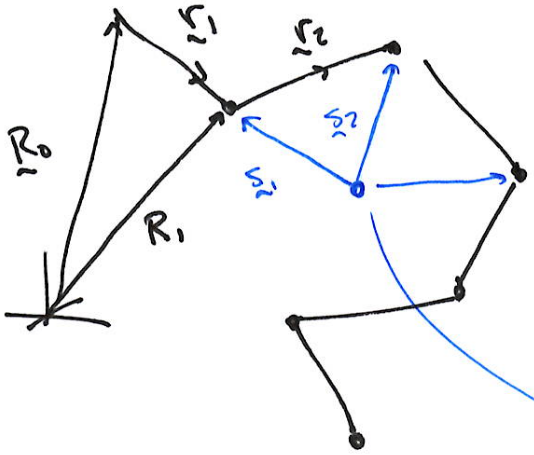
by symmetry

$$= N \langle b^2 \rangle = N b^2 \underbrace{\int dV \, p(r_1 \dots r_N)}_{=1 \text{ by defn of p.d.f}} = N b^2$$

$$\therefore \text{Root mean square } \sqrt{\langle \underset{\sim}{R}^2 \rangle} = b\sqrt{N}$$

Analogous to root mean square disp of random walker after N steps, ie Brownian motion

Defn The gyration radius, s, is the root mean square distance relative to centroid



Centroid $\underset{\sim}{S}$ (like centre of gravity)

$$= \frac{1}{N+1} \sum_{i=0}^{N} \underset{\sim}{R}_i$$

Define $\underset{\sim}{s}_i = \underset{\sim}{R}_i - \underset{\sim}{S}$. We want to compute

$$s^2 = \frac{1}{N+1} \sum_{i=0}^{N} \underset{\sim}{s}_i \cdot \underset{\sim}{s}_i \quad .$$ We'll use:

Theorem (Lagrange): $s^2 = \frac{1}{(N+1)^2} \sum_{0 \le i \le j \le N} \underset{\sim}{r}_{ij}^2$, $\underset{\sim}{r}_{ij} := \underset{\sim}{R}_j - \underset{\sim}{R}_i$

Proof: see problem sheets.

Let $j > i$. $\underset{\sim}{r}_{ij} = \underset{\sim}{R}_j - \underset{\sim}{R}_i = \sum_{p=i+1}^{j} \underset{\sim}{r}_p \Rightarrow \underset{\sim}{r}_{ij}^2 = \sum_{p,q=i+1}^{j} \underset{\sim}{r}_p \cdot \underset{\sim}{r}_q$

$$= \sum_{p=i+1}^{N} \underset{\sim}{r}_p \cdot \underset{\sim}{r}_p + \sum_{q \neq p \in (i+1,\dots,j)} \underset{\sim}{r}_p \cdot \underset{\sim}{r}_q$$

[We showed $\langle r_p \cdot r_q \rangle = \langle r_p \rangle \langle r_q \rangle = 0$ and $\langle r_p \cdot r_p \rangle = b^2$]

$$\therefore \quad \langle \underset{\sim}{r}_{ij}^2 \rangle = (j-i)\, b^2$$

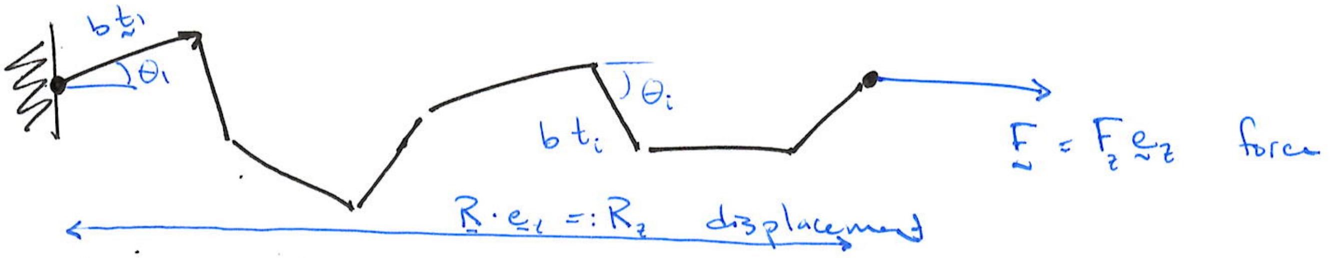
$$\therefore \quad \langle S^2 \rangle = \frac{1}{(N+1)^2} \sum_{0 \le i < j \le N} \langle \underset{\sim}{r}_{ij}^2 \rangle = \frac{b^2}{(N+1)^2} \sum_{j=1}^{N} \sum_{i=0}^{j-1} (j-i)$$

$$\overset{k=j-i}{=} \frac{b^2}{(N+1)^2} \sum_{j=1}^{N} \underbrace{\sum_{k=0}^{j} k}_{\frac{j(j+1)}{2}} = \frac{b^2}{2(N+1)^2} \left(\frac{N(N+1)(2N+1)}{6} + \frac{N(N+1)}{2} \right)$$

$$\rightarrow \langle S^2 \rangle = \frac{b^2 N(N+2)}{6(N+1)}$$

"In polymer physics - rad. of gyration used to describe dimensions of polymer chain
- can be computed experimentally by light scattering"

