Elastic knots

(elastic beam under finite rotation and self-contact)

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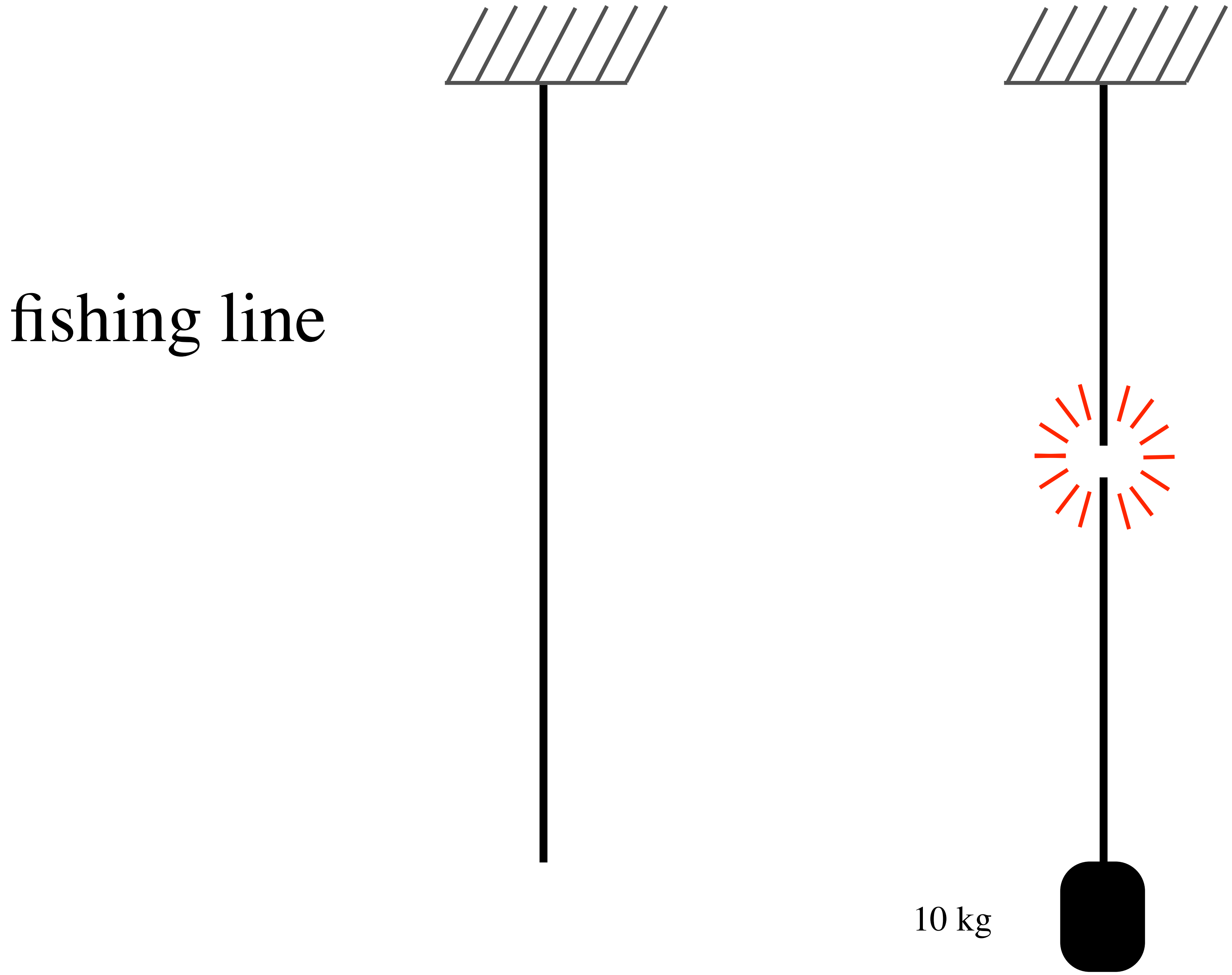
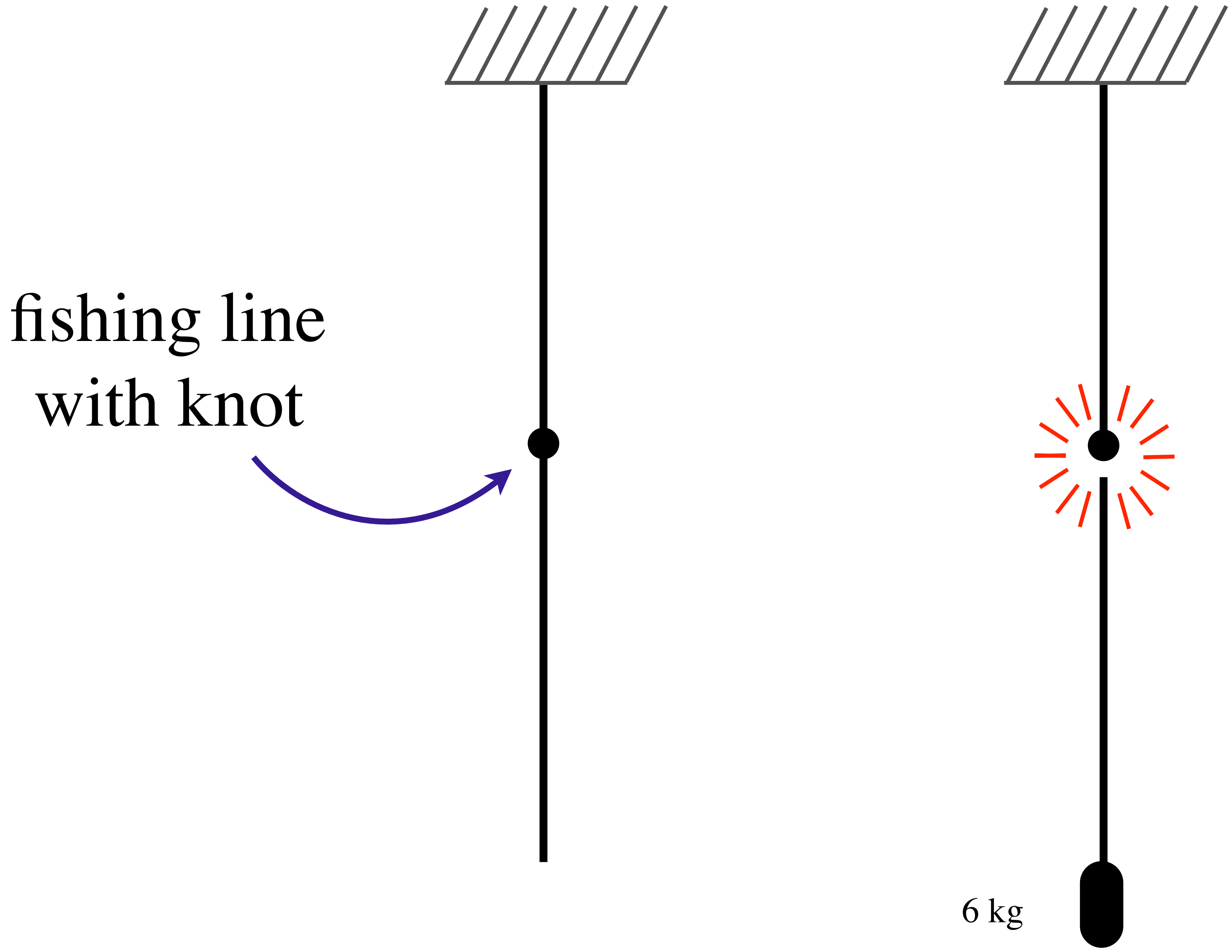
Tensile strength of a wire



Stasiak et al, *Science* (1999)

Tensile strength of a wire



Stasiak et al, *Science* (1999)

Knots are everywhere

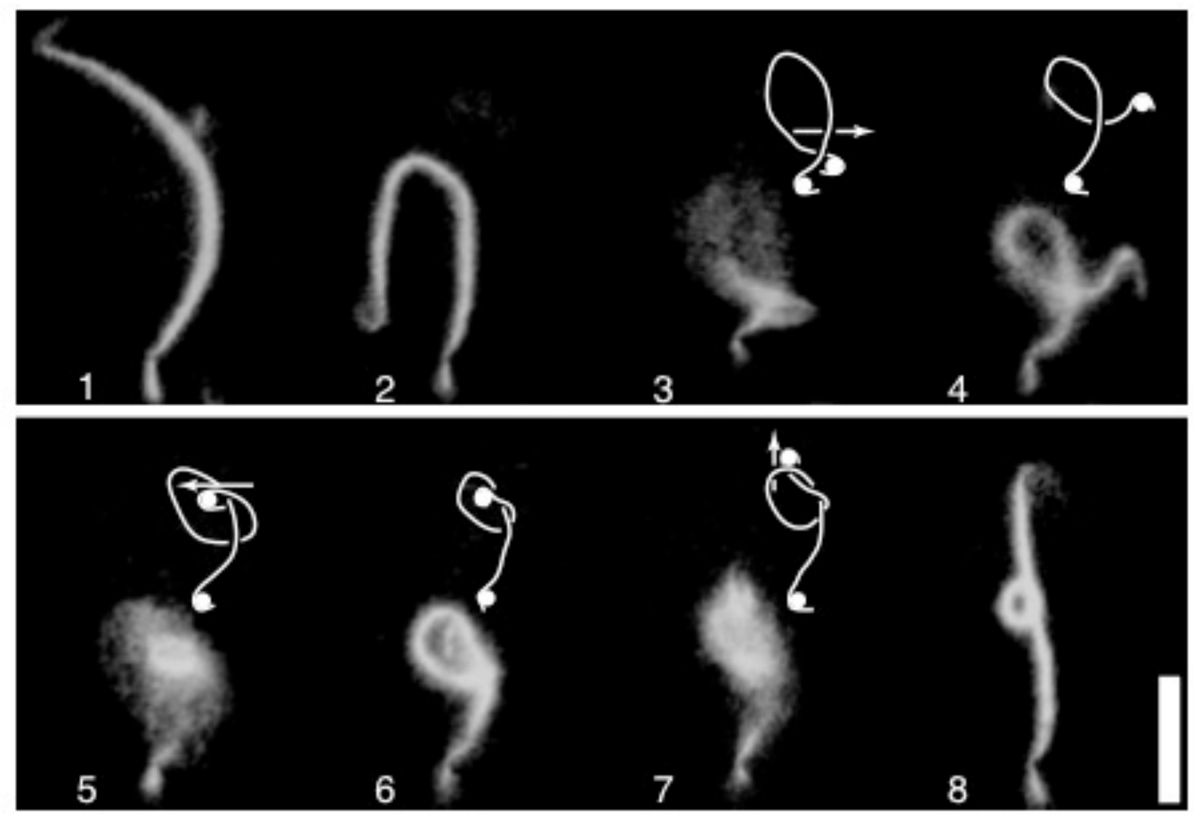
Long enough polymers are (almost) certainly knotted

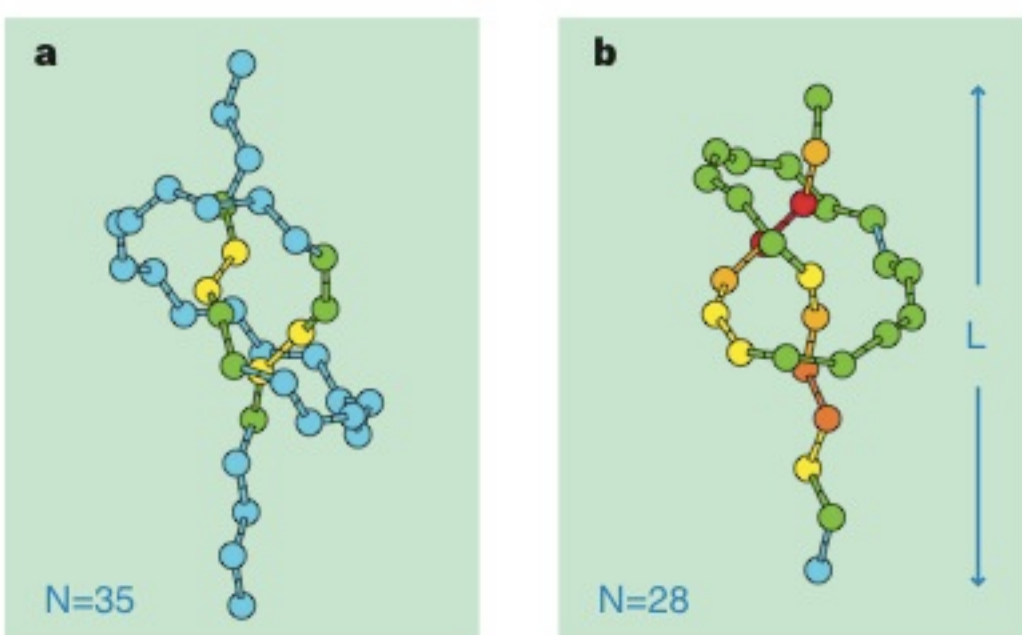
Sumners+Whittington, J. Phys. A : Math. Gen. 1988

273 knotted proteins in the ProteinDataBank (1%)

Single molecule experiment with knotted F-Actin filaments

Arai et al, *Nature* (1999)

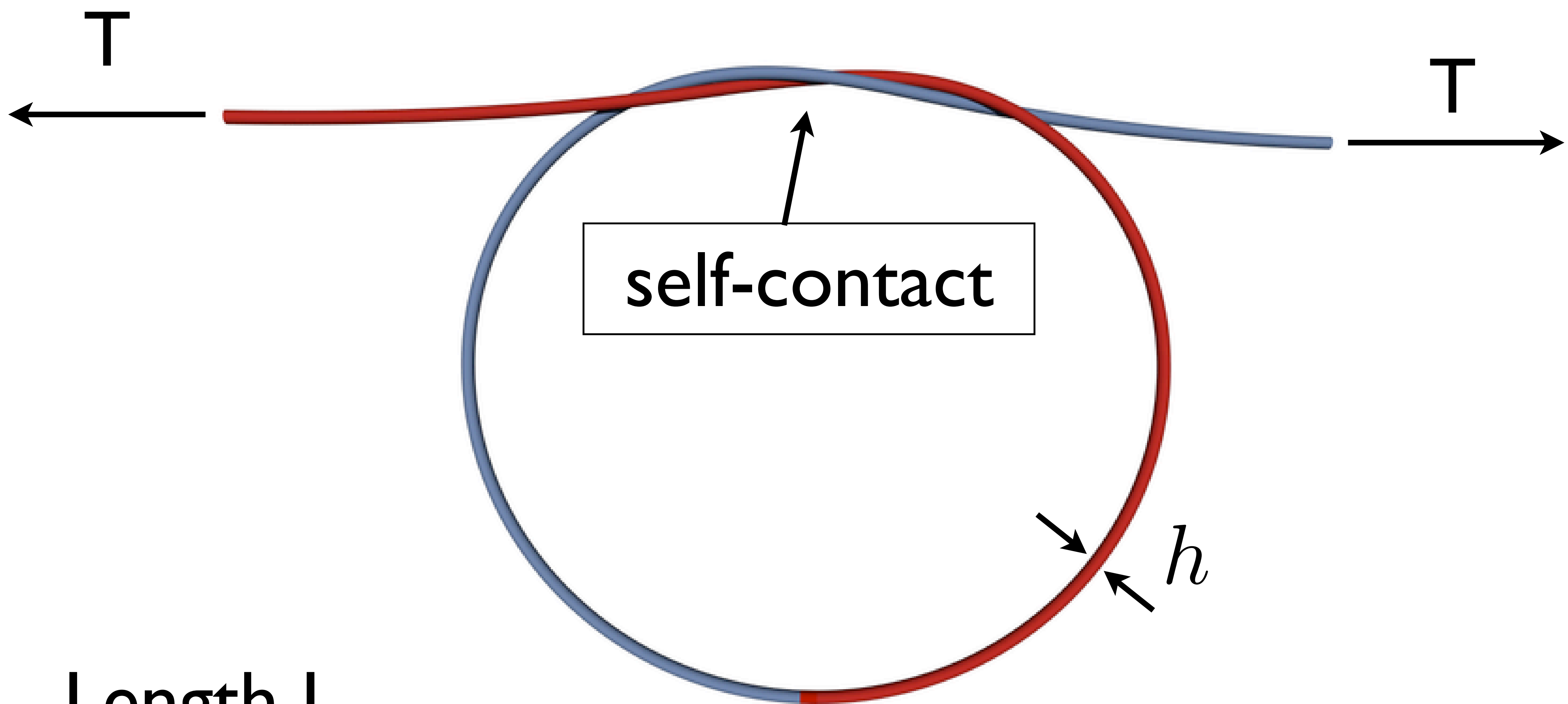




Ab-initio molecular simulations for alcane molecule ($C10H22$)

Saitta et al, *Nature* (1999)

Elastic knots



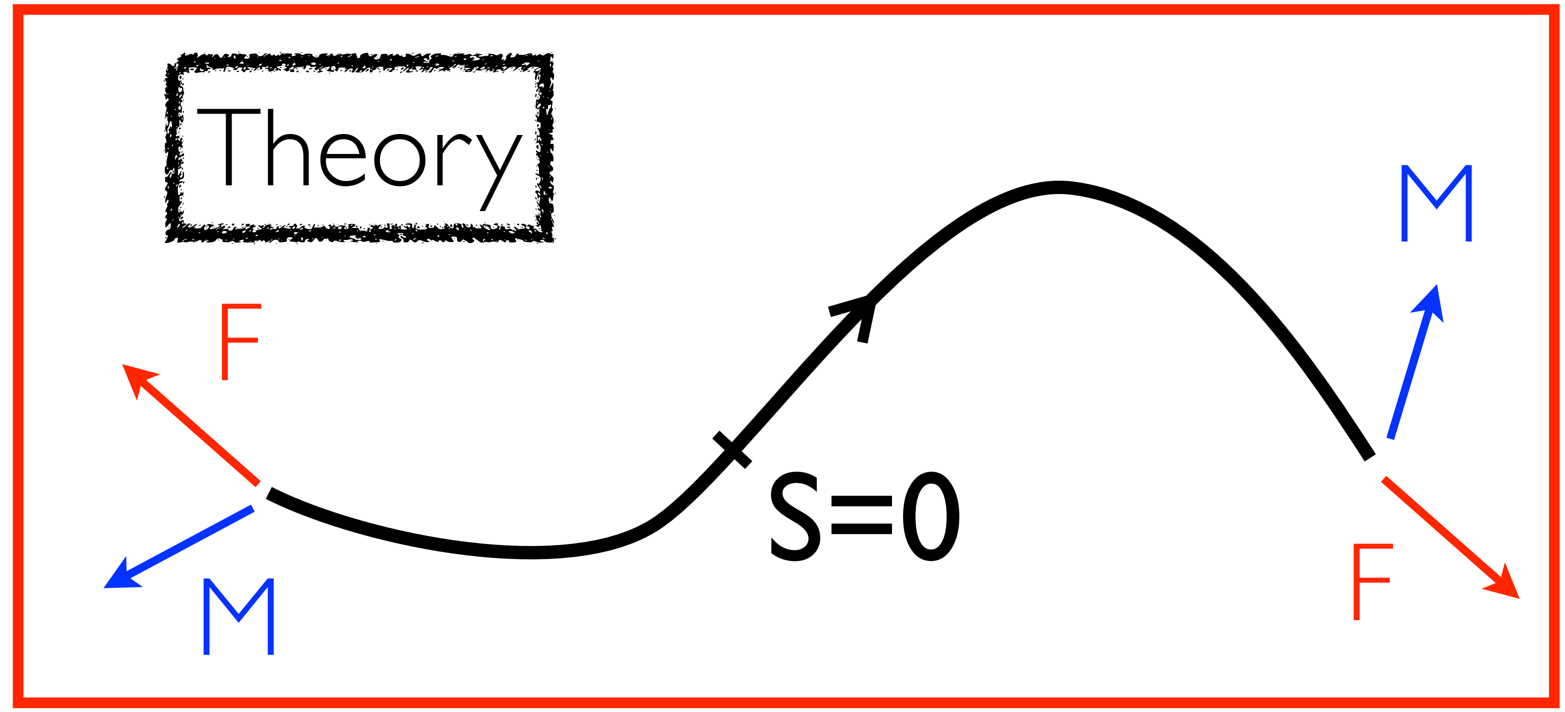
- Length L
- Circular cross-section: radius h
- Bending rigidity : E I
- Twist rigidity : G J

