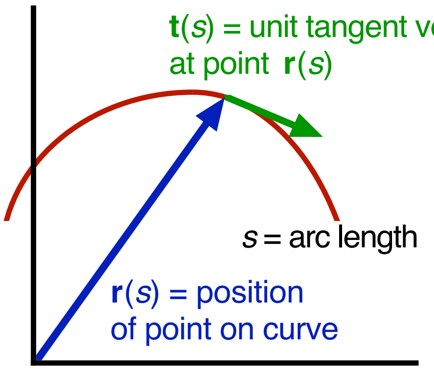
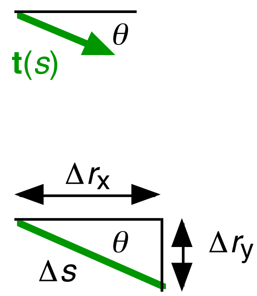
PHYS 4xx Flexible filaments

Mathematical description of curvature

- describe a line by positions $\mathbf{r}(s)$ where arc length s runs from 0 to L_c, the contour length



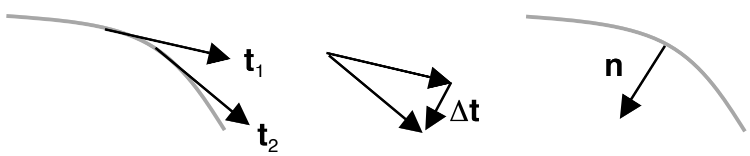


- unit tangent vector $\mathbf{t}$ has components $(\Delta r_x/\Delta s, \Delta r_y/\Delta s, \Delta r_z/\Delta s) = (\partial r_x/\partial s, \partial r_y/\partial s, \partial r_z/\partial s)$ in the infinitesimal limit. Hence

$$\mathbf{t}(s) = \partial \mathbf{r} / \partial s \qquad (1)$$

- curvature C measures the rate of change of $\mathbf{t}$ with s

$$\partial \mathbf{t}/\partial s \equiv C\mathbf{n} \qquad (2)$$



- $\Delta\mathbf{t} = \mathbf{t}_2 - \mathbf{t}_1$ is perpendicular to the curve at small separations
  ---> $\Delta\mathbf{t} \parallel \mathbf{n}$ ($\mathbf{n}$ = normal; hence, $\mathbf{n}$ points to center of curvature if $C > 0$)

- (1) + (2) gives

$$C\mathbf{n} = \partial^2\mathbf{r}/\partial s^2 \qquad (3)$$

or

$$C = 1/R_c \qquad (R = \text{the radius of curvature}) \qquad (4)$$

(proof: $\Delta s = R_c \,\Delta\theta$ + $\Delta\theta = |\Delta\mathbf{t}|$ ---> $1/R_c = \Delta t / \Delta s$)

Bending energy of a thin rod

A straight rod of length L_c with uniform density and cross section, bent into an arc with constant curvature C has a deformation energy per unit length which is quadratic in C

$$[energy] / [length] = (\kappa_f/2)C^2.$$

The energy per unit length is E_{arc}/L_c and the curvature is $1/R_c$, so we also have

$$E_{arc} / L_c = \kappa_f / 2R_c^2 = Y\mathcal{I} / 2R_c^2, \tag{5}$$

- κ_f ≡ flexural rigidity; units of [*energy*]•[*length*]
- one can show from continuum elasticity theory that $\kappa_f = Y\mathcal{I}$
  Y is Young's modulus; units of [*energy*] / [*length*]^3; [*stress*] = Y [*strain*]
  $Y \sim 10^9$ J/m^3 for plastics $\qquad$ $Y \sim 10^{11}$ J/m^3 for metals

  $\mathcal{I}$ = moment of inertia of the cross section (like moment of inertia of mass)
  area-weighted integral of the squared distance from an axis (of bending)
  where the *xy* plane of the integral is perpendicular to the length of the rod
  $$\mathcal{I}_y = \int x^2 \, dA \tag{6}$$
  For example: $\mathcal{I} = \pi R^4/4$ (solid cylinder)

- if the curvature varies along the arc, then the local energy per unit length is
  $$[\textit{energy / length}] = \kappa_f \, (\partial \mathbf{t}/\partial s)^2 /2 \tag{7}$$

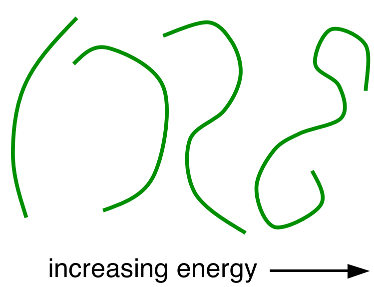
  and the general expression for the total energy becomes

  $$E_{bend} = (\kappa_f/2) \int_0^{L_c} (\partial \mathbf{t}/\partial s)^2 \, ds \qquad \text{(Kratky-Porod model)} \tag{8}$$

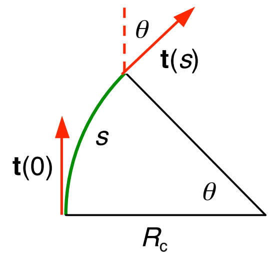
(doesn't include torsion resistance of rod)

Thermal fluctuations and persistence length

- at $T > 0$, shape of a filament can fluctuate:



- shape of a gentle curve of constant curvature is characterized by angle θ between the unit tangent vectors $\mathbf{t}(0)$ and $\mathbf{t}(s)$



