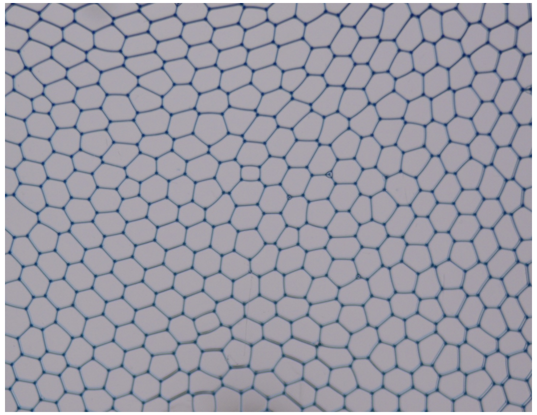
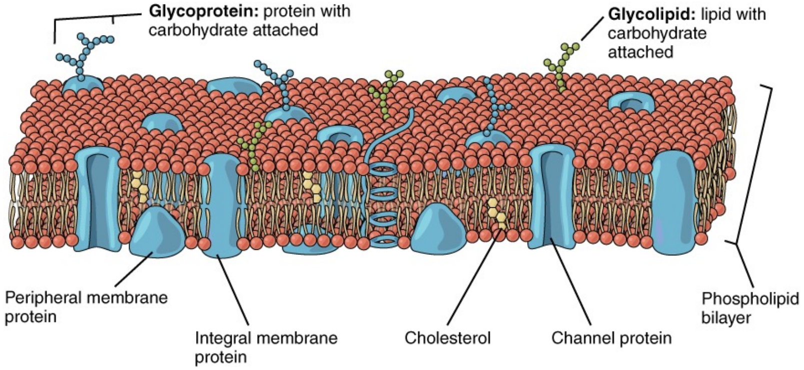
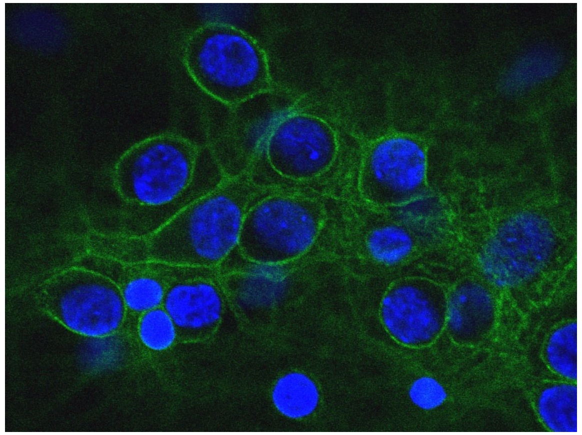
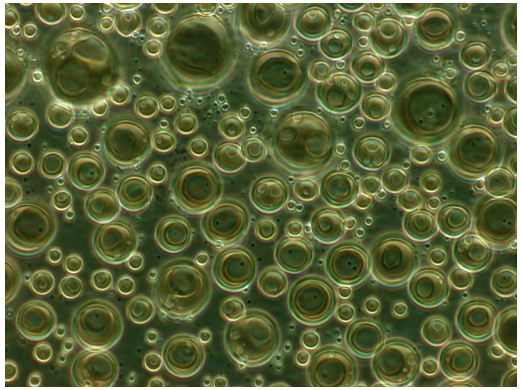
ME470: Mechanics of Soft and Biological Matter
Lecture3: 1D Elements









