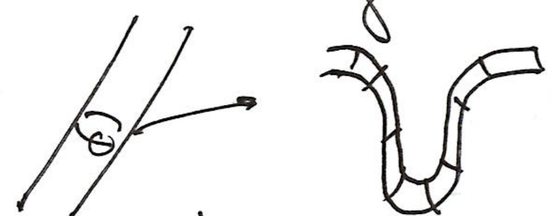
Biofilaments Overview

- Motivation - Filamentary structures (long and slender) with elastic properties are abundant in biology - appear across many lengthscales.

Ex.
- ▫ Subcellular DNA, protein filaments - eg make up cytoskeleton, give structure
  - axon . nerve fiber

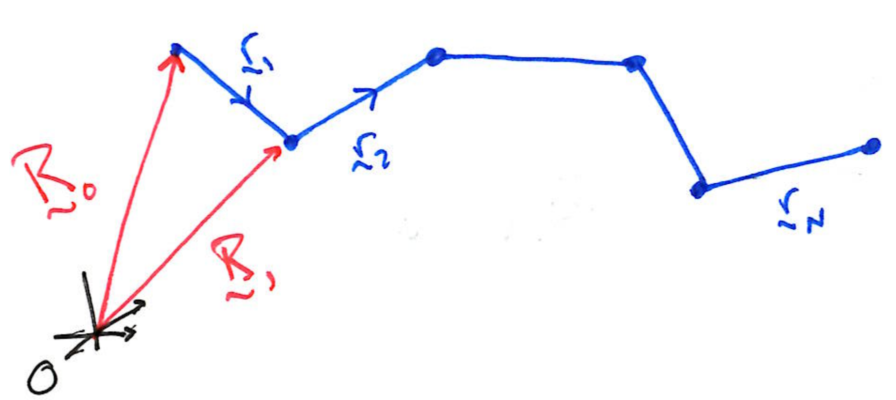
- ▫ Cellular . Mostly biomembrane (next module) - but a line of cells may behave as filament . eg crypts in intestine



- ▫ Tissue / organ . arteries, airways, umbilical cord muscle fibers, elephant's trunk, plant! branch, stem, roots
- ▫ Organism worm, snake

- The mechanical properties / behaviour crucial to function - natural shape . stiffness . resistance to bending, stretching, twisting

1.1 The freely-jointed chain model (FJC)



<u>Assume</u>: i) N links of fixed length b

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

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

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

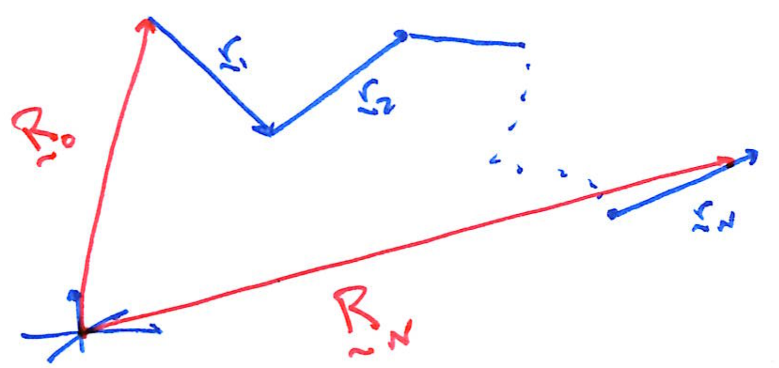
$$\langle \mathbf{a} \rangle := \int_{(\mathbb{R}^3)^N} dV\, \mathbf{a}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)\, p(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \quad \text{where}$$

$p(\mathbf{r}_1, \dots, \mathbf{r}_N)$ is the probability distribution function for <u>configuration</u> <u>state</u> $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N$

~~Foo~~ For our assumptions,

$$p = \prod_{i=1}^{N} \frac{1}{4\pi b^2}\, \delta\big(\overbrace{|\mathbf{r}_i| - b}^{\text{since } |\mathbf{r}_i| \text{ must } = b}\big)$$

$\mathbf{r}_i$ lives on sphere radius b



End-to-end displacement $\mathbf{R} := \mathbf{R}_N - \mathbf{R}_0$

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

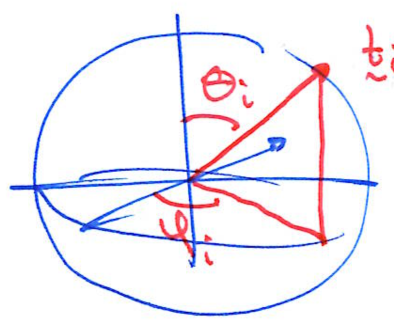
Its mean value (avg) is

$$\langle \mathbf{R} \rangle = \int_{(\mathbb{R}^3)^N} dV \left(\sum_{i=1}^{N} b\, \mathbf{t}_i \right) \frac{1}{(4\pi b^2)^N} \cdot \underbrace{\delta\big(|\mathbf{r}_1| - b\big)\, \delta\big(|\mathbf{r}_2| - b\big) \cdots \delta\big(|\mathbf{r}_N| - b\big)}_{\Downarrow}$$

integ. over sphere radius b

$$= \frac{(b^2)^N}{(4\pi b^2)^N} \cdot b \int d\Omega_1\, d\Omega_2 \dots d\Omega_N \cdot \sum_{i=1}^{N} \mathbf{t}_i$$

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



$$\mathbf{t}_i = \begin{pmatrix} \sin\theta_i \cos\varphi_i \\ \sin\theta_i \sin\varphi_i \\ \cos\theta_i \end{pmatrix}$$

Note: each integral indep.

and $\displaystyle\int d\Omega_i\, \mathbf{t}_i = \int_0^{2\pi}\!\!\int_0^{\pi} \mathbf{t}_i \sin\theta_i\, d\theta_i\, d\varphi_i = \mathbf{0}$

$\therefore \langle \mathbf{R} \rangle = \mathbf{0}$

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.

$$\underset{\sim}{R}^2 = \sum_{i=1}^{N} \underset{\sim}{r}_i \cdot \sum_{j=1}^{N} \underset{\sim}{r}_j = \sum_{i=1}^{N} \underset{\sim}{r}_i \cdot \underset{\sim}{r}_i + \sum_{i \neq j} \underset{\sim}{r}_i \cdot \underset{\sim}{r}_j$$

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

and $\langle \underset{\sim}{r}_i \rangle = \underset{\sim}{0}$ by similar calc as above

