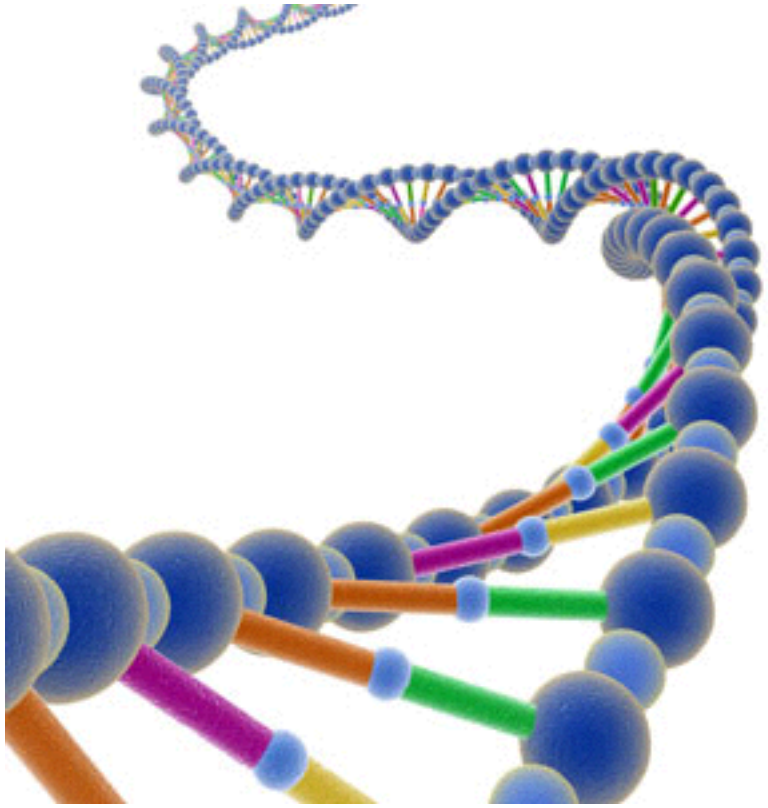
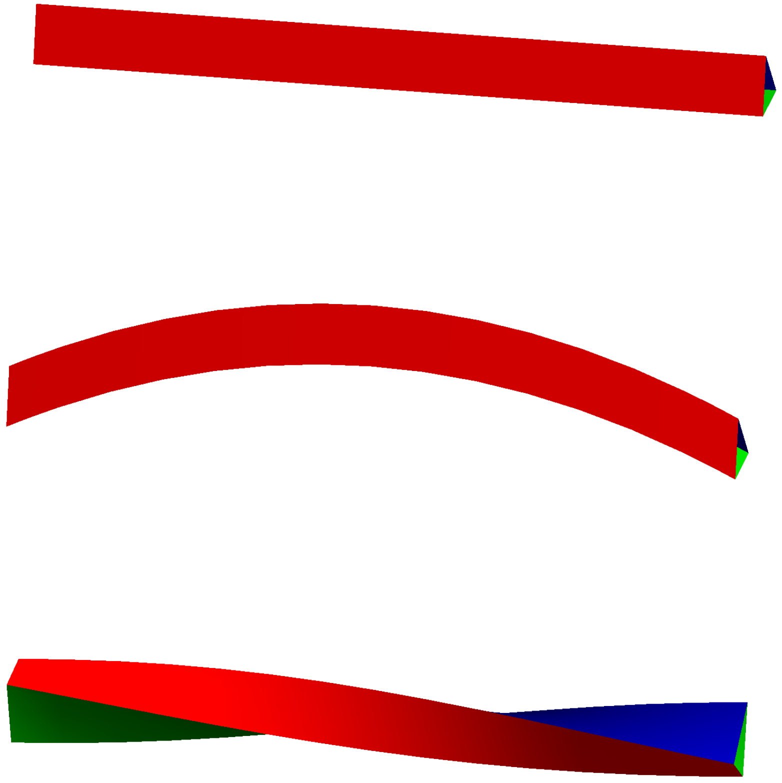
MAE 545: Lecture 13 (10/29)

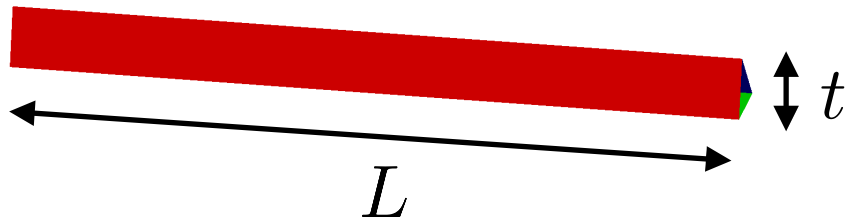
Elastic deformation energy for beams and thin filaments



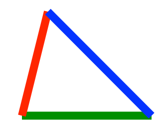


Deformations of macroscopic beams

undeformed beam



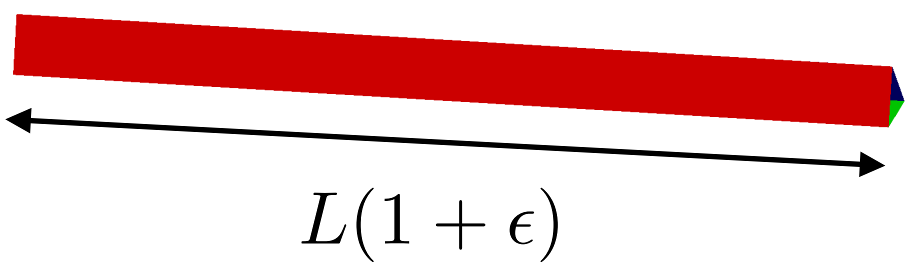
beam cross-section



beam made of material with Young's modulus

E_0

stretching

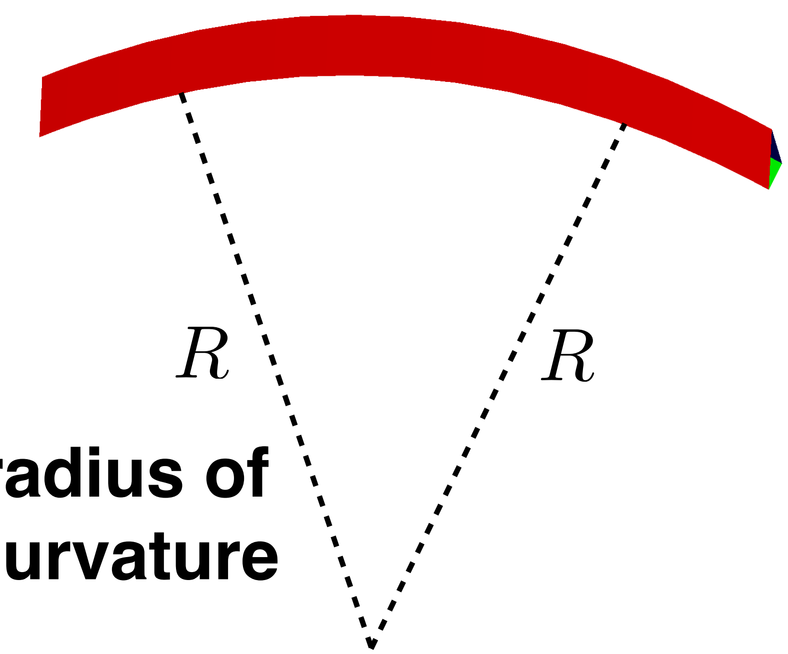


strain ϵ

$$\frac{E_s}{L} = \frac{k\epsilon^2}{2}$$

$$k \propto E_0 t^2$$

bending

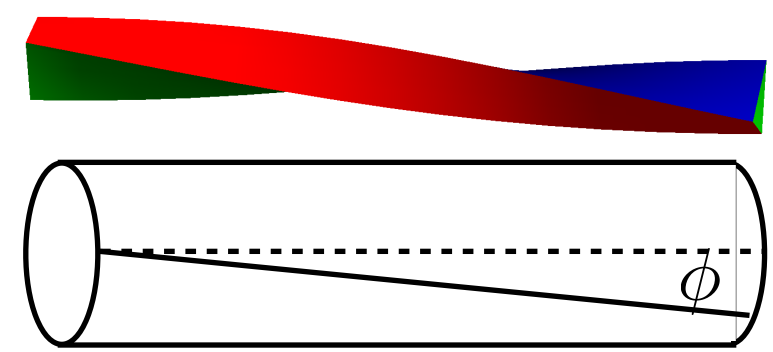


radius of curvature

$$\frac{E_b}{L} = \frac{A}{2R^2}$$

$$A \propto E_0 t^4$$

twisting



angle of twist

$\phi = \Omega L$

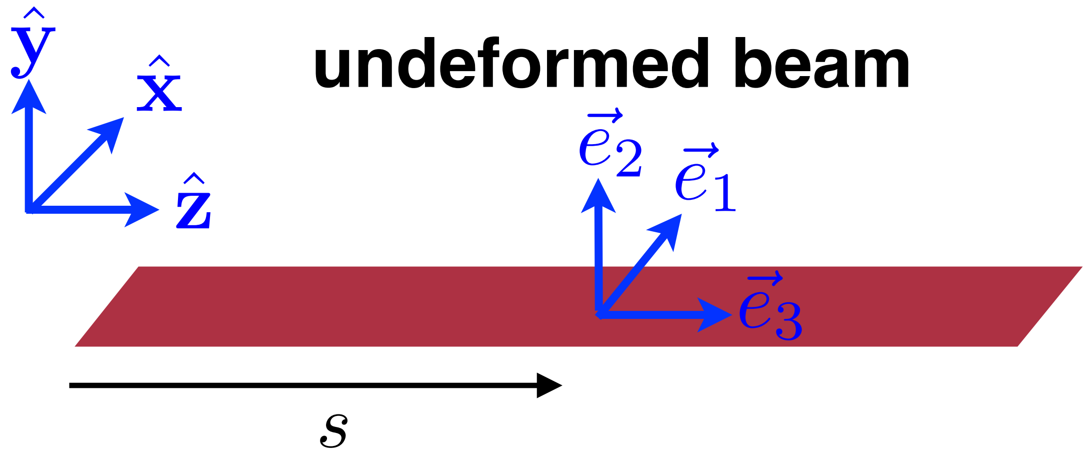
$$\frac{E_t}{L} = \frac{C\Omega^2}{2}$$

$$C \propto E_0 t^4$$

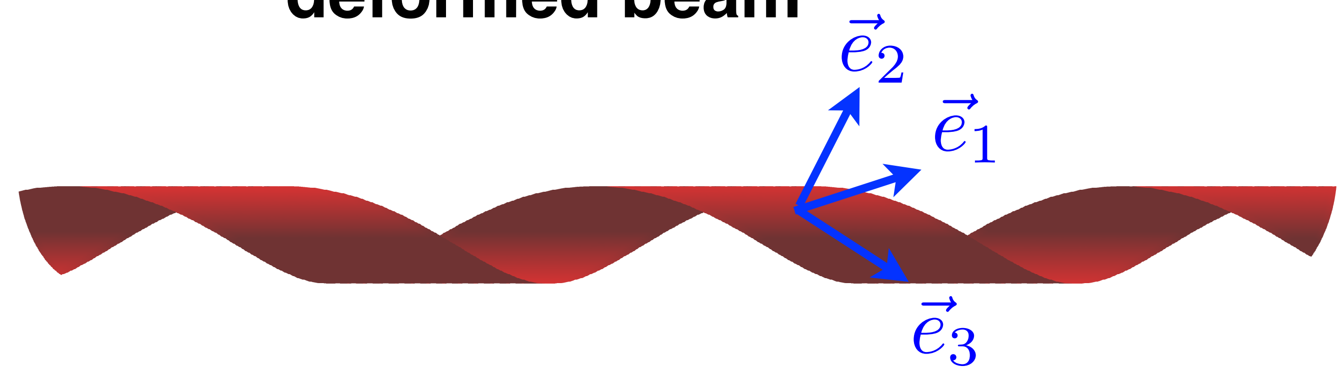
Bending and twisting is much easier than stretching for long and narrow beams!

Bending and twisting represented as rotations of material frame

undeformed beam



deformed beam



rotation rate of material frame

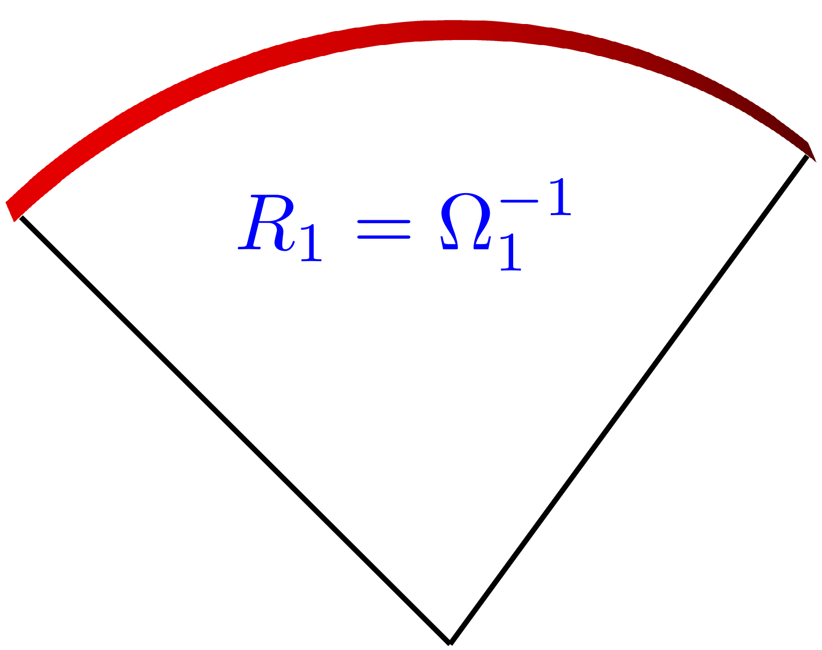
$$\frac{d\vec{e}_i}{ds} = \vec{\Omega} \times \vec{e}_i$$

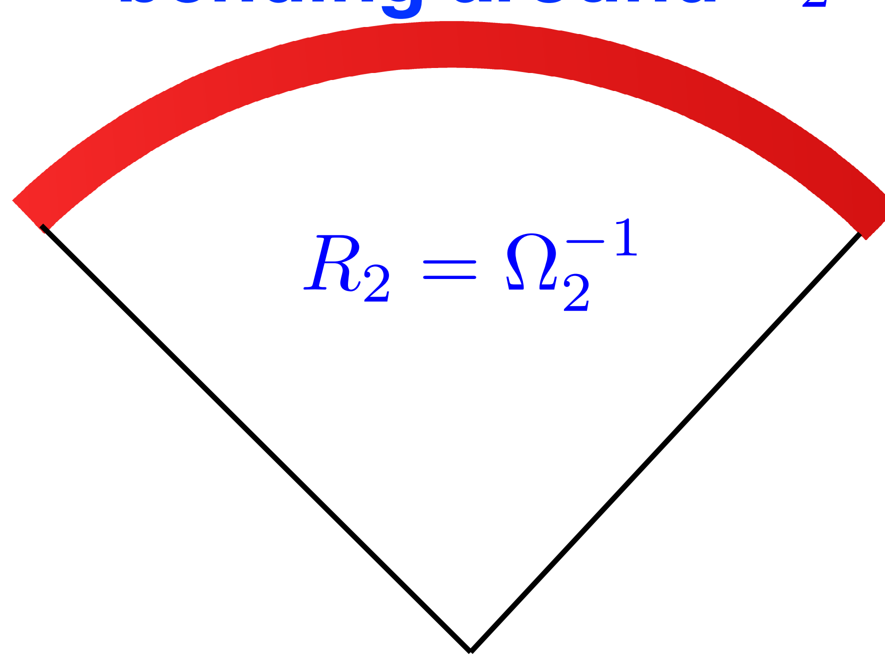
$$\vec{\Omega} = \Omega_1 \vec{e}_1 + \Omega_2 \vec{e}_2 + \Omega_3 \vec{e}_3$$

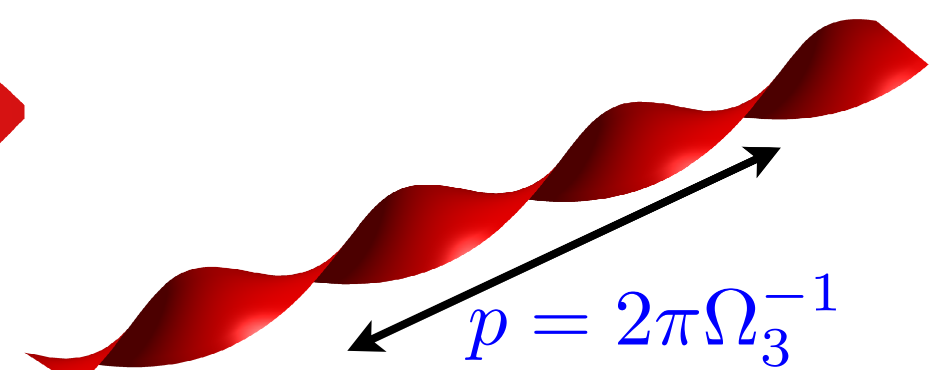
Energy cost of deformations

$$E = \int \frac{ds}{2} \left[A_1 \Omega_1^2 + A_2 \Omega_2^2 + C \Omega_3^2 \right]$$