FJC with external force



Assumptions i) FJC, fixed at one end

ii) Constant force

iii) Equilibrium w/ thermal bath, temp T

(Note: $\theta_1, \ldots \theta_N$ no longer unif. distrib)

Goal Find force-displacement relation

[Recall: $m\ddot{x} = F = -\nabla V \rightarrow m\ddot{x}\dot{x} = F\dot{x} = -V'(x)\dot{x}$

$\rightarrow \frac{1}{2}m\dot{x}^2 + \underset{\text{int. energy}}{V} = E = \frac{1}{2}m\dot{x}^2 - \underset{\text{work}}{Fx}$ $\therefore$ internal energy $= -Fx$]

The work to extend chain $W = \underset{\sim}{F} \cdot \underset{\sim}{R}$, so total internal energy is $E = -W = -F_z b \sum_{i=1}^{N} \cos\theta_i$

"Could add an additional constant energy for zero energy state, but can set 0 WLOG and doesn't change any result"

Statistical Mechanics

"same as thermodynamic equil"

By considering the maximisation of entropy for the combined system of the chain and heat bath,

$$\text{Prob}\begin{pmatrix}\text{system in state} \\ \{\theta_1, \dots \theta_N\}\end{pmatrix} = \frac{\exp\left(\frac{-E(\theta_1,\dots,\theta_N)}{k_b T}\right)}{Z}$$

where $E(\theta_1, \dots \theta_N)$ is internal energy of state $\{\theta_1 \dots \theta_N\}$,

k_b is Boltzmann's constant, and

$$Z = \int \underbrace{d\Omega_1 \dots d\Omega_N}_{\substack{\text{solid angles, } d\Omega_i = d\theta_i\, d\varphi_i \sin\theta_i \\ \text{for integ. over spheres}}} \exp\left(\frac{-E(\theta_1, \dots \theta_N)}{k_b T}\right)$$ is ~~so-called~~ partition function

weighted sum over all possible config. $\{\theta_1, \dots \theta_N\}$. normalization constant

- Observe : $E(\theta_1, \dots \theta_N)$ high $\Rightarrow P(\{\theta_1 \dots \theta_N\})$ low

We have $E = -F_z b \sum_{i=1}^{N} \cos\theta_i$

$$\Rightarrow Z = \int d\Omega_1 \dots d\Omega_N \exp\left(\frac{F_z b}{k_b T} \sum \cos\theta_i\right)$$

$$= \prod_{i=1}^{N} \int d\theta_i\, d\varphi_i\, e^{\alpha \cos\theta_i} \sin\theta_i \qquad \text{w/} \quad \alpha := \frac{F_z b}{k_b T}$$

$$= (2\pi)^N \left(\int_0^\pi d\theta\, e^{\alpha\cos\theta} \sin\theta\right)^N = \left(\frac{4\pi \sinh\alpha}{\alpha}\right)^N$$

$$\therefore \; P(\{\theta_1, \dots \theta_N\}) = \left(\frac{\alpha}{4\pi \sinh\alpha}\right)^N \cdot e^{\alpha \sum_{i=1}^N \cos\theta_i}$$

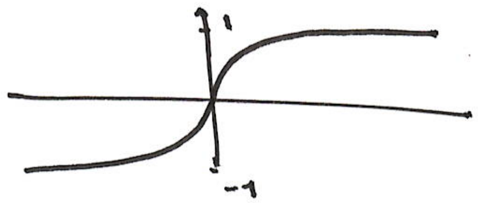
Now, average distance $\langle R_z \rangle = \int d\Omega_1 \dots d\Omega_N \left(b \sum \cos\theta_i\right) \dfrac{e^{\alpha \sum \cos\theta_i}}{Z}$

(A useful trick!)

$$\stackrel{\downarrow}{=} \frac{b}{Z} \frac{\partial}{\partial \alpha} \int d\Omega_1 \dots d\Omega_N \, e^{\alpha \sum \cos\theta_i} = \frac{b}{Z} \frac{\partial Z}{\partial \alpha} = b \frac{\partial}{\partial \alpha}(\ln Z)$$

$$= b \frac{\partial}{\partial \alpha}\left(\ln\left(\frac{4\pi \sinh\alpha}{\alpha}\right)^N\right) = bN\left[\coth\alpha - \frac{1}{\alpha}\right]$$

Def'n $\mathcal{L}(\alpha) := \coth\alpha - \frac{1}{\alpha}$ is called Langevin fn

(similar to $\tanh\alpha$ )

Then $\langle R_z \rangle = bN\,\mathcal{L}(\alpha)$, w/ $\alpha = \dfrac{F_z b}{k_b T}$

Limits: $\lim_{F_z \to \infty} \langle R_z \rangle = bN$ - max extension

- if F_z small so that $\alpha \ll 1$, $\langle R_z \rangle = Nb\left(\frac{\alpha}{3} + O(\alpha^2)\right)$

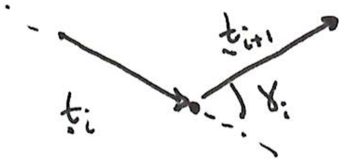
$$= \frac{Nb^2}{3k_bT} F_z + O(F_z^2)$$

Worm Like Chain Models

- FJC fails to explain experimental data at large forces → need to include bending stiffness

Discrete model (Kratky-Porod 1949)

Like FJC, but w/ internal energy to bend two links ~~proportional~~ w/ tangents $\underset{\sim}{t}_i$, $\underset{\sim}{t}_{i+1}$ proportional to $\underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+1}$



internal energy $E = -K \sum_{i=1}^{N} \underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+1} = -K \sum \cos\gamma_i$

(same form as FJC w/ ext. force!)