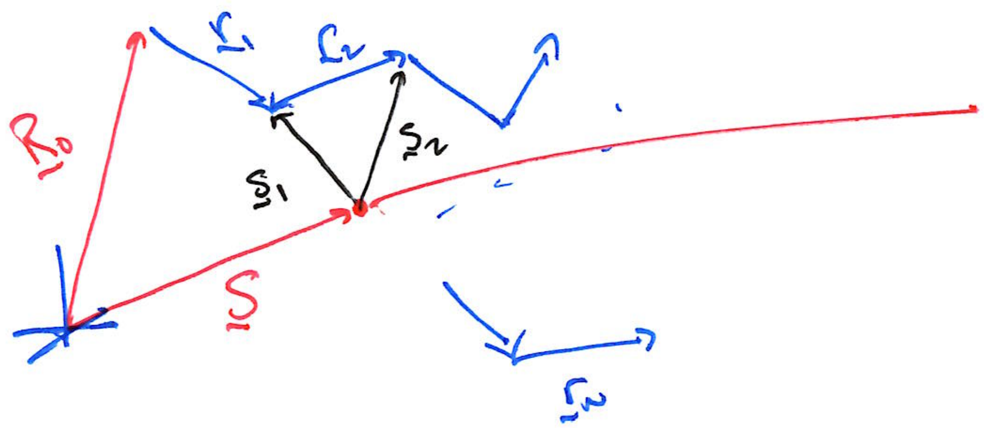
$$\therefore \langle \underset{\sim}{R}^2 \rangle = \langle \sum_{i=1}^{N} \underset{\sim}{r}_i \cdot \underset{\sim}{r}_i \rangle = N \langle \underset{\sim}{r}_1 \cdot \underset{\sim}{r}_1 \rangle \quad \text{by symmetry}$$

$$= N \langle b^2 \rangle = N b^2 \underbrace{\int_{(\mathbb{R}^3)^N} dV \, p(\underset{\sim}{r}_1, \ldots \underset{\sim}{r}_N)}_{=1 \text{ by defn of p.d.f.}} = N b^2$$

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

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

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



centroid $\underset{\sim}{S} = \frac{1}{N+1} \sum_{i=0}^{N} \underset{\sim}{R}_i$ Define $\underset{\sim}{s}_i = \underset{\sim}{R}_i - \underset{\sim}{S}$

we want to compute $s^2 = \frac{1}{N+1} \sum_{i=0}^{N} \underset{\sim}{s}_i \cdot \underset{\sim}{s}_i$

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

Proof: see problem sheets

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

We showed $\langle \underset{\sim}{r}_p \cdot \underset{\sim}{r}_q \rangle = 0$ if $p \ne q$, $\rightarrow \langle \underset{\sim}{r}_{ij}^2 \rangle = (j-i) b^2$

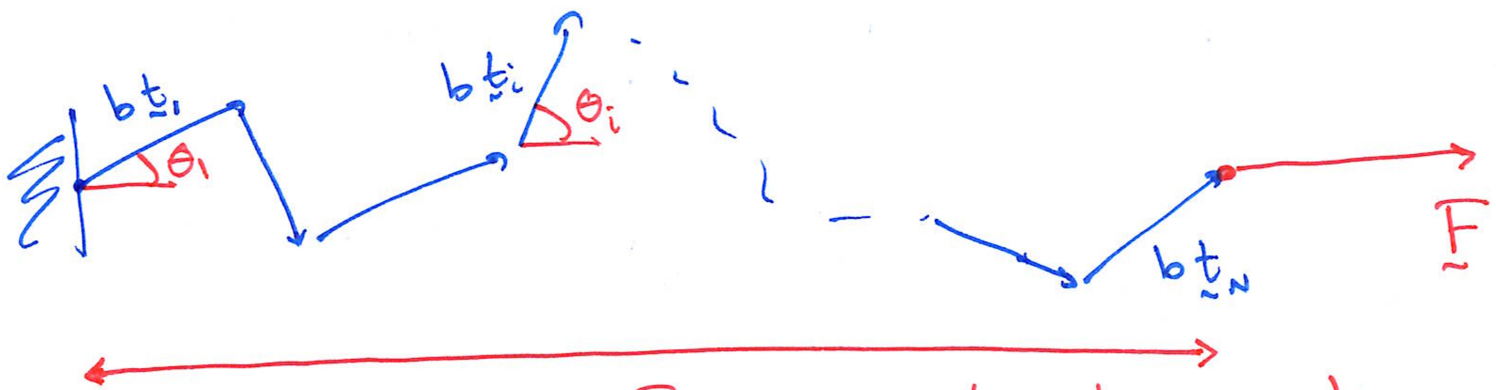
and $\langle \underset{\sim}{r}_p \cdot \underset{\sim}{r}_p \rangle = b^2$

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

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

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

FJC with external force



$\underset{\sim}{F} = F_z \underset{\sim}{e}_z$ force

$R_z = \underset{\sim}{R} \cdot \underset{\sim}{e}_z$ displacement

Assumptions

i) FJC with one end fixed

ii) Constant force

iii) Equilibrium w/ thermal bath, temp. T

Goal Find force - displacement relation

Note: $\theta_1, \theta_2, \cdots \theta_N$ no longer unif. distributed

[Recall: $m\ddot{x} = F = -\nabla V \rightarrow m\ddot{x}\dot{x} = F\dot{x} = -V'(x)\dot{x} \rightarrow \frac{1}{2}m\dot{x}^2 + \underbrace{V(x)}_{\text{internal energy}} = E = \frac{1}{2}m\dot{x}^2 \underbrace{- Fx}_{\text{work}}$

$\therefore$ internal energy $= -Fx$]

The work to extend chain is $W = \underset{\sim}{F} \cdot \underset{\sim}{R}$, so total internal energy is

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

Statistical Mechanics

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

$$\mathrm{Prob}\begin{pmatrix}\text{system in state} \\ \{\theta_1, \theta_2, \ldots \theta_N\}\end{pmatrix} = \frac{\exp\left(-\dfrac{E(\theta_1, \ldots, \theta_N)}{k_b T}\right)}{Z}$$

where $E(\theta_1, \ldots \theta_N)$ is internal energy of state,

k_b is Boltzmann's constant, and $Z = \int d\Omega_1 \ldots d\Omega_N \exp\left(-\dfrac{E(\theta_1, \ldots \theta_N)}{k_b T}\right)$

is partition function, $d\Omega_i = d\theta_i\, d\varphi_i \sin\theta_i$ are solid angles for integ. over spheres.