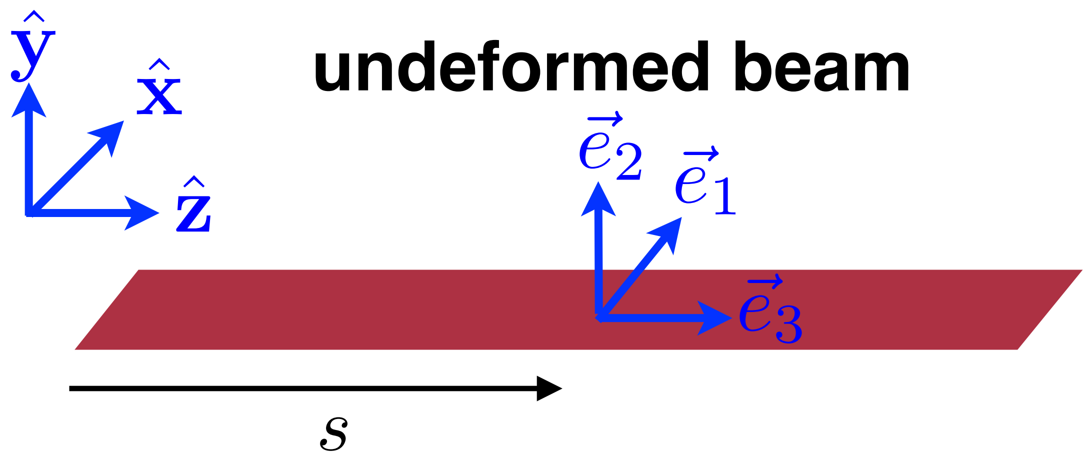
bending around $\mathbf{e}_1$ **bending around $\mathbf{e}_2$** **twisting around $\mathbf{e}_3$**

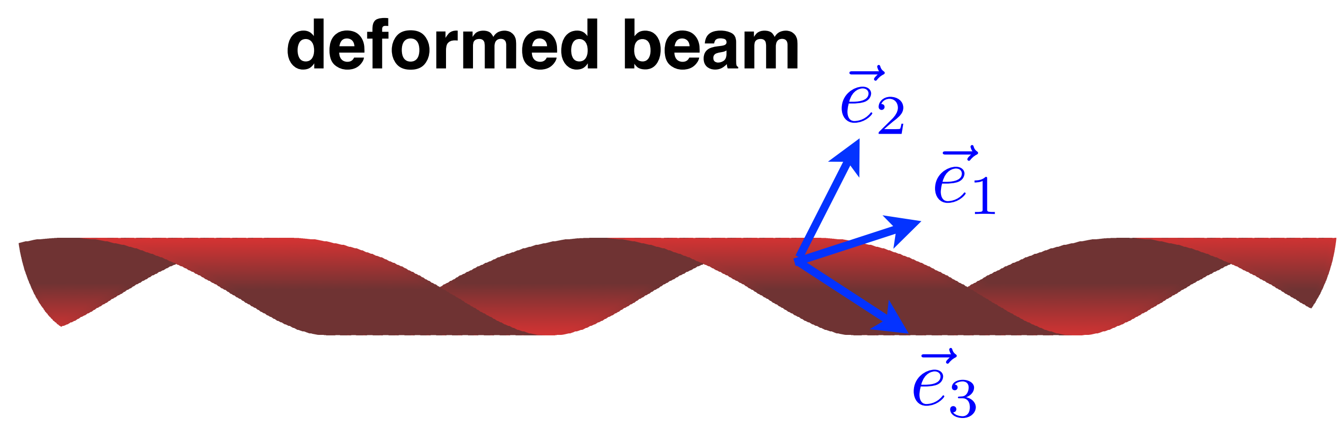






Bending and twisting represented as rotations of material frame





rotation rate of material frame

$$\frac{d\vec{e}_i}{ds} = \vec{\Omega} \times \vec{e}_i$$

$$\vec{\Omega} = \Omega_1 \vec{e}_1 + \Omega_2 \vec{e}_2 + \Omega_3 \vec{e}_3$$

Energy cost of deformations

$$E = \int \frac{ds}{2} \left[A_1 \Omega_1^2 + A_2 \Omega_2^2 + C \Omega_3^2 \right]$$

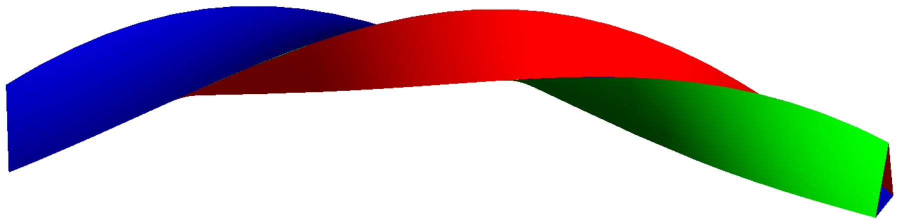
Bending and twisting modes are coupled, because successive rotations do not commute!

$$R_y\left(\frac{\pi}{2}\right) R_z\left(\frac{\pi}{2}\right) \hat{\mathbf{z}} = R_y\left(\frac{\pi}{2}\right) \hat{\mathbf{z}} = \hat{\mathbf{x}}$$

$$R_z\left(\frac{\pi}{2}\right) R_y\left(\frac{\pi}{2}\right) \hat{\mathbf{z}} = R_z\left(\frac{\pi}{2}\right) \hat{\mathbf{x}} = \hat{\mathbf{y}}$$

plectonemes

Elastic energy of deformations in the general form



Energy density for a deformed filament can be Taylor expanded around the minimum energy ground state

twist-bend coupling

$$E = \int_0^L \frac{ds}{2} \Big[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + 2A_{12}\Omega_1\Omega_2 + 2A_{13}\Omega_1\Omega_3 + 2A_{23}\Omega_2\Omega_3 + k\epsilon^2 + 2D_1\epsilon\Omega_1 + 2D_2\epsilon\Omega_2 + 2D_3\epsilon\Omega_3 \Big]$$

bend-stretch coupling

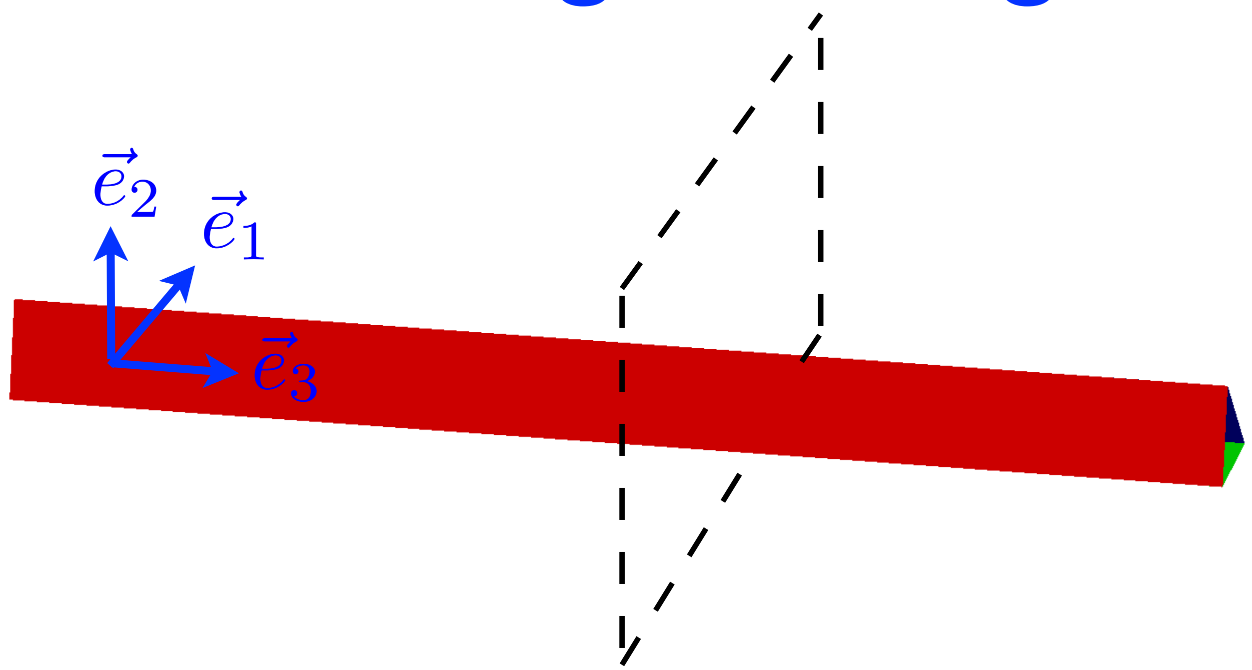
twist-stretch coupling

Energy density is positive definitive functional!

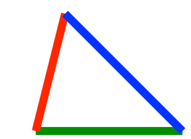
$$A_{11}, A_{22}, A_{33}, k > 0$$
$$A_{ij}^2 < A_{ii}A_{jj}$$
$$D_i^2 < kA_{ii}$$

In principle 10 elastic constants, but symmetries of filament shape determine how many independent elastic constants are allowed!

Beams with uniform cross-section along the long axis

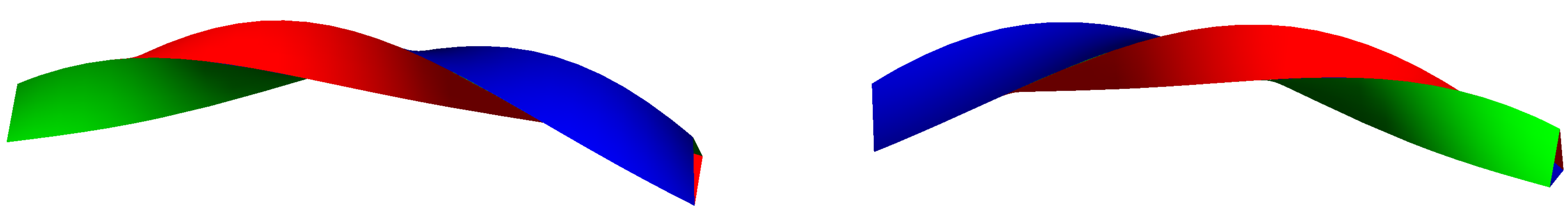


beam cross-section

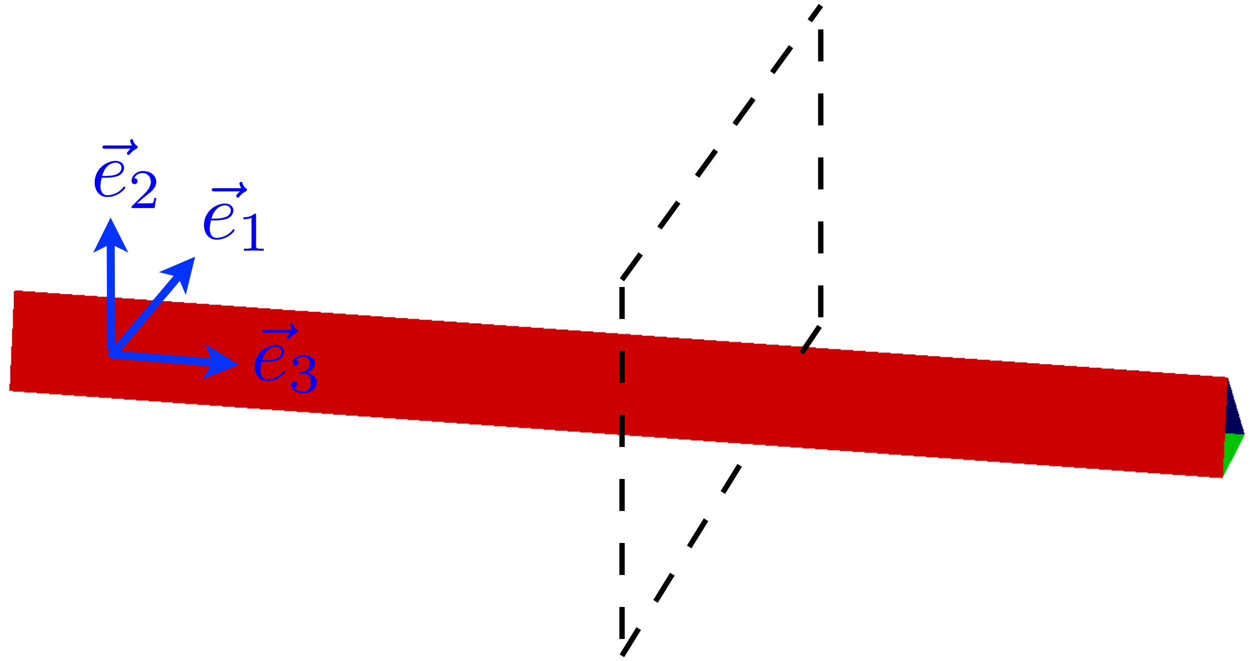


Beam has mirror symmetry through a plane perpendicular to $\vec{e}_3$.

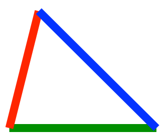
Two beam deformations that are mirror images of each other must have the same energy cost!



Beams with uniform cross-section along the long axis



beam cross-section



Beam has mirror symmetry through a plane perpendicular to $\vec{e}_3$.

$$E = \int_0^L \frac{ds}{2} \left[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + 2A_{12}\Omega_1\Omega_2 + k\epsilon^2 + 2D_1\epsilon\Omega_1 + 2D_2\epsilon\Omega_2 \right]$$

Twist is decoupled from bending and stretching!

$$A_{13} = A_{23} = D_3 = 0$$

Twist-bend coupling in propellers and turbines

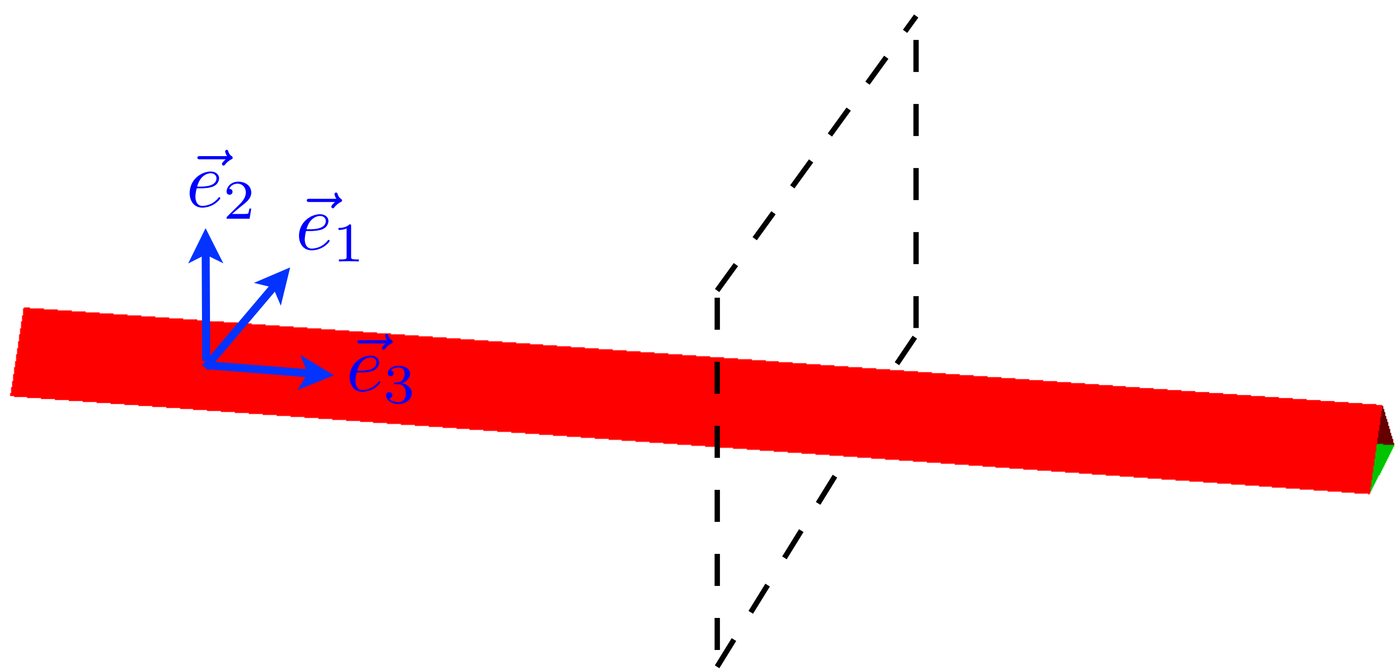
wind turbine

airplane propeller

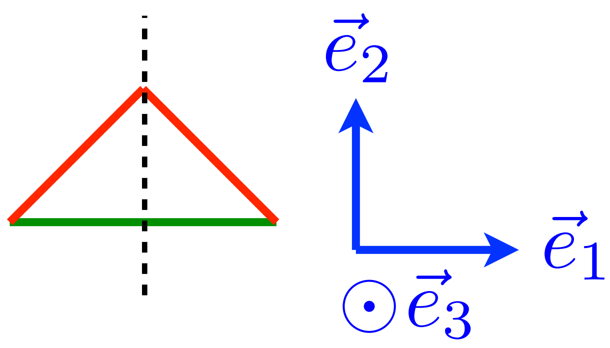
ship propeller

Blades of propellers and turbines are chiral, therefore there is coupling between twist and bend deformations!