Red Blood Cells

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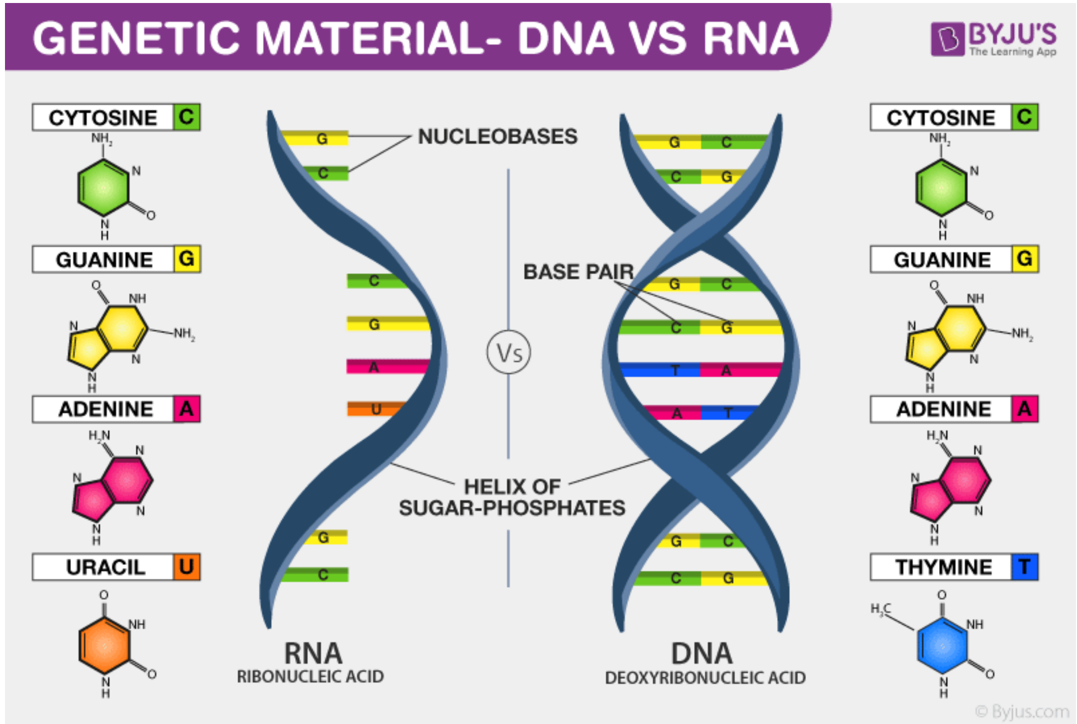
School of Engineering