→ Partition fn $\quad Z = \int d\Omega_1 \dots d\Omega_N \exp\left(\frac{K}{k_bT} \sum \cos\gamma_i \right)$

$$\overset{\text{as before}}{=} \left(\frac{4\pi \sinh\lambda}{\lambda} \right)^N \quad \text{w/} \quad \lambda := \frac{K}{k_bT}$$

To compute $\quad \langle \underset{\sim}{R}^2 \rangle = \langle \left(\sum b \underset{\sim}{t}_i \right)^2 \rangle = b^2 \sum_{i,j} \langle \underset{\sim}{t}_i \cdot \underset{\sim}{t}_j \rangle$

(1) Nearest neighbor

$$\omega_1 := \langle \underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+1} \rangle = \langle \cos\gamma_i \rangle = \frac{1}{Z} \int d\Omega_1 \dots d\Omega_N \cos\gamma_i \, e^{\lambda \sum_{j=1}^{N} \cos\gamma_j}$$

$$= \frac{\int d\gamma_i \sin\gamma_i \exp(\lambda \cos\gamma_i) \cos\gamma_i}{\int d\gamma_i \sin\gamma_i \exp(\lambda\cos\gamma_i)}$$

all other terms have matching term in Z, so cancel

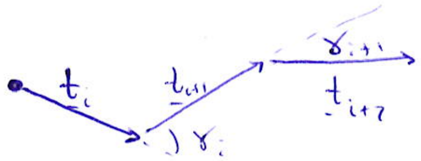
Observe: $\frac{\partial}{\partial\lambda}$(denom) = numer

$$= \frac{\partial}{\partial \lambda} \ln\left(\underbrace{\int d\gamma_i \sin\gamma_i \, e^{\lambda \cos\gamma_i}}_{\text{"} \iint d\phi_i \, d\gamma_i \sin\gamma_i \, e^{\lambda\cos\gamma_i}} \right) = \mathcal{L}(\lambda)$$

(Langevin fn)

(2) Consider <u>stiff</u> polymers, ie $\boxed{\lambda >> 1}$, & consider

$$\omega_n := \langle \underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+n} \rangle$$



$$\underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+n} = \cos\left(\gamma_i + \gamma_{i+1} \dots + \gamma_{i+n-1}\right)$$

$$= \cos\gamma_i \cos\left(\gamma_{i+1} + \dots \gamma_{i+n-1}\right) - \sin\gamma_i \sin\left(\gamma_{i+1} \dots \gamma_{i+n-1}\right)$$

- For $\lambda >> 1$, $|\gamma_i| << 1$ (stiff polymer can't bend much)

$$\rightarrow \langle \sin\gamma_i \rangle << \langle \cos\gamma_i \rangle$$

$$\therefore \omega_n \cong \langle \cos\gamma_i \rangle \langle \cos(\gamma_{i+1} \dots + \gamma_{i+n-1}) \rangle$$

$$= \omega_1 \cdot \omega_{|n|-1} \qquad \therefore \text{ By recursion } \boxed{\omega_n = (\omega_1)^{|n|}} = (\mathcal{L}(\lambda))^{|n|}$$

(* Modulus included as could have 'backwards' correlation, $n<0$)

(3) Back to $\langle \underset{\sim}{R}^2 \rangle$, for $\lambda >> 1$ (stiff)

$$\langle \underset{\sim}{R}^2 \rangle = b^2 \sum_{i,j=1}^{N} \langle \underset{\sim}{t}_i \cdot \underset{\sim}{t}_j \rangle = b^2 \sum_{i,j} \omega_1^{|i-j|}$$

$$= b^2 \sum_{i=1}^{N} \left[\sum_{j=1}^{i-1} \omega_1^{i-j} + 1 + \sum_{j=i+1}^{N} \omega_1^{j-i} \right]$$

from $t_i \cdot t_i = 1$

And $\omega_1 < 1$ since $\mathcal{L}(\lambda) < 1$ $\forall \lambda$

$\Rightarrow$ geometric series

$$= b^2 \sum_{i=1}^{N} \left[\frac{\omega_1 (1-\omega_1^{i-1})}{1-\omega_1} + \frac{1-\omega_1^{N+1-i}}{1-\omega_1} \right]$$

$$= \frac{b^2}{1-\omega_1} \left[\sum_{i=1}^{N} \omega_1 - \sum \omega_1^{i} + \sum 1 - \sum \omega_1^{N+1-i} \right]$$