"weighted sum" over all possible configurations

- Observe: $E(\theta_1, \ldots \theta_N)$ high $\rightarrow$ $P(\{\theta_1, \ldots \theta_N\})$ is low

- We have $E = -F_z\, b \sum_{i=1}^{N} \cos\theta_i \Rightarrow Z = \int d\Omega_1 \ldots d\Omega_N \exp\left(\dfrac{F_z b}{k_b T} \sum_{i=1}^{N} \cos\theta_i\right)$

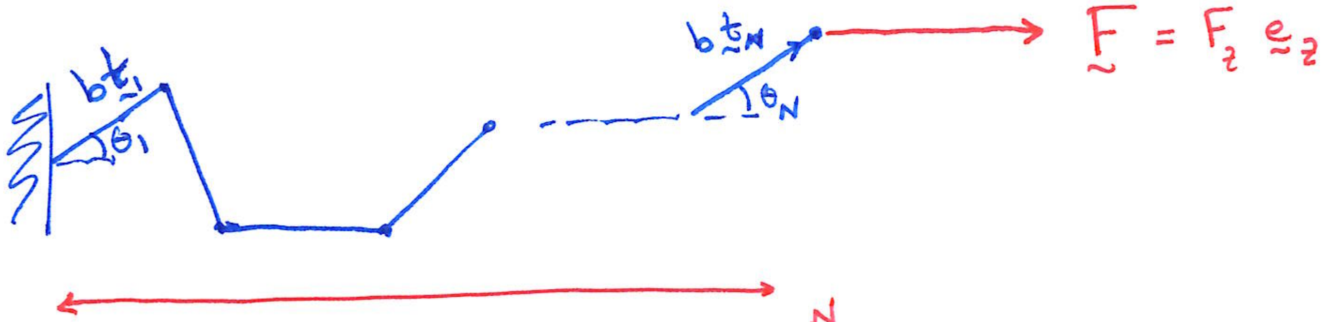
$$\rightarrow Z = \prod_{i=1}^{N} \int_0^{2\pi}\int_0^{\pi} e^{\alpha \cos\theta_i} \sin\theta_i \, d\theta_i \, d\varphi_i$$

w/ $\alpha := \dfrac{F_z b}{k_b T}$

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

$$\rightarrow \boxed{Z = \left(\frac{4\pi \sinh\alpha}{\alpha} \right)^N}$$

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



$$R_z = \underset{\sim}{R} \cdot \underset{\sim}{e}_z = b \sum_{i=1}^{N} \cos\theta_i$$

$$P(\{\theta_1, \dots \theta_N\}) = \frac{\exp\left(-\frac{E(\theta_1, \dots \theta_N)}{k_b T}\right)}{Z}$$

Recall

$$\left[\ Z = \int d\Omega_1 \dots d\Omega_N \exp\left(\alpha \sum_{i=1}^{N} \cos\theta_i\right)\ \right]$$

$$Z = \left(\frac{4\pi \sinh\alpha}{\alpha}\right)^N \quad \text{w/} \quad \alpha = \frac{F_z b}{k_b T}$$

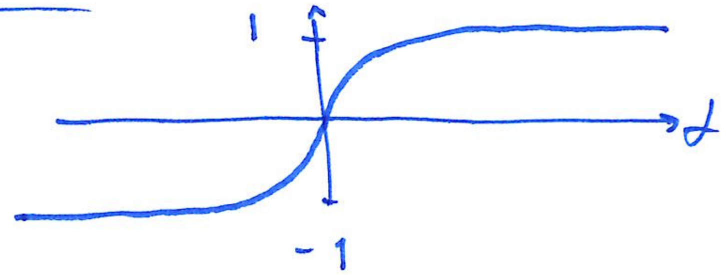
$$P(\{\theta_1, \dots \theta_N\}) = \left(\frac{\alpha}{4\pi \sinh\alpha}\right)^N e^{\alpha \sum_{i=1}^{N} \cos\theta_i}$$

Avg. displacement $\langle R_z \rangle = \int d\Omega_1 \dots d\Omega_N \left(b \sum_{i=1}^{N} \cos\theta_i\right) \frac{e^{\alpha \sum_{i=1}^{N} \cos\theta_i}}{Z}$

$$= \frac{b}{Z} \frac{\partial}{\partial\alpha} \int d\Omega_1 \dots d\Omega_N\, e^{\alpha \sum_{i=1}^{N} \cos\theta_i} = \frac{b}{Z} \frac{\partial}{\partial\alpha} Z = b \frac{\partial}{\partial\alpha} \ln Z = b \frac{\partial}{\partial\alpha}\left(\ln\left[\left(\frac{4\pi\sinh\alpha}{\alpha}\right)^N\right]\right)$$

$$= \boxed{bN\left[\coth\alpha - \frac{1}{\alpha}\right] = \langle R_z \rangle}$$

__Defn__ $\mathcal{L}(\alpha) := \coth\alpha - \frac{1}{\alpha}$ is called __Langevin function__ - similar to $\tanh\alpha$



$$\langle R_z \rangle = bN\,\mathcal{L}(\alpha)$$

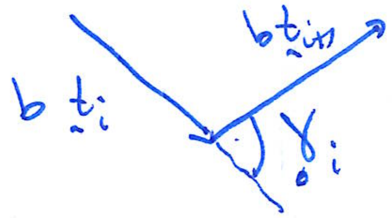
Limits: $\lim_{F_z \to \infty} \langle R_z \rangle = bN$ ← max extension

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

Worm Like Chain Model

FJC fails to explain exp't'al data at large forces → need to include bending stiffness

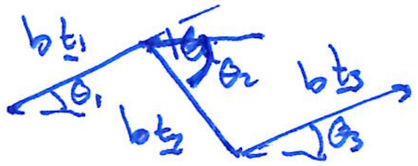
Discrete model (Kratky - Porod 1949) → Like FJC, but w/ internal energy to bend two links w/ tangents $\mathbf{t}_i$, $\mathbf{t}_{i+1}$ proportional to $\mathbf{t}_i \cdot \mathbf{t}_{i+1}$



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

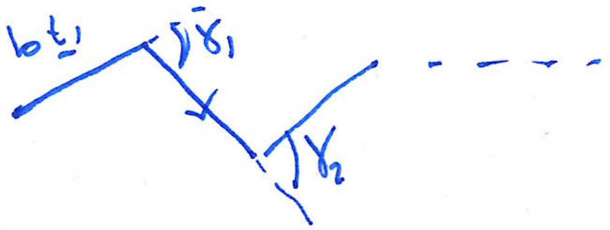
Compare:

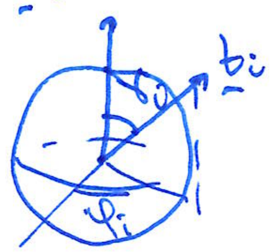
FJC w/ external force



→ Partition function

WLC





$$Z = \int d\Omega_1 \dots d\Omega_N \exp\left(\frac{K}{k_b T} \sum \cos\gamma_i\right)$$

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

$$\lambda := \frac{K}{k_b T}$$

$$\rightarrow Z = \left(\frac{4\pi \sinh\lambda}{\lambda}\right)^N$$

as before

. To compute $\langle \mathbf{R}^2 \rangle = \left\langle \left(\sum_{i=1}^{N} b\,\mathbf{t}_i\right)^2 \right\rangle = b^2 \sum_{i,j} \langle \mathbf{t}_i \cdot \mathbf{t}_j \rangle$

(i) Nearest neighbor: $w_1 := \langle \underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+1} \rangle = \langle \cos\gamma_i \rangle = \frac{1}{Z}\int d\Omega_1 \ldots d\Omega_N \cdot \cos\gamma_i \cdot \exp\left(\lambda \sum_j \cos\gamma_j\right)$

$$= \frac{\int d\Omega_i \cos\gamma_i \, e^{\lambda\cos\gamma_i}}{\int d\Omega_i \, e^{\lambda\cos\gamma_i}} = \frac{\partial}{\partial\lambda}\ln\left(\int_0^{2\pi}\int_0^{\pi} d\gamma_i \, d\varphi_i \sin\gamma_i \, e^{\lambda\cos\gamma_i}\right)$$

$= \mathcal{L}(\lambda)$ Langevin fn.

all other terms have matching term in Z, so cancel

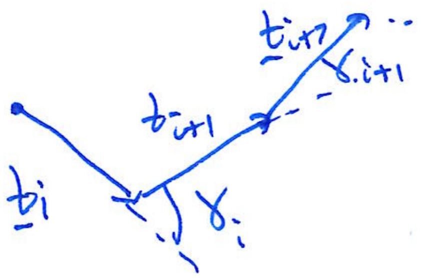
Observe: numer $= \frac{\partial}{\partial\lambda}$ (denom)

(ii) Consider stiff polymers, ie $\boxed{\lambda \gg 1}$, consider:

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

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

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



$\cdot\ \lambda \gg 1 \Rightarrow |\gamma_i| \ll 1$ (stiff polymer can't bend much)

$\rightarrow |\sin\gamma_i| \ll |\cos\gamma_i|$ $\therefore$ $w_n \cong \langle \cos\gamma_i \rangle \langle \cos(\gamma_{i+1} + \cdots + \gamma_{i+n-1}) \rangle$

$= w_1 \cdot w_{|n|-1}$ ← Modulus allows for $n<0$, "backwards" correlation

$\therefore$ By recursion, $\boxed{w_n \cong (w_1)^{|n|} = (\mathcal{L}(\lambda))^{|n|}}$

(iii) Back to $\langle \underset{\sim}{R}^2 \rangle$, in limit $\lambda \gg 1$,

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

Note $|\omega_1| < 1$ since $|\mathcal{L}(\lambda)| < 1$ $\Rightarrow$ geom. series

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

small in comparison as $N \to \infty$

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

Persistance length ($\lambda \gg 1$), consider $\langle \underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+n} \rangle \approx (\mathcal{L}(\lambda))^{|n|} \sim \left(1 - \frac{1}{\lambda}\right)^{|n|}$

$\mathcal{L}(\lambda) = \coth \lambda - \frac{1}{\lambda}$

$$= \exp\left(|n| \ln \left(1 - \frac{1}{\lambda}\right)\right) \underset{\text{expand log}}{\approx} \exp\left(\frac{-|n|}{\lambda}\right) = \exp\left(\frac{-|n| k_b T}{K}\right) = \exp\left(\frac{-|n| b}{\xi_p}\right), \quad \xi_p := \frac{K b}{k_b T}$$

ξ_p gives scale on which tangent-tangent correlations decay.

- If L is polymer length (or scale at which viewing) is persistance length
- $\xi_p \gg L$ - stiff chain
- $\xi_p \ll L$ flexible chain (FJC valid)

$\uparrow$ DNA

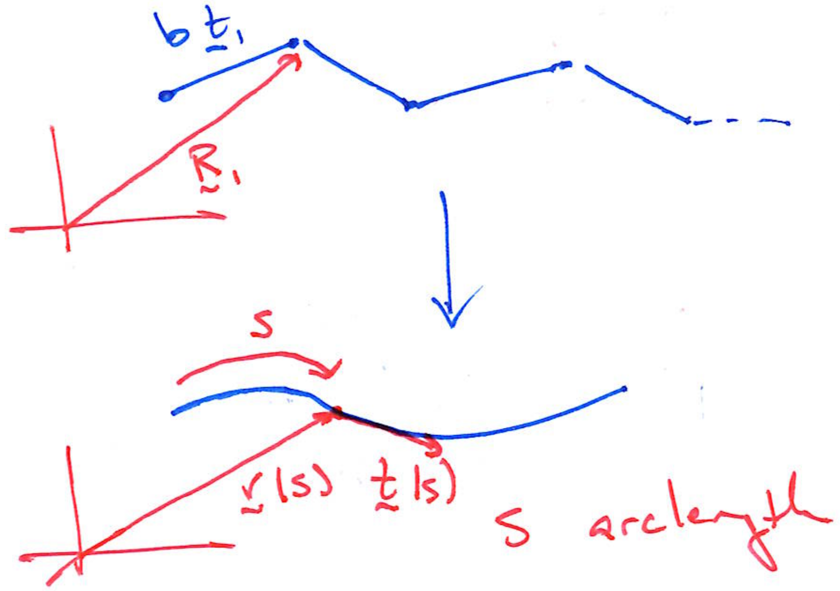
Continuous Limit

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

Consider energy $H = -K \sum_{i=1}^{N} \left(\underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+1} - 1 \right)$ ← shifts energy by constant so that min energy $= 0$.