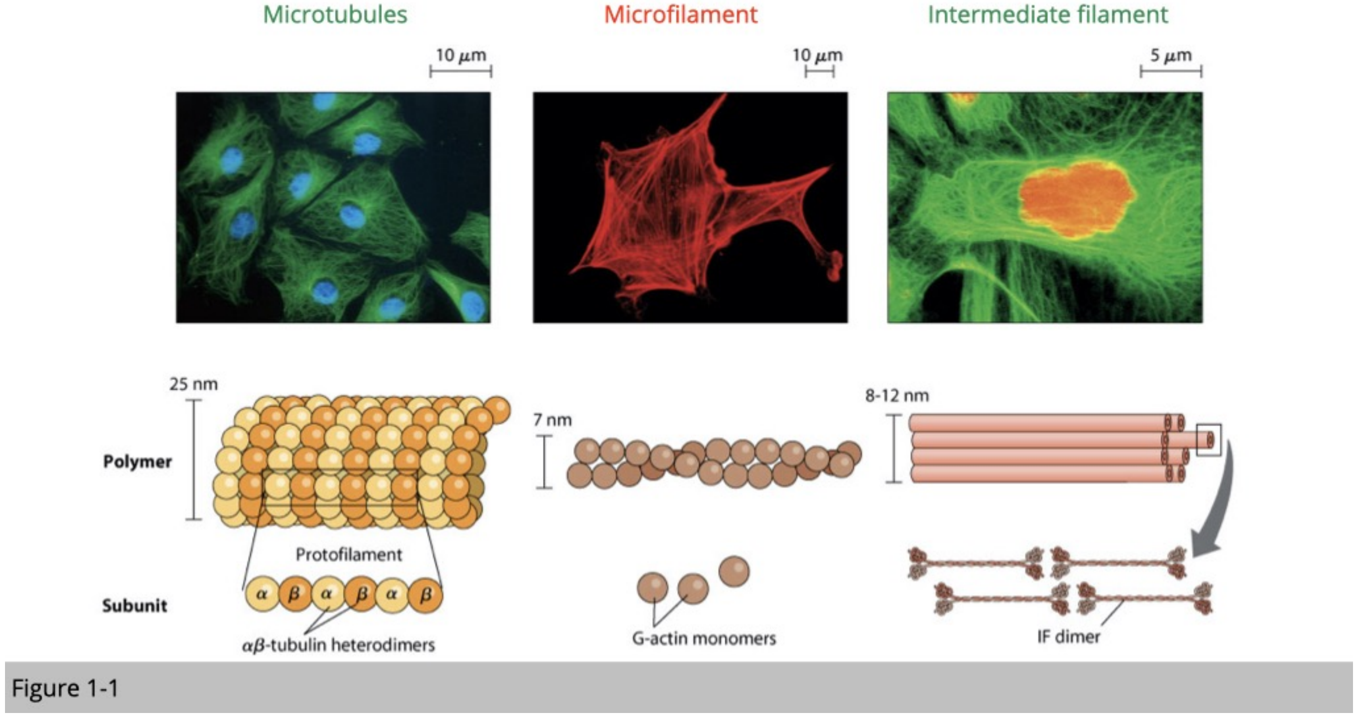
Motivation

Genetic materials



(https://byjus.com/biology/genetic-material-dna-rna/)

Cytoskeleton



(https://medicine.nus.edu.sg/phys/lab/TsaiSY_Lab/LSM4232-L1.html)

Goal: How can we describe mechanics of one-dimensional filaments?

Motivation

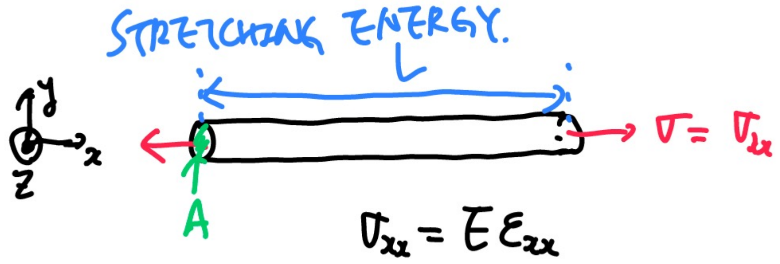
Biopolymer is one of the most important structural elements for cells

- DNA, RNA: Nucleotides
- Microfilament (actin filament): actin
- Microtubule: tubulin dimers
- Intermediate filament: diverse composition (keratins, vimentins)

1D elements (filaments, fibers, springs) can contribute to soft behaviors by

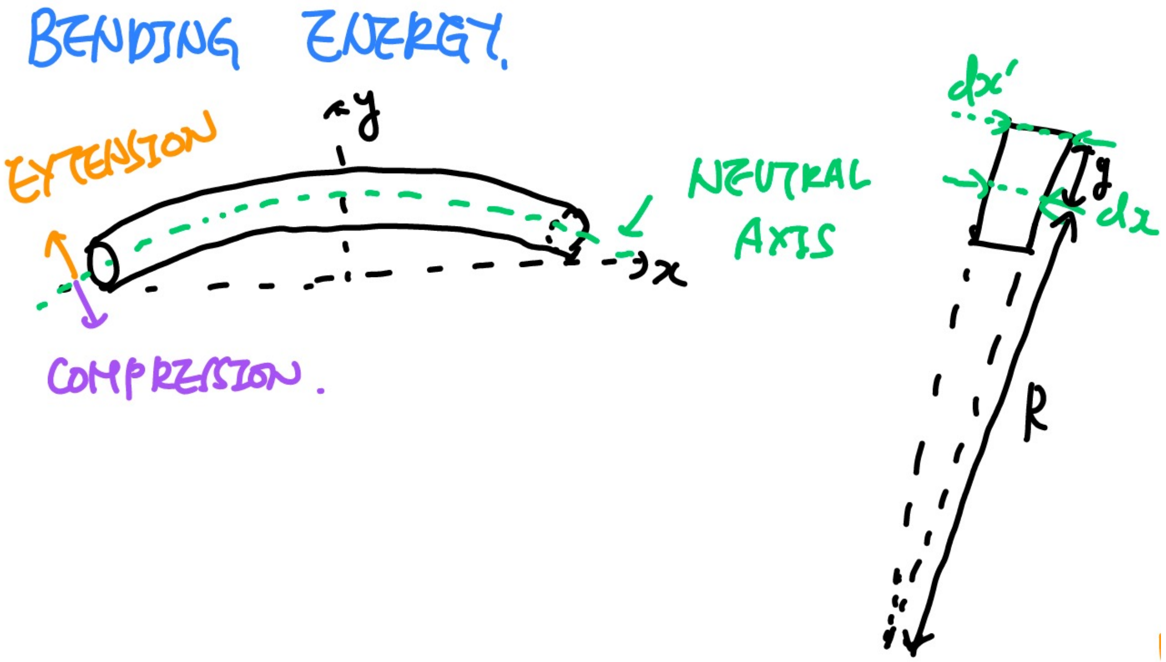
- Elastic response (bending dominant)
- Entropic response

