ME 470: Mechanics of Soft and biological matter.

LECTURE 3: 1D ELEMENTS

CONTENTS

- Why 1D ELEMENT?
- How to describe 1D filament shape?
    - Persistence length.
- Ideal chain model

2.1. MOTIVATION.

BIOPOLYMER: ONE OF THE MOST IMPORTANT

e.g.) DNA, RNA: NUCLEOTIDES.

MICROFILAMENT (ACTIN FILAMENT): ACTIN

MICROTUBULE: TUBULIN DIMERS

INTERMEDIATE FILAMENT: DIVERSE COMPOSITION (KERATINS, VIMENTINS)

1D ELEMENTS (FILAMENT, FIBERS, SPRINGS) CAN CONTRIBUTE TO SOFT BEHAVIOR BY

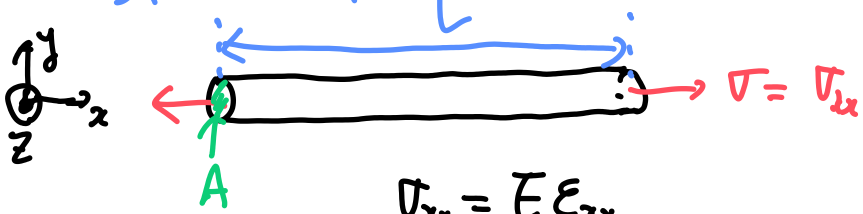
(a) ELASTIC RESPONSE (Bending dominant)

(b) ENTROPIC RESPONSE

(STRECHING IN NETWORK IN PART 3)

2.2. ELASTIC RESPONSE: STRETCHING vs BENDING.

STRETCHING ENERGY.



$$\sigma_{xx} = E\,\varepsilon_{xx}$$

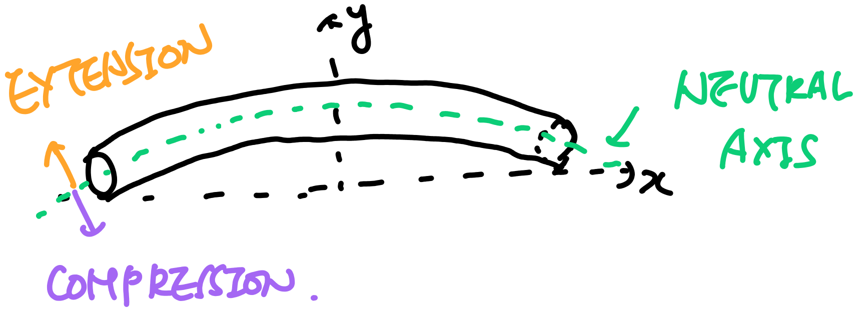
CONSTANT

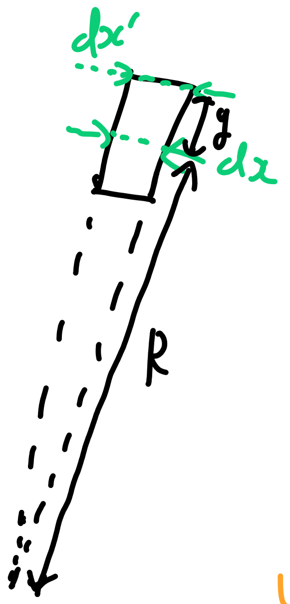
$$\underbrace{U}_{\text{STRETCH}} = \int u\, dV = V \int \sigma_{xx}\, d\varepsilon_{xx}$$

$$= LA \cdot E \int \varepsilon_{xx}\, d\varepsilon_{xx} = \frac{1}{2} L \cdot A \cdot E \cdot \varepsilon^2$$

TYPICAL ENERGY TO STRETCH BY $\varepsilon = \frac{\Delta L}{L}$

BENDING ENERGY.





$$\frac{dx'}{dx} = \frac{R+y}{R} \Rightarrow \frac{dx' - dx}{dx} = \frac{y}{R} = \varepsilon_{xx}$$

$$\Rightarrow U = \int \frac{1}{2} E \cdot \left(\frac{y^2}{R^2}\right) dV$$

UNIFORM ALONG AXIS

$$= \frac{1}{2} L E \int \frac{y^2}{R^2}\, dA$$

UNIFORM CURVATURE

$$\boxed{= \frac{1}{2} \cdot E \cdot \left(\frac{L}{R^2}\right) \underbrace{\int y^2 dA}_{\text{AREA MOMENT OF INERTIA, } I}}$$