- arc s of a circle with radius R_c: $\theta = s/R_c$
- (5) says this configuration has an energy:
  $E_{arc} = \kappa_f s / 2R_c^2 = \kappa_f \theta^2 / 2s$ (9)
- probability $\mathcal{P}(E)$ of the filament being found with energy E is proportional to the Boltzmann factor $\exp(-\beta E)$, where $\beta = k_B T$
- for arcs of circles, the probability of each configuration is equal to $\mathcal{P}(E_{arc})$, and
  $<\theta^2> = \int \theta^2 \mathcal{P}(E_{arc}) d\Omega \,/\, \int \mathcal{P}(E_{arc}) d\Omega$, (10)

- fixed end of the filament defines the z-axis, free end is described by the angles θ and ϕ; integral over the solid angle $d\Omega = \sin\theta \, d\theta \, d\phi$ (in 3D)
- E_{arc} is independent of ϕ, so the azimuthal integral cancels out, leaving

$$<\theta^2> = \int \theta^2 \exp(-\beta E_{arc}) \sin\theta \, d\theta \,/\, \int \exp(-\beta E_{arc}) \sin\theta \, d\theta \quad (11)$$

- using the small angle approximation $\sin\theta \sim \theta$.

$$<\theta^2> = \int \theta^3 \exp(-[\beta\kappa_f/2s]\theta^2) \, d\theta \;/\; \int \theta \exp(-[\beta\kappa_f/2s]\theta^2) \, d\theta$$
$$= (2s / \beta\kappa_f) \int x^3 \exp(-x^2) \, dx / \int x \exp(-x^2) \, dx, \quad (12)$$

where $x = (\beta\kappa_f/2s)^{1/2}\theta$

- in the small oscillation approximation, the upper limits of the integrals in (12) can be taken to be infinite, whence
  $\int x^3 \exp(-x^2) \, dx = \int x \exp(-x^2) \, dx = 1/2$

----> $<\theta^2> \cong 2s / \beta\kappa_f$ (small oscillations in 3D). (13)

- combination $\beta\kappa_f$ is defined as the persistence length ξ_p of the filament:
  $\xi_p \equiv \beta\kappa_f$ (units of [*length*]) (14)

- Note that the persistence length decreases with increasing temperature.

Correlation function

The correlation function $<\mathbf{t}(0)\cdot\mathbf{t}(s)> = <\cos\theta>$ describes the correlation between the direction of the tangent vectors at different positions along the curve. At low temperature, θ is small and $\cos\theta \sim 1 - \theta^2/2$, so

$$<\mathbf{t}(0)\bullet\mathbf{t}(s)> \sim 1 - <\theta^2>/2$$
$$= 1 - s / \xi_p \qquad (s/\xi_p << 1). \qquad (15)$$

This is a first-order approximation to an exponential *via* $\exp(-x) \sim 1 - x$ at small x; the complete correlation function is

$$<\mathbf{t}(0)\bullet\mathbf{t}(s)> = \exp(-s / \xi_p) \qquad (16)$$

(which can also be built up segment by segment).

Extras

1. *Filament in 2D*

For the fluctuating filament problem, if the tip is confined to a plane, the angular integral in the calculation of $<\theta^2>$ involves $d\theta$, not the solid angle $d\Omega$. Thus,

$$<\theta^2> = (2s / \beta\kappa_f) \int x^2 \exp(-x^2)\, dx / \int \exp(-x^2)\, dx$$

where $x = (\beta\kappa_f/2s)^{1/2}\theta$

Integrated from 0 to ∞, the integrals are

$$\int x^2 \exp(-x^2)\, dx = \sqrt{\pi} / 4 \qquad \int \exp(-x^2)\, dx = \sqrt{\pi} / 2$$

so

$$<\theta^2> = (2s / \beta\kappa_f) \cdot 1/2 = s / \beta\kappa_f.$$

This is half of $<\theta^2>$ in 3D, meaning that the persistence length is

$$\xi_p = 2\beta\kappa_f \qquad \text{(2 dimensions).}$$

2. *Tangent correlations in 2D*

The tangent correlation function is easy to obtain in 2D without recourse to the small angle expansion $\sin\theta \sim \theta$. Starting with $<\mathbf{t}(0)\cdot\mathbf{t}(s)> = <\cos\theta>$, the correlation function is

$$<\mathbf{t}(0)\cdot\mathbf{t}(s)> = \int \cos\theta \exp(-\gamma\theta^2)\, d\theta / \int \exp(-\gamma\theta^2)\, d\theta \quad \text{(two dimensions)}$$

where $\gamma = \beta\kappa_f / 2s$.

With the limits $0 \leq \theta \leq \infty$, the integrals are

$$\int \exp(-\gamma\theta^2)\, d\theta = \sqrt{\pi} / 2\sqrt{\gamma}$$

$$\int \cos\theta \exp(-\gamma\theta^2)\, d\theta = \{\sqrt{\pi} / 2\sqrt{\gamma}\} \exp(-1 / 4\gamma) \qquad \text{Gradshteyn and Ryzhik, 3.896}$$

so we have exactly

$$<\cos\theta> = \exp(-2s / 4\beta\kappa_f)$$

or

$$<\mathbf{t}(0)\cdot\mathbf{t}(s)> = \exp(-s / 2\beta\kappa_f) \quad \text{and} \quad \xi_p = 2\beta\kappa_f \quad \text{(2 dimensions)}$$

3. *Equipartition theorem*

Some students may be familiar with the theorem for the equipartition of energy

$<E> = k_B T/2$ per degree of freedom.

This can be applied directly to $<\theta^2>$ using

$<\theta^2> = (2s/\kappa_f) <E_{arc}>$

two dimensions	three dimensions
$<E_{arc}> = k_B T/2$ for 1 angle	$<E_{arc}> = k_B T$ for 2 angles
$<\theta^2> = s / \beta\kappa_f$	$<\theta^2> = 2s / \beta\kappa_f$.
$\xi_p = 2\beta\kappa_f$	$\xi_p = \beta\kappa_f$.