Beams with isosceles triangle cross-section



beam cross-section



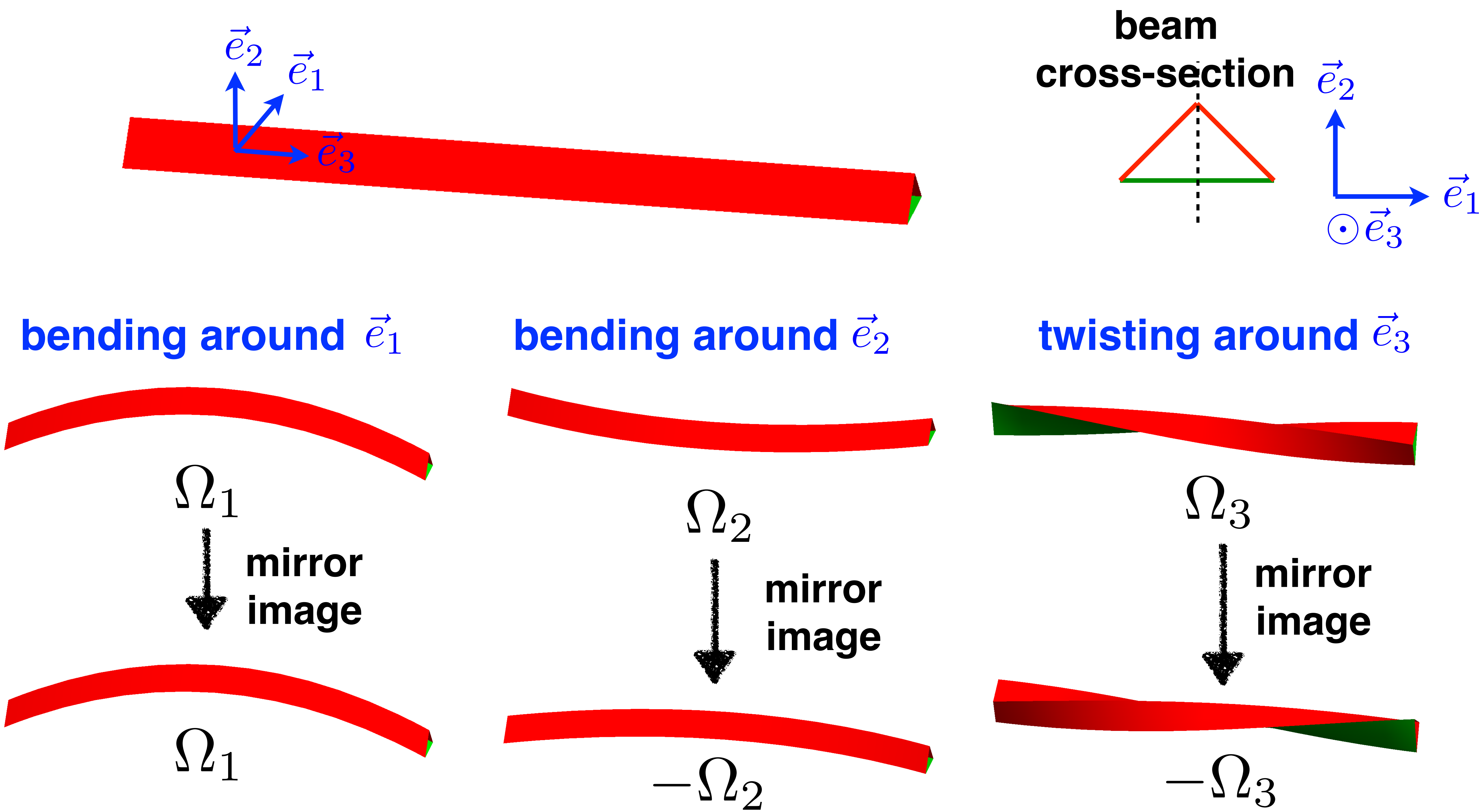
Beam has mirror symmetry through a plane perpendicular to $\vec{e}_3$.

Beam has mirror symmetry through a plane perpendicular to $\vec{e}_1$.

Beam has 2-fold rotational symmetry around axis $\vec{e}_2$.

Note: n-fold rotational symmetry is symmetry due to rotation by angle $2\pi/n$.

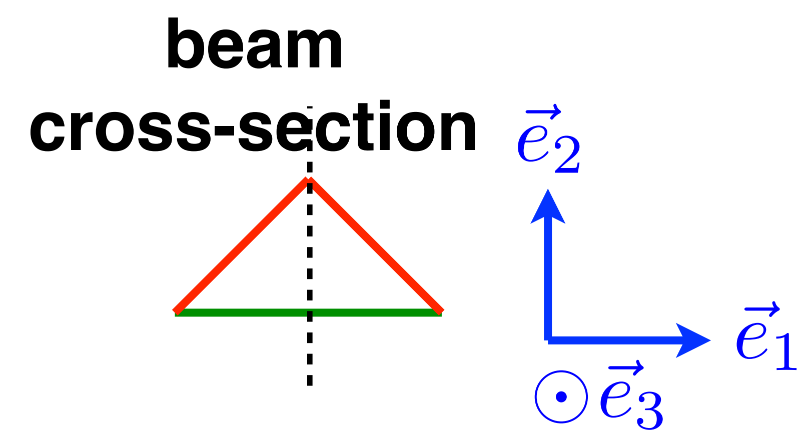
How mirroring around $\vec{e}_1$ affects bending and twisting?



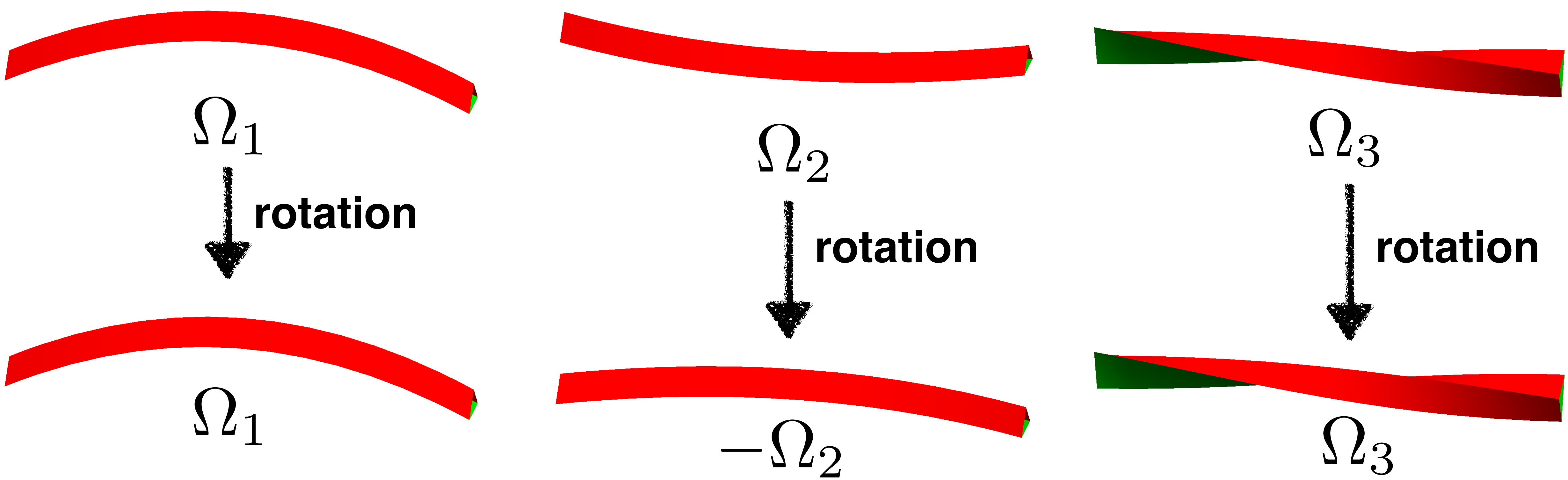
Note: mirroring doesn't affect stretching

$$A_{12} = A_{13} = D_2 = D_3 = 0$$

How rotation by π around $\vec{e}_2$ affects bending and twisting?



bending around $\vec{e}_1$ | **bending around $\vec{e}_2$** | **twisting around $\vec{e}_3$**

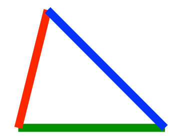


Note: rotation doesn't affect stretching

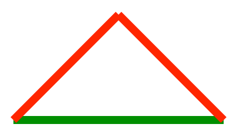
$$A_{12} = A_{23} = D_2 = 0$$

Elastic energy for beams of various cross-sections

beam cross-section

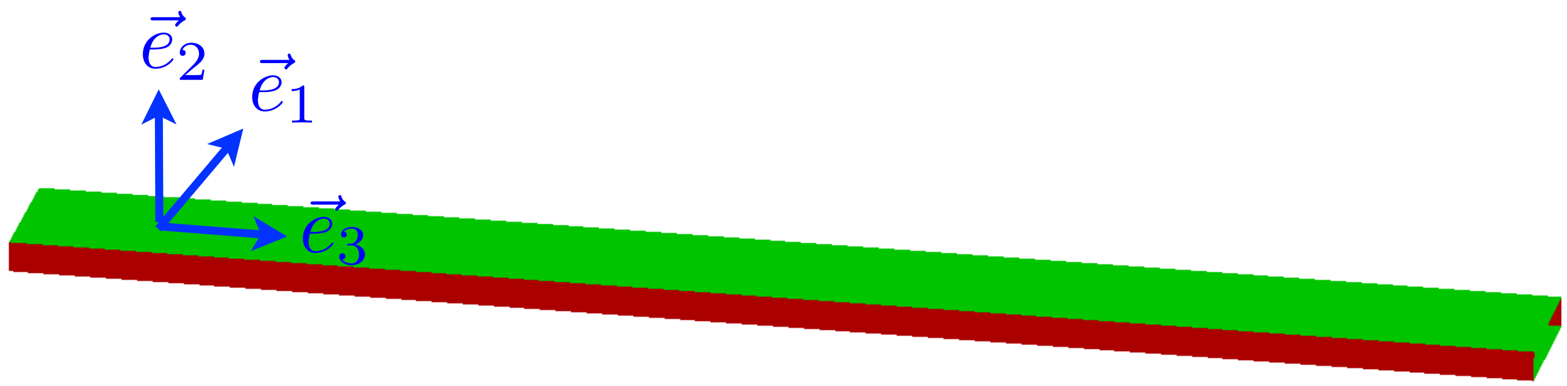



$$E = \int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + 2A_{12}\Omega_1\Omega_2 + k\epsilon^2 + 2D_1\epsilon\Omega_1 + 2D_2\epsilon\Omega_2\Big]$$

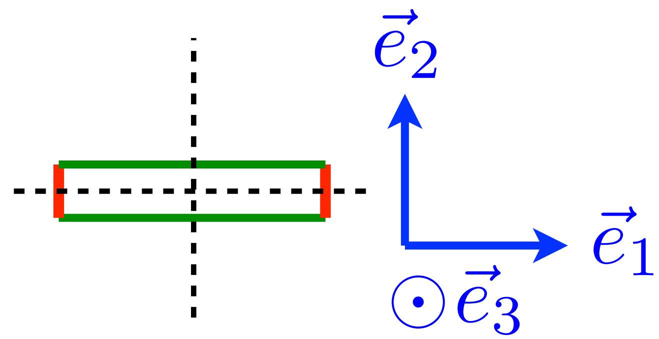



$$E = \int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + k\epsilon^2 + 2D_1\epsilon\Omega_1\Big]$$

Beams with rectangular cross-section



beam
cross-section



Beam has mirror symmetry through a plane perpendicular to $\vec{e}_3$.

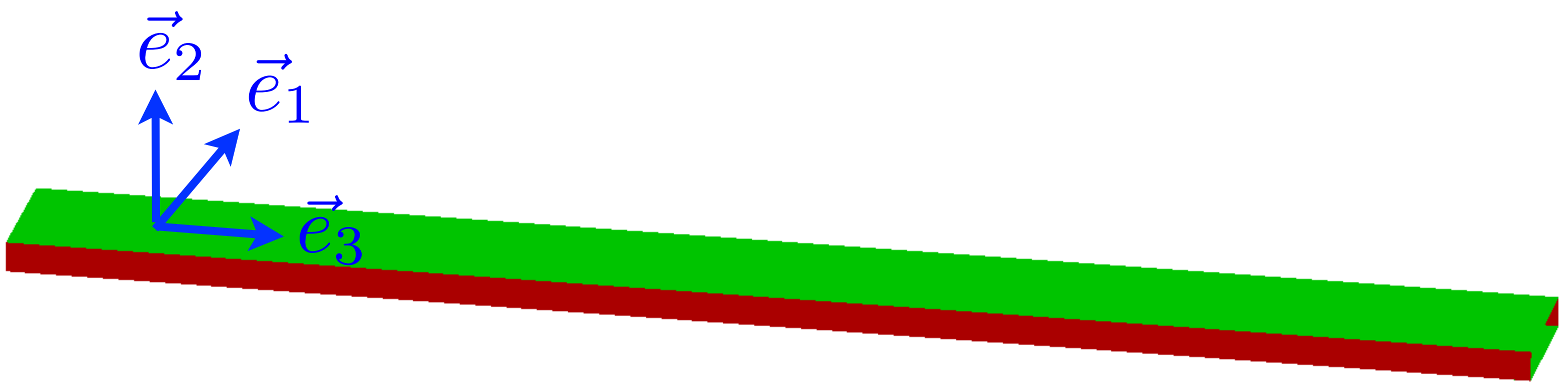
Beam has mirror symmetry through a plane perpendicular to $\vec{e}_1$.

Beam has 2-fold rotational symmetry around axis $\vec{e}_2$.

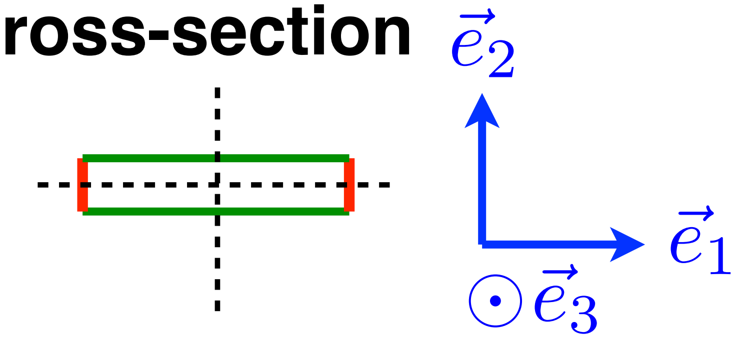
Beam has mirror symmetry through a plane perpendicular to $\vec{e}_2$.

Beam has 2-fold rotational symmetry around axis $\vec{e}_3$.