IF RELEVANT LENGTH SCALE OF BEAM IS $\sim d$ IN y AND z, $I \sim d^4$

(e.g. CIRCULAR CROSS SECTION WITH DIAMETER d

$I = \frac{\pi}{64} d^4$)

FOR LARGE BENDING DEFORMATION, $K \sim L$

$A \sim d^2$

$$\Rightarrow U_{bend} \sim \frac{1}{2} E \cdot \frac{1}{L} \cdot d^4 \sim \boxed{\frac{1}{2} \cdot L \cdot E \cdot A \cdot \left(\frac{d^2}{L^2}\right)}$$

COMPARE WITH STRONG STRETCHING $(\varepsilon \sim 1)$, $\frac{U_{STRETCH}}{U_{bend}} \sim \left(\frac{d^2}{L^2}\right) \ll 1$

$\Rightarrow$ Inextensible assumption is good for 1D element!

(e.g. fixed contour length)

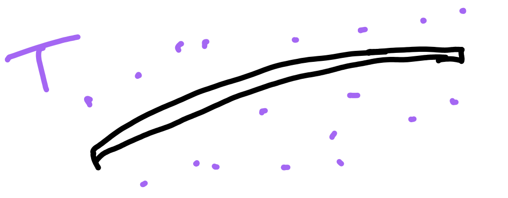
2.3. Persistence length.

2.3.1. Definition

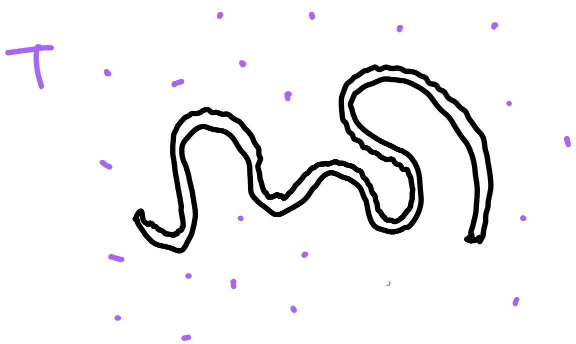
$\boxed{\text{Q:}}$ WHAT DETERMINES EQUILIBRIUM CONFIGURATION OF 1D ELEMENT?

⇒ COMPETITION BETWEEN ENERGETIC INFLUENCE (BENDING) AND ENTROPIC INFLUENCE (THERMAL FLUCTUATION)