$$\approx \frac{b^2 N (\omega_1 + 1)}{1-\omega_1} \quad \text{as} \quad N \to \infty$$

small in comparison as $N \to \infty$

Persistence length - take $\lambda \gg 1$, consider

$$\langle \underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+n} \rangle \sim \big(\underbrace{\mathcal{L}(\lambda)}_{=\coth\lambda - \frac{1}{\lambda}}\big)^{|n|} \sim \left(1 - \frac{1}{\lambda}\right)^{|n|} = \exp\left[|n| \ln\left(1 - \frac{1}{\lambda}\right)\right]$$

$$\underset{\text{expand log}}{\approx} \exp\left(-\frac{|n|}{\lambda}\right) = \exp\left(\frac{-|n| k_B T}{K}\right)$$

$$= \exp\left(-\frac{|n| b}{\xi_p}\right) \quad \text{w/} \quad \xi_p := \frac{K b}{k_B T}$$ the persistence length,

the scale on which tangent-tangent correlations decay

- If L is polymer length: (or scale at which you're viewing)
  - $\xi_p \gg L$ Stiff chain

[DNA] $\xi_p \ll L$ flexible chain - well modelled by FJC

[Microtubule] $\xi_p \simeq L$ semi-flexible

Continuous limit

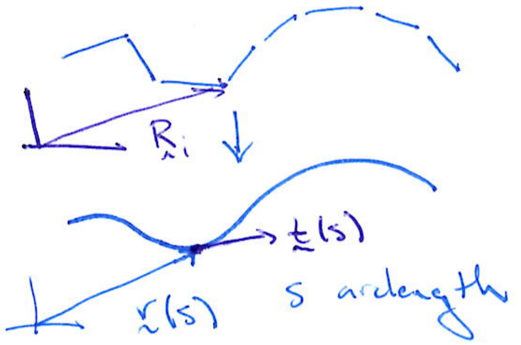
Goal: take limit $N \to \infty$, $b \to 0$ w/ $Nb = L$ fixed

Consider energy $H = -K \sum_{i=1}^{N} (\underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+1} - 1)$ shifted by constant so that energy $= 0$ in minimum

Now use $\frac{(\underset{\sim}{t}_{i+1} - \underset{\sim}{t}_i)^2}{2} = \frac{1}{2}\left(1 - 2\,\underset{\sim}{t}_{i+1} \cdot \underset{\sim}{t}_i + 1\right) = 1 - \underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+1}$

$$\Rightarrow H = \frac{K}{2} \sum (\underset{\sim}{t}_{i+1} - \underset{\sim}{t}_i)^2 = \frac{Kb}{2} \sum \underbrace{b}_{\to\, ds} \underbrace{\left(\frac{\underset{\sim}{t}_{i+1} - \underset{\sim}{t}_i}{b} \right)^2}_{\to \left(\frac{\partial \underset{\sim}{t}}{\partial s}\right)^2}$$

in the limit



$$\xrightarrow[N\to\infty,\ b\to 0]{} \frac{Kb}{2} \int_0^{L(=Nb)} \kappa^2(s)\, ds$$

where $|\kappa| = \left|\frac{\partial \underset{\sim}{t}}{\partial s}\right|$

is the <u>curvature</u>

Compare to 'classic result': elastic energy of an unstretchable, unshearable" beam

$$\mathcal{E}_{el} = \frac{EI}{2} \int_0^L \kappa^2\, ds\,, \quad EI = B \text{ is } \underline{\text{bending}} \text{ stiffness}$$

$\therefore$ we identify $Kb = B$, and persistence length

$$\xi_p = \frac{Kb}{k_bT} = \frac{B}{k_bT}$$

"so if know persis. length, can define bending stiffness"

Statistical Mech in Continuous Limit

Internal energy $H = \frac{B}{2}\int_0^L \left(\frac{\partial \underset{\sim}{t}}{\partial s}\right)^2 ds$

Partition function $Z = \int \underbrace{\mathcal{D}(\underset{\sim}{t}(s))}_{\text{defined via limiting process}} e^{-\beta H} \, \delta(|\underset{\sim}{t}(s)| - 1)$

$\langle \underset{\sim}{t}(s) \cdot \underset{\sim}{t}(s') \rangle = \exp\left(-\frac{|s-s'|}{\xi_p}\right)$ ← by taking limit of

$\langle t_i \cdot t_{i+n} \rangle \sim \exp\left(-\frac{|n| b}{\xi_p}\right)$

$$\therefore \langle \underset{\sim}{R}^2 \rangle = \left\langle \left(\int_0^L \underset{\sim}{t}(s)\, ds\right)^2 \right\rangle = \int_0^L ds \int_0^L ds' \langle \underset{\sim}{t}(s) \cdot \underset{\sim}{t}(s') \rangle$$

$$= \int_0^L\int_0^L ds\, ds' \exp\left(-\frac{|s-s'|}{\xi_p}\right) = 2\xi_p^2 \left(\frac{L}{\xi_p} - 1 + e^{-L/\xi_p}\right)$$

messy but doable integ.