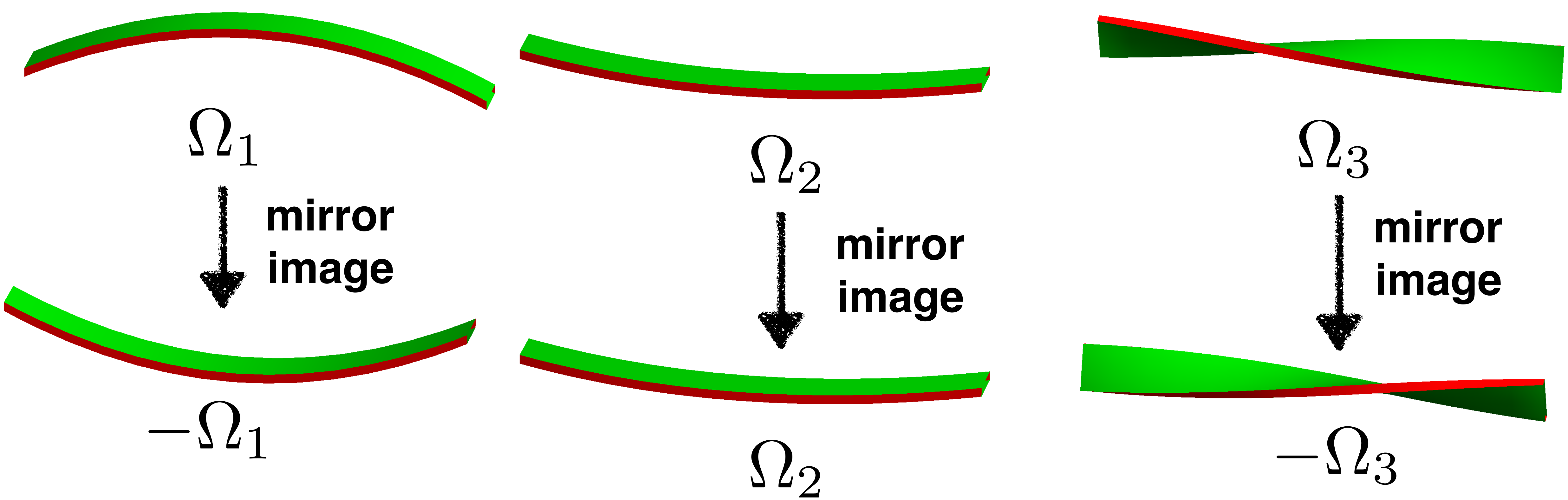
How mirroring around $\vec{e}_2$ affects bending and twisting?



beam cross-section



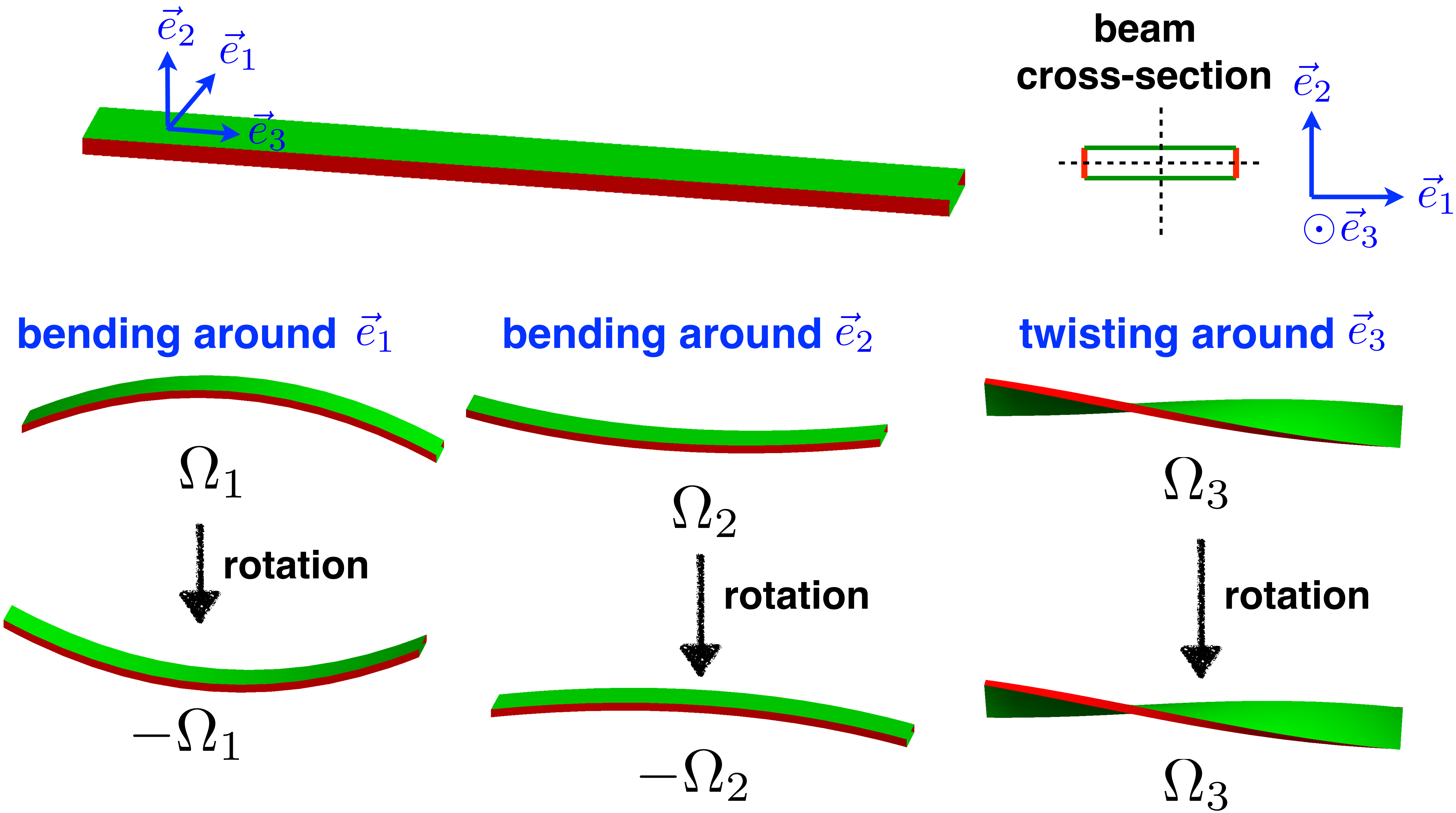
bending around $\vec{e}_1$ | **bending around $\vec{e}_2$** | **twisting around $\vec{e}_3$**



Note: mirroring doesn't affect stretching

$$A_{12} = A_{23} = D_1 = D_3 = 0$$

How rotation by π around $\vec{e}_3$ affects bending and twisting?



Note: rotation doesn't affect stretching

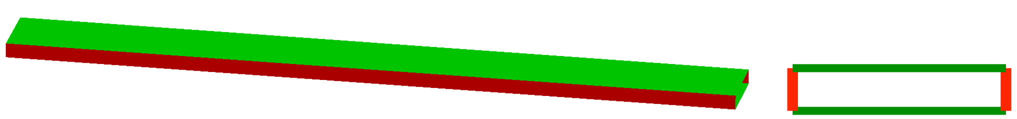
$$A_{13} = A_{23} = D_1 = D_2 = 0$$

Elastic energy for beams of various cross-sections

beam cross-section

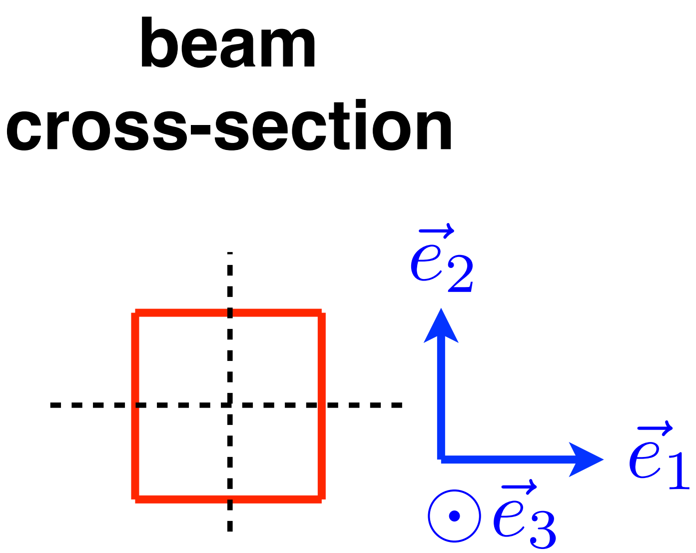
$$E = \int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + 2A_{12}\Omega_1\Omega_2 + k\epsilon^2 + 2D_1\epsilon\Omega_1 + 2D_2\epsilon\Omega_2\Big]$$

$$E = \int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + k\epsilon^2 + 2D_1\epsilon\Omega_1\Big]$$



$$E = \int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + k\epsilon^2\Big]$$

Beams with square cross-section



Beam has mirror symmetry through a plane perpendicular to $\vec{e}_3$.

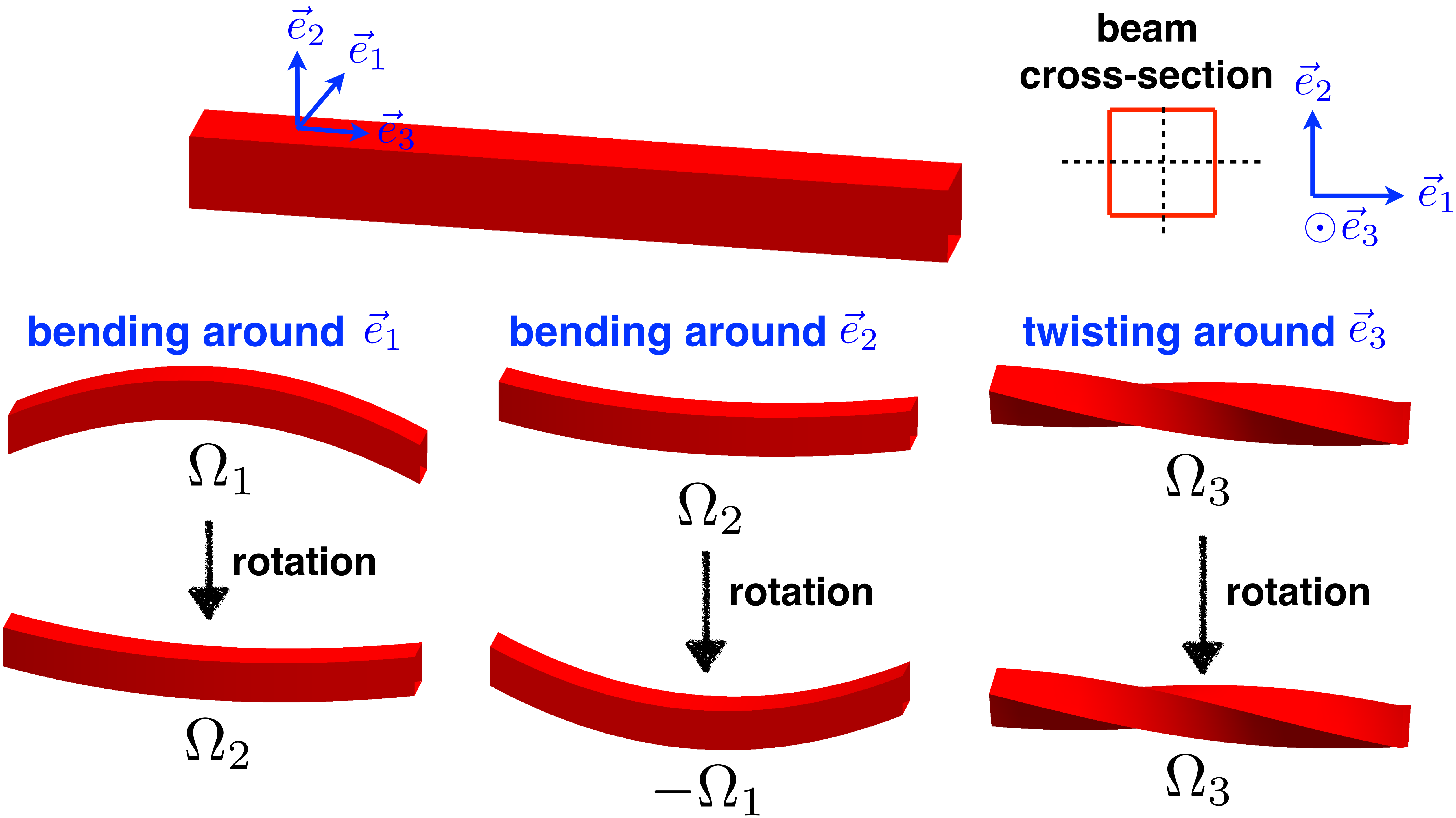
Beam has mirror symmetry through a plane perpendicular to $\vec{e}_1$.

Beam has 2-fold rotational symmetry around axis $\vec{e}_2$.

Beam has mirror symmetry through a plane perpendicular to $\vec{e}_2$.

Beam has 4-fold rotational symmetry around axis $\vec{e}_3$.

How rotation by $\pi/2$ around $\vec{e}_3$ affects bending and twisting?



Note: rotation doesn't affect stretching

$$A_{11} = A_{22}, \quad A_{12} = D_1 = D_2 = 0$$

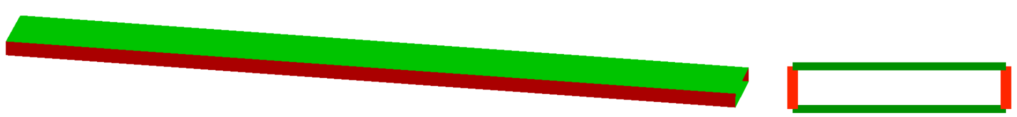
Elastic energy for beams of various cross-sections

beam

cross-section

$$E=\int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2+A_{22}\Omega_2^2+C\Omega_3^2+2A_{12}\Omega_1\Omega_2 +k\epsilon^2+2D_1\epsilon\Omega_1+2D_2\epsilon\Omega_2\Big]$$

$$E=\int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2+A_{22}\Omega_2^2+C\Omega_3^2 +k\epsilon^2+2D_1\epsilon\Omega_1\Big]$$



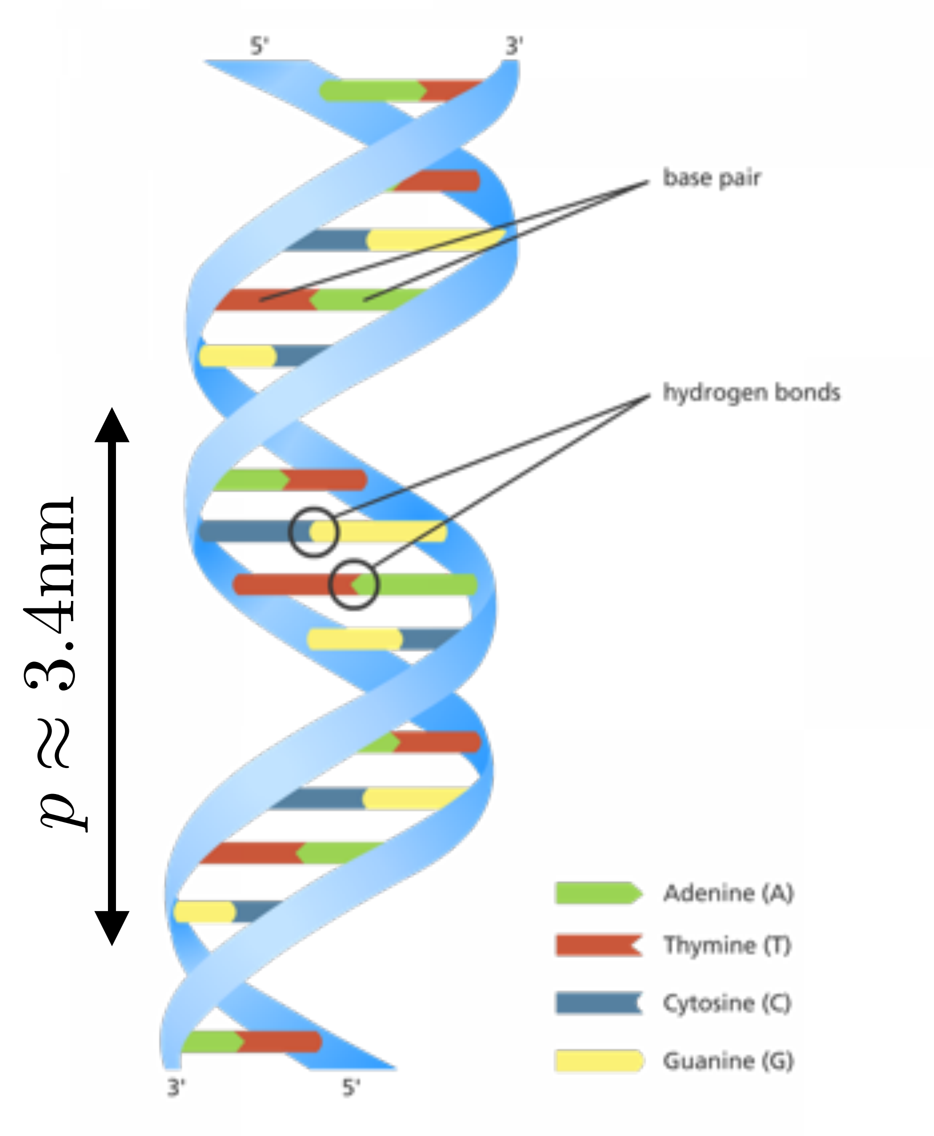
$$E=\int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2+A_{22}\Omega_2^2+C\Omega_3^2+k\epsilon^2\Big]$$