E : Young's modulus G : shear modulus

$$I = \frac{\pi h^4}{4}$$

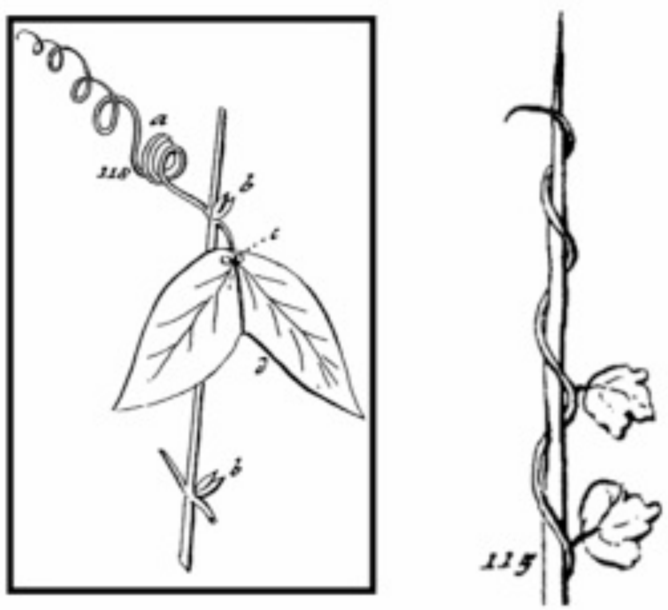
$$J = \frac{\pi h^4}{2}$$

Elastic filaments

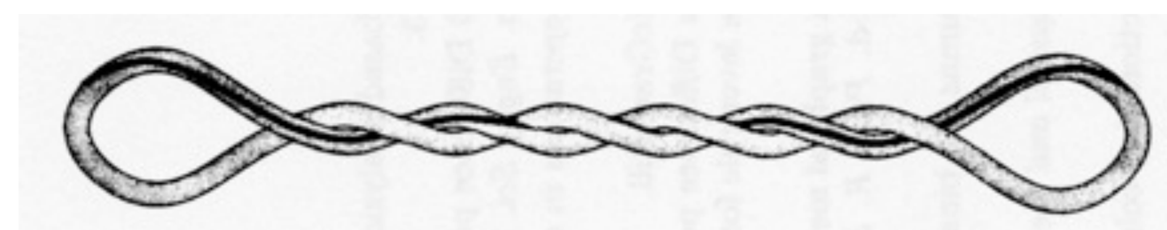


Applications

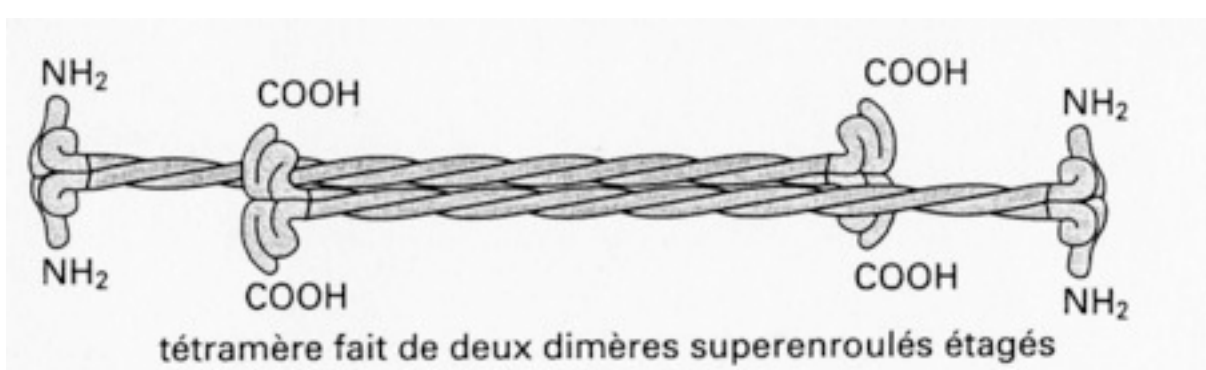
climbing plants



DNA supercoiling

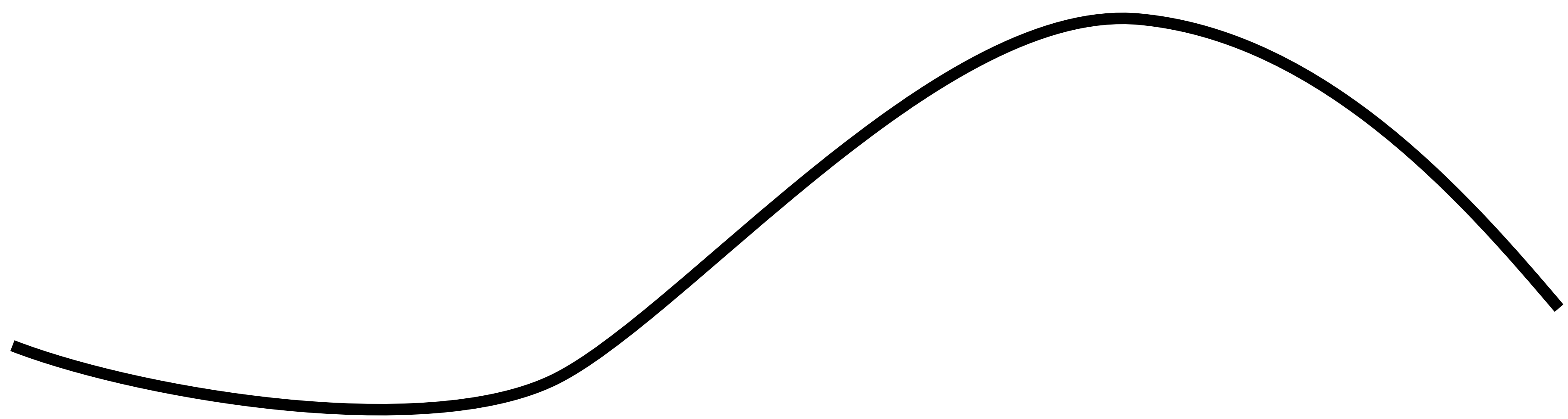


fibrous proteins



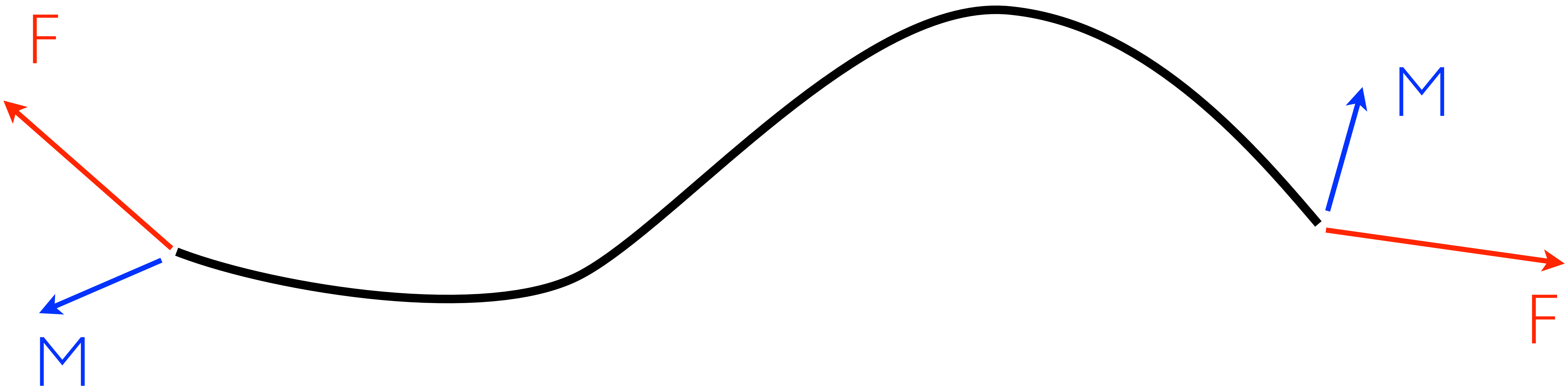
cables

Kirchhoff equations

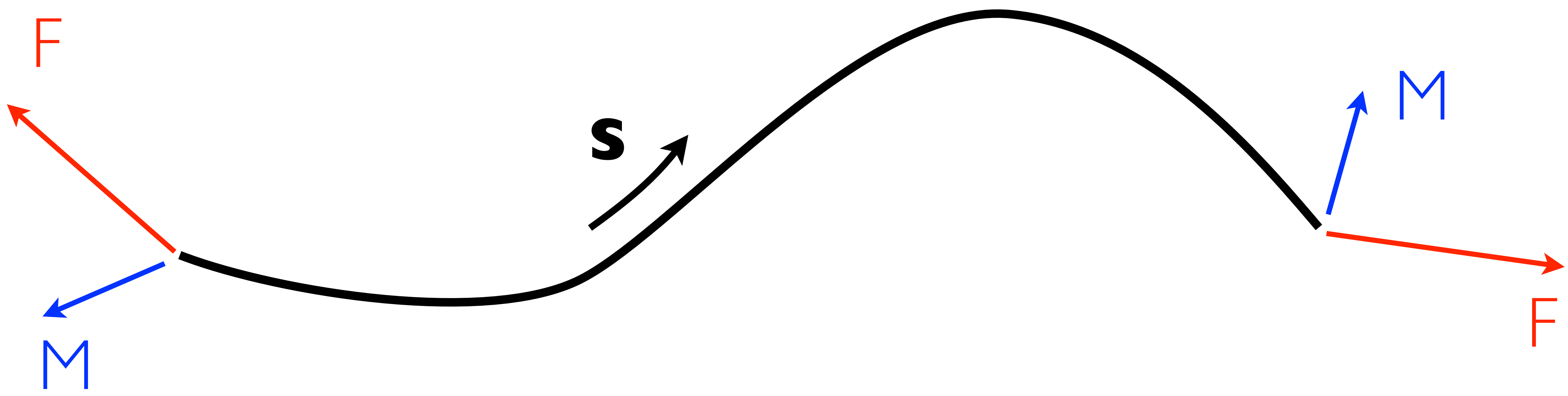


apply to :
- slender bodies
- not too bent

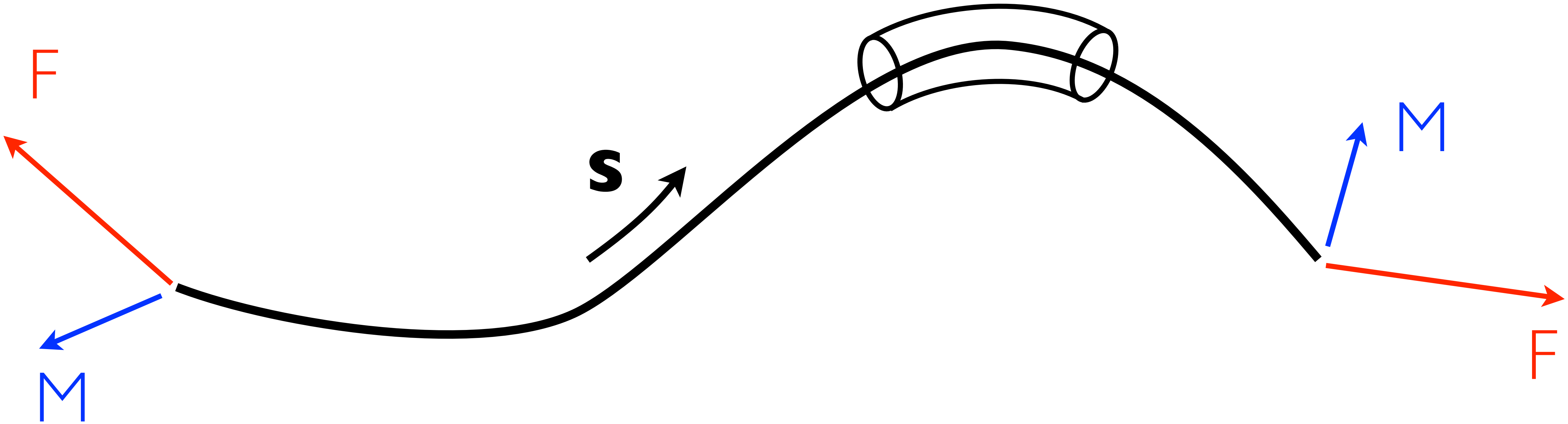
Kirchhoff equations



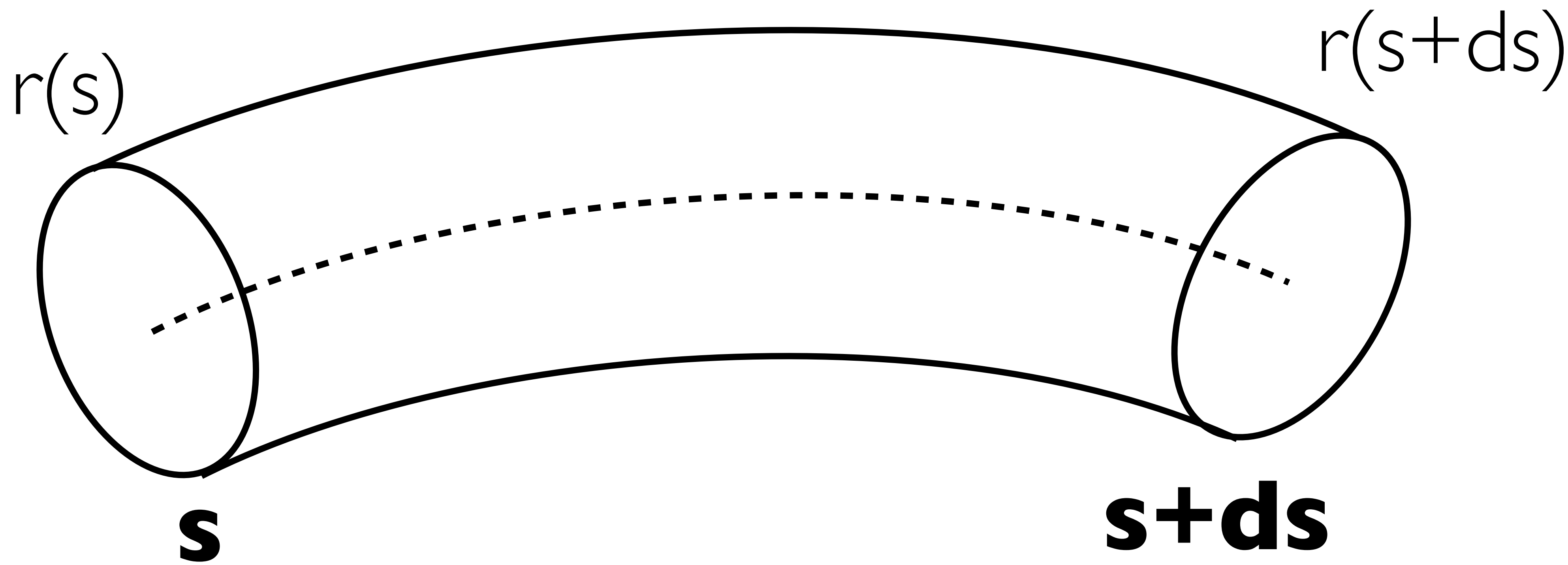
Kirchhoff equations



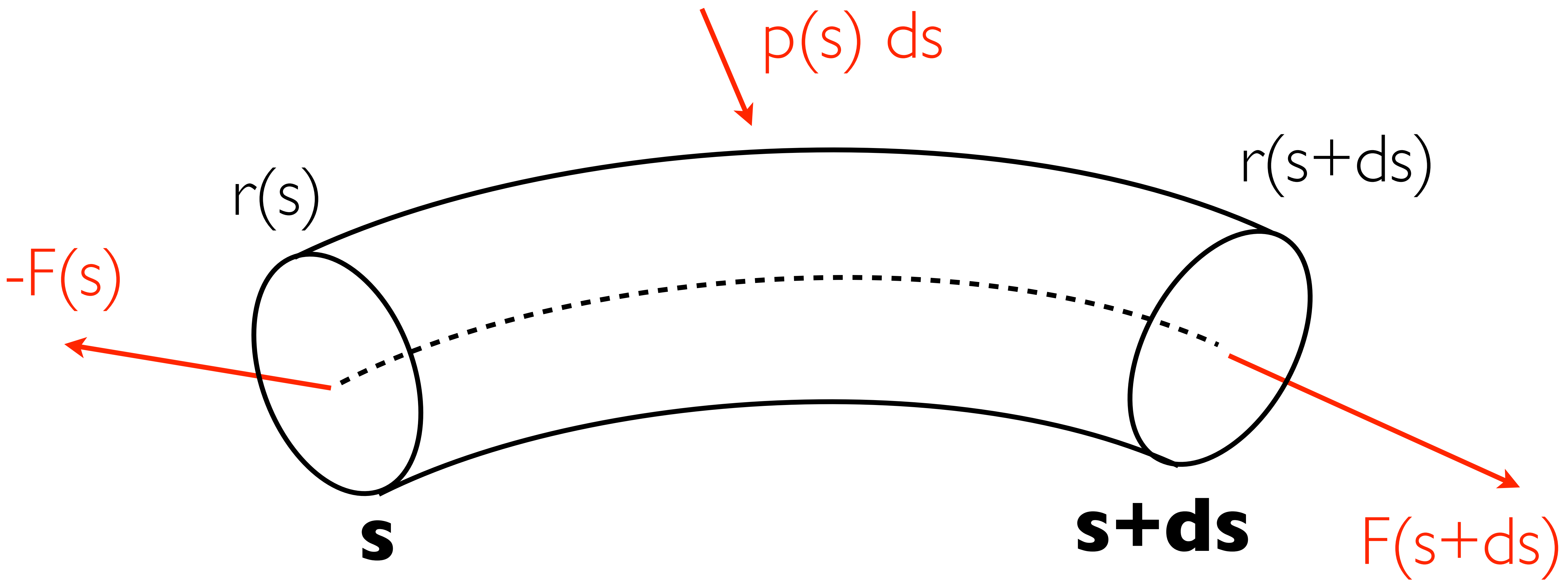
Kirchhoff equations



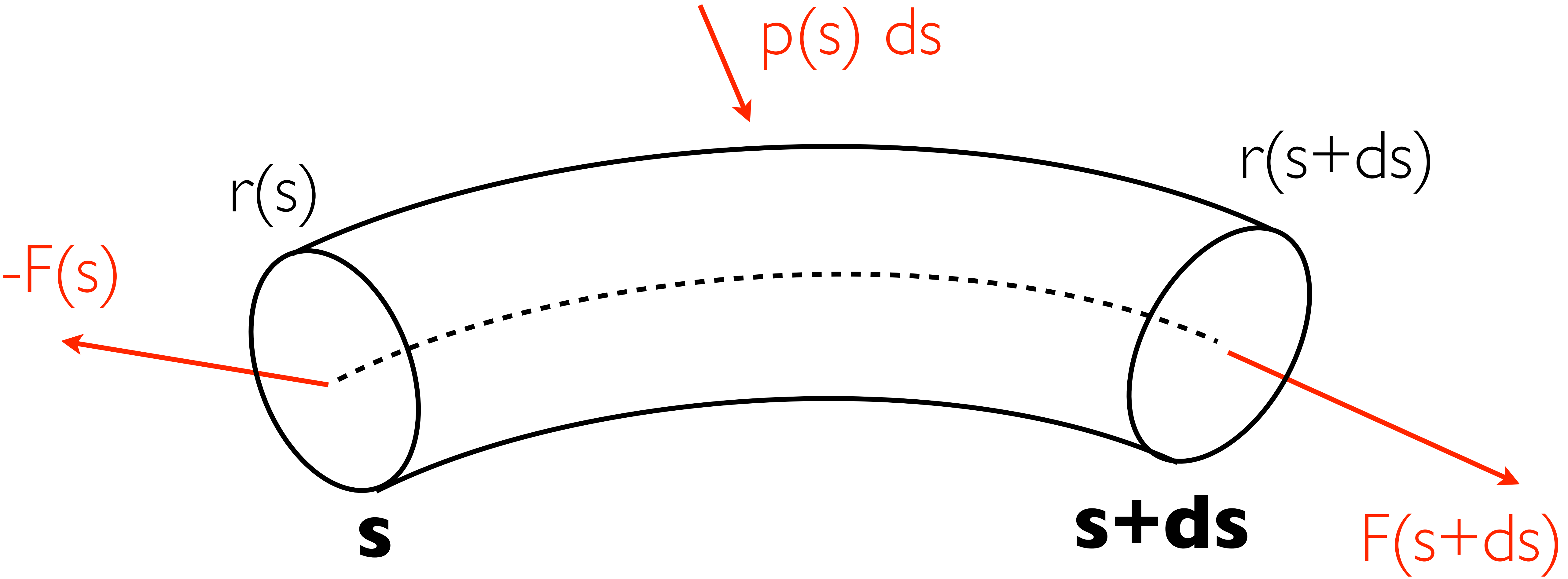
Kirchhoff equations



Kirchhoff equations



Kirchhoff equations

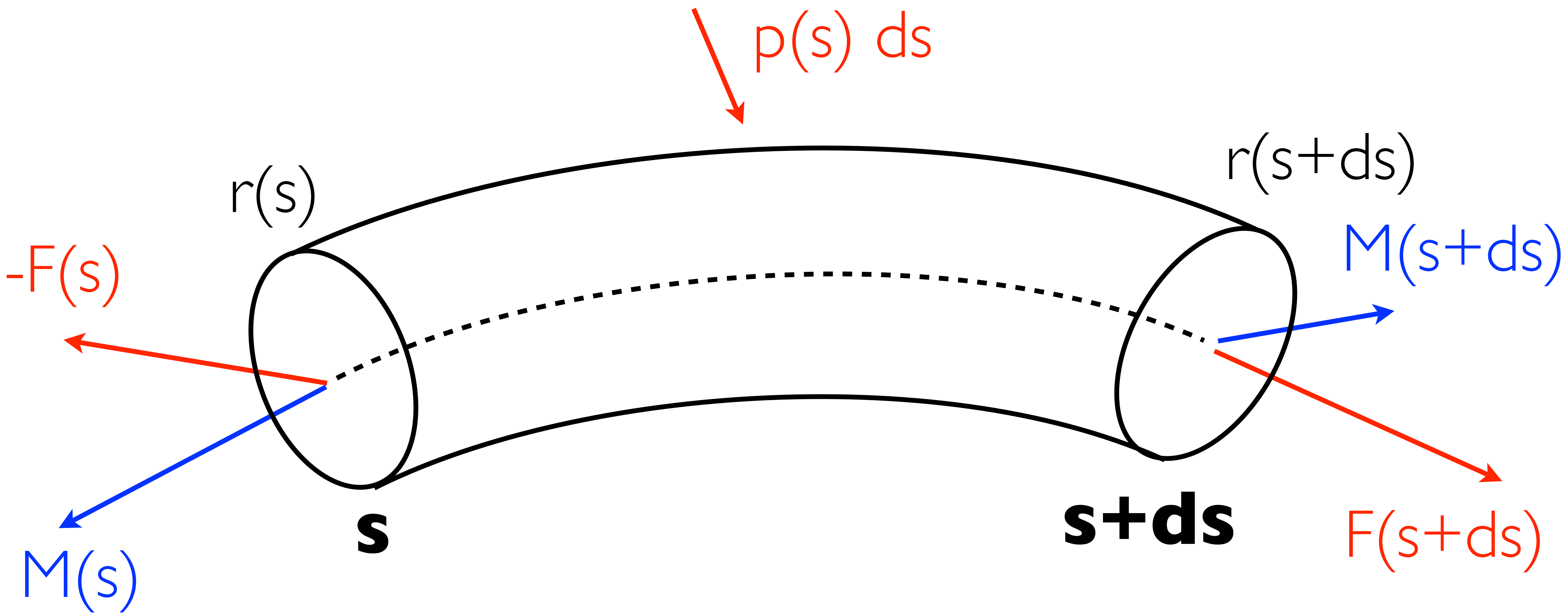


$$F(s+ds) - F(s) + p(s)\, ds = 0$$

Equilibrium

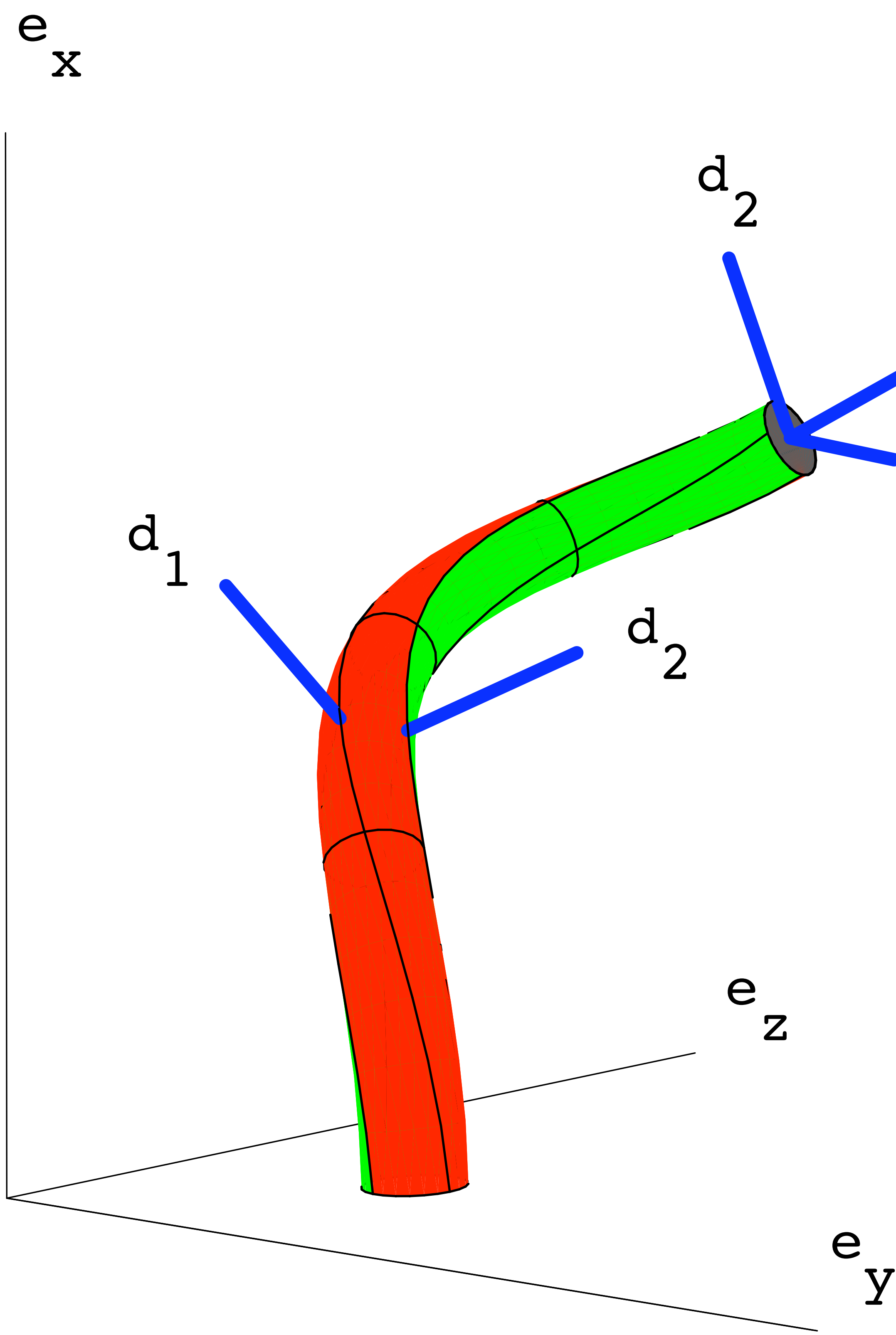
$$F'(s) + p(s) = 0$$

Kirchhoff equations