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

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



in limit $N \to \infty$, $b \to 0$:

$$H \to \frac{Kb}{2} \int_0^L \kappa^2(s)\, ds \quad \text{where } |\kappa| = \left| \frac{\partial \underset{\sim}{t}}{\partial s} \right| \text{ is the } \underline{\text{curvature}}$$

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

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

$\boxed{Kb = B}$ so persistance length $\xi_p = \frac{Kb}{k_B T} = \frac{B}{k_B T}$

Statistical Mechanics in Continuous Limit

Internal energy $H = \frac{B}{2}\int_0^L \kappa^2(s)\,ds$. Compute $\langle \underset{\sim}{R}^2 \rangle$

Partition fn $Z = \int D(\underset{\sim}{t}(s))\, e^{-\beta H}\, \delta(|\underset{\sim}{t}(s)| - 1)$

↳ defined via limiting process

$\langle \underset{\sim}{t}(s) \cdot \underset{\sim}{t}(s') \rangle = \exp\left(-\frac{|s-s'|}{\xi_p}\right)$ by taking limit of $\langle \underset{\sim}{t}_i \cdot \underset{\sim}{t}_{i+n} \rangle \sim \exp\left(\frac{-|n|\, b}{\xi_p}\right)$

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

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

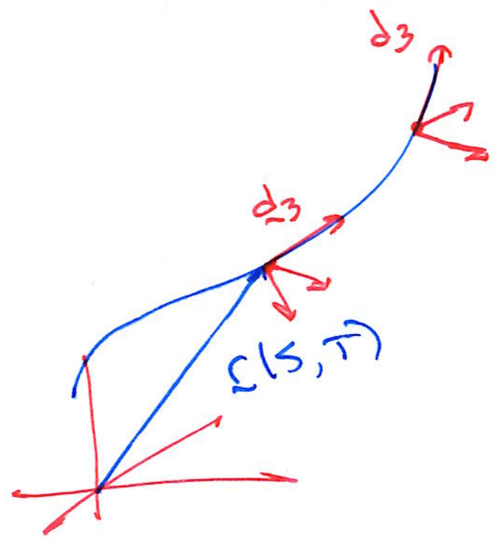
messy but doable integral

w/ $f_D(x) = \frac{2(x - 1 + e^{-x})}{x^2}$ is Debye fn

Continuous filaments - We now develop a theory of elastic rods. - Suitable when stochastic motion irrelevant - (elastic energy much higher than k_bT). good model for some biopolymers, many macrostructures, eg vine, hair, umbilical cord, etc..

Ingredients: 1) Geometry 2) Mechanics 3) Constitutive Law

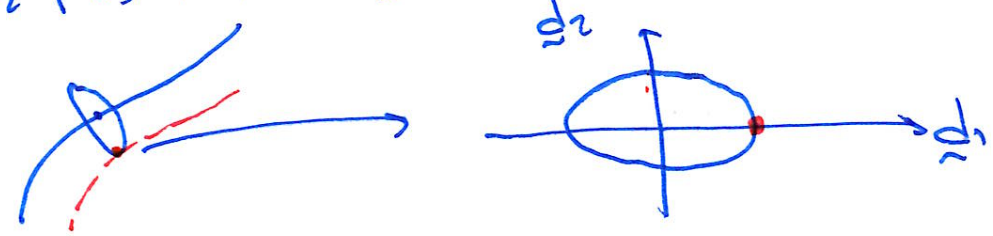
1. Geometry. A rod is defined geometrically by a **central curve** $\underset{\sim}{r}(S,T)$, S is arclength in stress-free configuration, and T is time.



- The **current** arclength $s = \int_0^S \left| \frac{\partial \underset{\sim}{r}}{\partial \tilde{S}} \right| d\tilde{S}$. for **unstretchable** or **inextensible** rod, $s = S$

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

Let $\underset{\sim}{d}_1(S,T)$, $\underset{\sim}{d}_2(S,T)$ be unit vectors **fixed** in each material cross-section



, $\underset{\sim}{d}_3 = \underset{\sim}{d}_1 \wedge \underset{\sim}{d}_2$

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

· we can write any vector in basis $\{\underset{\sim}{d}_1, \underset{\sim}{d}_2, \underset{\sim}{d}_3\}$ or in an fixed lab frame $\{\underset{\sim}{e}_1, \underset{\sim}{e}_2, \underset{\sim}{e}_3\}$. $\underset{\sim}{a} = \sum a_i \underset{\sim}{d}_i = \sum a_j \underset{\sim}{e}_j \Rightarrow a_j = \sum_i (\underset{\sim}{d}_i \cdot \underset{\sim}{e}_j) a_i$

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,

$$D^T D = D D^T = \mathbb{1}$$

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

Also, $\frac{\partial \underset{\sim}{d}_i}{\partial S} = \alpha \underset{\sim}{d}_1 + \beta \underset{\sim}{d}_2 + \gamma \underset{\sim}{d}_3$

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

$$\therefore 0 = DUD^T + D(DU)^T = DUD^T + DU^T D^T = D(U + U^T) D^T \Rightarrow U + U^T = 0$$

ie U is antisymmetric

Similarly, $\frac{\partial D}{\partial T} = DW$ for some antisymm. W → can define axial vectors

$\underset{\sim}{u} = \sum u_i \underset{\sim}{d}_i$ so that $U = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}$, $W = \begin{pmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{pmatrix}$

$\underset{\sim}{w} = \sum w_i \underset{\sim}{d}_i$

equivalently,

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

$\underset{\sim}{u}, \underset{\sim}{w}$ describe how material frame rotates

in S, T

<u>Compatibility</u> . Require $\dfrac{\partial^2 D}{\partial S \partial T} = \dfrac{\partial^2 D}{\partial T \partial S}$

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

$$- \frac{\partial D}{\partial S}W - D\frac{\partial W}{\partial S} = D(WU - UW) + D\left(\frac{\partial U}{\partial T} - \frac{\partial W}{\partial S}\right)$$

$$\Rightarrow \boxed{\frac{\partial U}{\partial T} - \frac{\partial W}{\partial S} = -WU + UW}$$

Full Kinematics Description

$$\left\{\begin{array}{ll} \dfrac{\partial \boldsymbol{r}}{\partial S} = \boldsymbol{v} & \boldsymbol{v} \text{ stretch vector} \\[2ex] \dfrac{\partial \boldsymbol{d}_i}{\partial S} = \boldsymbol{u} \wedge \boldsymbol{d}_i \quad i=1,2,3 & \boldsymbol{u} \text{ strain (curvature) vector} \\[2ex] \dfrac{\partial \boldsymbol{d}_i}{\partial T} = \boldsymbol{w} \wedge \boldsymbol{d}_i & \boldsymbol{w} \text{ spin vector} \end{array}\right.$$

★ Unshearable $\Rightarrow v_1 = v_2 = 0$

$\left(\boldsymbol{v} = \sum v_i \boldsymbol{d}_i \right)$

★ Inextensible $\Rightarrow v_3 = 1$

no axial stretch allowed.