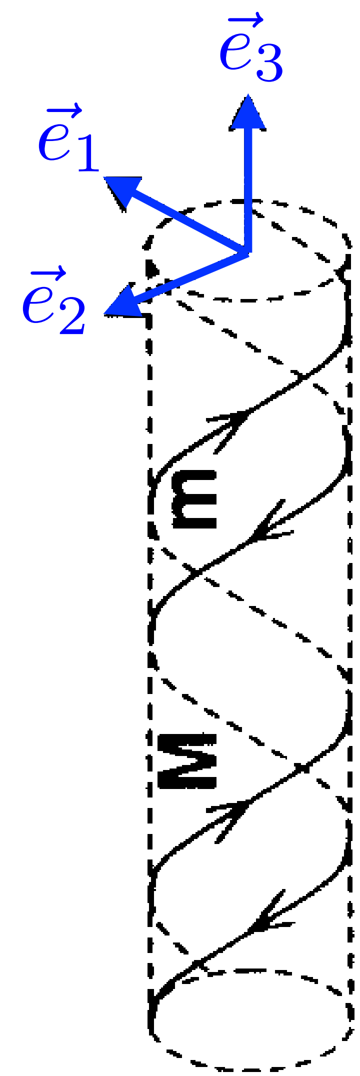
$$E=\int_0^L \frac{ds}{2}\Big[A\left(\Omega_1^2+\Omega_2^2\right)+C\Omega_3^2+k\epsilon^2\Big]$$

$$E=\int_0^L \frac{ds}{2}\Big[A_{11}(s)\Omega_1^2(s)+A_{22}(s)\Omega_2^2(s)+C(s)\Omega_3^2(s) +2A_{12}(s)\Omega_1(s)\Omega_2(s)+2A_{13}(s)\Omega_1(s)\Omega_3(s)+2A_{23}(s)\Omega_2(s)\Omega_3(s) +k(s)\epsilon(s)^2+2D_1(s)\epsilon(s)\Omega_1(s)+2D_2(s)\epsilon(s)\Omega_2(s)+2D_3(s)\epsilon(s)\Omega_3(s)\Big]$$

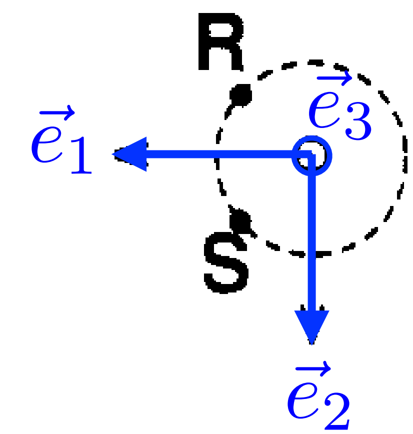
DNA

DNA is chiral and has right-handed helical structure





cross section



In the undeformed state DNA has spontaneous twist

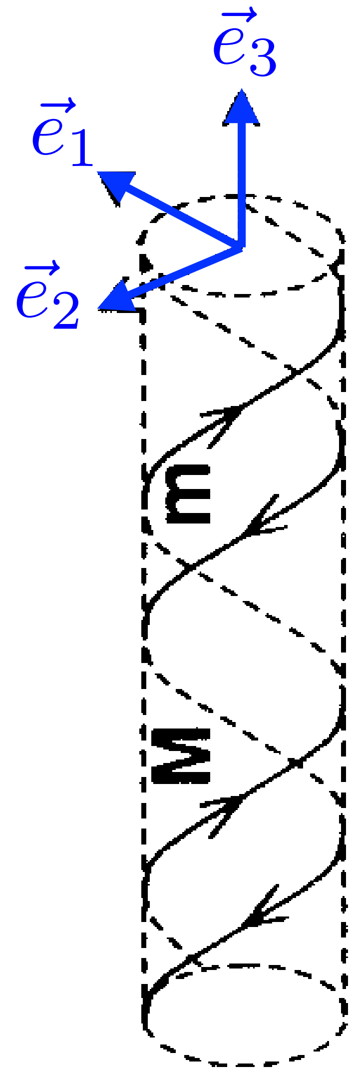
$$\omega_0 = 2\pi/p \approx 1.8\,\mathrm{nm}^{-1}$$

Twist strain Ω_3 is measured relative to the spontaneous twist

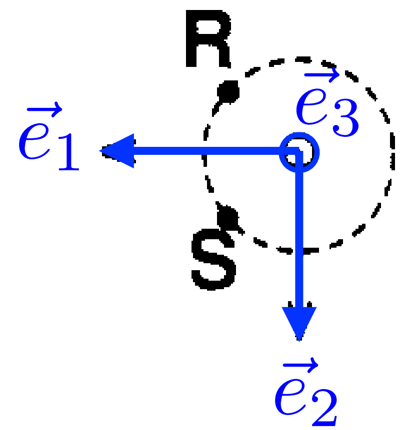
$$\frac{d\vec{e}_i}{ds} = \left(\vec{\Omega} + \omega_0 \vec{e}_3\right) \times \vec{e}_i$$

For simplicity we ignore DNA sequence dependence of elastic constants!

DNA



cross section



DNA has 2-fold rotational symmetry around axis $\vec{e}_1$.

$$A_{12} = A_{13} = D_1 = 0$$

Twist strain Ω_3 is measured relative to the spontaneous twist

$$\frac{d\vec{e}_i}{ds} = \left(\vec{\Omega} + \omega_0 \vec{e}_3\right) \times \vec{e}_i$$

Elastic energy for deforming DNA

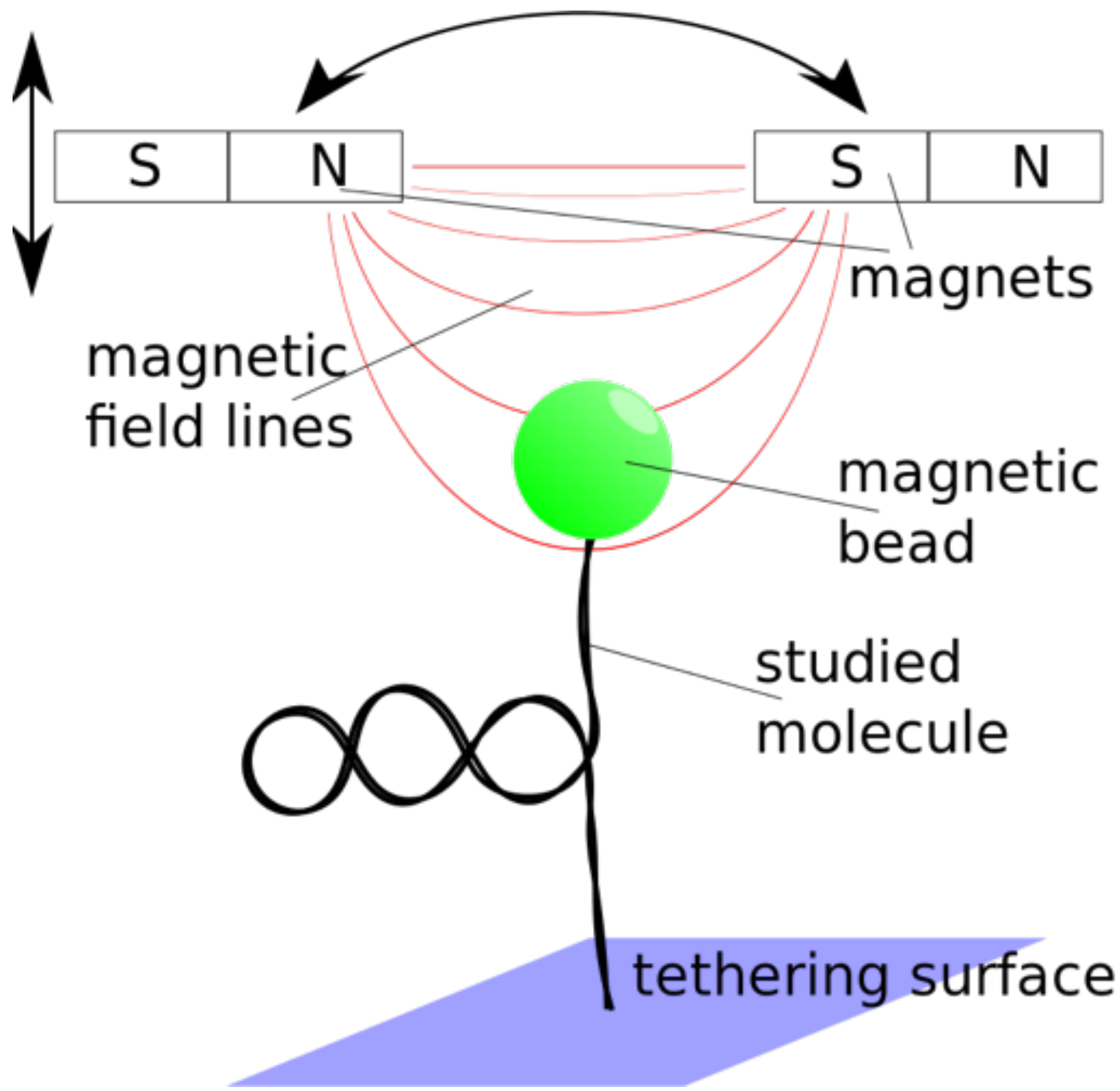
$$E = \int_0^L \frac{ds}{2}\Big[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + 2A_{23}\Omega_2\Omega_3 + k\epsilon^2 + 2D_2\epsilon\Omega_2 + 2D_3\epsilon\Omega_3\Big]$$

$$A_{11}/k_BT \approx A_{22}/k_BT = \ell_p \sim 50\text{nm}$$
$$C/k_BT \sim 100\text{nm}$$
$$k \sim 1000\text{pN}$$
$$D_3/k_BT \sim -20$$
$$A_{23}, D_2 \sim 0$$

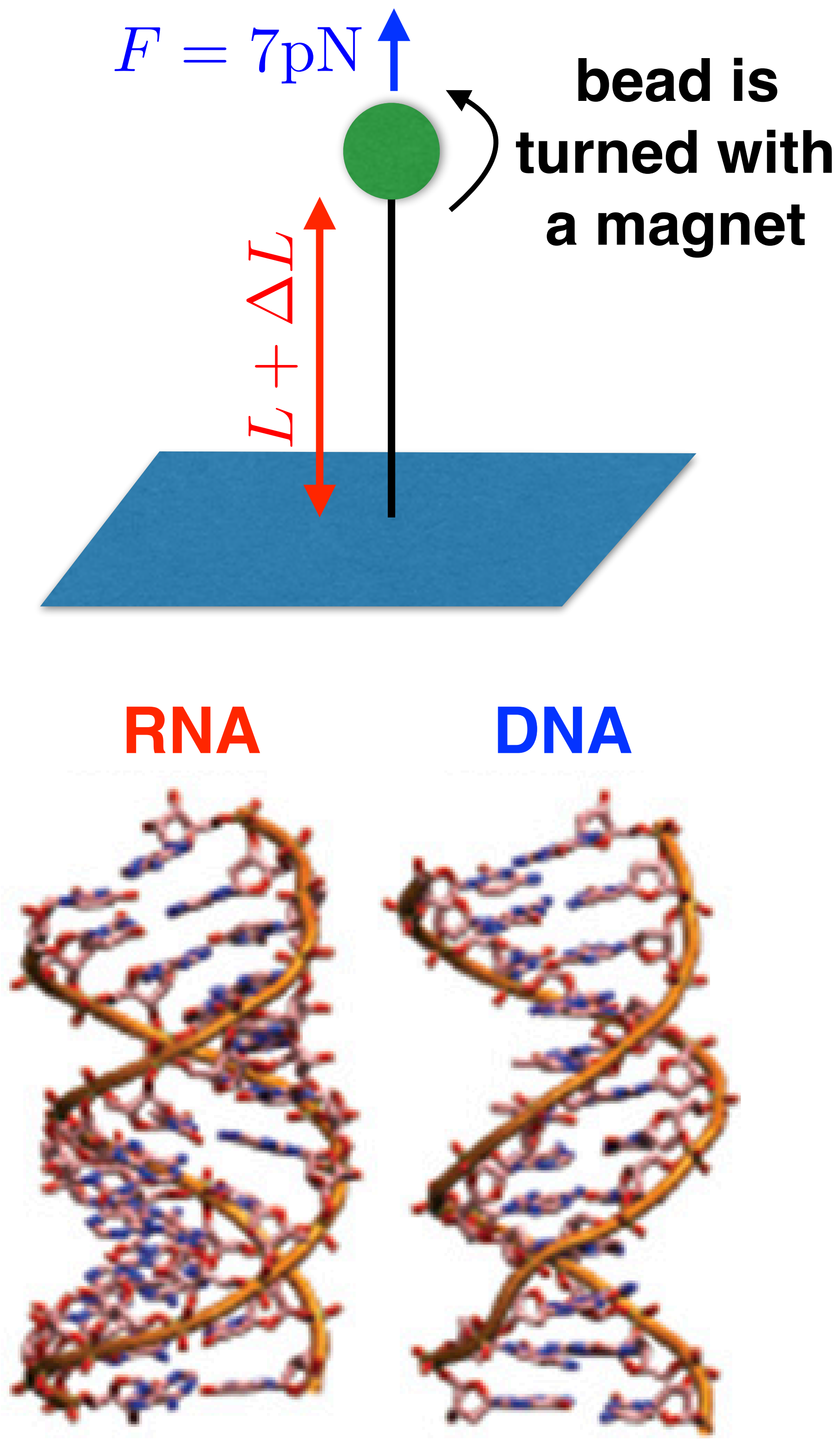
Magnetic tweezers

Torque on magnetic bead can be produced by rotating the magnet.

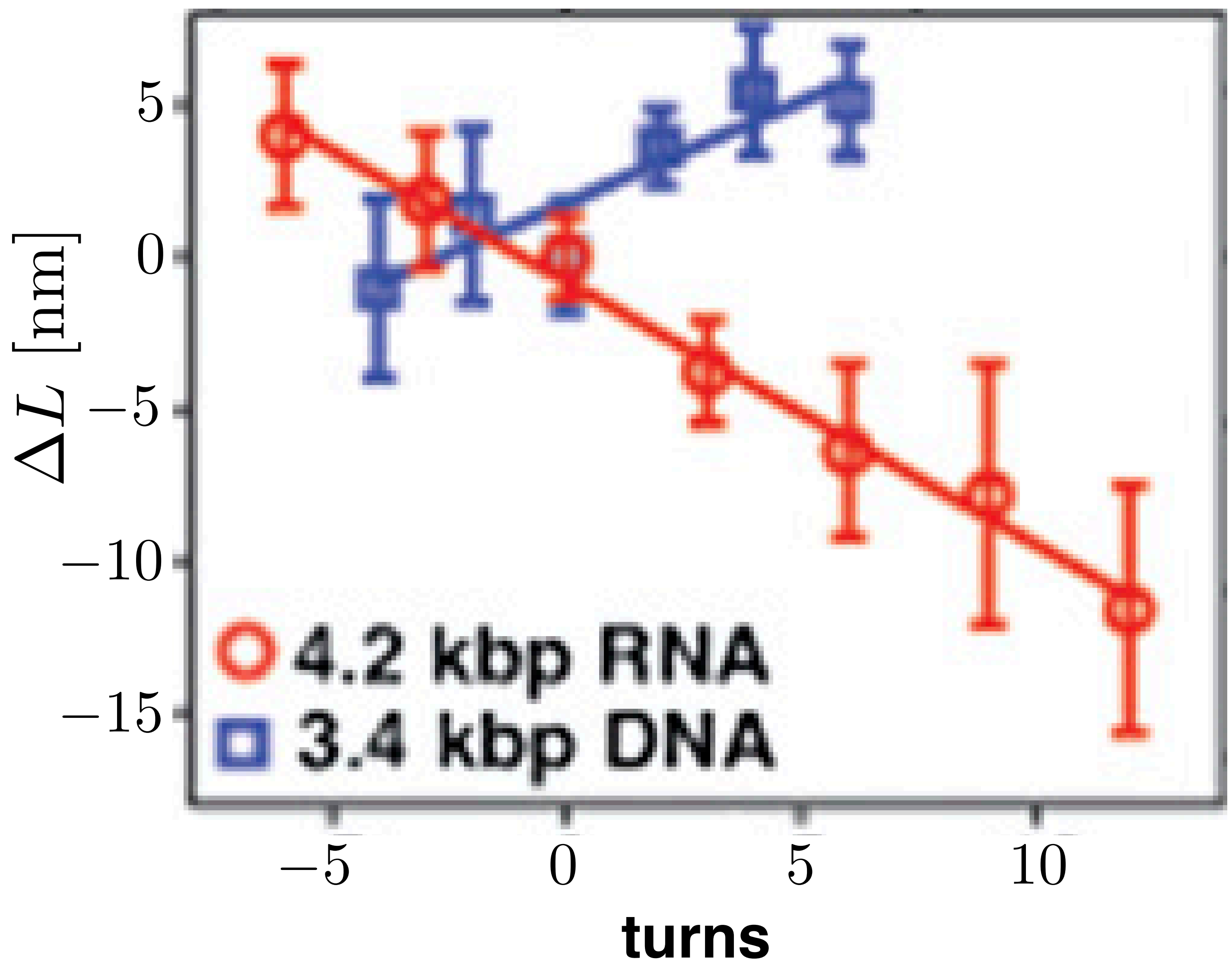
Force on magnetic bead is proportional to the gradient of magnetic field and can be adjusted by raising or lowering the magnet