$$= L^2 f_D\left(\frac{L}{\xi_p}\right) \quad \text{w/} \quad f_D(x) = \frac{2(x - 1 + e^{-x})}{x^2}$$

is Debye fn

Continuous filaments

We now develop a theory of elastic rods

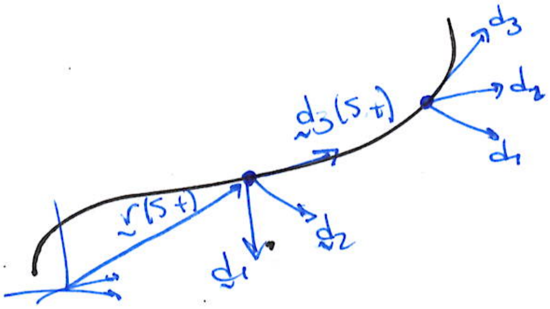
- suitable when stochastic motion irrelevant, ie when elastic energy much higher than $k_B T$
- good model for some bio polymers, and many 'macro structures', eg vine, hair, ~~axon~~ umbilical cord, elephant trunk, ..

1. Geometry

A rod is defined geometrically by a centreline curve $\underset{\sim}{r}(S,T)$, S is arclength in the stress-free configuration, and a material parameter, and T is time

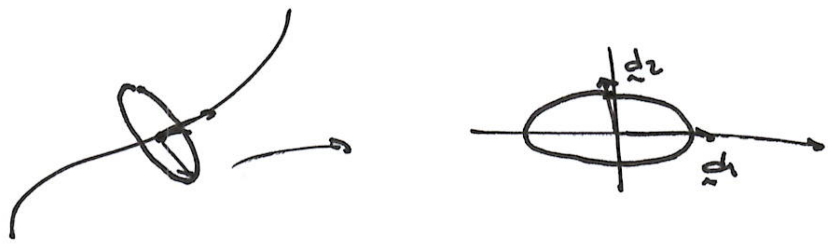
- The current arclength $s = \int_0^S \left| \frac{\partial \underset{\sim}{r}}{\partial S} \right| dS$
  - for unstretchable, ie inextensible rod, $s = S$

At each S, the rod is equipped w/ an orthonormal frame $\{\underset{\sim}{d}_1, \underset{\sim}{d}_2, \underset{\sim}{d}_3\}$



Discuss the point: take a 3D structure, which is slender, & collapse description to a central curve.

Let $\underset{\sim}{d}_1(S,T)$, $\underset{\sim}{d}_2(S,T)$ be unit vectors fixed in the material cross-section, and $\underset{\sim}{d}_3 = \underset{\sim}{d}_1 \wedge \underset{\sim}{d}_2$



For unshearable rod (most common) $\underset{\sim}{d}_3$ aligned w/ tangent $\frac{d\underset{\sim}{r}}{dS}$

- We can write a vector in local basis $\{\underset{\sim}{d}_1, \underset{\sim}{d}_2, \underset{\sim}{d}_3\}$ or in an inertial frame $\{\underset{\sim}{e}_1, \underset{\sim}{e}_2, \underset{\sim}{e}_3\}$

$$\underset{\sim}{a} = \sum a_i \underset{\sim}{d}_i = \sum a_j \underset{\sim}{e}_j \Rightarrow a_j = \sum_i (\underset{\sim}{d}_i \cdot \underset{\sim}{e}_j) a_i$$

$$\therefore \quad \text{ie} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \underbrace{\left(\underset{\sim}{d}_1 \,\middle|\, \underset{\sim}{d}_2 \,\middle|\, \underset{\sim}{d}_3 \right)}_{= D} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

Since frame orthonormal, $D^T D = D D^T = \mathbb{1}$

Alt - next page

$$\Rightarrow \frac{\partial D}{\partial S} D^T + D \frac{\partial D^T}{\partial S} = 0$$

Also, $\frac{\partial \underset{\sim}{d}_1}{\partial S} = \alpha \underset{\sim}{d}_1 + \beta \underset{\sim}{d}_2 + \gamma \underset{\sim}{d}_3$ since it's a basis

$$\Rightarrow \frac{\partial D}{\partial S} = \frac{\partial}{\partial S} \left(\underset{\sim}{d}_1 \,\middle|\, \underset{\sim}{d}_2 \,\middle|\, \underset{\sim}{d}_3 \right) = D U \quad \text{for some } U$$

Alt:

$$D^T D = \mathbb{1} \Rightarrow D^T D' + \underbrace{D^{T'} D}_{(D^T D')^T} = 0$$

$$\Rightarrow D^T D' + (D^T D')^T = 0$$

$$\Rightarrow D^T D' = U \quad \text{skew symmetric}$$

$$\Rightarrow D' = DU$$

$\therefore$ we have $0 = DUD^T + D(DU)^T$

$= DUD^T + DU^TD^T = D(U+U^T)D^T$,

$\Rightarrow U + U^T = 0$ (since $DD^T = \mathbb{1}$)

ie U anti-symmetric

Similarly, $\frac{\partial D}{\partial T} = DW$ w/ W antisymm $\left(\frac{\partial}{\partial S} \to \frac{\partial}{\partial T}\right)$