Standard Frenet equations

$\{\boldsymbol{\tau}, \boldsymbol{\nu}, \boldsymbol{\beta}\}$ orthon. basis for space curve, satisfying:

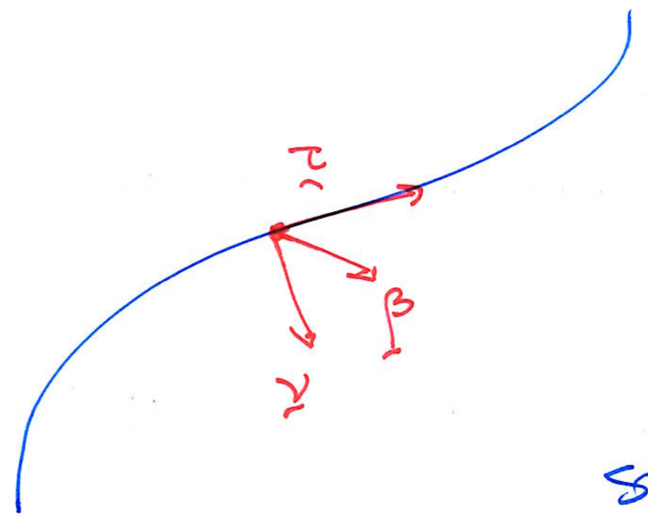
tangent, normal, binormal

$$\frac{\partial \boldsymbol{r}}{\partial S} = \boldsymbol{\tau}$$

$$\left\{\begin{array}{l} \dfrac{\partial \boldsymbol{\tau}}{\partial S} = \kappa \boldsymbol{\nu} \\[2ex] \dfrac{\partial \boldsymbol{\nu}}{\partial S} = \tau \boldsymbol{\beta} - \kappa \boldsymbol{\tau} \\[2ex] \dfrac{\partial \boldsymbol{\beta}}{\partial S} = -\tau \boldsymbol{\nu} \end{array}\right.$$

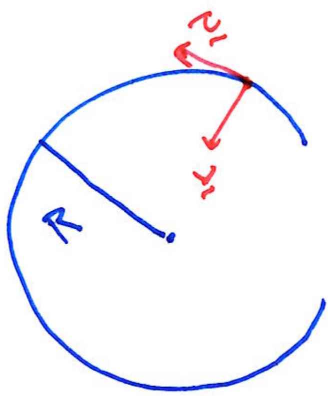
$\kappa = \left| \dfrac{\partial \boldsymbol{\tau}}{\partial S} \right|$ is curvature,

τ is torsion & a measure of non-planarity



• Properties only of space curve

Ex 1 Ring (constant curvature)



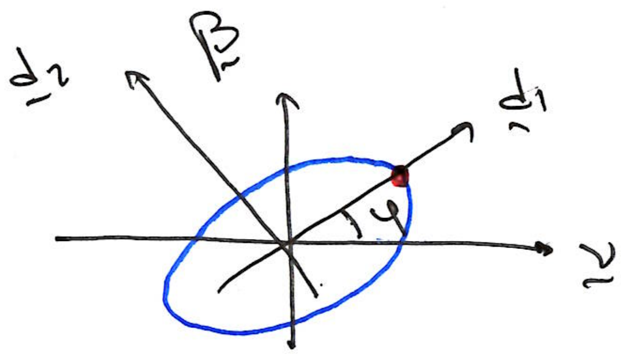
$\kappa = \frac{1}{R}$, $\tau = 0$

Under assumptions of inext., unshearable,

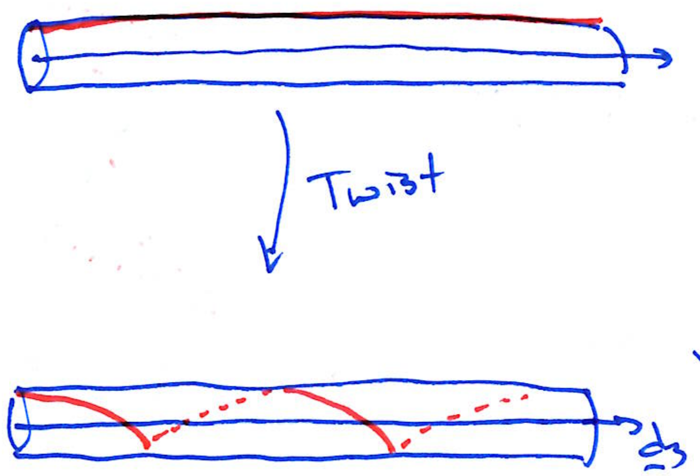
$\underset{\sim}{\tau} = \underset{\sim}{d}_3$, and

$\underset{\sim}{d}_1 = \underset{\sim}{\nu} \cos\varphi + \underset{\sim}{\beta} \sin\varphi$

$\underset{\sim}{d}_2 = -\underset{\sim}{\nu} \sin\varphi + \underset{\sim}{\beta} \cos\varphi$



Ex2



$\kappa = \tau = 0$

$\kappa = \tau = 0$

$\frac{\partial \varphi}{\partial s} \neq 0$

$u_1 = u_2 = 0$, $u_3 \neq 0$

- if $\frac{\partial \varphi}{\partial s} = 0$, we can define $\underset{\sim}{d}_1, \underset{\sim}{d}_2$ by $\varphi \equiv 0 \rightarrow \underset{\sim}{d}_1 = \underset{\sim}{\nu}$, $\underset{\sim}{d}_2 = \underset{\sim}{\beta}$

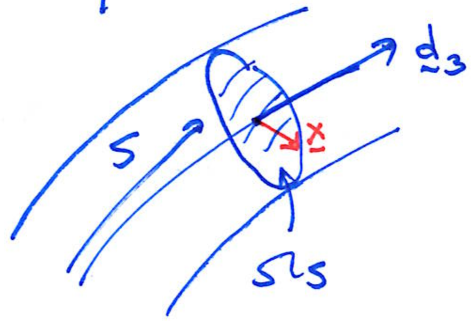
  Then $\underset{\sim}{u} = (0, \kappa, \tau)$