Elastic response: stretching vs bending



$$U_{stretch} = \int u\, dV = V \int \sigma_{xx} d\varepsilon_{xx} = LAE \int \varepsilon_{xx} d\varepsilon_{xx} = \frac{1}{2} LAE\varepsilon^2$$

Typical energy to stretch by $\varepsilon = \frac{\Delta L}{L}$



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

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

$$= \frac{1}{2} EL \int \frac{y^2}{R^2} dV$$ (uniform along x axis)

$$\boxed{= \frac{1}{2} E \frac{L}{R^2} \int y^2 dV}$$ (uniform curvature)

Area moment of inertia, I

EPFL

Elastic response: stretching vs bending

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, $R \sim L$

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

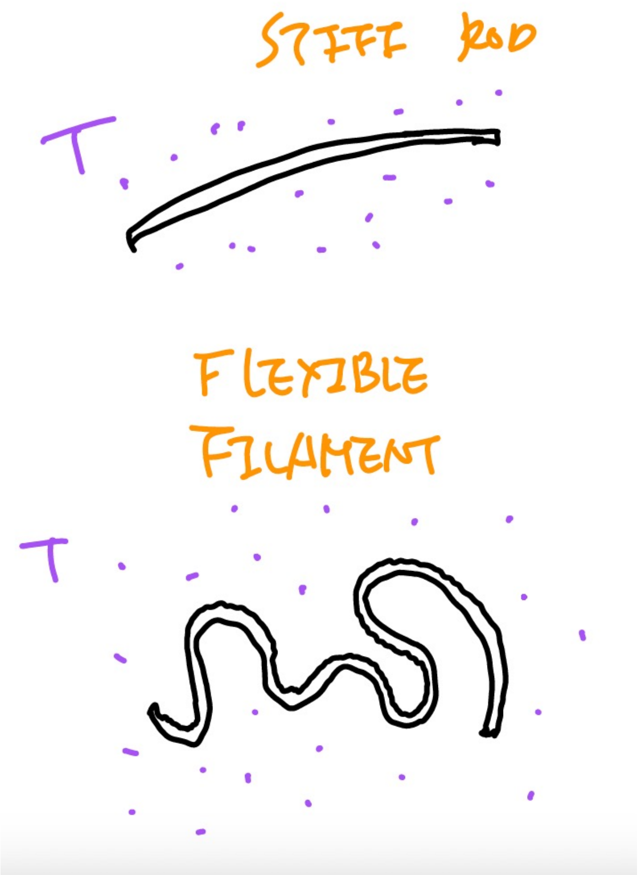
Compare with strong stretching ($\varepsilon \sim 1$) $\Rightarrow$ $\frac{U_{stretch}}{U_{bend}} \sim \frac{d^2}{L^2} \ll 1$

Inextensible assumption is good for 1D element! (e.g. fixed contour length)