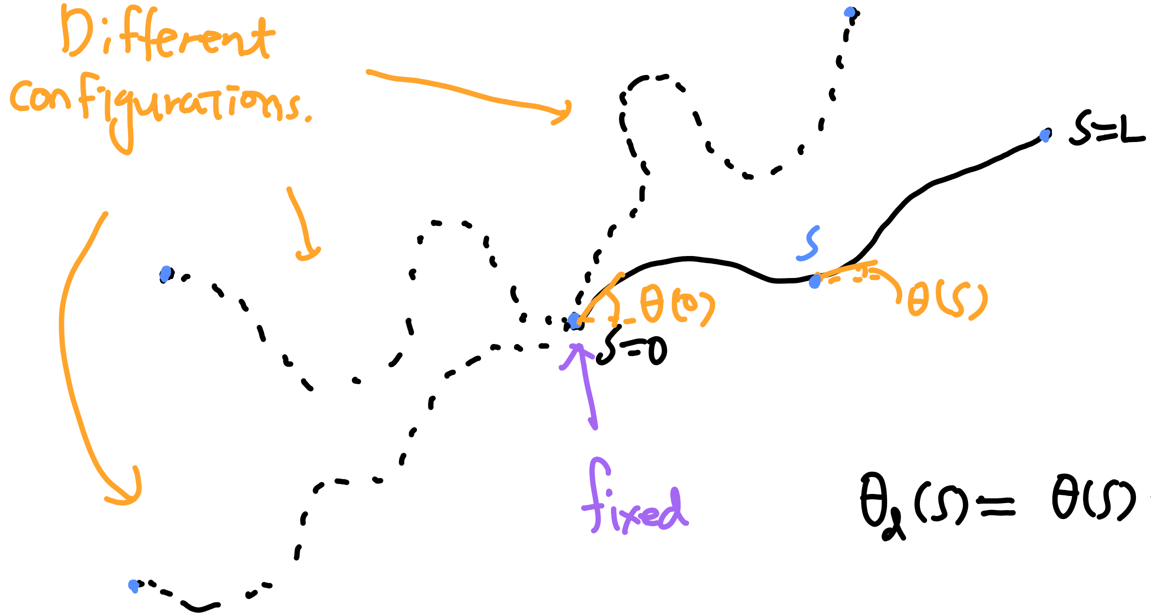
STIFF ROD



FLEXIBLE FILAMENT

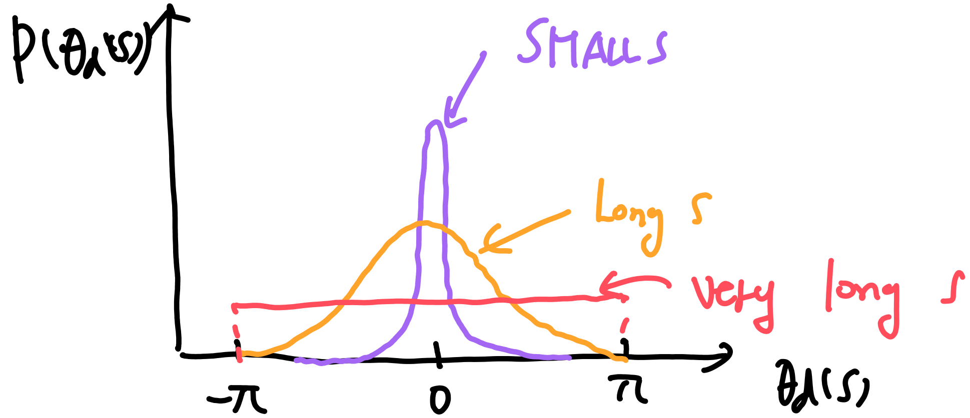


- MEASURE FLEXIBILITY OF 1D ELEMENT.



$$\theta_d(s) = \theta(s) - \theta(0)$$

$\Delta\theta(s)$ EXHIBIT DISTINCT DISTRIBUTION.



DEFINE $f(s) = \langle \cos(\theta_d(s)) \rangle$: Orientation correlation function

($\langle \cdot \rangle$ means average over multiple configuration)

$$\frac{df(s)}{ds} \simeq \frac{f(s+\Delta s) - f(s)}{\Delta s}$$

$$= \frac{\langle \cos(\theta_d(s+\Delta s)) \rangle - \langle \cos(\theta_d(s)) \rangle}{\Delta s}$$

HERE,

$$\theta_d(s+\Delta s) \simeq \theta_d(s) + \frac{d\theta_d(s)}{ds}\cdot\Delta s = \theta_d(s) + \Delta\theta_d(s)$$

$$\Rightarrow \frac{df(s)}{ds} \simeq \frac{\langle \cos(\theta_d(s)+\Delta\theta_d(s))\rangle - \langle \cos(\theta_d(s))\rangle}{\Delta s}$$

cosine rule

$$= \frac{\langle \cos(\theta_d(s))\cdot\cos(\Delta\theta_d(s)) - \sin(\theta_d(s))\cdot\sin(\Delta\theta_d(s))\rangle - \langle \cos(\theta_d(s))\rangle}{\Delta s}$$

θ_d, $\Delta\theta_d$ INDEPENDENT

odd function

$$= \frac{\langle \cos(\theta_d(s))\rangle\langle \cos(\Delta\theta_d(s))\rangle - \cancelto{0}{\langle \sin(\theta_d(s))\rangle}\cancelto{0}{\langle \sin(\Delta\theta_d(s))\rangle} - \langle \cos(\theta_d(s))\rangle}{\Delta s}$$

$$= \frac{\langle \cos(\theta_d(s))\rangle\langle \cos(\Delta\theta_d(s))\rangle - \langle \cos(\theta_d(s))\rangle}{\Delta s}$$

INDEPENDENT OF s, constant.

$$\Rightarrow \boxed{\frac{df(s)}{ds} \simeq \left(\frac{\langle \cos(\Delta\theta_d(s))\rangle - 1}{\Delta s}\right) f(s) = -c\, f(s)}$$

SOLUTION : $f(s) = e^{-cs} \equiv e^{-s/\ell_p}$

PERSISTENCE LENGTH.