$\to$ can define axial vectors $\underset{\sim}{u} = \sum u_i \underset{\sim}{d}_i$, $\underset{\sim}{w} = \sum w_i \underset{\sim}{d}_i$

so that $U = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}$, $W = \begin{pmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{pmatrix}$ ★

$\underset{\sim}{u}, \underset{\sim}{w}$ describe how frame rotates in S, T

eg u_3 is rotation about $\underset{\sim}{d}_3$ along curve

Compatibility We must have $\frac{\partial^2 D}{\partial S \partial T} = \frac{\partial^2 D}{\partial T \partial S}$

$\Rightarrow 0 = \frac{\partial}{\partial T}(DU) - \frac{\partial}{\partial S}(DW) = \frac{\partial D}{\partial T} U + D\frac{\partial U}{\partial T} - \frac{\partial D}{\partial S} W - D\frac{\partial W}{\partial S}$

$= D[WU - UW] + D\left[\frac{\partial U}{\partial T} - \frac{\partial W}{\partial S}\right] \Rightarrow \frac{\partial U}{\partial T} - \frac{\partial W}{\partial S} = UW - WU$

★ $\frac{\partial \underset{\sim}{d}_i}{\partial S} = \underset{\sim}{u} \wedge \underset{\sim}{d}_i$, $\frac{\partial \underset{\sim}{d}_i}{\partial T} = \underset{\sim}{w} \wedge \underset{\sim}{d}_i$

Full kinematic description

$$\begin{cases} \dfrac{\partial \underset{\sim}{r}}{\partial S} = \underset{\sim}{v} \\[2ex] \dfrac{\partial \underset{\sim}{d_i}}{\partial S} = \underset{\sim}{u} \wedge \underset{\sim}{d_i} \qquad i = 1,2,3 \\[2ex] \dfrac{\partial \underset{\sim}{d_i}}{\partial T} = \underset{\sim}{w} \wedge \underset{\sim}{d_i} \end{cases}$$

$\underset{\sim}{v}$ stretch vector

$\underset{\sim}{u}$ strain (curvature) vector

$\underset{\sim}{w}$ spin vector

$$\star \left| \begin{array}{l} \text{Unshearable} \Rightarrow v_1 = v_2 = 0 \\ \text{Inextensible} \Rightarrow v_3 = 1 \quad \leftarrow \text{No axial stretch} \end{array} \right.$$

If $\{ \underset{\sim}{\tau}, \underset{\sim}{\nu}, \underset{\sim}{\beta} \}$ is standard Frenet-frame,

tangent normal binormal

then under $\star$, $\underset{\sim}{\tau} = \underset{\sim}{d_3}$ & $\underset{\sim}{d_1} = \underset{\sim}{\nu} \cos\varphi + \underset{\sim}{\beta} \sin\varphi$

$\underset{\sim}{d_2} = -\underset{\sim}{\nu} \sin\varphi + \underset{\sim}{\beta} \cos\varphi$

Frenet eq'ns

$$\begin{cases} \dfrac{\partial \underset{\sim}{\tau}}{\partial S} = \kappa \underset{\sim}{\nu} \\[2ex] \dfrac{\partial \underset{\sim}{\nu}}{\partial S} = \tau \underset{\sim}{\beta} - \kappa \underset{\sim}{\tau} \\[2ex] \dfrac{\partial \underset{\sim}{\beta}}{\partial S} = -\tau \underset{\sim}{\nu} \end{cases}$$

where $\kappa = \left| \dfrac{\partial \underset{\sim}{\tau}}{\partial S} \right|$ is curvature, and torsion τ is a measure of non-planarity.

- if $\dfrac{\partial \varphi}{\partial S} = 0$, can define $\underset{\sim}{d_1}, \underset{\sim}{d_2}$ by $\varphi = 0$, so $\underset{\sim}{d_1} = \underset{\sim}{\nu}$, $\underset{\sim}{d_2} = \underset{\sim}{\beta}$

then $\underset{\sim}{u} = (0, \kappa, \tau)$

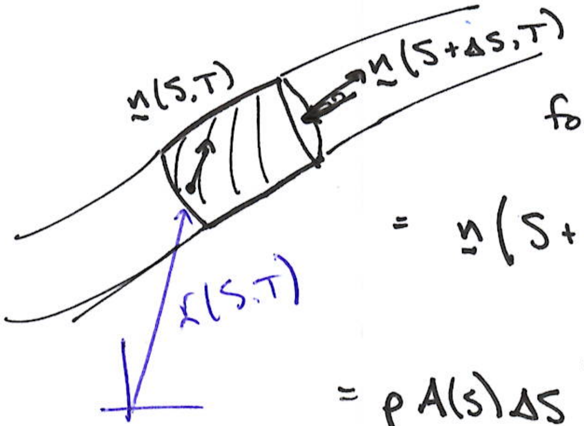
"excess twist"