Equilibrium $\quad M' + r' \times F = 0$

Kirchhoff equations



Cosserat frame

$$d_1' = u \times d_1$$
$$d_2' = u \times d_2$$
$$d_3' = u \times d_3$$

$$u = \{\kappa_1, \kappa_2, \tau\}_{d_i}$$

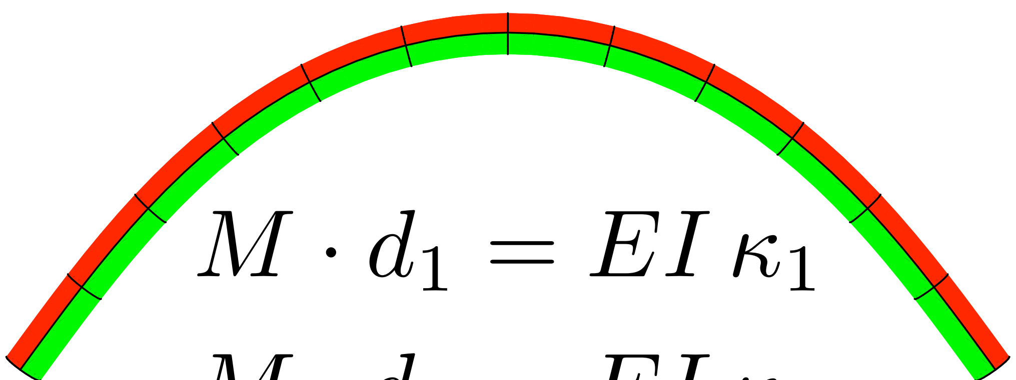
curvatures

twist

Kirchhoff equations

constitutive relations

curvature

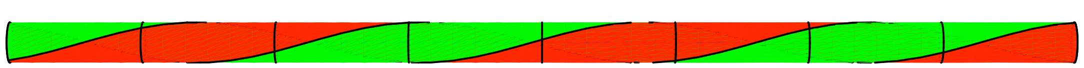


$$M \cdot d_1 = EI\,\kappa_1$$
$$M \cdot d_2 = EI\,\kappa_2$$

E Young's modulus

I second moment of area

twist



$$M \cdot d_3 = GJ\,\tau$$

G shear modulus

J polar moment of area

Kirchhoff equations

21 ODEs with variable : s

ordinary differential equations

$$\frac{d}{ds}\vec{F}=\vec{p}$$

$$\frac{d}{ds}\vec{M}=\vec{F}\wedge\vec{d}_3$$

$$\frac{d}{ds}\vec{r}=\vec{d}_3$$

$$\frac{d}{ds}\vec{d}_i=\vec{u}\wedge\vec{d}_i$$

$$m_i=K_i u_i$$

linear elasticity

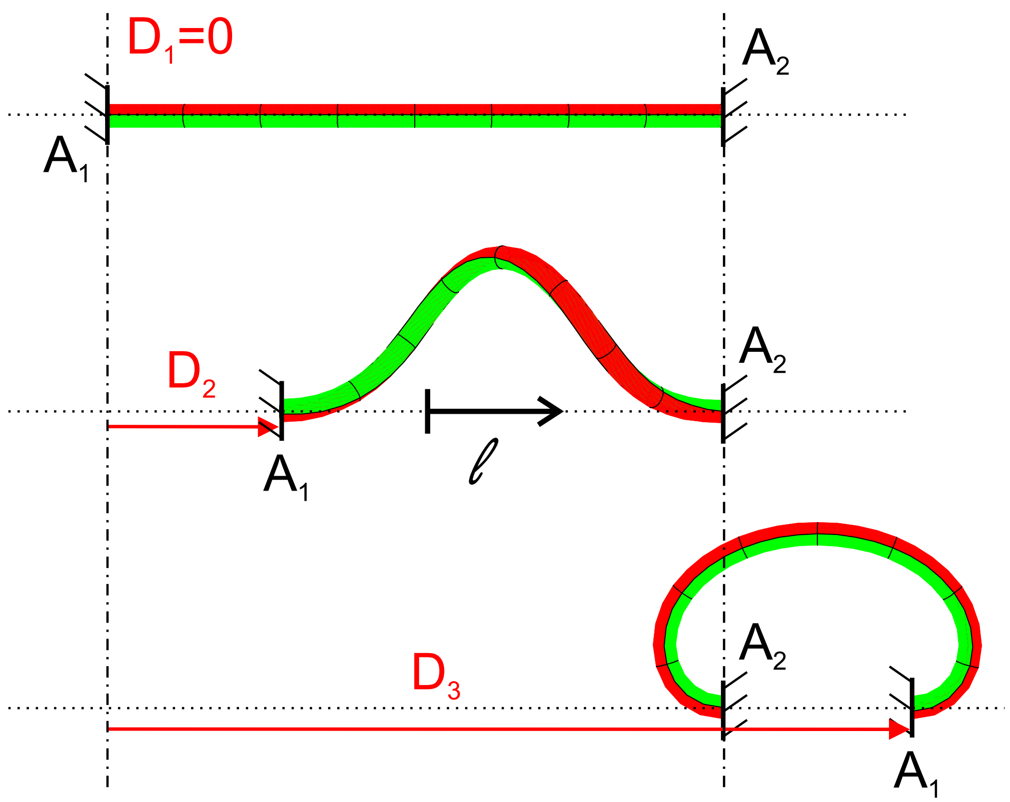
21 unknowns

$\vec{F}(s)$
$\vec{M}(s)$
$\vec{r}(s)$
$\vec{d}_3(s)$
$\vec{d}_2(s)$
$\vec{d}_1(s)$
$\vec{u}(s)$