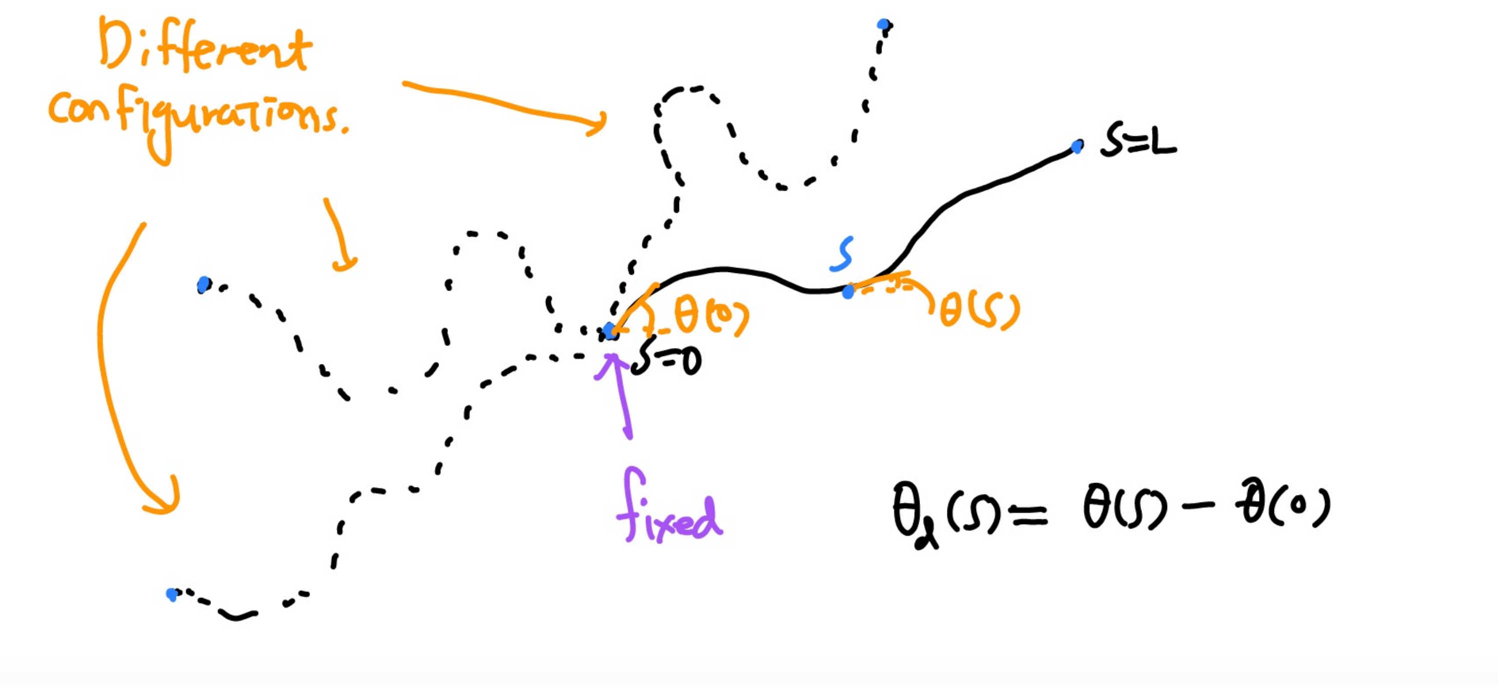
Persistence length

Q: what determines equilibrium configuration of 1D element?

A: competition between energetic influence (bending) and entropic influence (thermal fluctuations)