PERSISTENCE LENGTH GIVES A CHARACTERISTIC LENGTH scale over which the orientation of a thermally undulating polymer become mostly uncorrelated.

2.3.2. RELATION TO BENDING STIFFNESS.

CONSIDER 3D ELASTIC BEAM WITH BENDING STIFFNESS (FLEXURAL RIGIDITY) EI,

$$U_b = \frac{1}{2}(EI)\cdot\frac{s}{R^2} \qquad \left(\Leftarrow \ \theta = \frac{s}{R}\right)$$

$$= \frac{1}{2}(EI)\cdot\frac{\theta^2}{s}$$

USE CANONICAL ENSEMBLE. (CONSTANT T, BOLTZMANN DISTRIBUTION)

$$p(\theta) = \frac{1}{Z_1} \exp\left[-\frac{U_b(\theta)}{k_B T}\right]$$

$$Z_1 = \int_0^{2\pi}\int_0^{\pi} \exp\left[-\frac{U_b(\theta)}{k_B T}\right] \cdot \sin\theta \, d\theta \, d\phi$$

($\Leftarrow$ USE SPHERICAL COORDINATE. CONSIDER ALL POSSIBLE ANGLE IN 3D)

$$\langle \theta^2 \rangle = \frac{1}{Z_1}\int_0^{2\pi}\int_0^{\pi} \theta^2 \cdot p(\theta) \cdot \sin\theta \, d\theta \, d\phi$$

(EXERCISE) $\rightarrow$

$$= \frac{2 k_B T s}{EI}$$

WE KNOW THAT.

$$\langle \cos(\Delta\theta_d(s)) \rangle \simeq \left\langle 1 - \frac{\Delta\theta_d^2(s)}{2} \right\rangle = 1 - \frac{\langle \Delta\theta_d^2(s) \rangle}{2} = 1 - \frac{k_B T}{EI} s$$

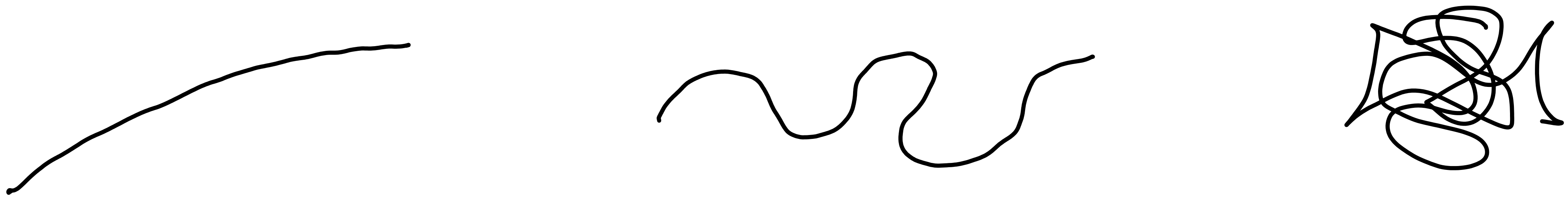
Also. $$\langle \cos(\Delta\theta_d(s))\rangle = e^{-s/l_p} \simeq 1 - \frac{s}{l_p}$$

$$\Rightarrow \boxed{l_p = \frac{EI}{k_B T}}$$

2.3.3 CLASSIFICATION.

	F-actin	Microtubule	Intermediate filament.	DNA
l_p	10 μm	6 mm	1 μm	53 nm
L	1 μm ~ 20 μm	1 ~ 20 μm	1 ~ 20 μm	$0.34 \cdot N_{bp}$ nm
	Semi-flexible	Stiff	Usually flexible	Flexible for large enough N_{bp}

STIFF SEMI- FLEXIBLE FLEXIBLE



BENDING ENERGY DOMINANT

ENTROPY DOMINATE.