More generally, $\underset{\sim}{u} = \left(\kappa \sin\varphi, \kappa \cos\varphi, \tau + \dfrac{\partial \varphi}{\partial S} \right)$

2. Mechanics

Let $\mathbf{n}(S,T)$ be the resultant force and $\mathbf{m}(S,T)$ resultant moment exerted by rod section $(S, L]$ on $[0, S)$

Balance of force:



force on section $(S, S+\Delta S)$

$$= \mathbf{n}(S+\Delta S, T) - \mathbf{n}(S,T) + \mathbf{f}\,\Delta S$$

force per unit length

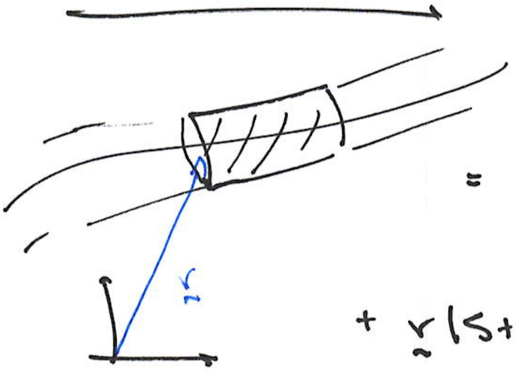
$$= \rho A(S)\Delta S \frac{\partial^2 \mathbf{r}}{\partial T^2}$$

density (ρ), area ($A(S)$)

Divide by ΔS,
Take $\Delta S \to 0$:

$$\boxed{\frac{\partial \mathbf{n}}{\partial S} + \mathbf{f} = \rho A \frac{\partial^2 \mathbf{r}}{\partial T^2}} \qquad (FB)$$

Balance of moments



Total moment on $(S, S+\Delta S)$

$$= \mathbf{m}(S+\Delta S, T) - \mathbf{m}(S,T)$$

$$+ \underbrace{\mathbf{r}(S+\Delta S, T)\wedge \mathbf{n}(S+\Delta S, T) - \mathbf{r}(S,T)\wedge\mathbf{n}(S,T)}_{*}$$

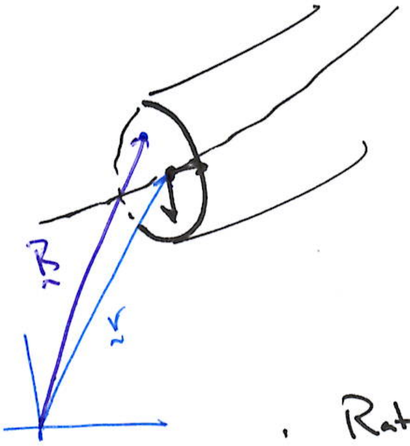
$$+ (\mathbf{r}\wedge\mathbf{f})\Delta S + \mathbf{l}\,\Delta S$$

external couple per unit length

Divide by ΔS, take $\Delta S \to 0$:

$$\frac{\partial}{\partial S}\left(\mathbf{m} + \mathbf{r}\wedge\mathbf{n}\right) + \mathbf{r}\wedge\mathbf{f} + \mathbf{l} = \text{Rate of chg of angul. mom'm per length}$$

Points in material given by $\mathbf{R} = \mathbf{r} + x_1 \mathbf{d}_1 + x_2 \mathbf{d}_2$



Ang mom per unit length $= \cancel{}\left[\int\!\!\int dx_1\, dx_2\; \mathbf{R}\wedge\rho\,\dot{\mathbf{R}}\right]$

i.e. $\dfrac{\partial \mathbf{R}}{\partial T}$

$\therefore$ Rate chg Ang Mom. per length $= \rho\int dx_1 dx_2\; \mathbf{R}\wedge\ddot{\mathbf{R}}$

⋮

$$\to \frac{\partial}{\partial S}\left(\mathbf{m} + \mathbf{r}\wedge\mathbf{n}\right) + \mathbf{r}\wedge\mathbf{f} + \mathbf{l} = \rho A\, \mathbf{r}\wedge\ddot{\mathbf{r}} + \rho I_2\, \mathbf{d}_1\wedge\ddot{\mathbf{d}}_1 + \rho I_1\, \mathbf{d}_2\wedge\ddot{\mathbf{d}}_2$$

where $I_1 = \int x_1^2\, dx_1 dx_2$, $I_2 = \int x_2^2\, dx_1 dx_2$ are 2^{nd} moments of area.

$$\Rightarrow \boxed{\frac{\partial \mathbf{m}}{\partial S} + \frac{\partial \mathbf{r}}{\partial S}\wedge\mathbf{n} + \mathbf{l} = \rho I_2\, \mathbf{d}_1\wedge\ddot{\mathbf{d}}_1 + \rho I_1\, \mathbf{d}_2\wedge\ddot{\mathbf{d}}_2} \quad \text{(MB)}$$

↑ by FB

3. Constitutive Laws

To close the system we must relate force $\underset{\sim}{n}$ and moment $\underset{\sim}{m}$ to strain $\underset{\sim}{v}$ and $\underset{\sim}{u}$.