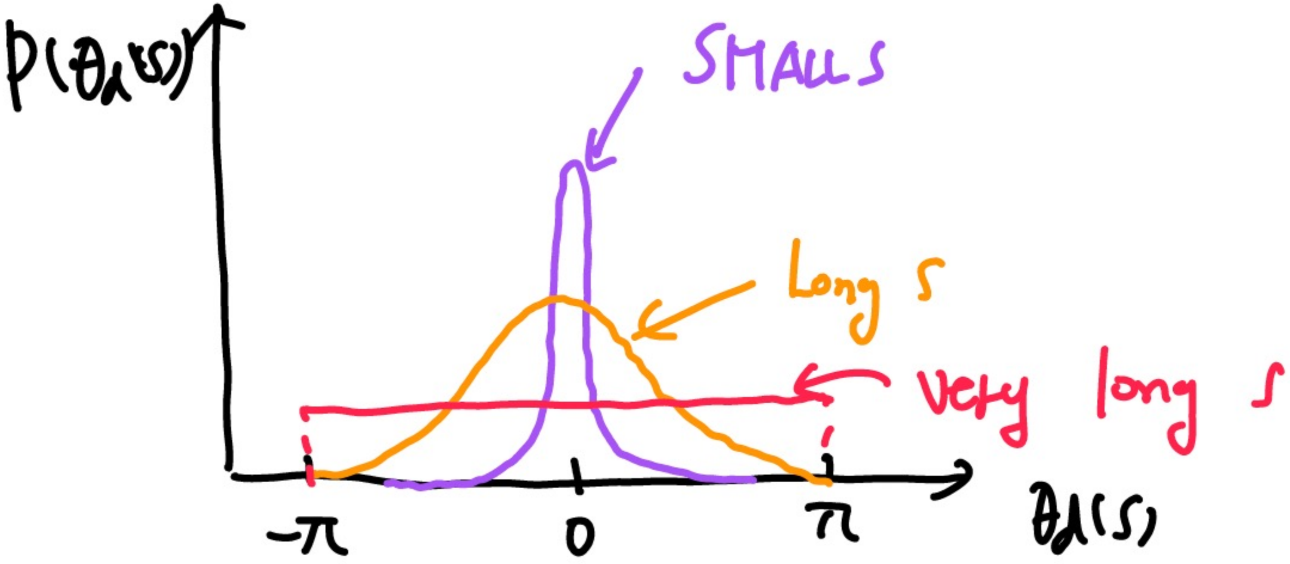


Measure flexibility of 1D element



Persistence length

$\theta_d(s)$ exhibit distinct distributions



Define $f(s) = \langle \cos(\theta_d(s)) \rangle$: orientation correlation function ($\langle \cdot \rangle$ means average over multiple configurations)

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

Persistence length

Here $$\theta_d(s+\Delta s) \approx \theta_d(s) + \frac{d\theta_d(s)}{ds}\Delta s = \theta_d(s) + \Delta\theta_d(s)$$

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

$$\boxed{\frac{df(s)}{ds} \approx \left(\frac{\langle \cos(\Delta\theta_d(s))\rangle - 1}{\Delta s}\right) f(s) = -cf(s)}$$

Independent of s, constant

Solution: $$f(s) = e^{-cs} = e^{-\frac{s}{l_p}}$$ Persistence length

Persistence length gives a characteristic length scale over which the orientation of a thermally undulating polymer become mostly uncorrelated

Persistence length: relation to bending stiffness

Consider 3D elastic beam with bending stiffness (flexural rigidity), EI

$$U_b = \frac{1}{2} EI \frac{s}{R^2} = \frac{1}{2} EI \frac{\theta^2}{s} \Leftarrow \theta = \frac{s}{R}$$

Use canonical ensemble (constant T, Boltzmann distribution)

$$P(\theta) = \frac{1}{Z} exp\left(-\frac{U_b(\theta)}{k_B T}\right)$$

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

(Use spherical coordinate, consider all possible angle in 3D)

$$\langle\theta^2\rangle = \frac{1}{Z} \int_0^{2\pi} \int_0^{\pi} \theta^2 P(\theta) \sin\theta \, d\theta d\phi = \frac{2k_B T s}{EI}$$

Exercise

Persistence length: relation to bending stiffness

We also know that for small $\theta_d(s)$,

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

Also,

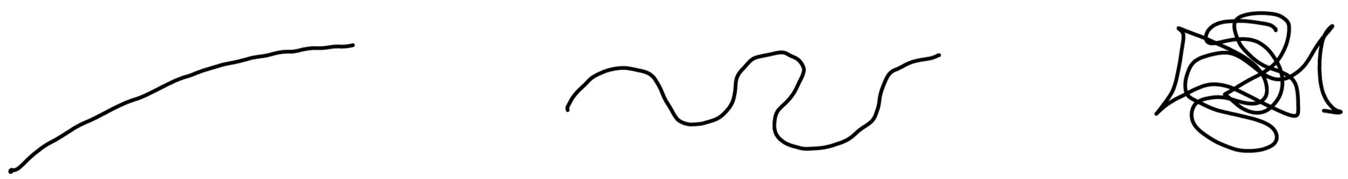
$$\langle\cos(\theta_d(s))\rangle = e^{-s/l_p} \approx 1 - \frac{s}{l_p}$$

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

Classification

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

STIFF SEMI- FLEXIBLE FLEXIBLE



BENDING ENERGY DOMINANT

ENTROPY DOMINATE.