Twist-stretch coupling

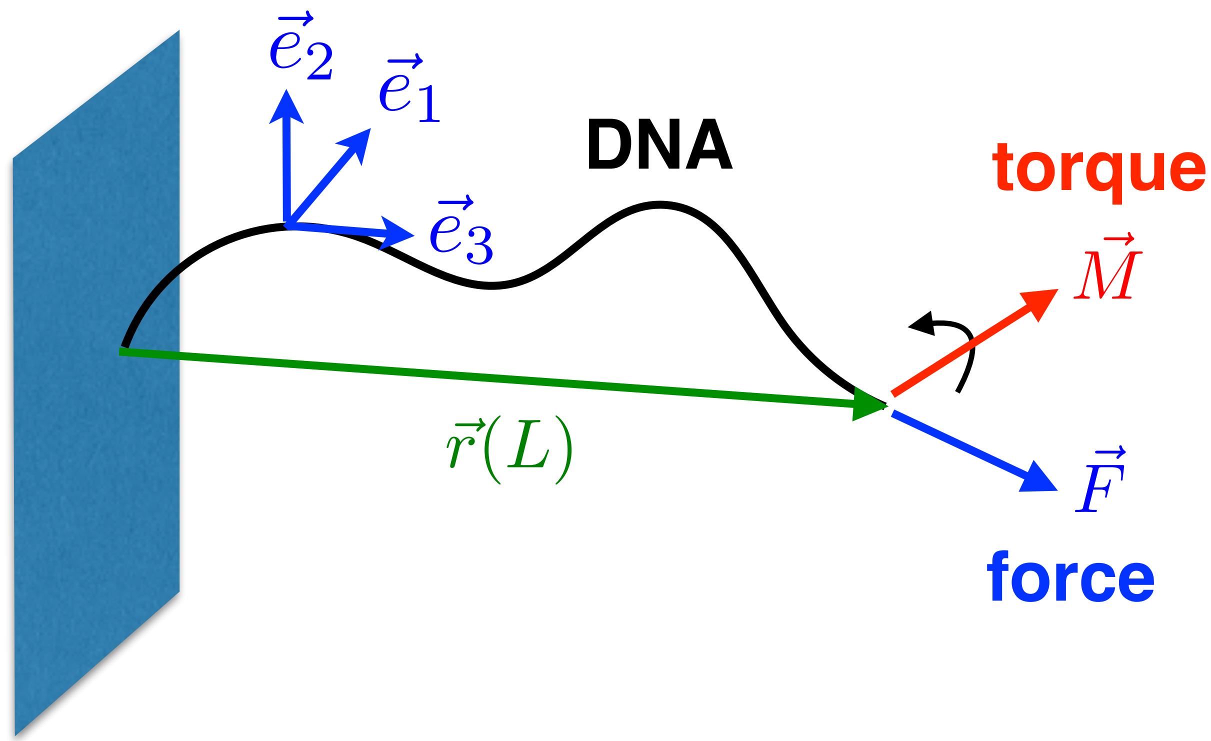


Twist-stretch coupling has opposite sign for double stranded RNA and DNA!



J. Lipfert *et al.*, PNAS 111, 15408 (2014)

Response of DNA to external forces and torques



$$E = \int_0^L \frac{ds}{2}\left[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + k\epsilon^2 + 2D_3\epsilon\Omega_3\right] - \vec{F}\cdot\vec{r}(L) - \vec{M}\cdot\vec{\phi}(L)$$

work due to external force and torque

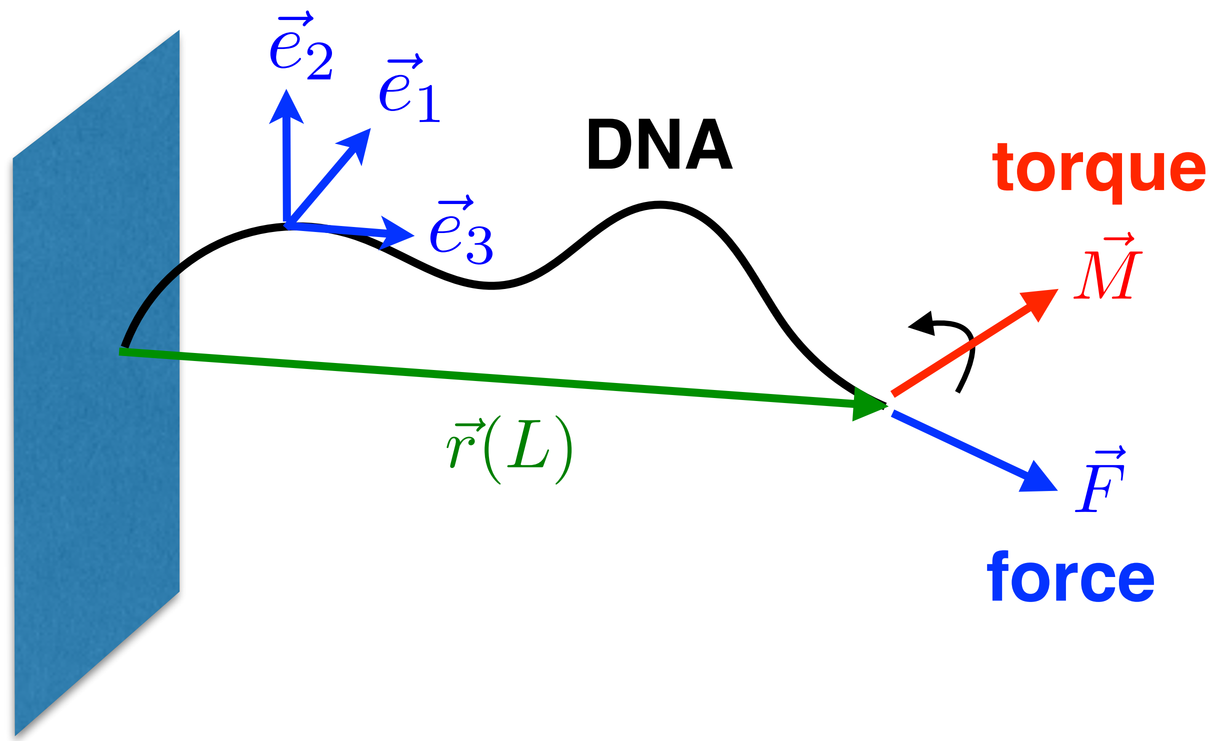
DNA end to end distance

$$\vec{r}(L) = \int_0^L ds\,\frac{d\vec{r}}{ds} = \int_0^L ds\;\vec{e}_3(1+\epsilon)$$

rotation of DNA end

$$\vec{\phi}(L) = \int_0^L ds\,\frac{d\vec{\phi}}{ds} = \int_0^L ds\;\vec{\Omega}$$

Response of DNA to external forces and torques



$$E = \int_0^L ds \left(\frac{1}{2} \left[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + k\epsilon^2 + 2D_3\epsilon\Omega_3 \right] - \vec{F}\cdot\vec{e}_3(1+\epsilon) - \vec{M}\cdot\vec{\Omega} \right)$$

$$E = \int_0^L ds\ g(\epsilon, \Omega_1, \Omega_2, \Omega_3)$$

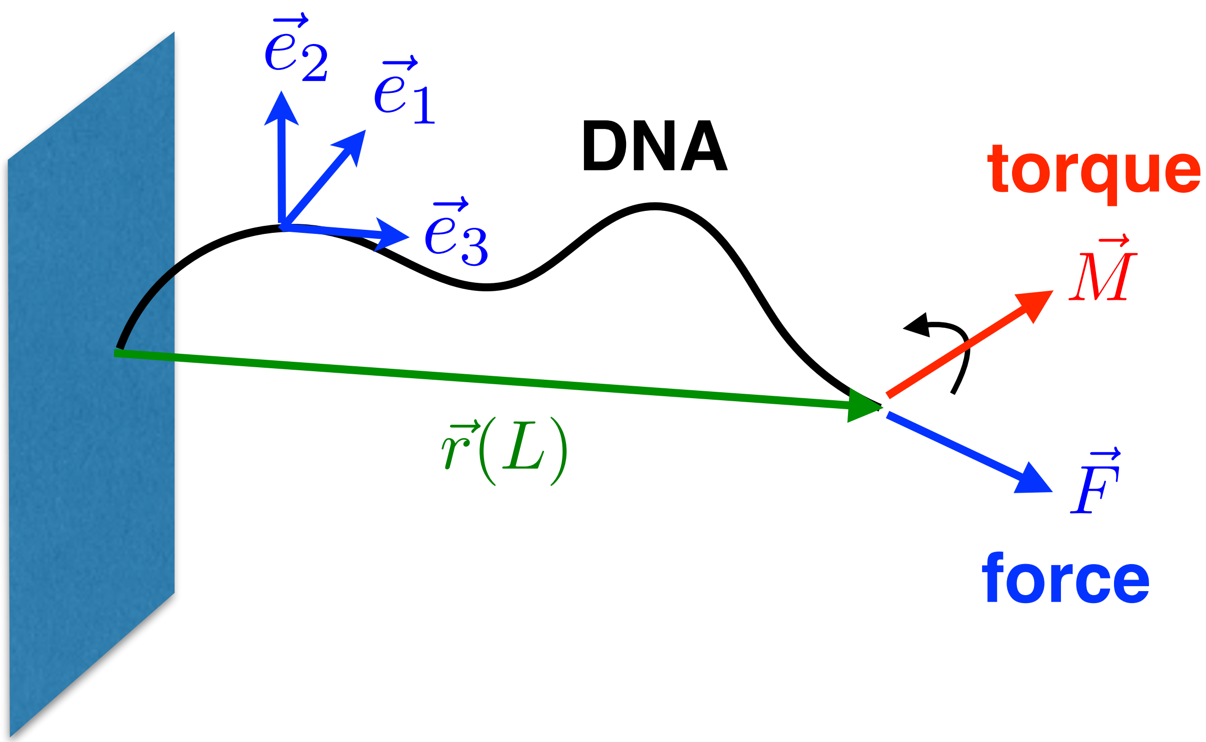
The configuration of DNA that minimizes energy is described by Euler-Lagrange equations

$$0 = \frac{d}{ds}\left(\frac{\partial g}{\partial (d\epsilon/ds)} \right) - \frac{\partial g}{\partial \epsilon}$$

$$0 = \frac{d}{ds}\left(\frac{\partial g}{\partial (d\phi_i/ds)} \right) - \frac{\partial g}{\partial \phi_i}$$

$$\Omega_i = d\phi/ds$$

Tension and torque along DNA backbone



$$E = \int_0^L ds \left(\frac{1}{2} \left[A_{11}\Omega_1^2 + A_{22}\Omega_2^2 + C\Omega_3^2 + k\epsilon^2 + 2D_3\epsilon\Omega_3 \right] - \vec{F}\cdot\vec{e}_3(1+\epsilon) - \vec{M}\cdot\vec{\Omega} \right)$$

Euler-Lagrange equations

$$0 = \frac{d}{ds}\left(\frac{\partial g}{\partial(d\epsilon/ds)}\right) - \frac{\partial g}{\partial \epsilon} \longrightarrow$$

tension along DNA

$$k\epsilon(s) + D_3\Omega_3(s) = \vec{F}\cdot\vec{e}_3(s)$$

$$0 = \frac{d}{ds}\left(\frac{\partial g}{\partial(d\phi_i/ds)}\right) - \frac{\partial g}{\partial \phi_i} \longrightarrow$$

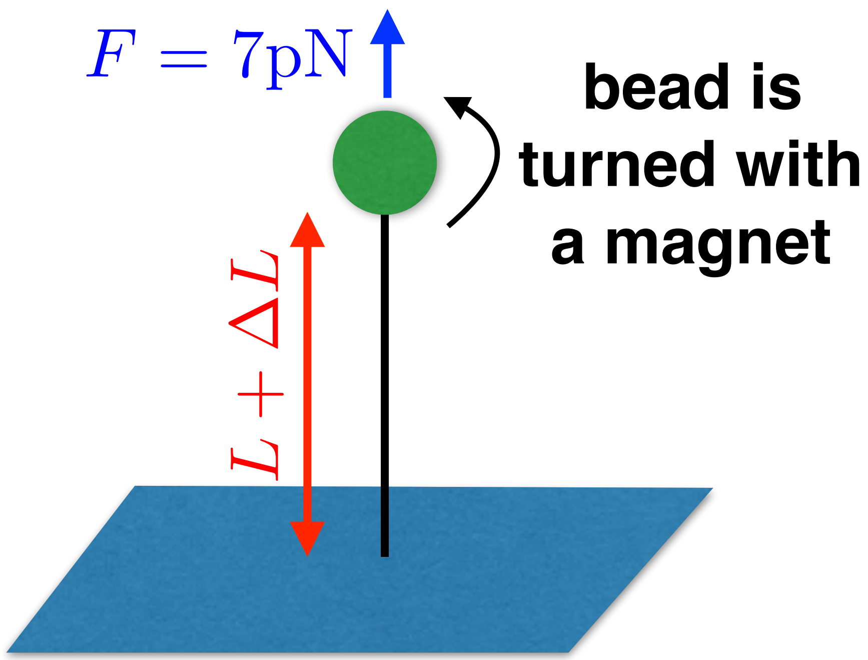
torque along DNA

$$A_{11}\Omega_1(s)\vec{e}_1(s) + A_{22}\Omega_2(s)\vec{e}_2(s) + \left[C\Omega_3(s) + D_3\epsilon(s)\right]\vec{e}_3(s) = \vec{M}$$

$$\Omega_i = d\phi/ds$$

Euler-Lagrange equations thus describe local force and torque balance!

Twist-stretch coupling

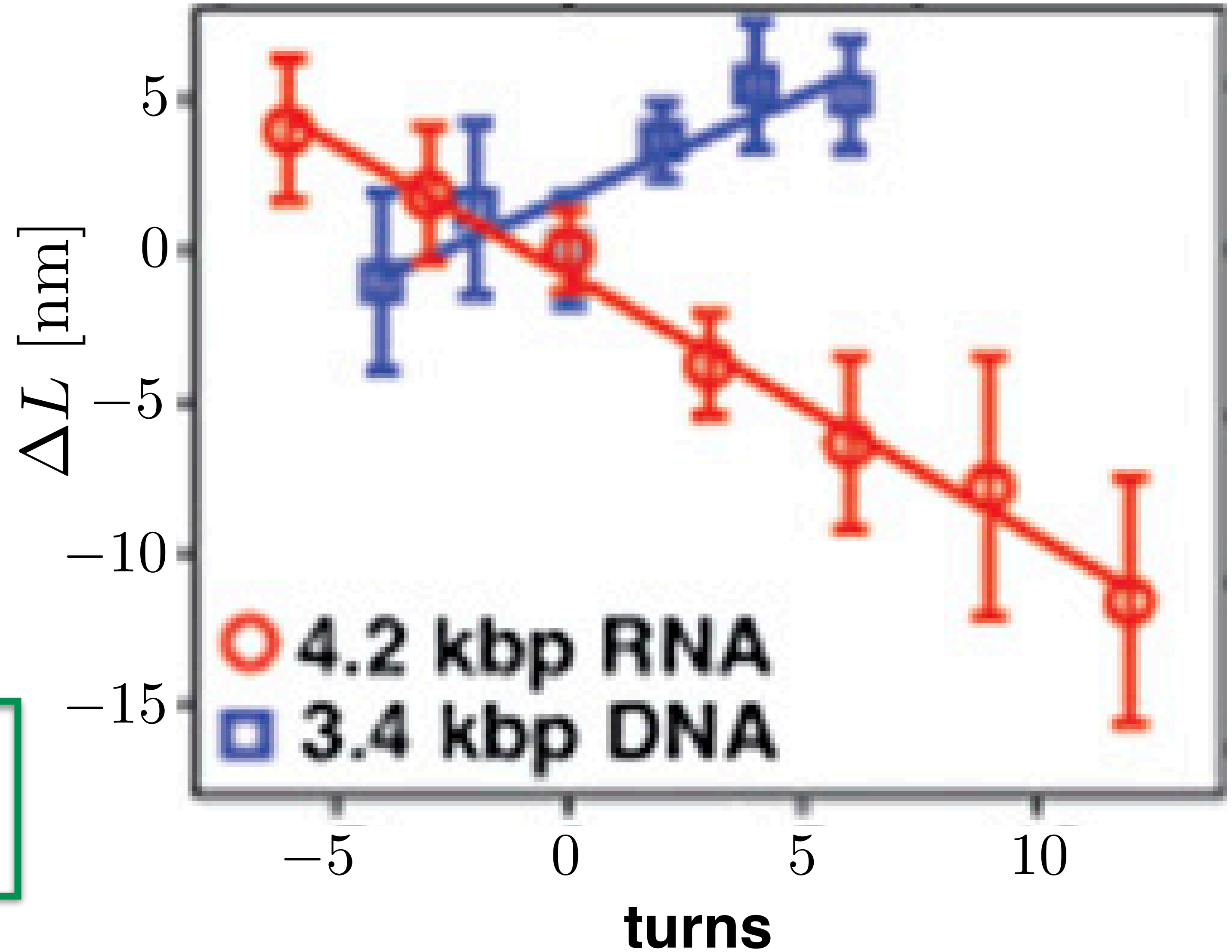


$$k\epsilon(s) + D_3\Omega_3(s) = \vec{F}\cdot\vec{e}_3(s)$$

$$\Omega_3 = 2\pi N_{\text{turns}}/L$$

$$\Delta L = L\epsilon = \frac{FL}{k} - \frac{2\pi D_3}{k} N_{\text{turns}}$$

Twist-stretch coupling has opposite sign for double stranded RNA and DNA!