$i=1,2,3$

boundary conditions

- how the rod is held
- few solutions are admissibles

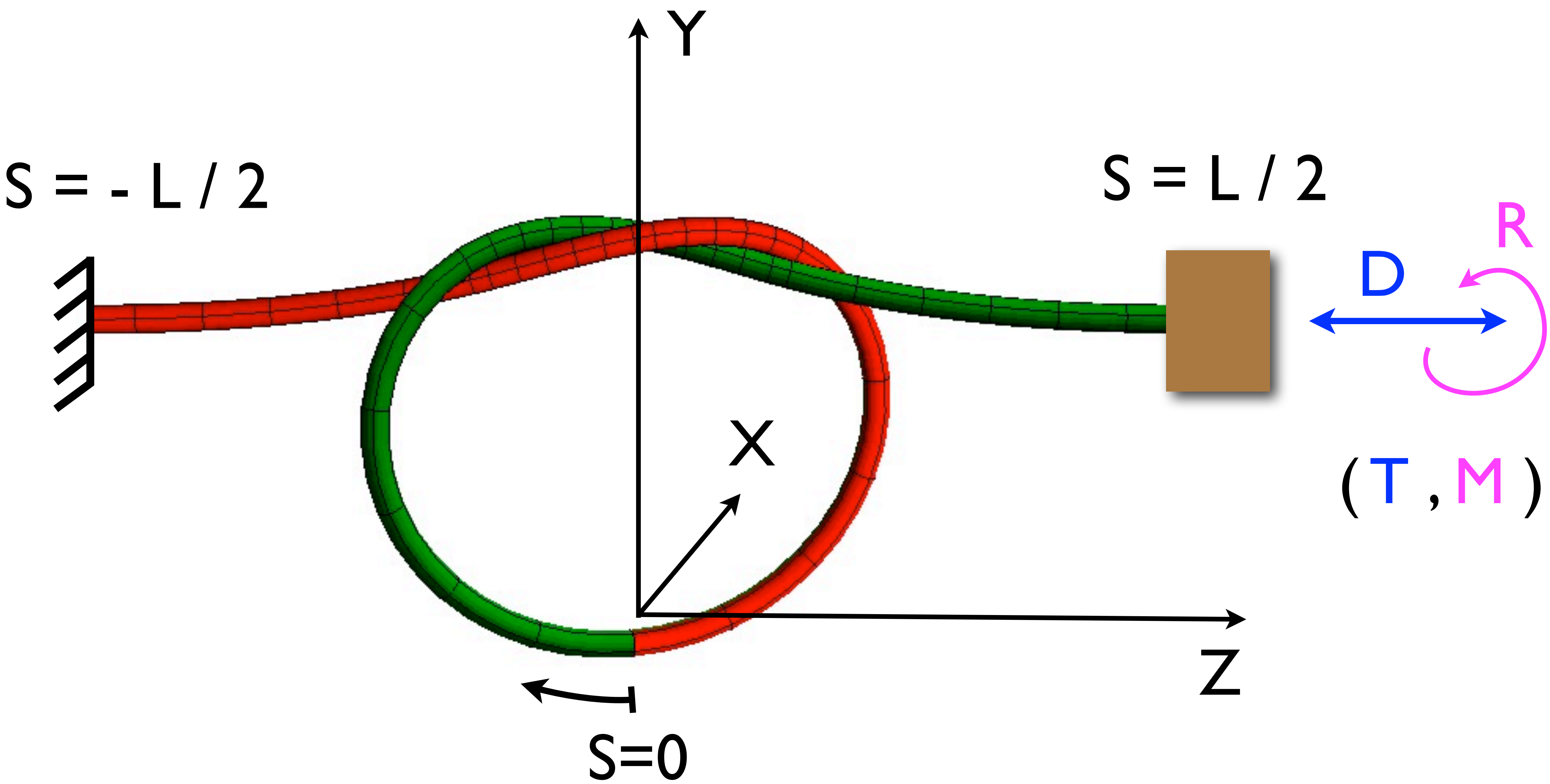


$$\vec{d}_3(A_1)=\vec{d}_3(A_2)$$

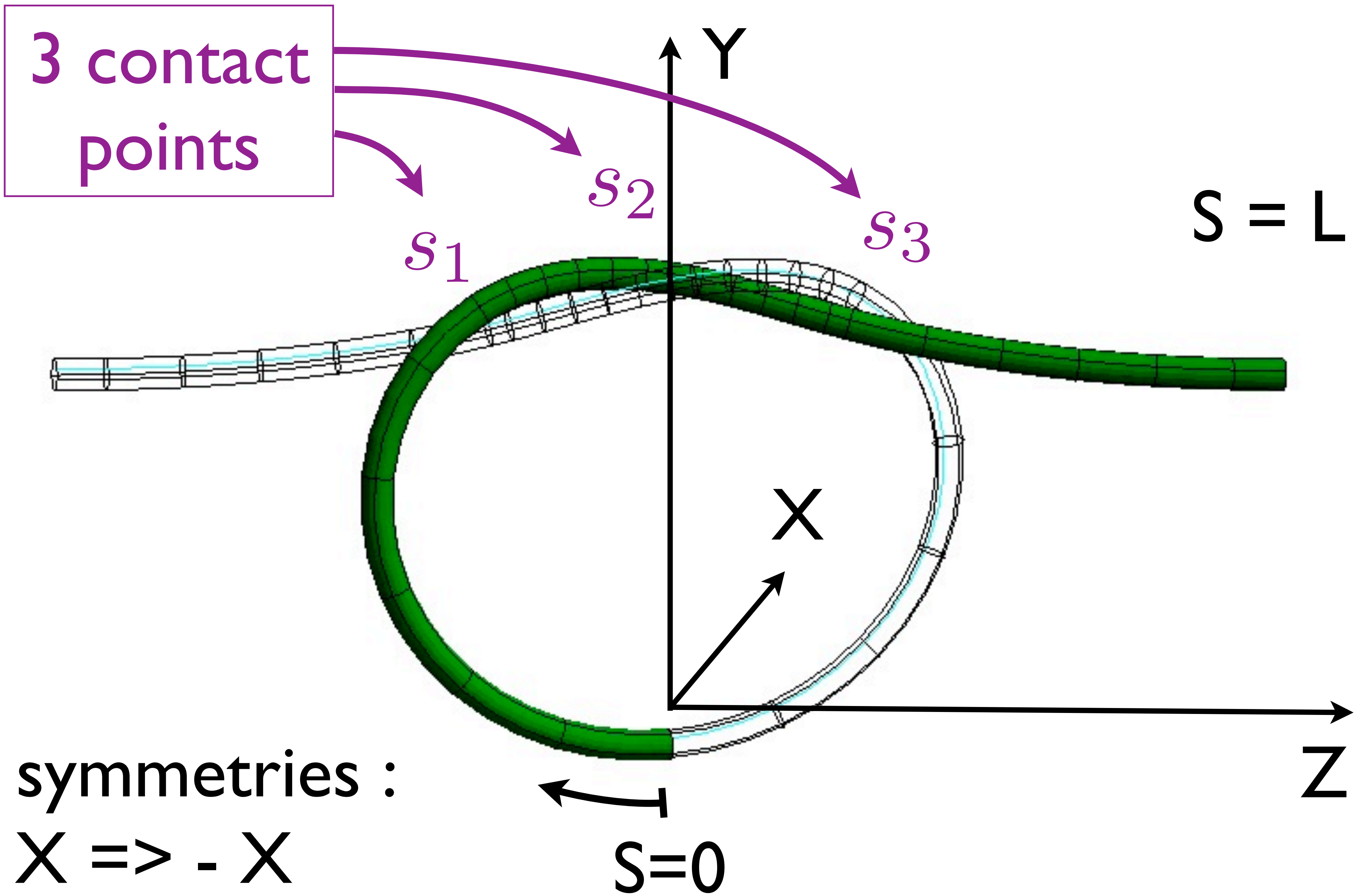
$$\vec{r}(A_2)-\vec{r}(A_1)=k\,\vec{d}_3(A_2)$$

$$(D=L-k)$$

Boundary value problem



Boundary value problem



S = L / 2

symmetries :

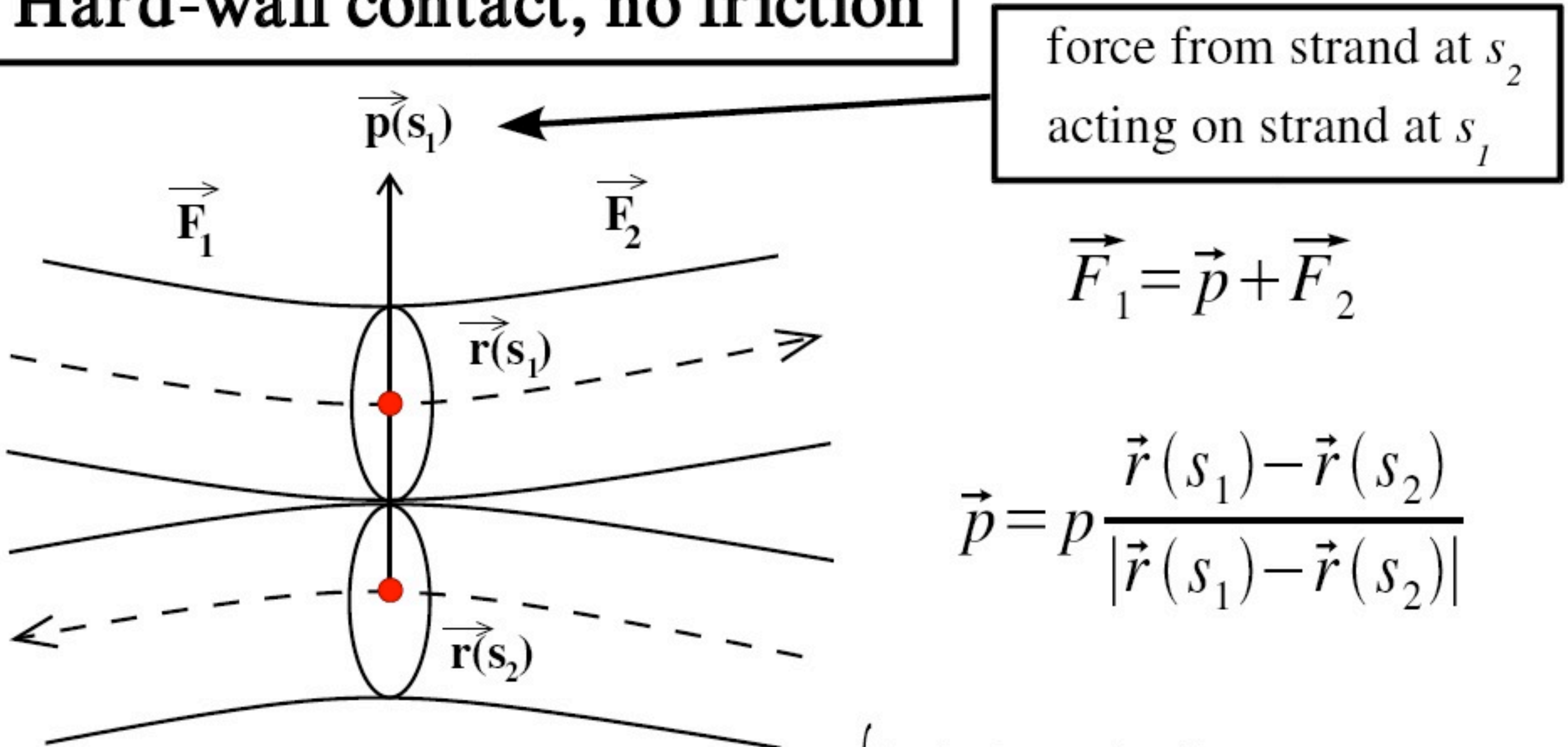
X => - X

Y => Y

Z => - Z

- Shooting method (Mathematica)
- Gauss colocation (AUTO)

Hard-wall contact, no friction



$$\vec{F}_1 = \vec{p} + \vec{F}_2$$

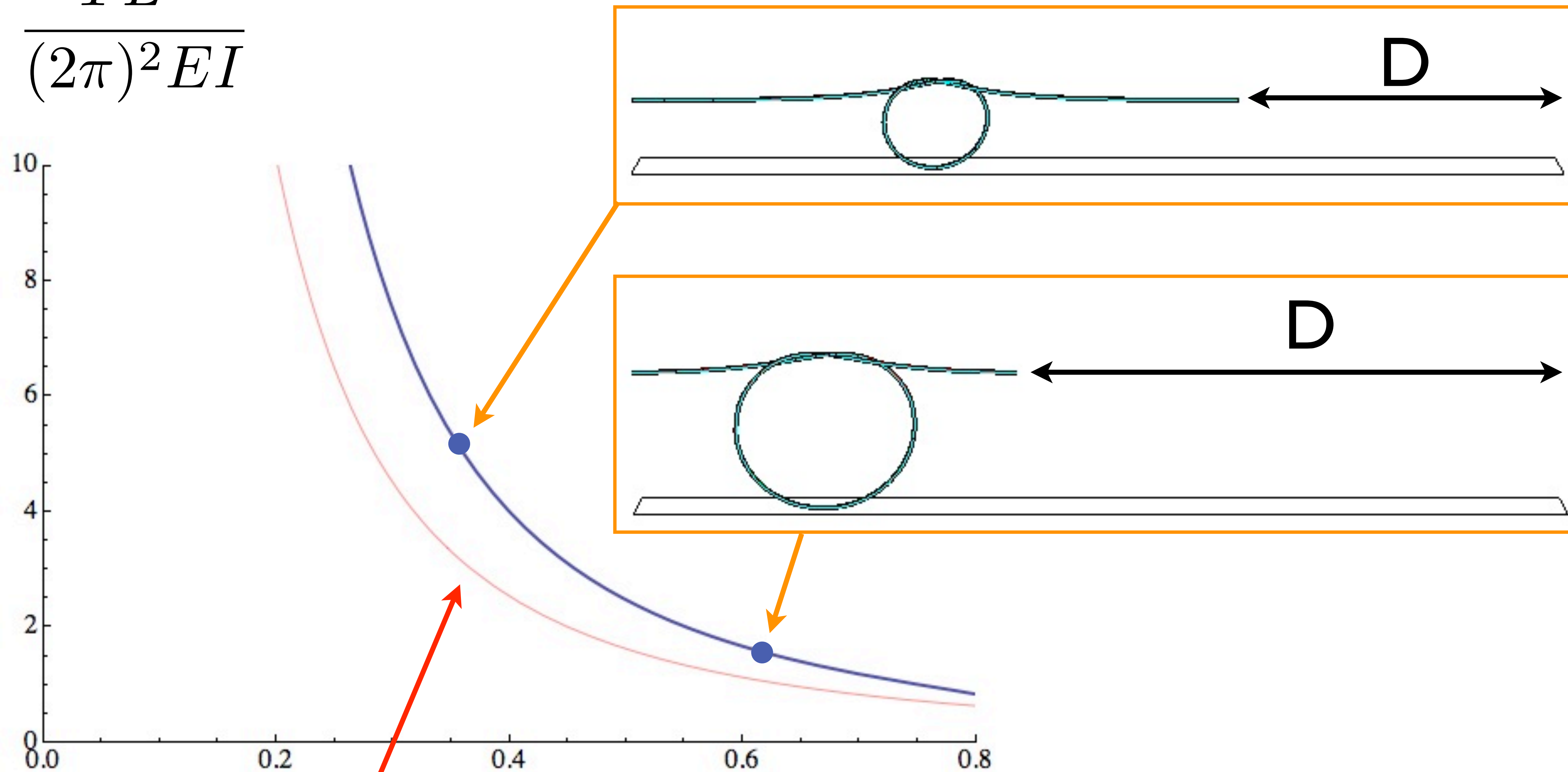
$$\vec{p} = p\,\frac{\vec{r}(s_1) - \vec{r}(s_2)}{|\vec{r}(s_1) - \vec{r}(s_2)|}$$

touching conditions :

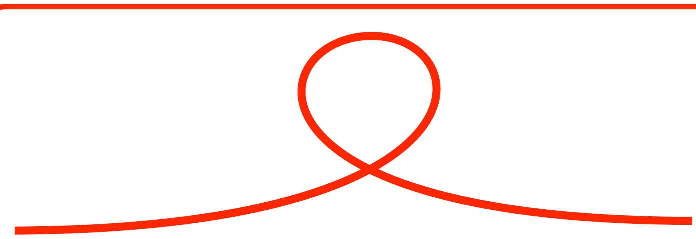
$$\begin{cases} |\vec{r}(s_1) - \vec{r}(s_2)| = \text{thickness} \\ (\vec{r}(s_1) - \vec{r}(s_2)) \perp \vec{d}_3(s_1) \\ (\vec{r}(s_1) - \vec{r}(s_2)) \perp \vec{d}_3(s_2) \end{cases}$$