- if $\frac{\partial \varphi}{\partial s} \neq 0$, can express $\underset{\sim}{u} = \left(\underbrace{\kappa \sin\varphi}_{u_1}, \underbrace{\kappa \cos\varphi}_{u_2}, \underbrace{\tau + \frac{\partial \varphi}{\partial s}}_{u_3}\right)$

2. Elastic Rod Mechanics

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

[3D to 1D : suppose σ is stress tensor

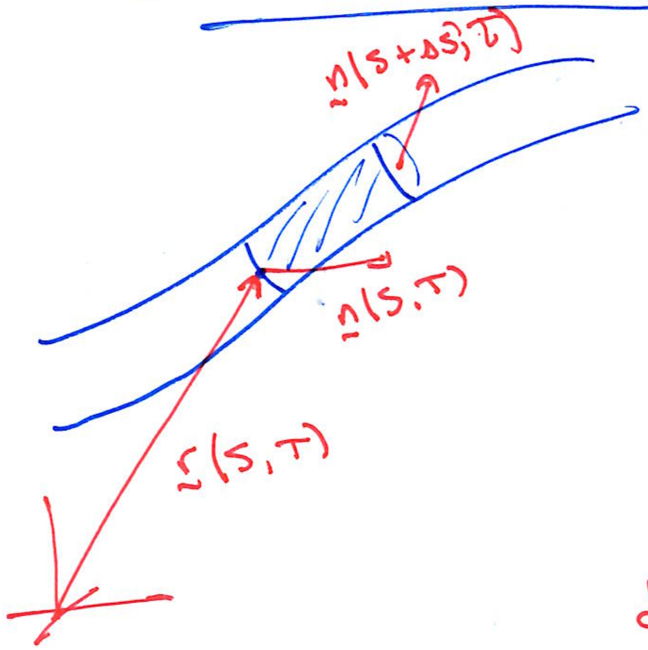


$$\underset{\sim}{n} = \int_{\Omega_S} \sigma \cdot \underset{\sim}{d}_3 \, dA$$

$$\underset{\sim}{m} = \int_{\Omega_S} (\sigma \cdot \underset{\sim}{d}_3) \wedge \underset{\sim}{x} \, dA \Big]$$

Balance of force

on section $[S, S+\Delta S]$:



$$\underset{\sim}{n}(S+\Delta S,T) - \underset{\sim}{n}(S,T) + \underset{\sim}{f}\,\Delta S$$

external force per unit length

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

density Area

Divide by ΔS, send $\Delta S \to 0$:

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

Balance of moments (PS1)

on section $[S, S+\Delta S]$: Total moment on section

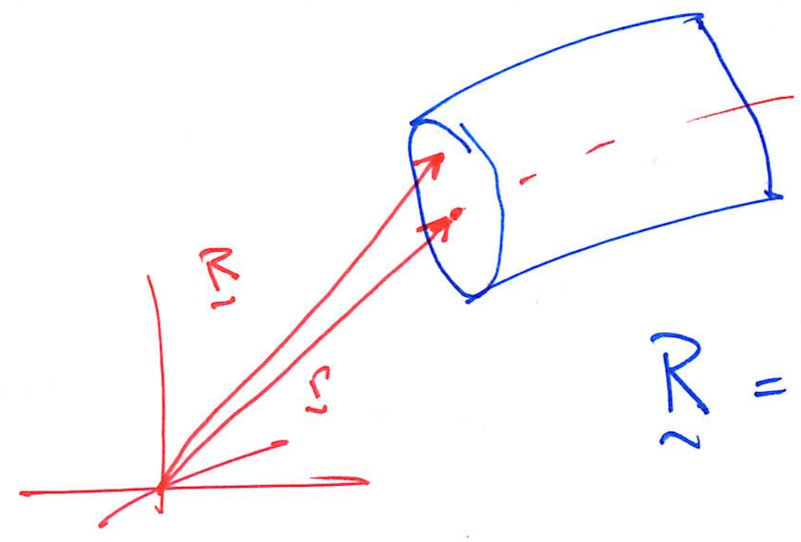
$$= \underset{\sim}{m}(S+\Delta S,T) - \underset{\sim}{m}(S,T) + \underset{\sim}{r}(S+\Delta S,T) \wedge \underset{\sim}{n}(S+\Delta S,T)$$

$$- \underset{\sim}{r}(S,T) \wedge \underset{\sim}{n}(S,T) + \underset{\sim}{r} \wedge \underset{\sim}{f}\,\Delta S + \underset{\sim}{l}\,\Delta S$$

external couple

Divide by ΔS, $\Delta S \searrow 0$: $\quad \dfrac{\partial}{\partial S}\left(\underset{\sim}{m} + \underset{\sim}{r} \wedge \underset{\sim}{n}\right) + \underset{\sim}{r} \wedge \underset{\sim}{f} + \underset{\sim}{l}$

= Rate of change of angular momentum per unit length



Material points in section:

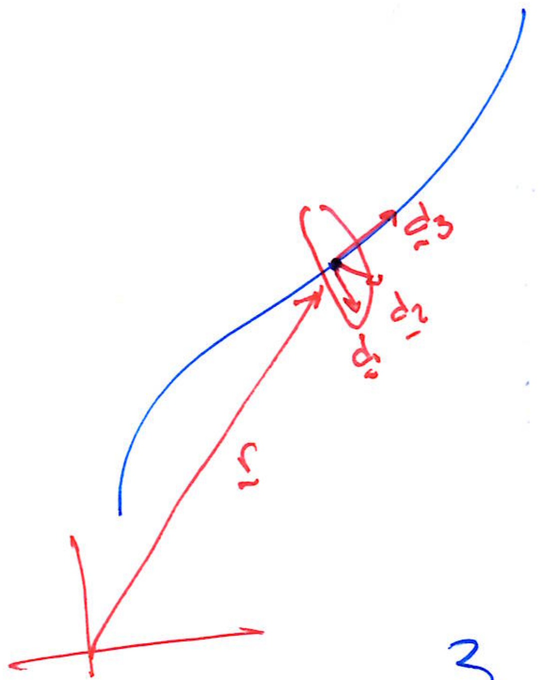
$$\underset{\sim}{R} = \underset{\sim}{r} + x_1 \underset{\sim}{d}_1 + x_2 \underset{\sim}{d}_2$$

Ang. momentum per unit length $= \displaystyle\int dx_1 dx_2\, \underset{\sim}{R} \wedge \rho \dot{\underset{\sim}{R}} \leftarrow \dfrac{\partial \underset{\sim}{R}}{\partial T}$