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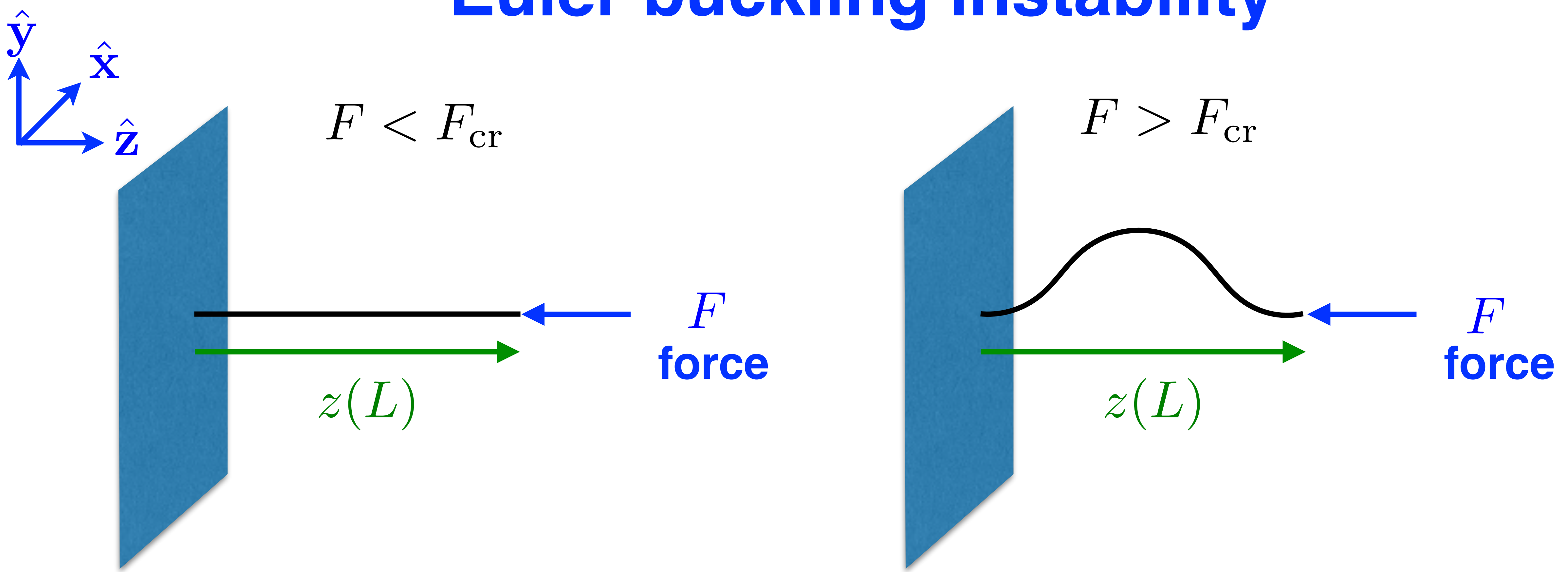
Euler buckling instability



Analyze the stability of flat configuration by investigating the energy cost of slightly deformed profile with

$$\vec{r}(s) = (0, y(s), z(s))$$

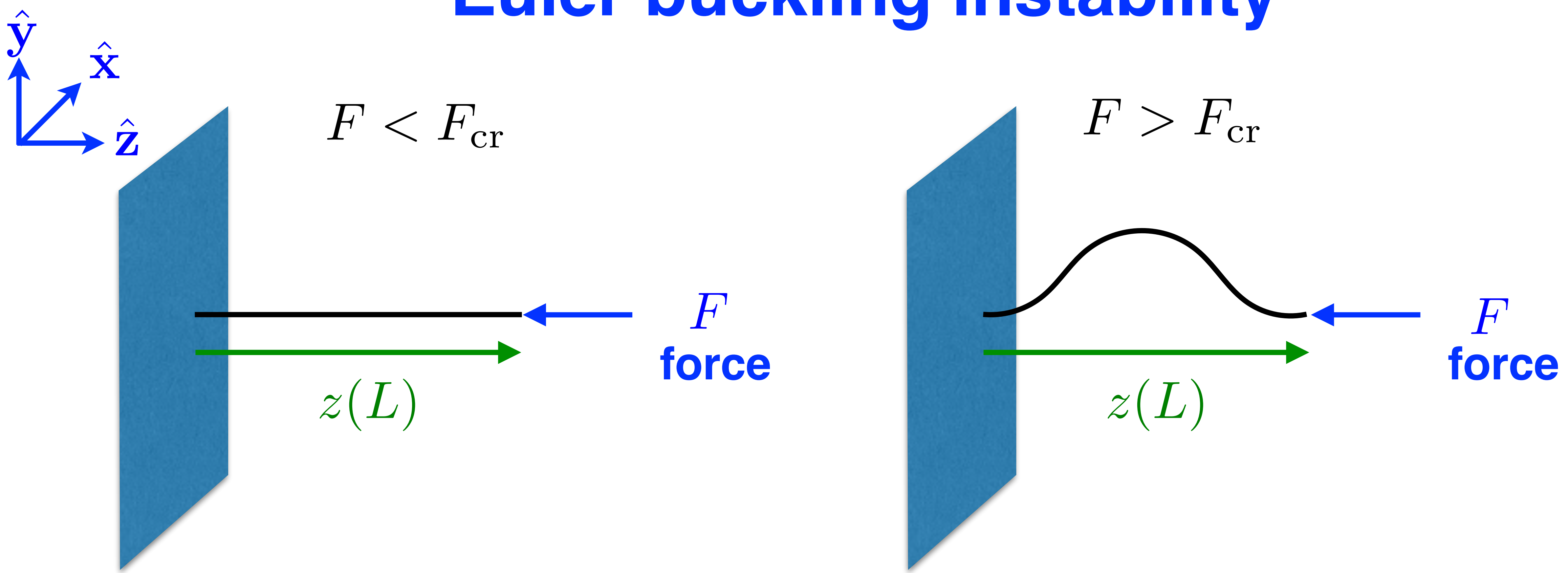
Assume the very thin beam (filament) limit with $\epsilon \to 0$

$$\vec{e}_3 = \frac{d\vec{r}}{ds} = (0, y', z') \longrightarrow z' = \sqrt{1 - y'^2} \longrightarrow z(s) = \int_0^s d\ell \sqrt{1 - y'(\ell)^2}$$

Bending strain

$$\Omega^2 = \frac{1}{R^2} = \left(\frac{d^2\vec{r}}{ds^2}\right)^2 = y''^2 + z''^2 = \frac{y''^2}{1 - y'^2}$$

Euler buckling instability



$$E = \int_0^L ds \frac{A}{2}\Omega^2 + F z(L) = \int_0^L ds \left[\frac{A}{2} \frac{y''^2}{(1-y'^2)} + F\sqrt{1-y'^2} \right]$$

Assume small deformations around the flat configuration

$$E \approx \int_0^L ds \left[\frac{1}{2} A y''^2 - \frac{1}{2} F y'^2 + F \right]$$

$$y(s) = \sum_q e^{iqs} \tilde{y}(q)$$

analyze with Fourier modes

$$E \approx +FL + \sum_q \frac{1}{2} \left(Aq^4 - Fq^2 \right) |\tilde{y}(s)|^2$$

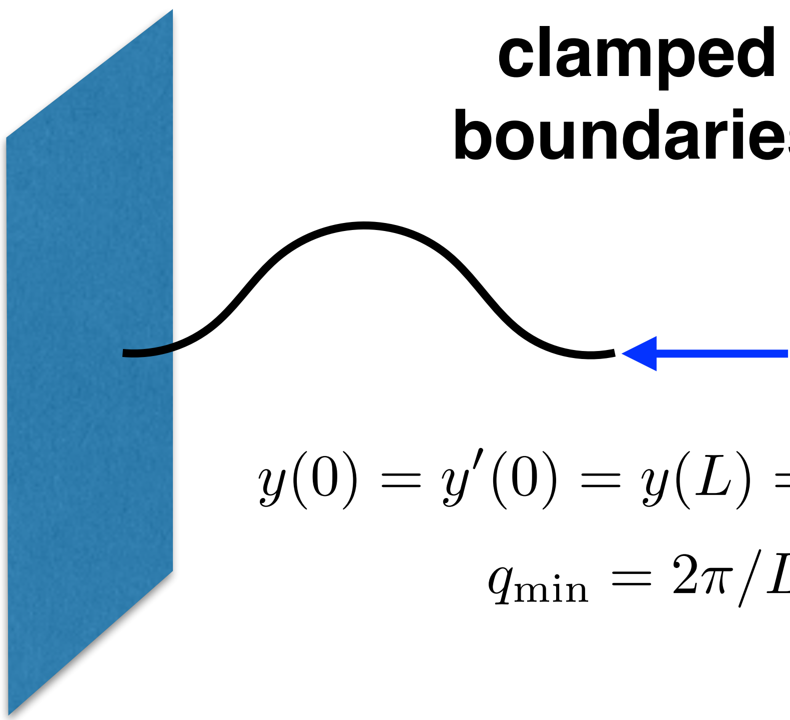
Buckled configurations have lover energy for

$$F > F_{\rm cr} = A q_{\rm min}^2$$

Note: buckling direction corresponds to the lower value of bending rigidity *A*

Euler buckling instability

clamped boundaries

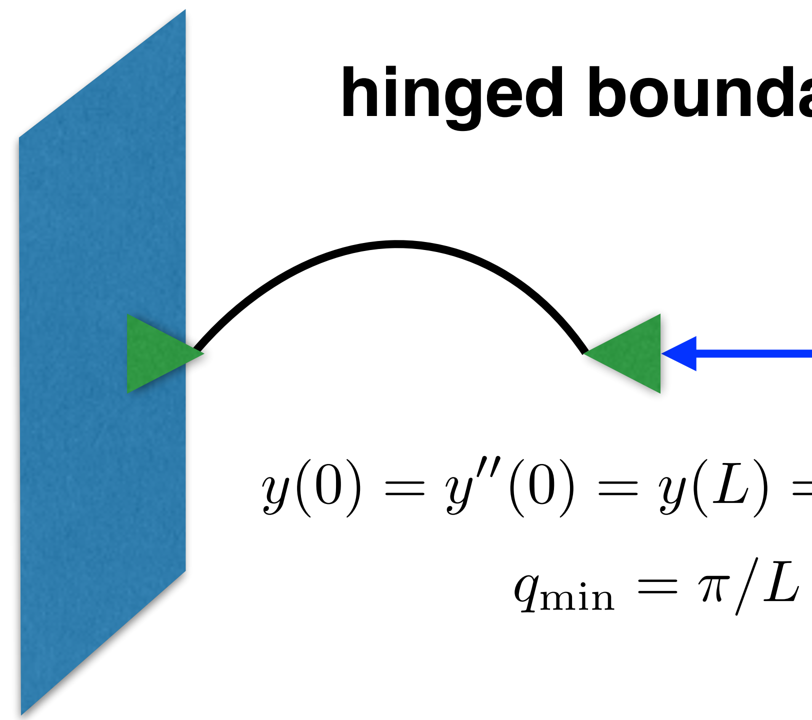


$$F_{\rm cr} = \frac{4\pi^2 A}{L^2}$$

$$y(0) = y'(0) = y(L) = y'(L) = 0$$

$$q_{\rm min} = 2\pi/L$$

hinged boundaries

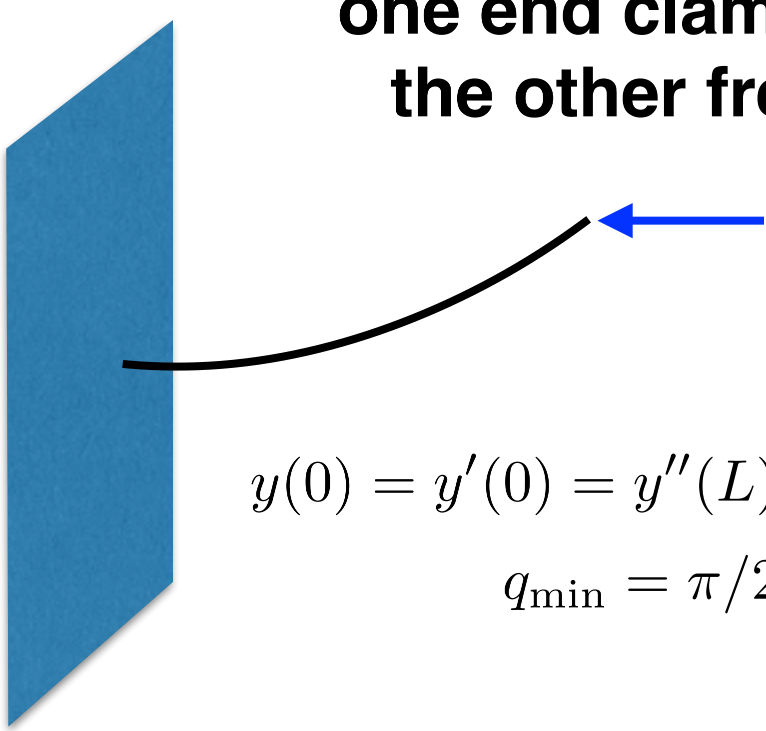


$$F_{\rm cr} = \frac{\pi^2 A}{L^2}$$

$$y(0) = y''(0) = y(L) = y''(L) = 0$$

$$q_{\rm min} = \pi/L$$

one end clamped
the other free



$$F_{\rm cr} = \frac{\pi^2 A}{4L^2}$$

$$y(0) = y'(0) = y''(L) = y'''(L) = 0$$

$$q_{\rm min} = \pi/2L$$

The amplitudes of buckled modes are determined by the 4th order terms in energy functional that we ignored