Numerical Path Following : Results

$$t = \frac{TL^2}{(2\pi)^2 EI}$$



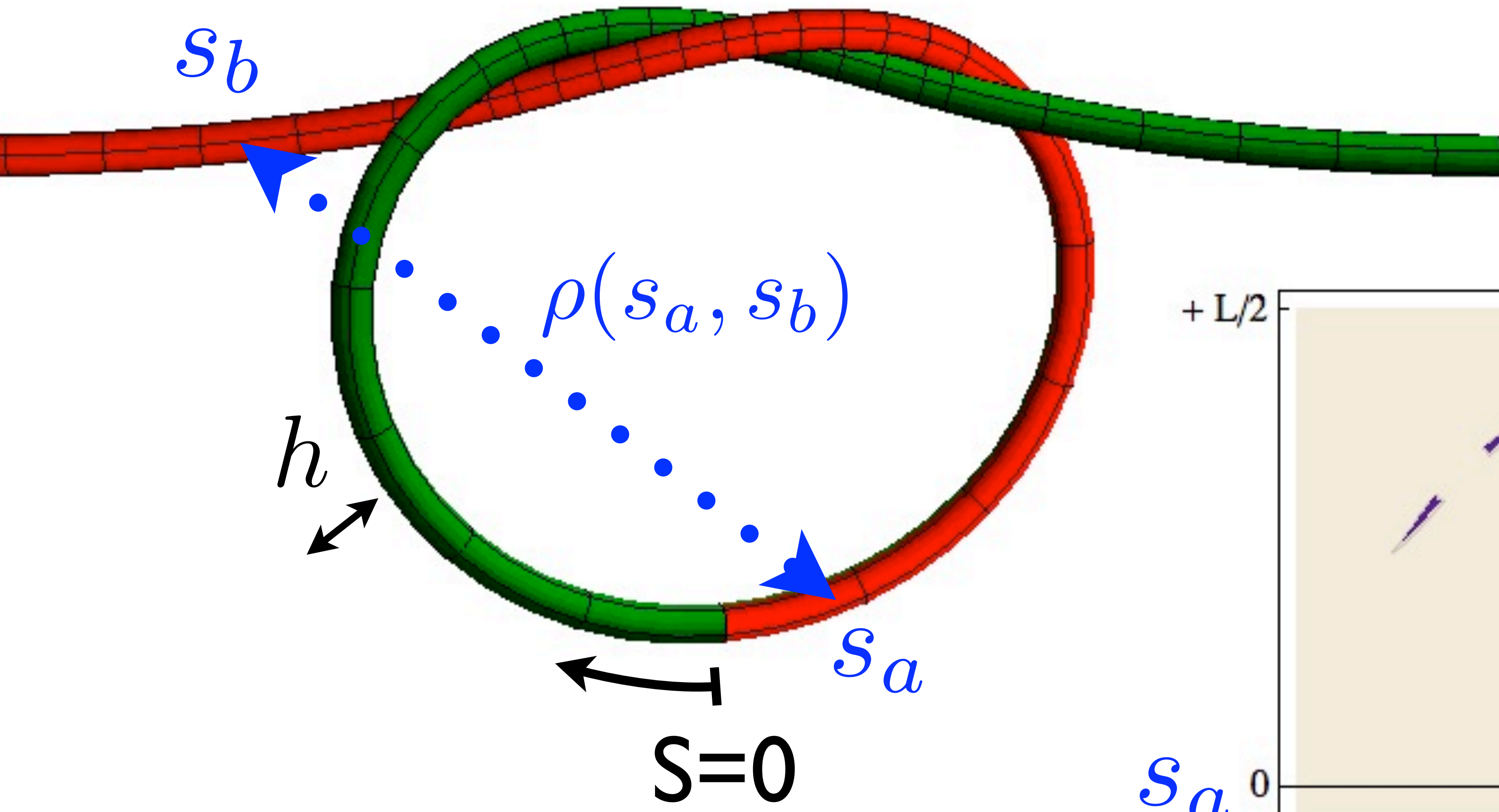
$$d = \frac{D}{L}$$

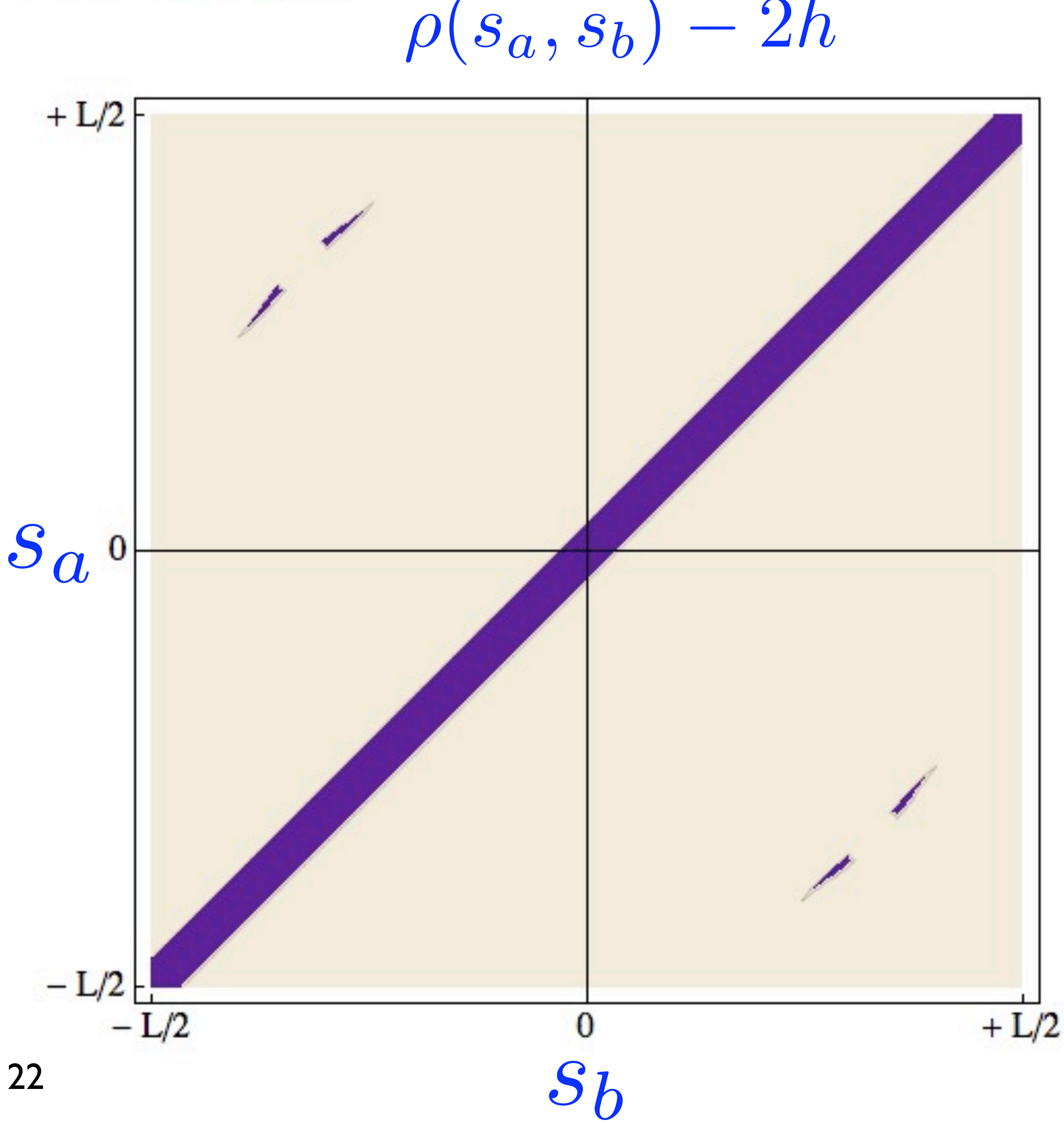


Planar Elastica

$$t = \left(\frac{2/\pi}{d}\right)^2$$

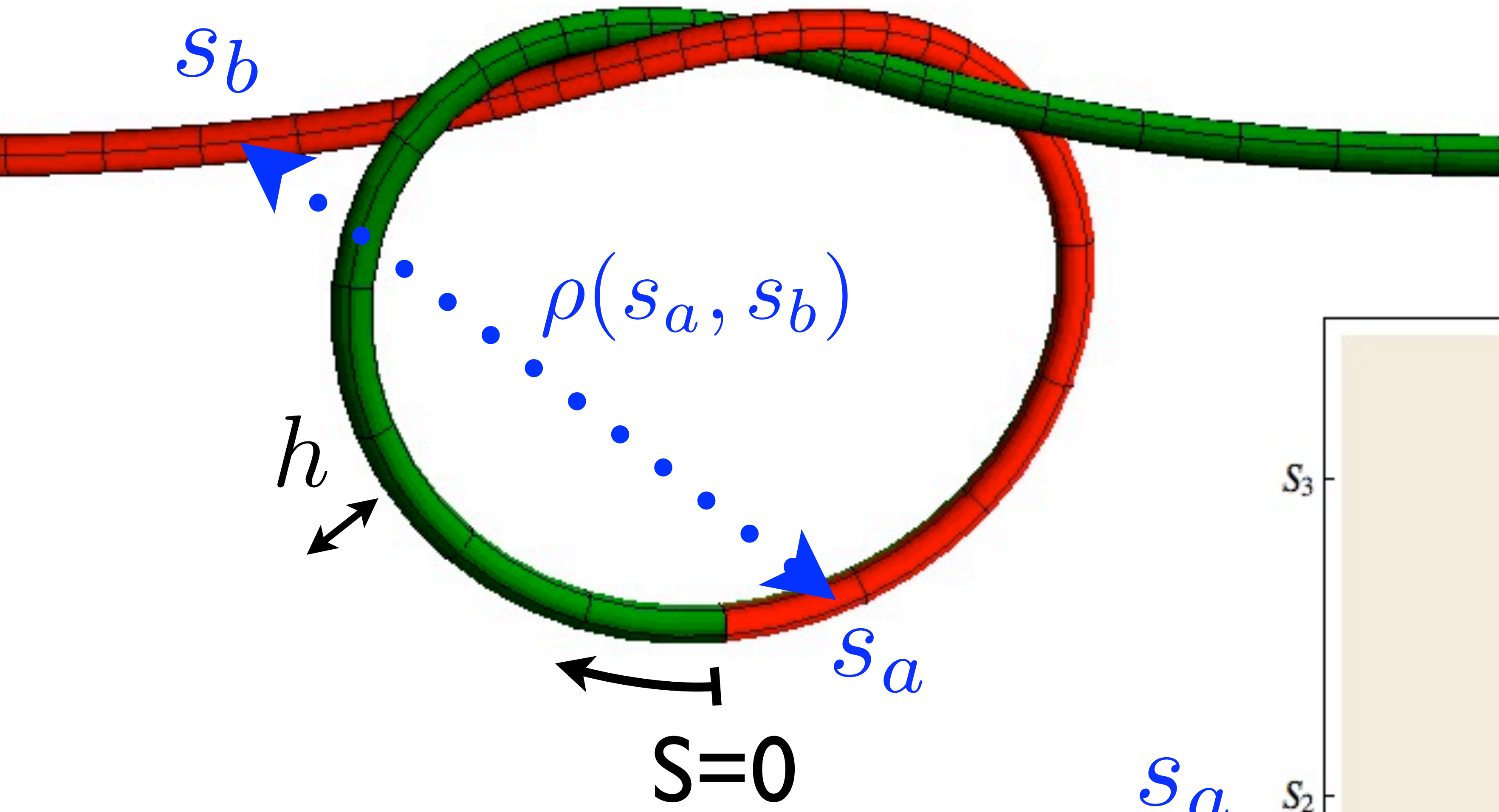
Distance of self-approach

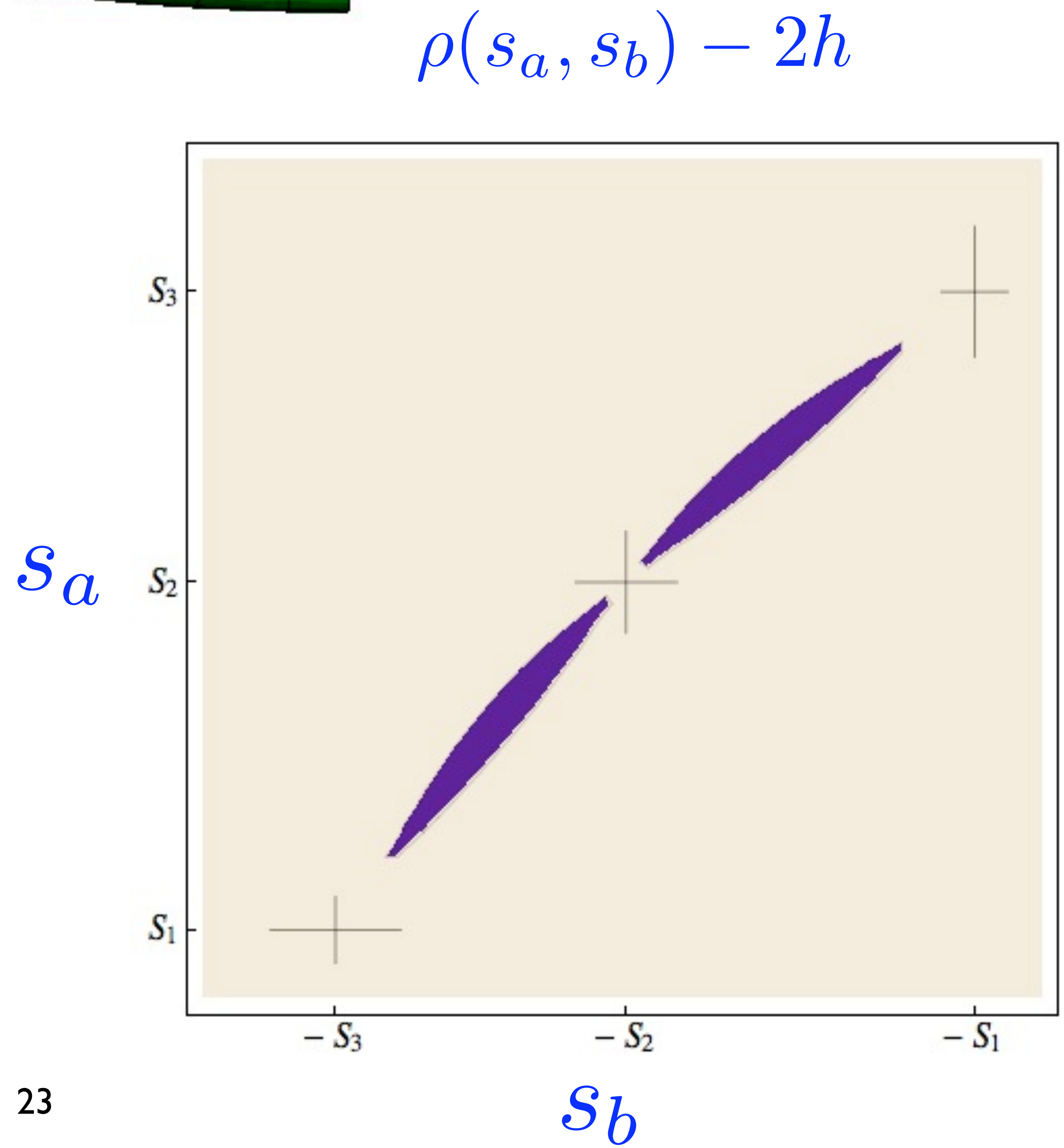




$\rho(s_a, s_b) < 2h$

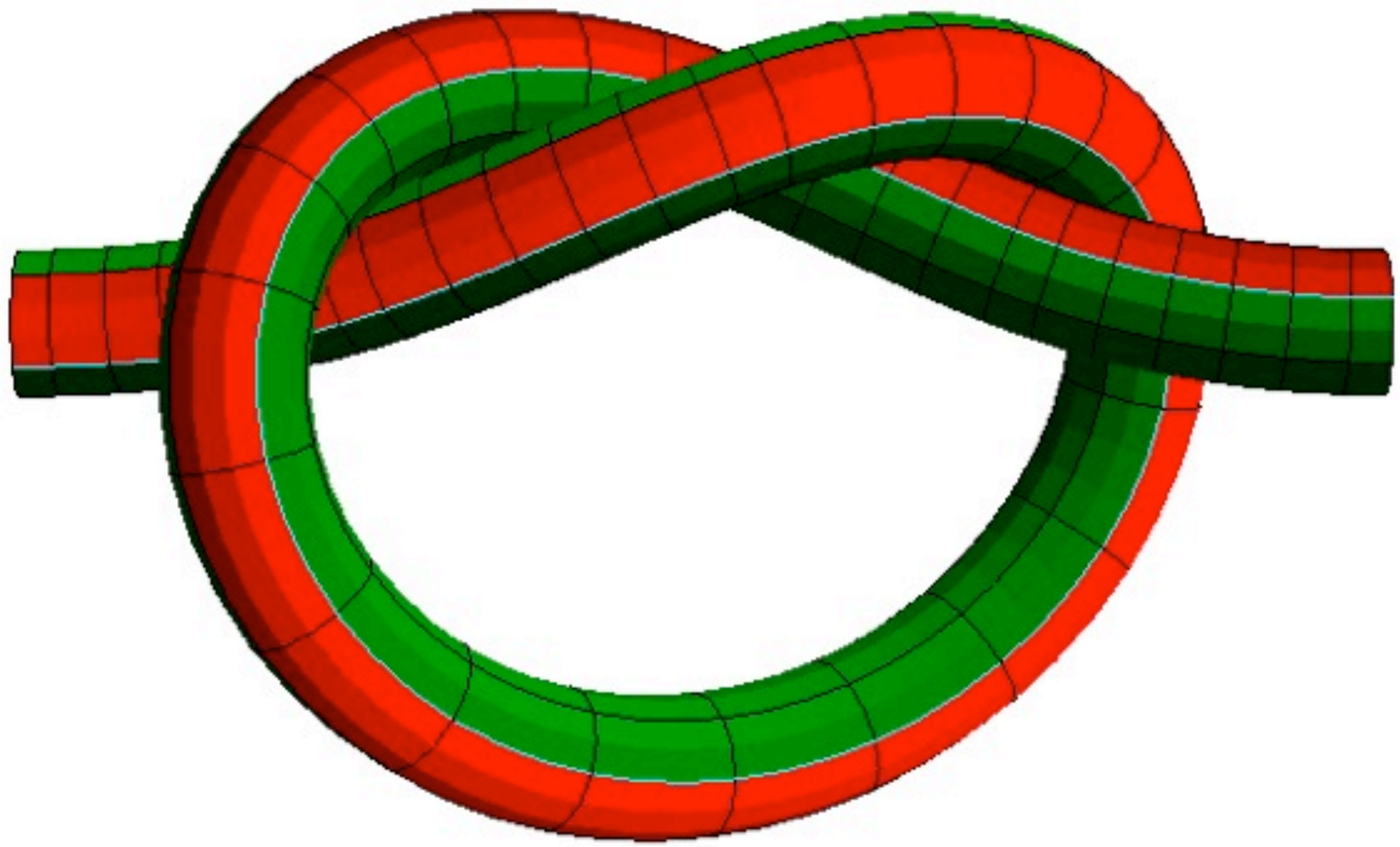
Distance of self-approach



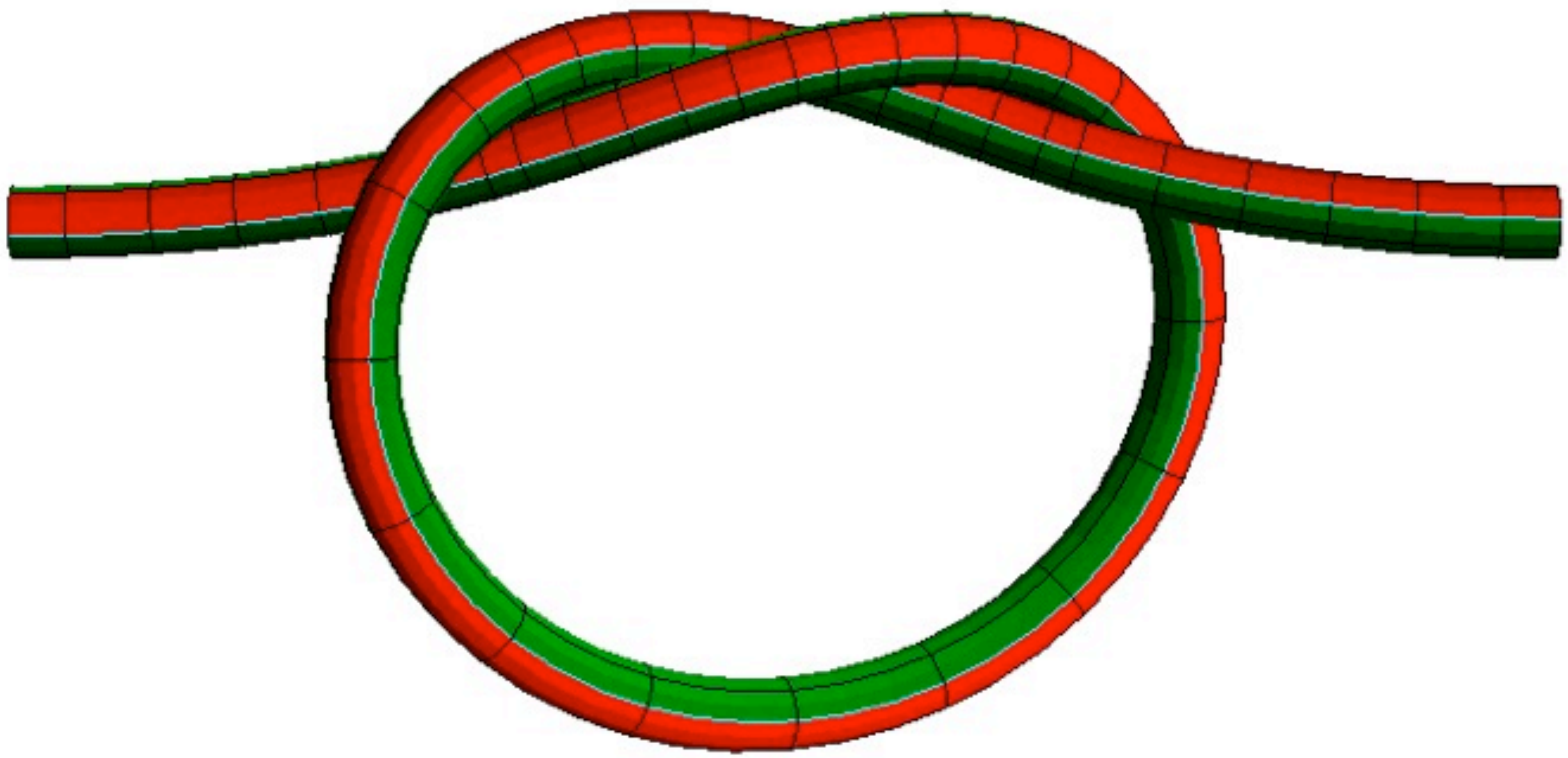


$\rho(s_a, s_b) < 2h$

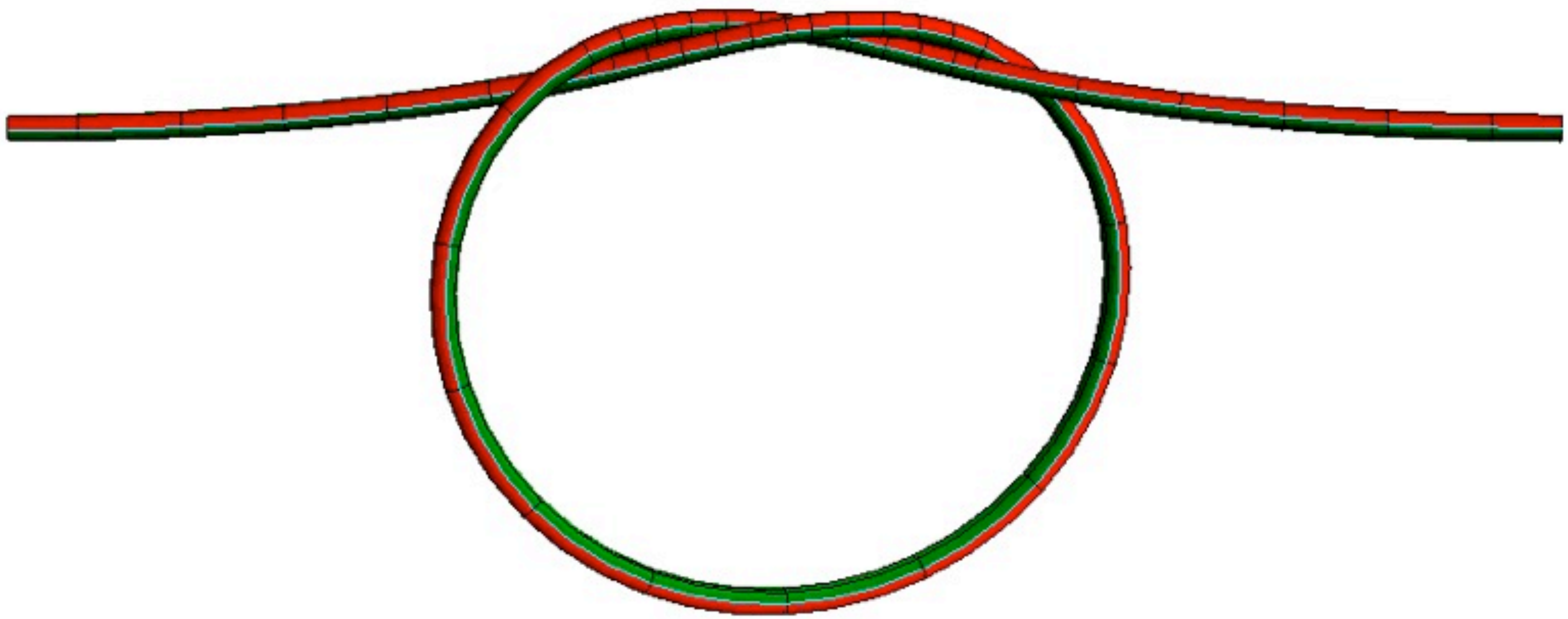
Making the rod thinner



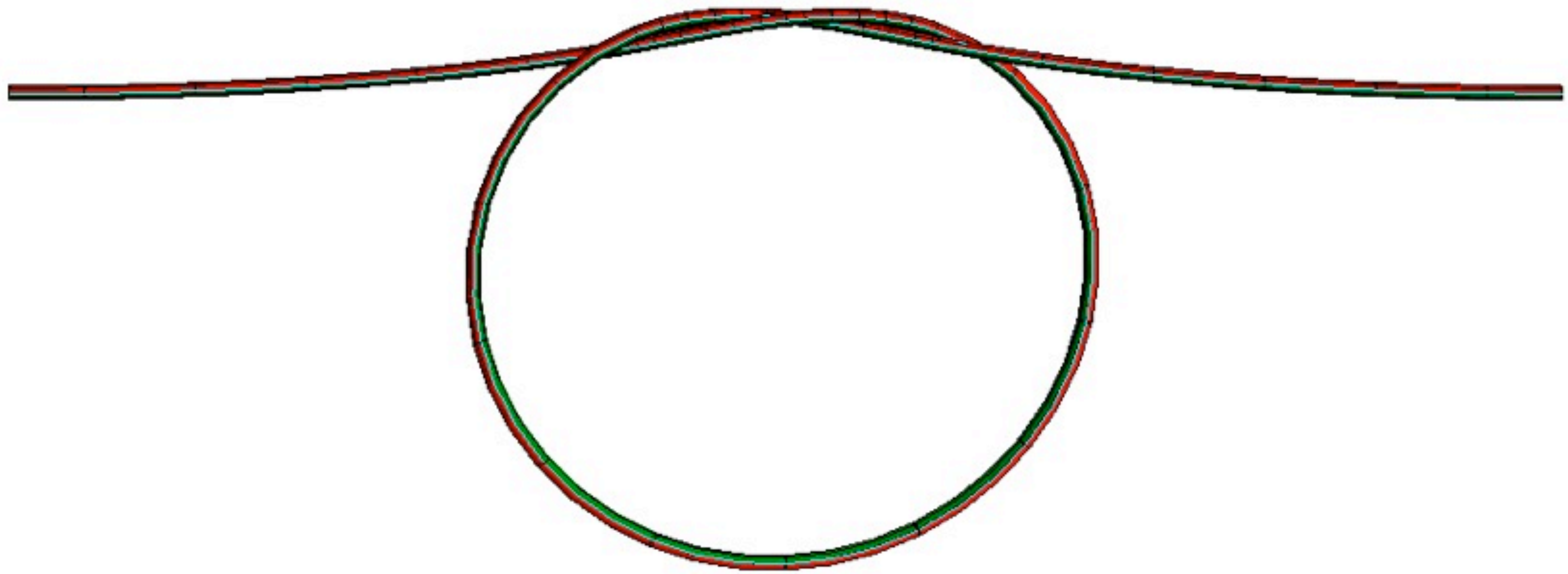
Making the rod thinner