$\therefore$ Rate of change Ang. mom'm per unit length $= \rho \displaystyle\int dx_1 dx_2\, \underset{\sim}{R} \wedge \ddot{\underset{\sim}{R}}$

$\vdots$

$$\boxed{\frac{\partial \underset{\sim}{m}}{\partial S} + \frac{\partial \underset{\sim}{r}}{\partial S} \wedge \underset{\sim}{n} + \underset{\sim}{l} = \rho I_2\, \underset{\sim}{d}_1 \wedge \ddot{\underset{\sim}{d}}_1 + \rho I_1\, \underset{\sim}{d}_2 \wedge \ddot{\underset{\sim}{d}}_2} \qquad (MB)$$



$$\left\{\begin{aligned} \frac{\partial \underset{\sim}{r}}{\partial S} &= \alpha\, \underset{\sim}{d}_3 \\ \frac{\partial \underset{\sim}{d}_i}{\partial S} &= \underset{\sim}{u} \wedge \underset{\sim}{d}_i \\ \frac{\partial \underset{\sim}{d}_i}{\partial T} &= \underset{\sim}{w} \wedge \underset{\sim}{d}_i \end{aligned}\right.
\qquad
\left\{\begin{aligned} &\frac{\partial \underset{\sim}{n}}{\partial S} + \underset{\sim}{f} = \rho A \frac{\partial^2 \underset{\sim}{r}}{\partial T^2} \\ &\frac{\partial \underset{\sim}{m}}{\partial S} + \frac{\partial \underset{\sim}{r}}{\partial S} \wedge \underset{\sim}{n} + \underset{\sim}{l} = \rho I_2\, \underset{\sim}{d}_1 \wedge \ddot{\underset{\sim}{d}}_1 + \rho I_1\, \underset{\sim}{d}_2 \wedge \ddot{\underset{\sim}{d}}_2 \end{aligned}\right.$$

3. Constitutive Laws. To close the system, we must relate $\underset{\sim}{n}$ and $\underset{\sim}{m}$ to strain α, $\underset{\sim}{u}$. The simplest (& 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 parameters

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

$\hat{u}_i = \hat{u}_i(S, T)$ - intrinsic curvatures $\leftarrow$ when $u_i = \hat{u}_i$, $\underset{\sim}{m} = \underset{\sim}{0}$

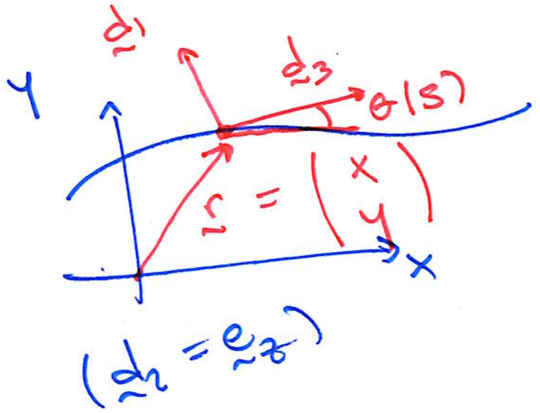
$\hat{u}_i$ describe shape rod "wants to be"

- For extensible rod, we have
  - $n_3 = \underset{\sim}{n} \cdot \underset{\sim}{d}_3 = EA(\alpha - 1)$ "Hooke's Law" A cross-sec. Area

$\alpha := \frac{\partial s}{\partial S}$ axial stretch

$\alpha \equiv 1$ for inextensible

Ex. Planar inextensible rod



$$\underset{\sim}{d}_3 = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \qquad \underset{\sim}{d}_1 = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}$$

Geometry $\quad \underset{\sim}{r}' = \underset{\sim}{d}_3$

$$\begin{cases} x'(s,\tau) = \cos\theta & (1) \\ y'(s,\tau) = \sin\theta & (2) \end{cases}$$

$$\underset{\sim}{d}_i' = \underset{\sim}{u} \wedge \underset{\sim}{d}_i \longrightarrow \underset{\sim}{u} = u_2 \underset{\sim}{d}_2 = \theta'(s,\tau)\, \underset{\sim}{d}_2 = (0, \kappa, 0)$$

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

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

$(\underset{\sim}{f} = \underset{\sim}{0}, \underset{\sim}{l} = \underset{\sim}{0})$

MB $\rightarrow \quad \underset{\sim}{m}' + \underset{\sim}{r}' \wedge \underset{\sim}{n} = \rho I_2 \underset{\sim}{d}_1 \wedge \ddot{\underset{\sim}{d}}_1$

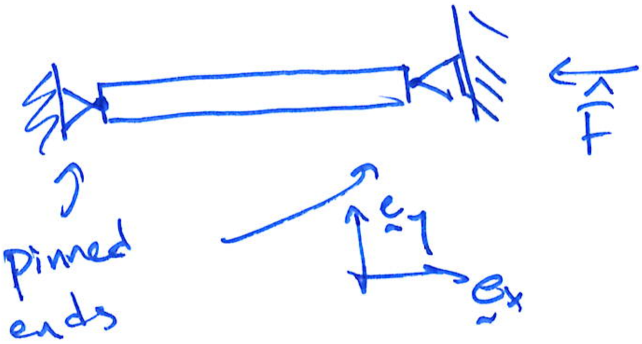
$\rightarrow m' + G\cos\theta - F\sin\theta = \rho I_2 \ddot{\theta} \qquad (5)$

variables: $\{x, y, \theta, F, G, m\}$

Constit $\quad m = EI_2 u_2 = EI_2 \theta' \qquad (6)$

Need 6 BC + initial profile

Euler Buckling



- apply compressive force
- At which $\hat{F}$ does rod buckle?

Static $\rightarrow$ drop time deriv's.

$(3,4) \Rightarrow F, G$ const.

- if align $\hat{F}$ w/ $\underset{\sim}{e}_x$, then $F = \hat{F}$, $G = 0$

(for compressive, $\hat{F} < 0$)

- $|\theta| \ll 1 \rightarrow \sin\theta \approx \theta, \quad \cos\theta \approx 1$

$\xrightarrow{(1,2)} x \approx s, \quad y' \approx \theta$

MB: $m' - \hat{F}\theta \approx 0 \rightarrow EI_2\,\theta'' - \hat{F}\theta \approx 0$

BC: $\theta' = 0$ at $s = 0, L$

has sol'ns $\theta(s) = a\cos\left(\frac{n\pi s}{L}\right)$

if $\hat{F} = \hat{F}_n = \dfrac{-EI n^2\pi^2}{L^2}$