We'll consider the simplest and most common form:

$$\underset{\sim}{m} = EI_1 (u_1 - \hat{u}_1) \underset{\sim}{d}_1 + EI_2 (u_2 - \hat{u}_2) \underset{\sim}{d}_2 + \mu J (u_3 - \hat{u}_3) \underset{\sim}{d}_3$$

E - Young's modulus
μ - shear modulus
} Mechanical par's

I_1, I_2, J - depend on cross-section geometry

$\hat{u}_i$ - intrinsic curvatures

For extensible rod, we also have $n_3 = \underset{\sim}{n} \cdot \underset{\sim}{d}_3 = EA(\alpha - 1)$

w/ $\alpha := \frac{\partial s}{\partial S}$ axial stretch, A is area

"Hooke's law for stretching rod"

($\alpha \equiv 1$ for inextensible)

4. Boundary, initial conditions

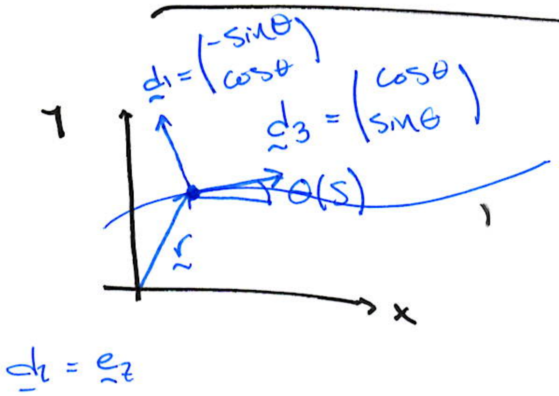
Many possibilities ...

eg clamped bdy $\Rightarrow$ impose $\underset{\sim}{r}$, $\{\underset{\sim}{d}_i\}$

pinned bdy $\Rightarrow$ impose $\underset{\sim}{r}$, $\underset{\sim}{m} = \underset{\sim}{0}$

free bdy $\Rightarrow$ impose $\underset{\sim}{n} = \underset{\sim}{m} = \underset{\sim}{0}$

Ex. - Planar inextensible rod



Geometry: $\underset{\sim}{r} = \begin{pmatrix} x(s,t) \\ y(s,t) \end{pmatrix}$

$\underset{\sim}{r}' = \underset{\sim}{d}_3 \rightarrow \quad x' = \cos\theta \quad (1)$

$y' = \sin\theta \quad (2)$

$\underset{\sim}{d}_3' = \theta' \underset{\sim}{d}_1 \rightarrow \quad \underset{\sim}{u} = (0, \underset{\theta'}{\underset{\shortparallel}{\kappa}}, 0)$

Mech Let $\underset{\sim}{n} = F \underset{\sim}{e}_x + G \underset{\sim}{e}_y, \quad \underset{\sim}{m} = m \underset{\sim}{e}_z$

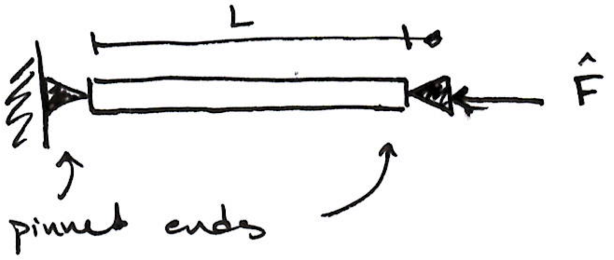
FB $\rightarrow \quad F' = \rho A \ddot{x}, \quad G' = \rho A \ddot{y} \quad (3), (4)$

MB $\rightarrow \quad m' + G\cos\theta - F\sin\theta = \rho I_2 \ddot{\theta} \quad (5)$

Constit $\quad m = EI_2 \kappa = EI_2 \theta' \quad (6)$

+ 6 BC & initial profile for $\{x, y, \theta\}$

Euler Buckling



- impose compressive force $\hat{F}$
- At which $\hat{F}$ does beam buckle?

- Static $\rightarrow$ drop time deriv's. $\overset{3,4}{\Rightarrow} F' = G' = 0$
- align $\hat{F}$ w/ $\underset{\sim}{e}_x \Rightarrow F = \hat{F}, \; G = 0$ (compressive $\Leftrightarrow \hat{F} < 0$)
- $|\theta| \ll 1 \rightarrow \sin\theta \approx \theta, \; \cos\theta \approx 1 \overset{1,2}{\Rightarrow} x \approx s, \; y' \approx \theta$

$\rightarrow$ BVP $\quad EI\theta'' - \hat{F}\theta = 0, \quad \theta' = 0$ at $s = 0, L$

(↑ pinned)

has sol'ns $\Theta(S) = a\cos\left(\frac{n\pi S}{L}\right)$ if $\hat{F} = F_n = \frac{-EI n^2 \pi^2}{L^2}$

Reduction to Beam Eq'n (static)

Assumption: θ small. Same steps but treat y as dep. var.

- $X \approx S \rightarrow$ can write $y = w(x)$
- $y' \approx \theta$ and $EI\theta'' - F\theta + G = 0$

take $\frac{d}{dS}$:

$EIw'''' - Fw''(x) = 0$ ← classic beam eq'n (F unknown)