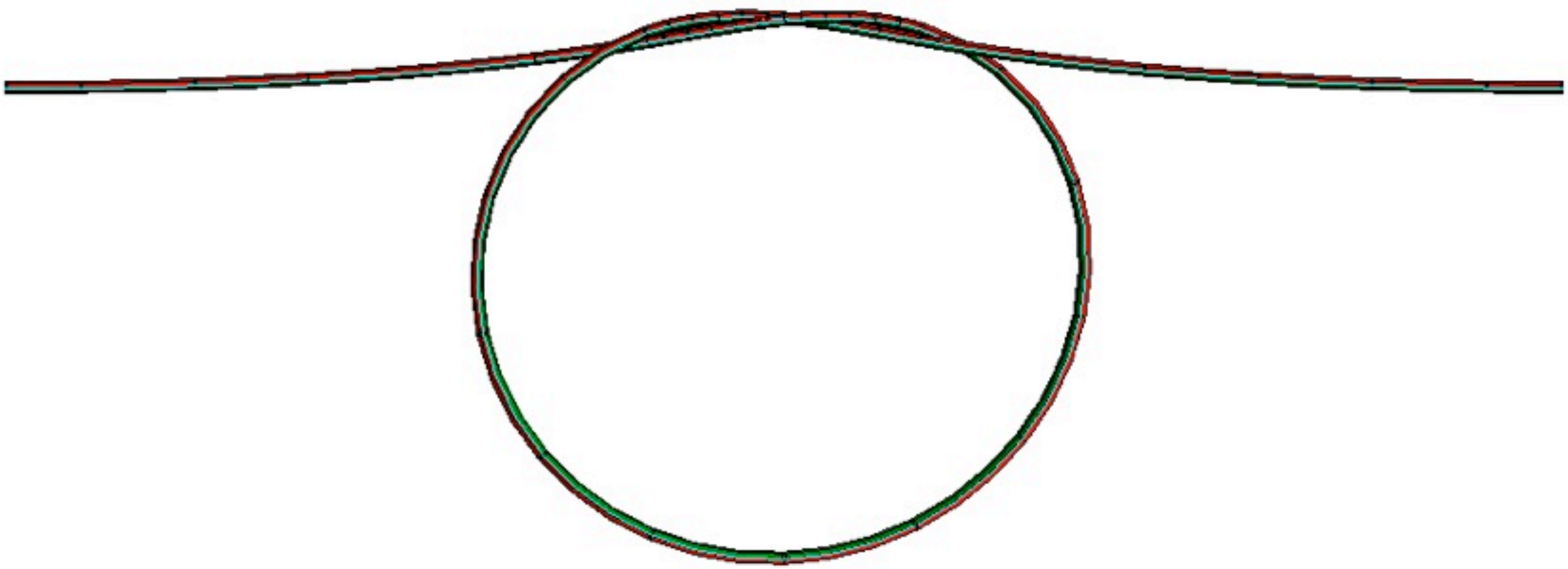
Making the rod thinner



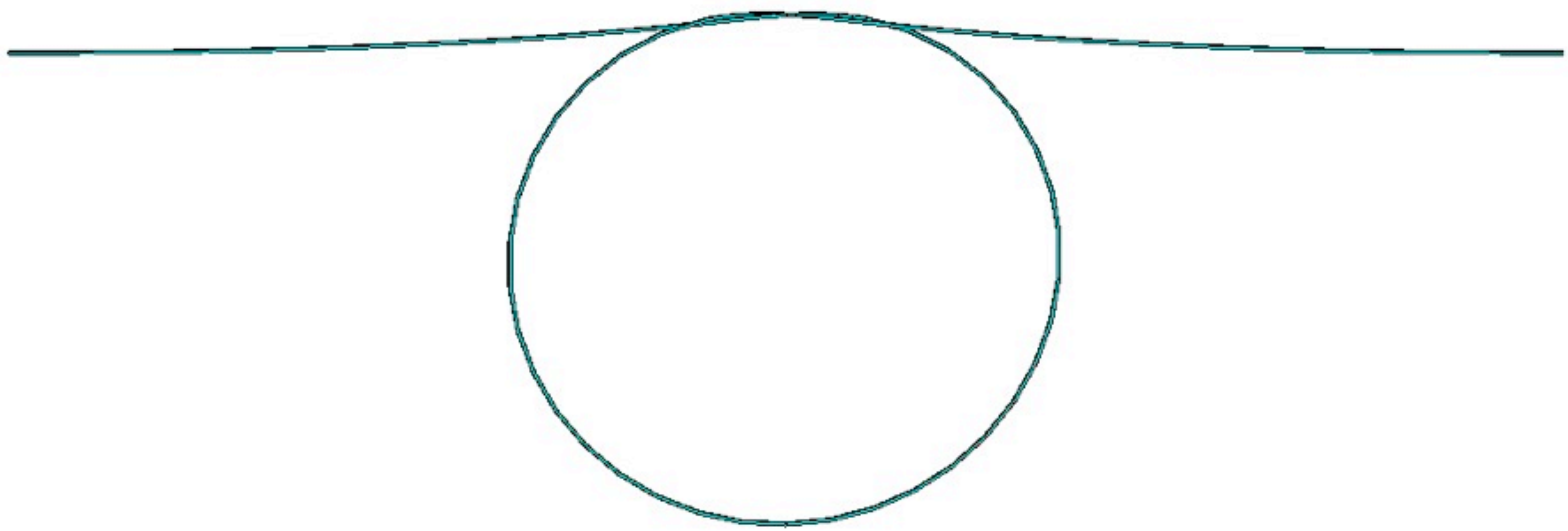
Making the rod thinner



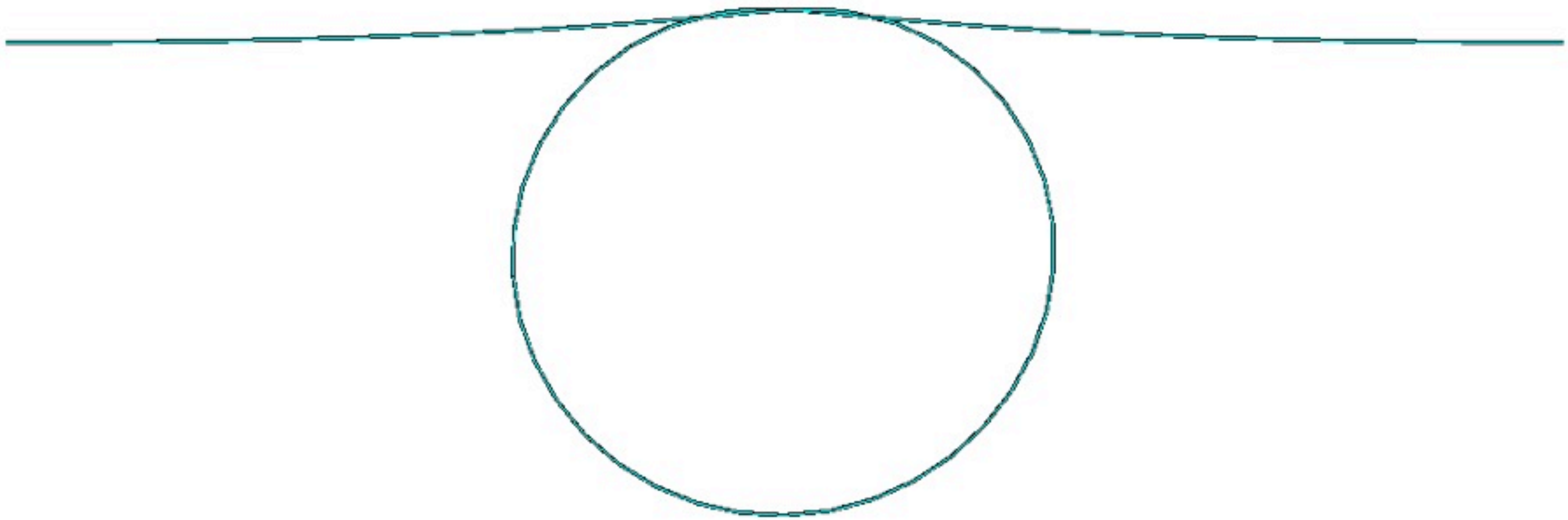
Making the rod thinner



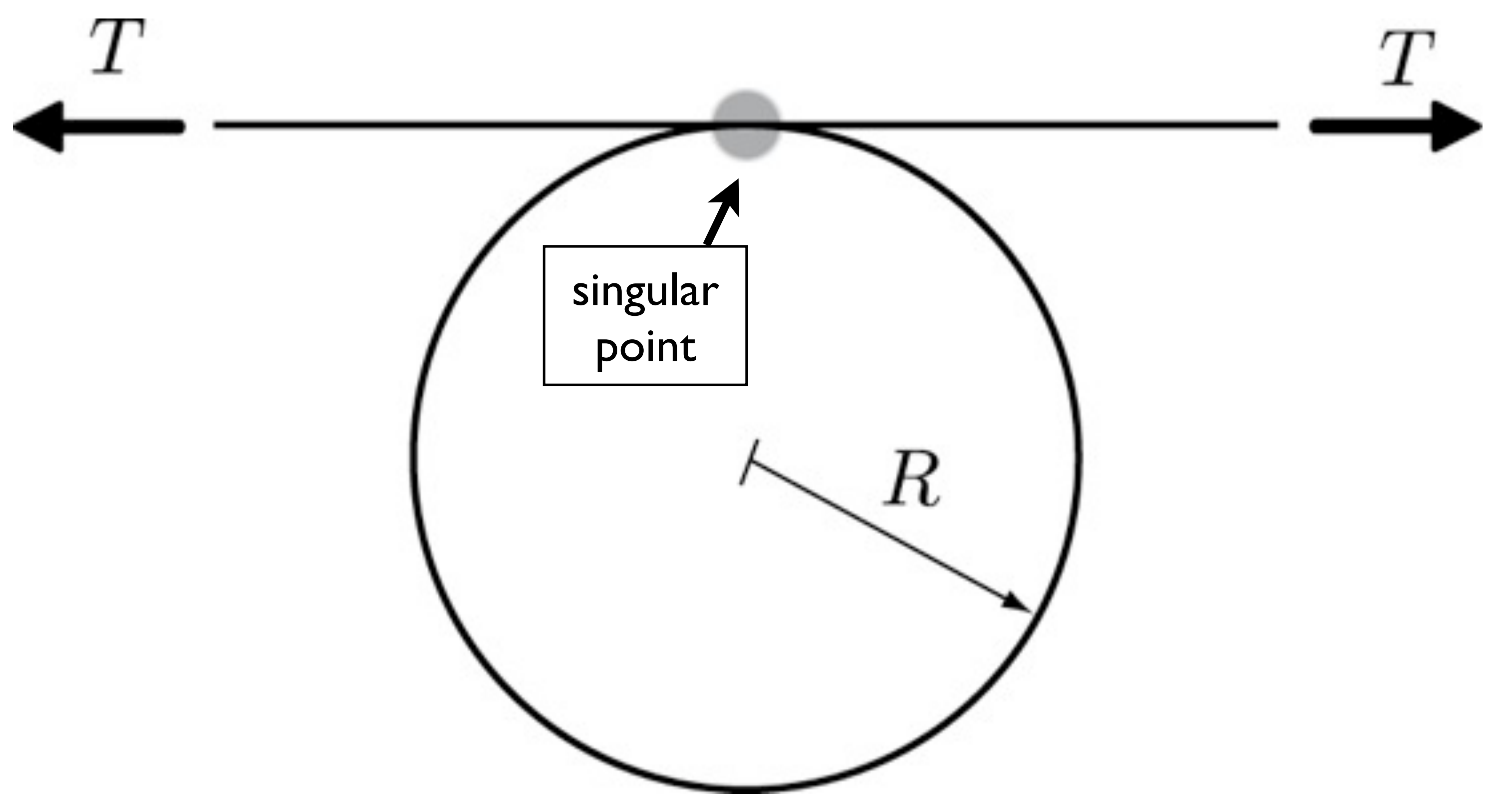
Making the rod thinner



Making the rod thinner



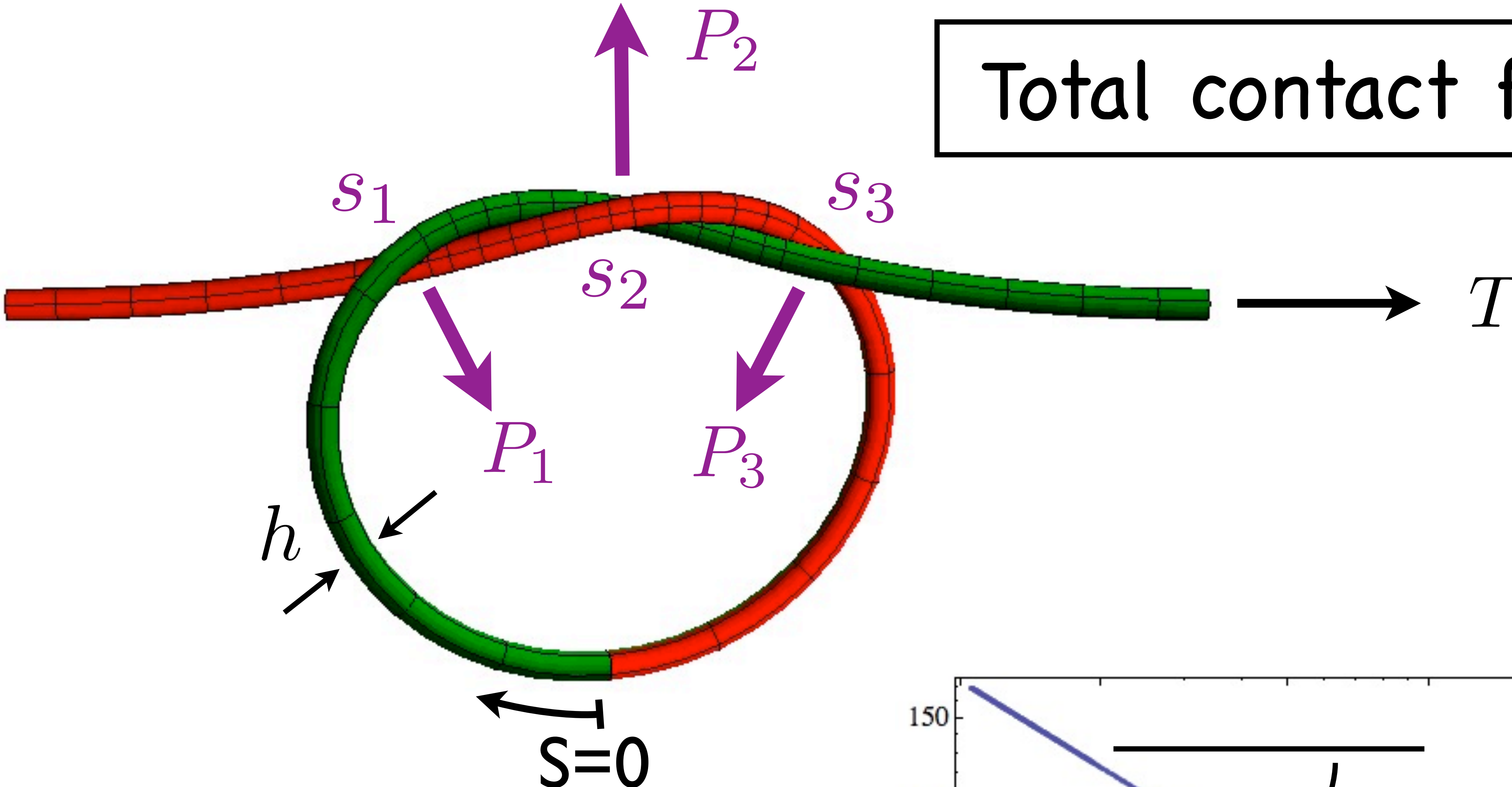
Zero thickness limit

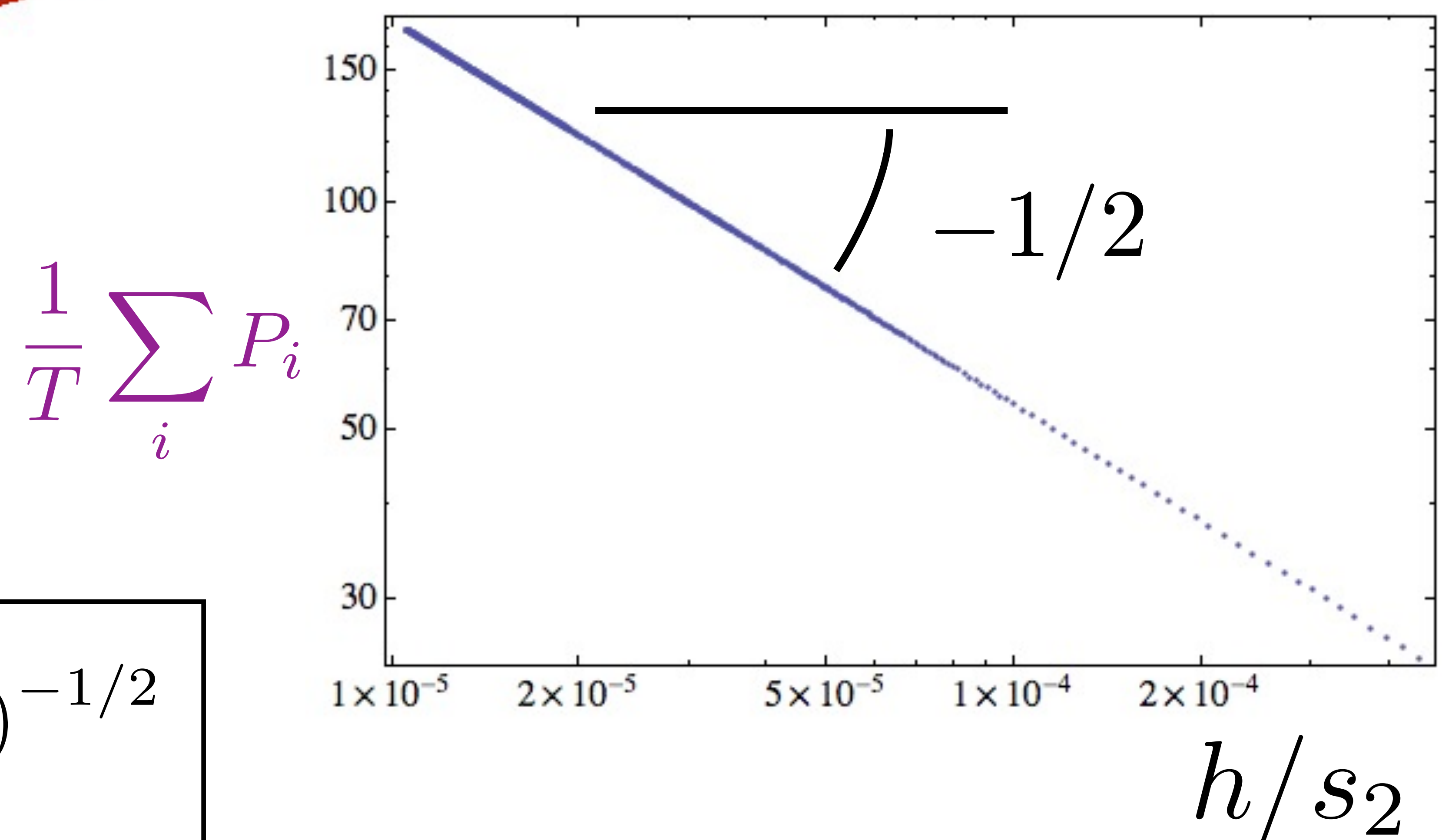


equilibrium : $T = \dfrac{EI}{2R^2}$ Arai et al (1999)

tensile force T → (singular point) → bending moment $\dfrac{EI}{R}$

Total contact force





$$\frac{1}{T}\sum_i P_i \simeq 0.55\,(h/s_2)^{-1/2}$$

Kirchhoff Equations

$$
\begin{cases}
\vec{F}' &= -\vec{p} \\