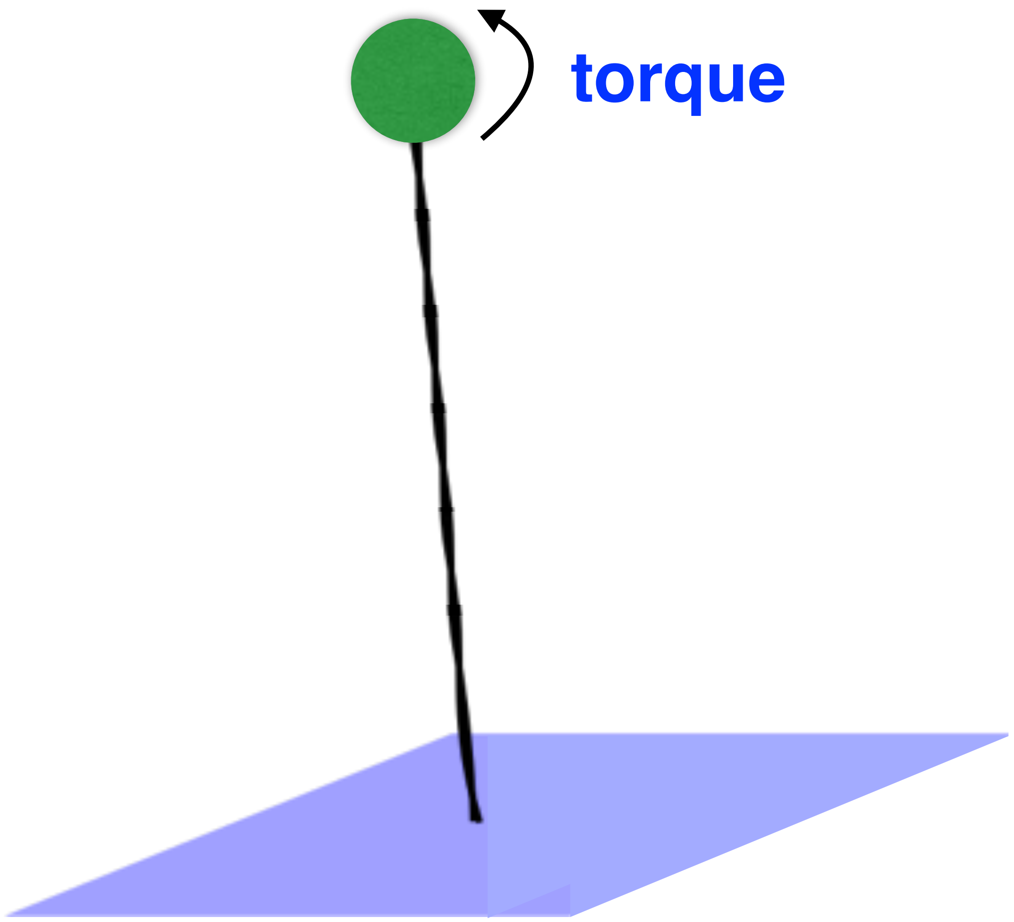
$$E \approx \int_0^L ds \left[\frac{A}{2} y''^2 (1 + y'^2) + F\left(1 - \frac{1}{2} y'^2 + \frac{1}{8} y'^4\right)\right]$$

$$\downarrow$$

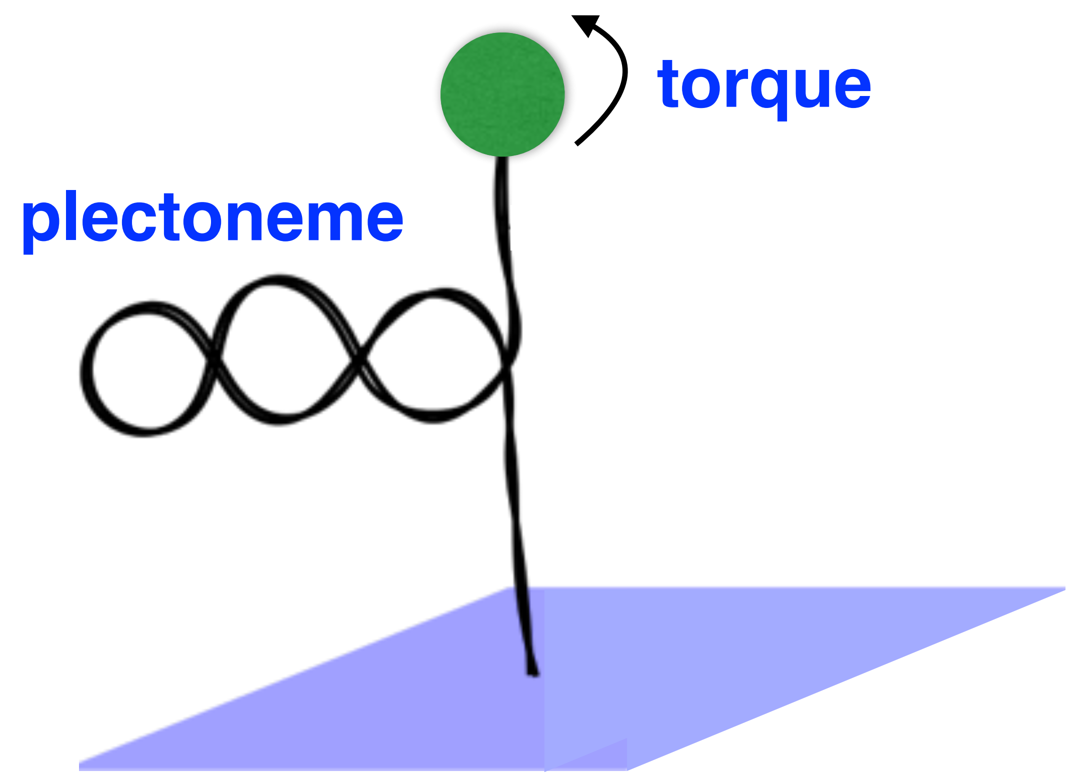
$$\tilde{y}(q_{\rm min}) \propto \sqrt{(F - Aq_{\rm min}^2)/(Aq_{\rm min}^4)}$$

Torsional instability

$M < M_{\mathrm{cr}}$



$M > M_{\mathrm{cr}}$



critical torque for clamped boundaries

$$M_{\mathrm{cr}} \approx 9\frac{A}{L}$$

number of turns that lead to torsional instability

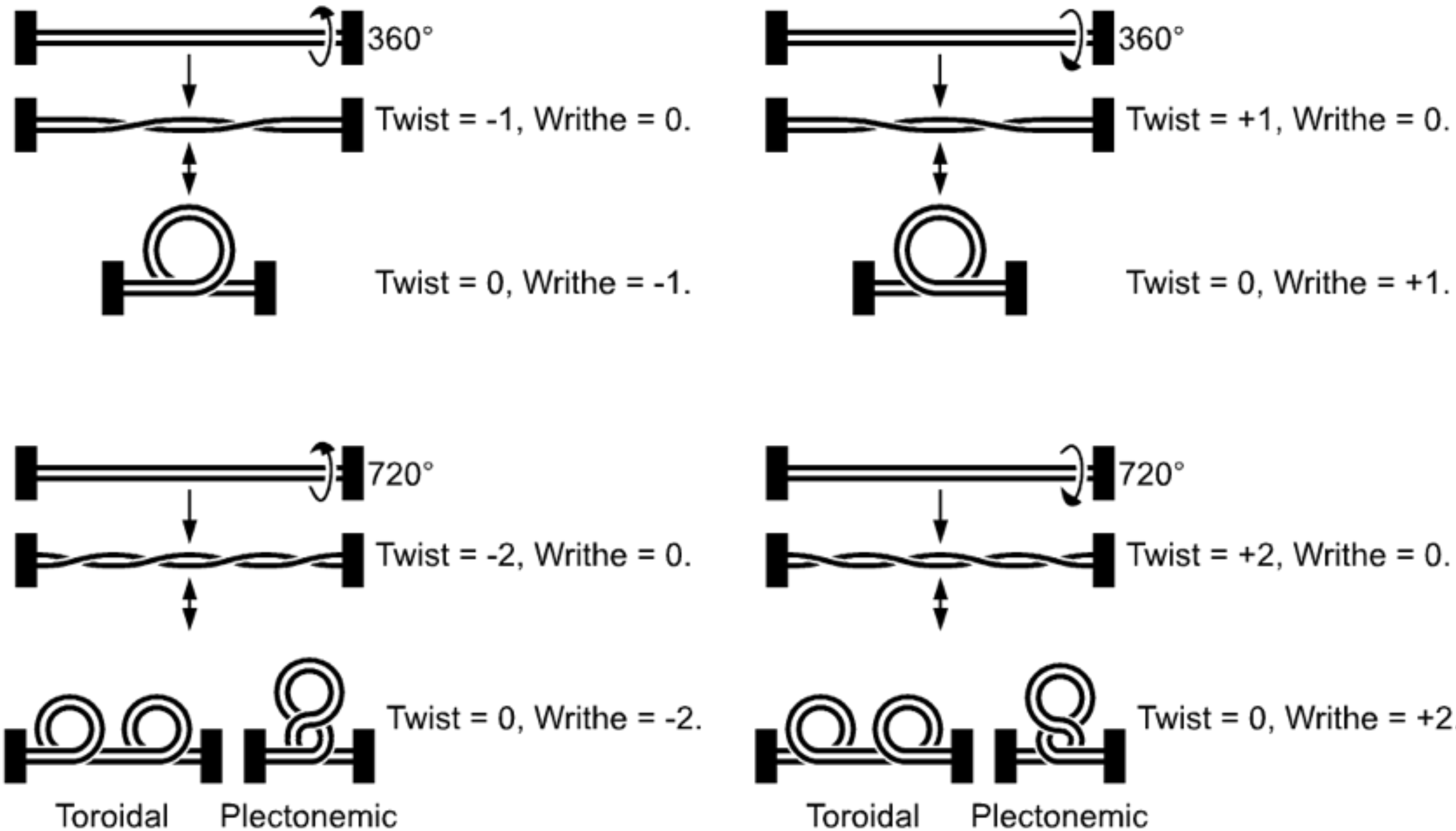
$$N_{\mathrm{turns}} = \frac{L\Omega_3}{2\pi} = \frac{LM_{\mathrm{cr}}}{2\pi C} \approx 1.4\frac{A}{C}$$

Twist, Writhe and Linking numbers

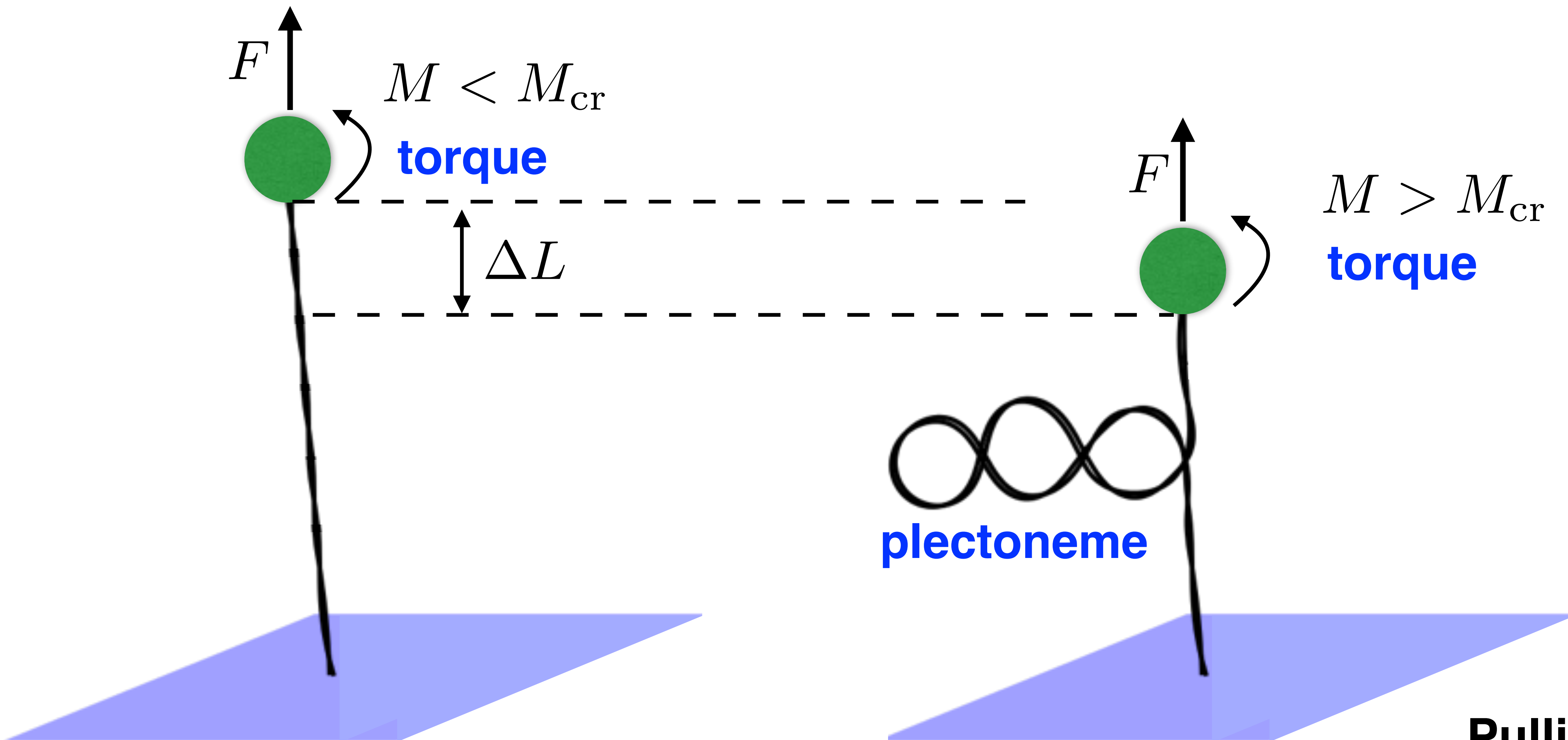
Ln=Tw+Wr **linking number: total number of turns of a particular end**

$\mathrm{Tw} = \int_0^L ds\, \Omega_3(s)/2\pi$ **twist: number of turns due to twisting the beam**

Wr **writhe: number of crossings when curve is projected on a plane**



Torsional instability



Pulling force suppresses instability.

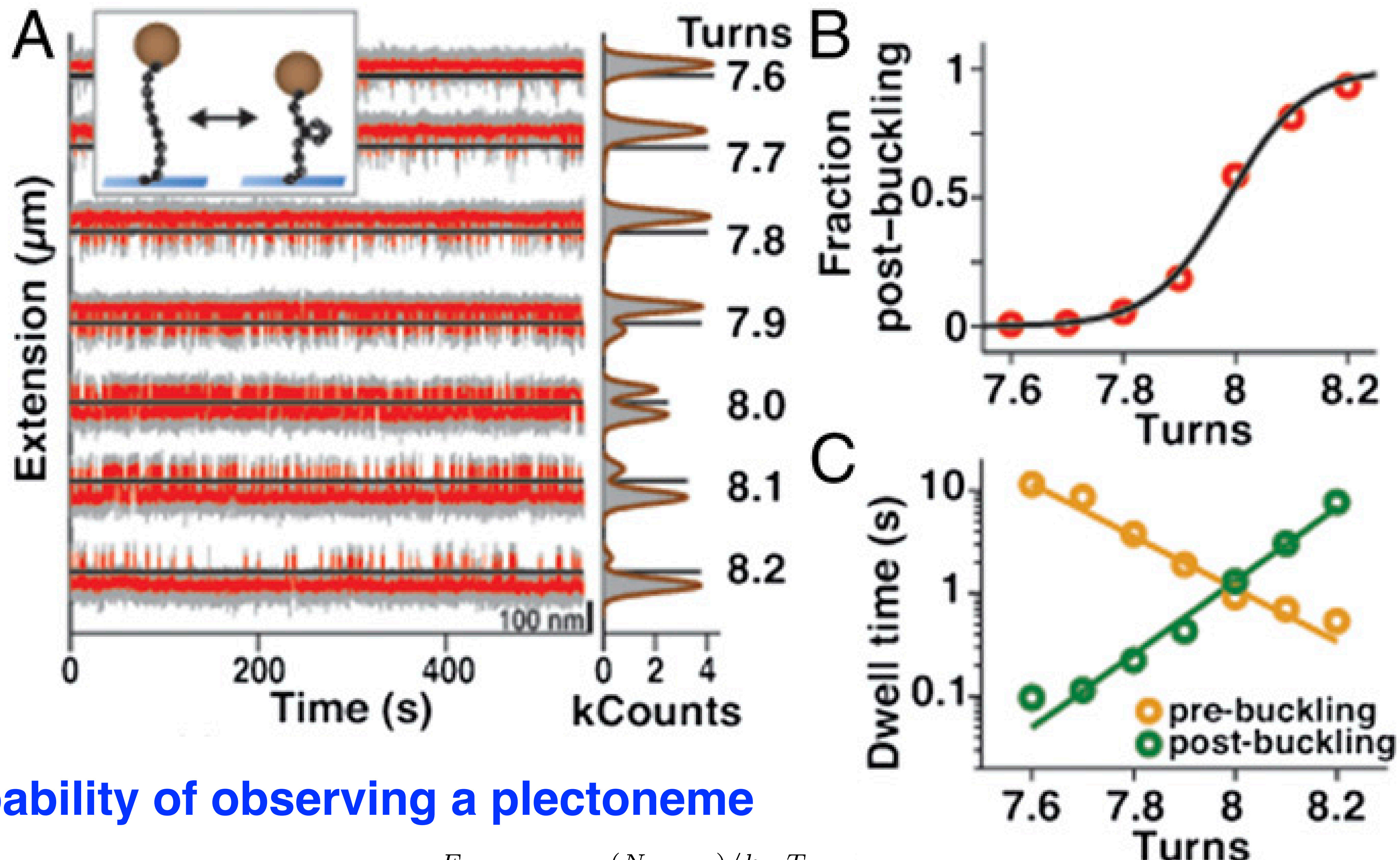
$$E = \frac{CL[2\pi \mathrm{Ln}]^2}{2}$$

$$E = \frac{CL[2\pi\,(\mathrm{Ln} - \mathrm{Wr})]^2}{2} + E_{\rm bend} + F\Delta L$$

Torsional instability occurs, because part of the twisting energy can be released by bending and forming a plectoneme.

Stochastic switching between two states near instability for twisting RNA

puling force $F = 2\text{pN}$



probability of observing a plectoneme

$$p_{\text{plectoneme}}(N_{\text{turns}}) = \frac{e^{-E_{\text{plectoneme}}(N_{\text{turns}})/k_B T}}{e^{-E_{\text{straight}}(N_{\text{turns}})/k_B T} + e^{-E_{\text{plectoneme}}(N_{\text{turns}})/k_B T}}$$

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