\vec{M}' &= \vec{F} \times \vec{t} \\
\vec{t}' &= \dfrac{1}{EI}\,\vec{M} \times \vec{t} \\
\vec{R}' &= \vec{t}
\end{cases}
$$

forces equil.

moments equil.

kinematics

tangent def.

$$' \equiv \frac{d}{ds}$$

$\vec{p}(s)$ ext. pressure

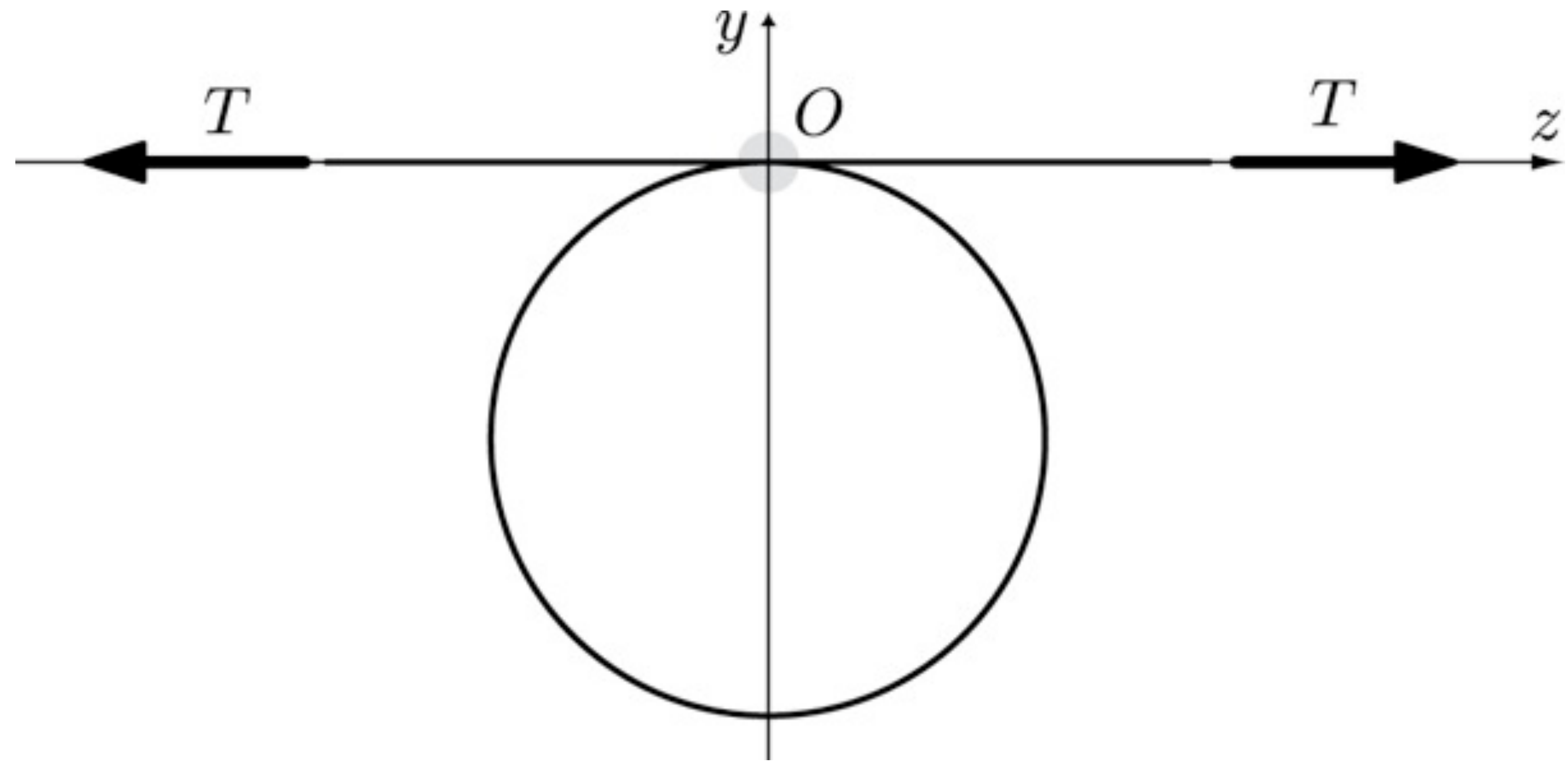
$\vec{M}(s)$ internal moment

$\vec{F}(s)$ internal force

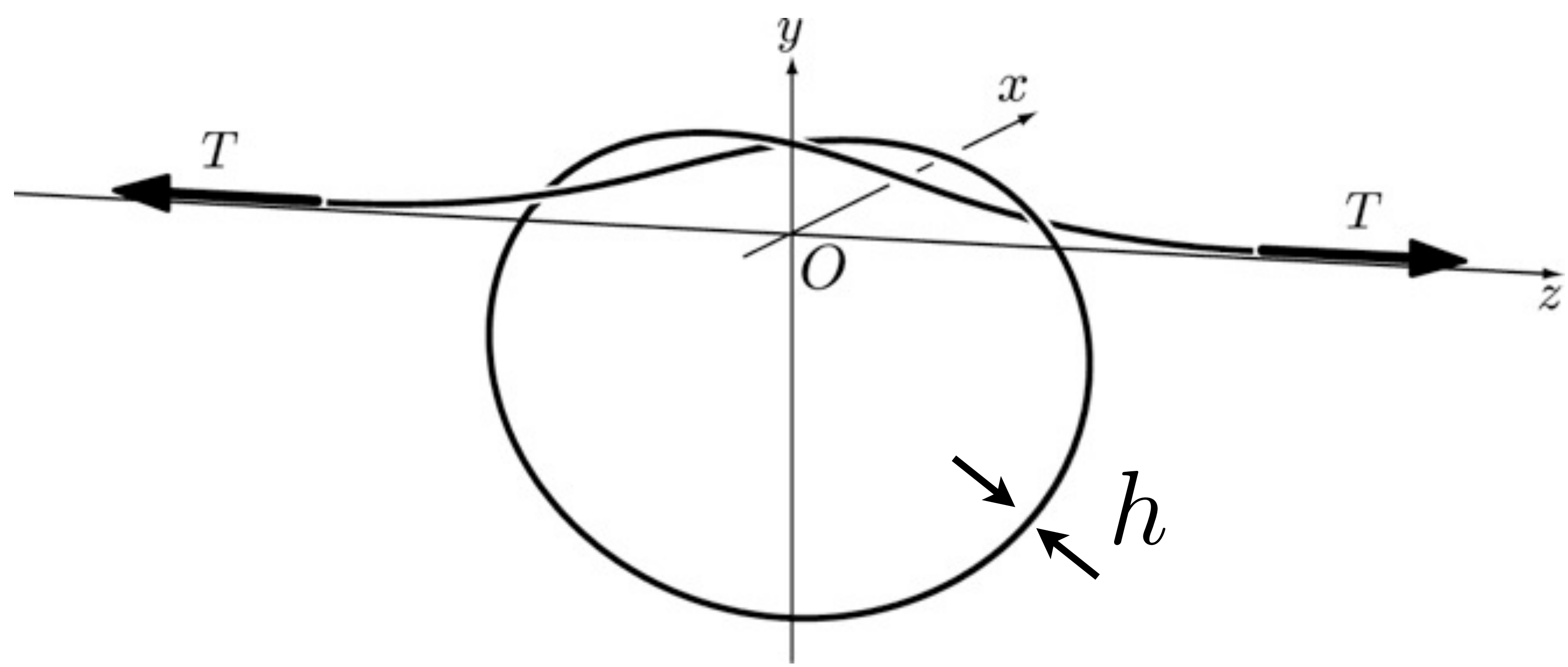
$\vec{R}(s)$ position

$\vec{t}(s)$ tangent

Perturbative problem



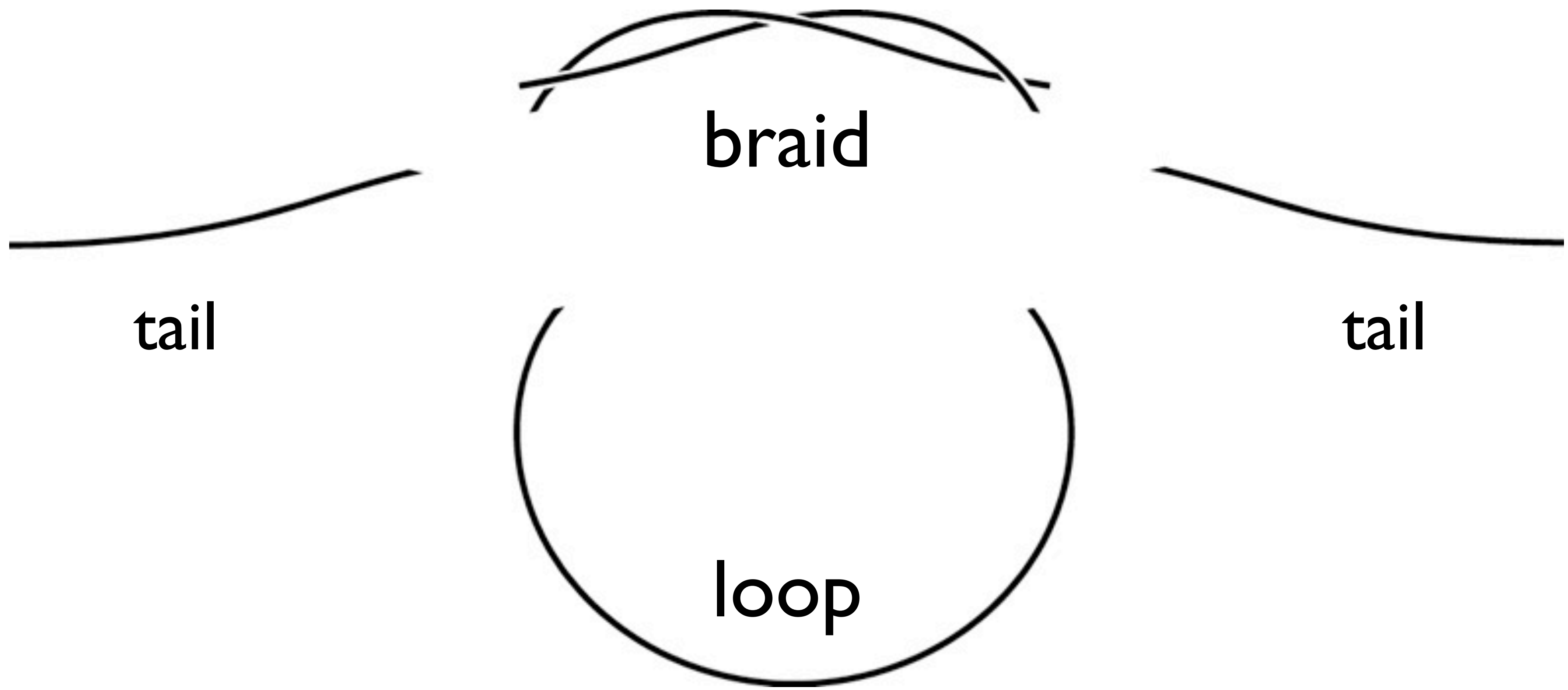
$$\epsilon = 0$$
$$(h = 0)$$



small parameter

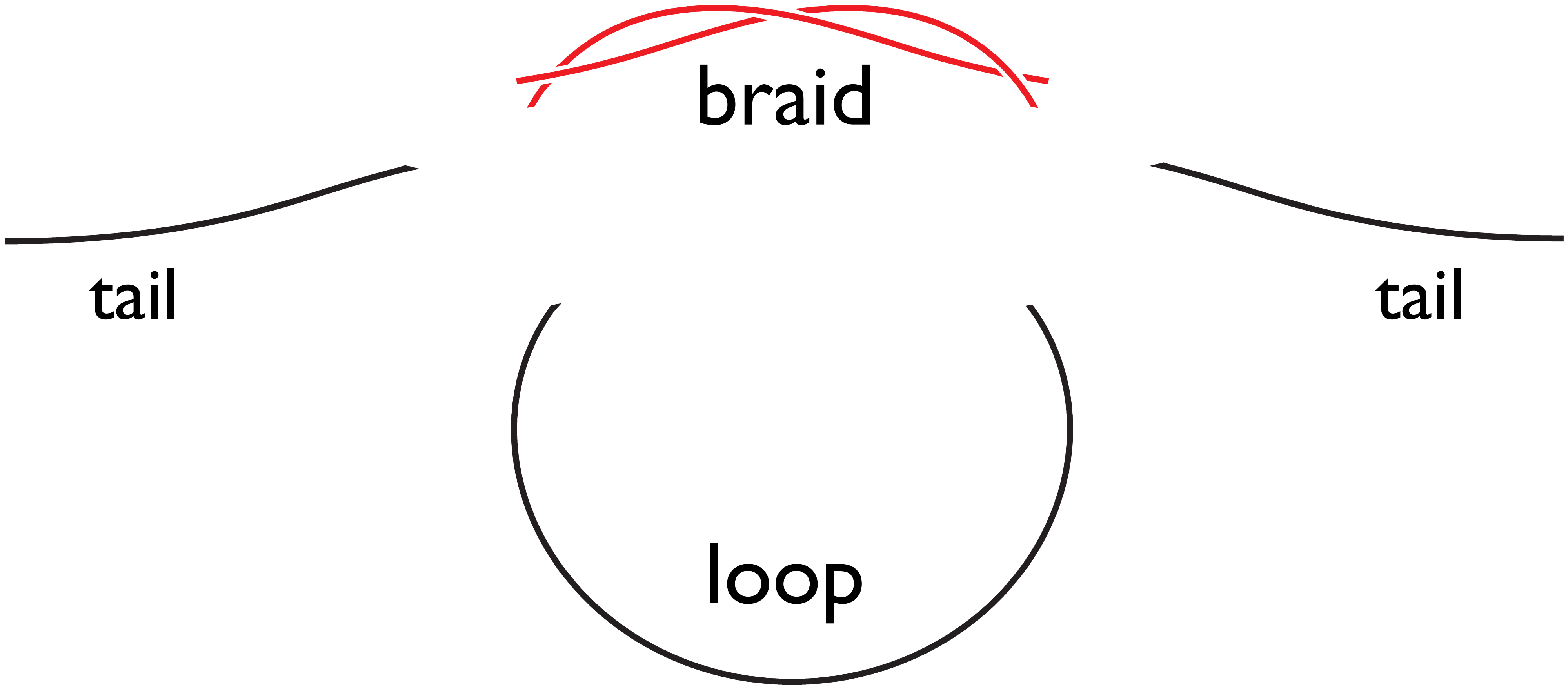
$$\epsilon = \left(\frac{2h^2 T}{EI}\right)^{1/4} \ll 1$$

Matched asymptotic expansions

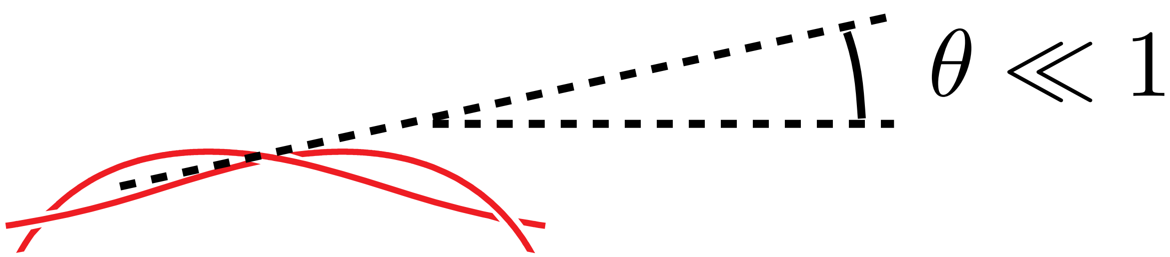


small parameter : $\epsilon = \left(\frac{2h^2 T}{EI} \right)^{1/4} \ll 1$

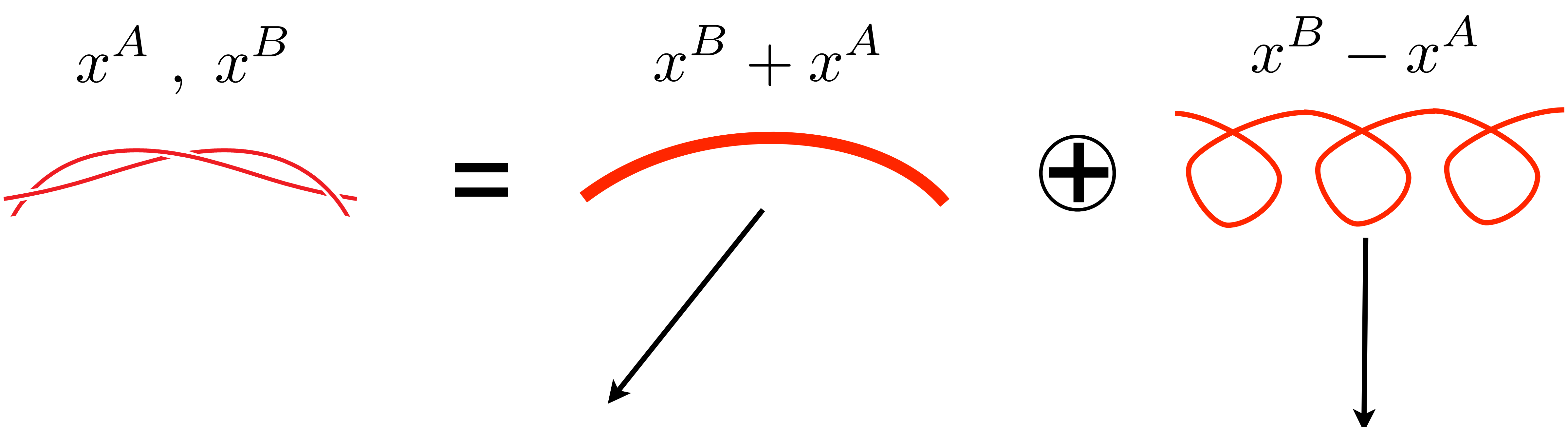
Braid : self-contact zone



Braid : linear superposition



small deflections => linear problem



twice more rigid

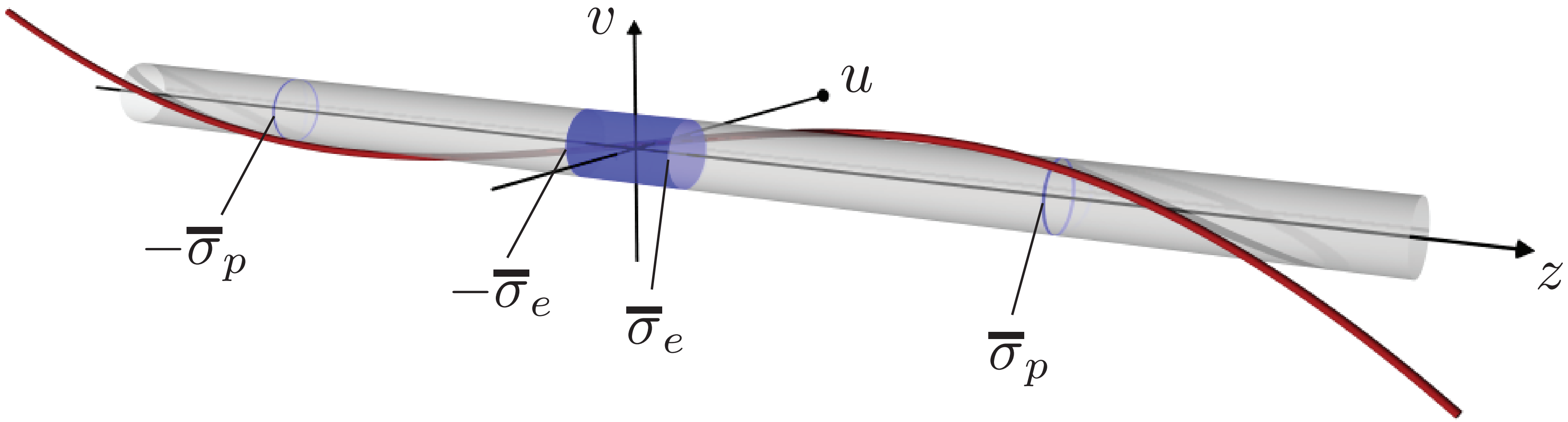
curvature: $\frac{1}{2}\frac{1}{R}$

self-contact

=>

contact with obstacle

Braid : variational formulation



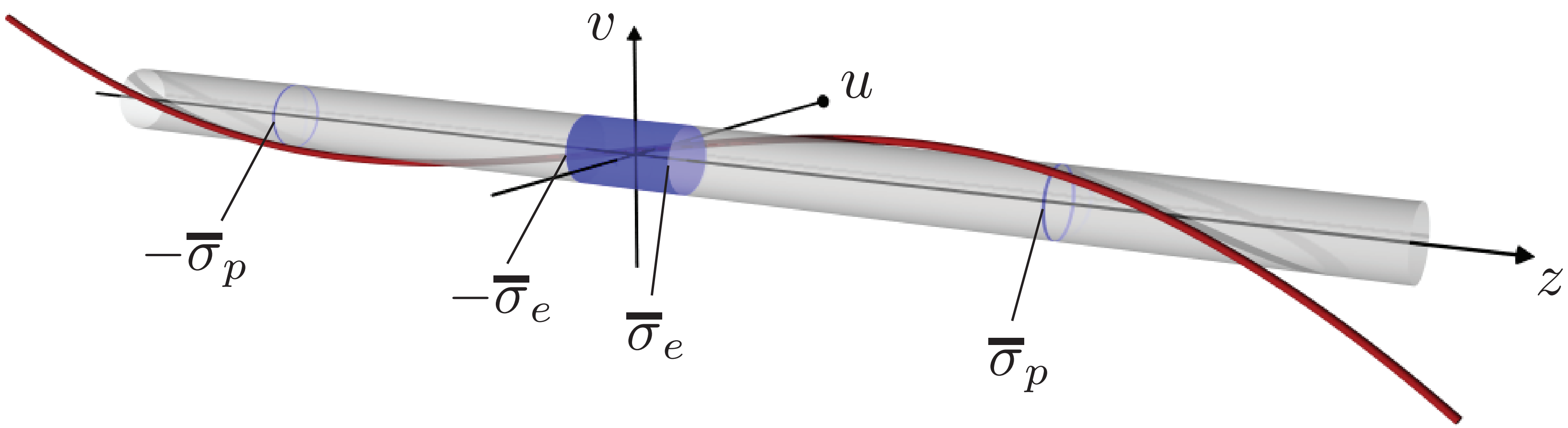
Kirchhoff equations => minimizing an energy

$$V = \frac{1}{2}\int_{-\infty}^{+\infty}\left(u''^2 + v''^2\right) d\sigma \; + \underbrace{v'(+\infty) + v'(-\infty)}_{\text{work of external applied moments}}$$

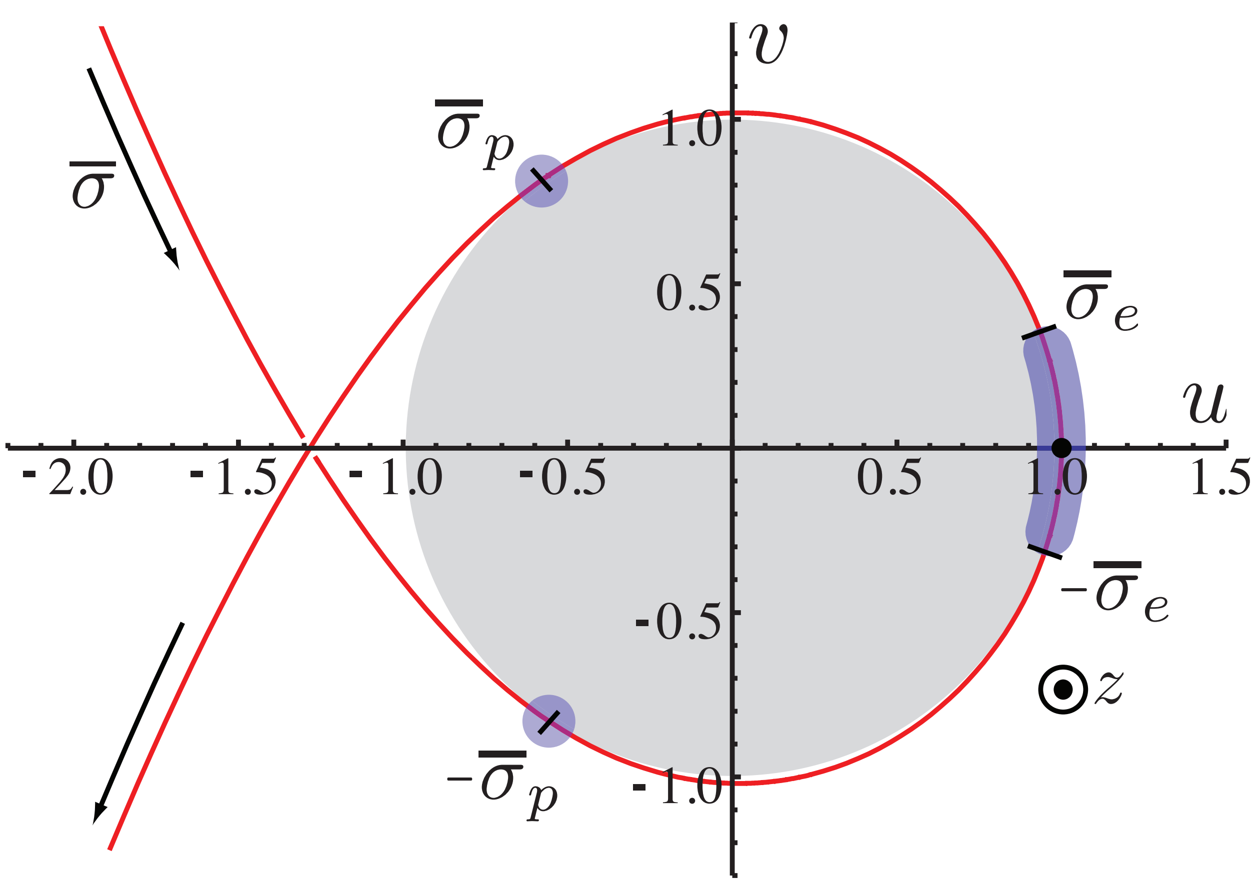
work of external applied moments

with constraint:
$u^2(\sigma) + v^2(\sigma) \geq 1 \;,\; \forall\sigma$

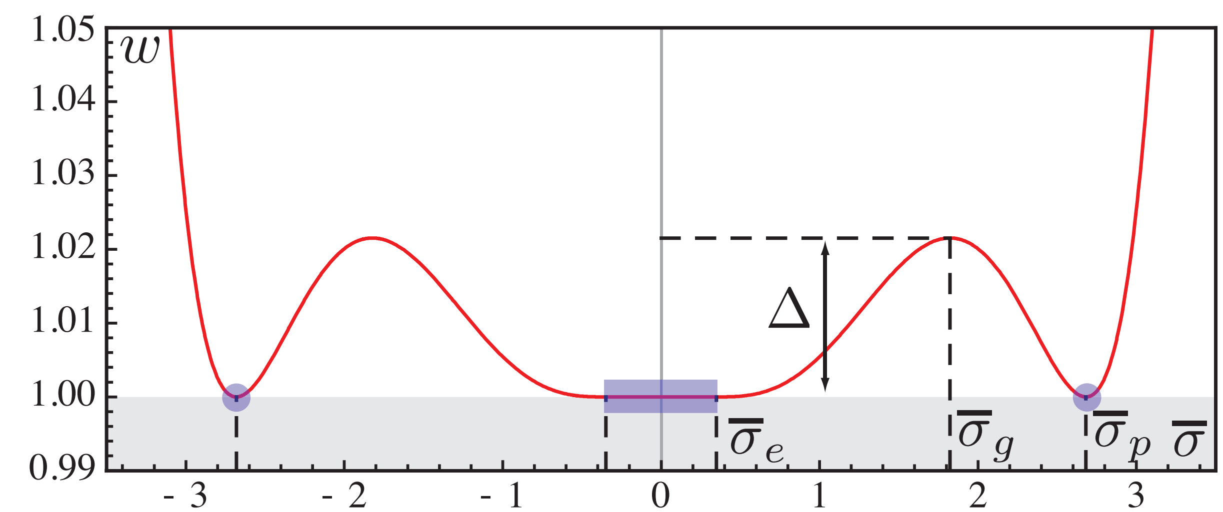
Braid : contact topology



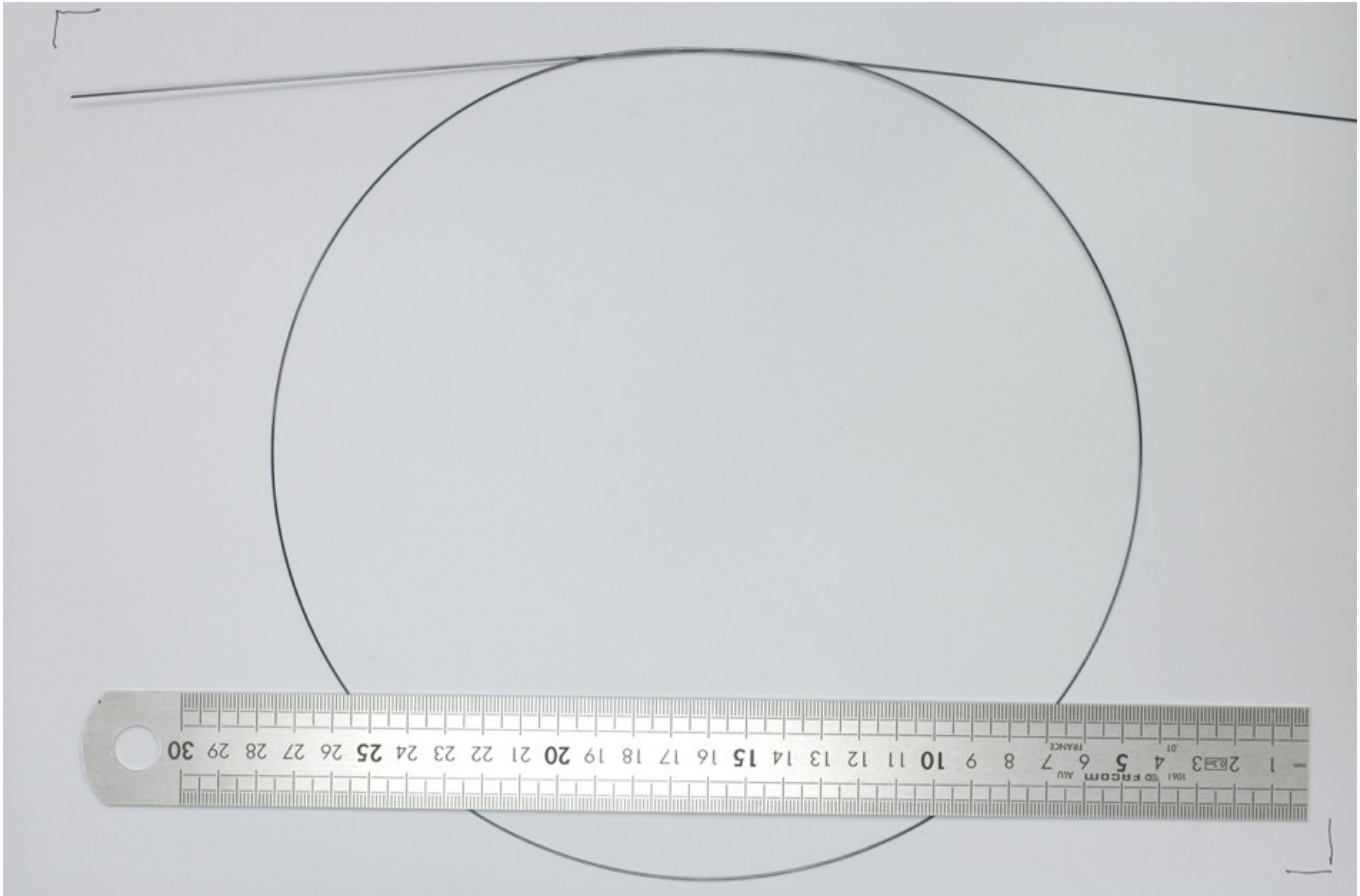
side view



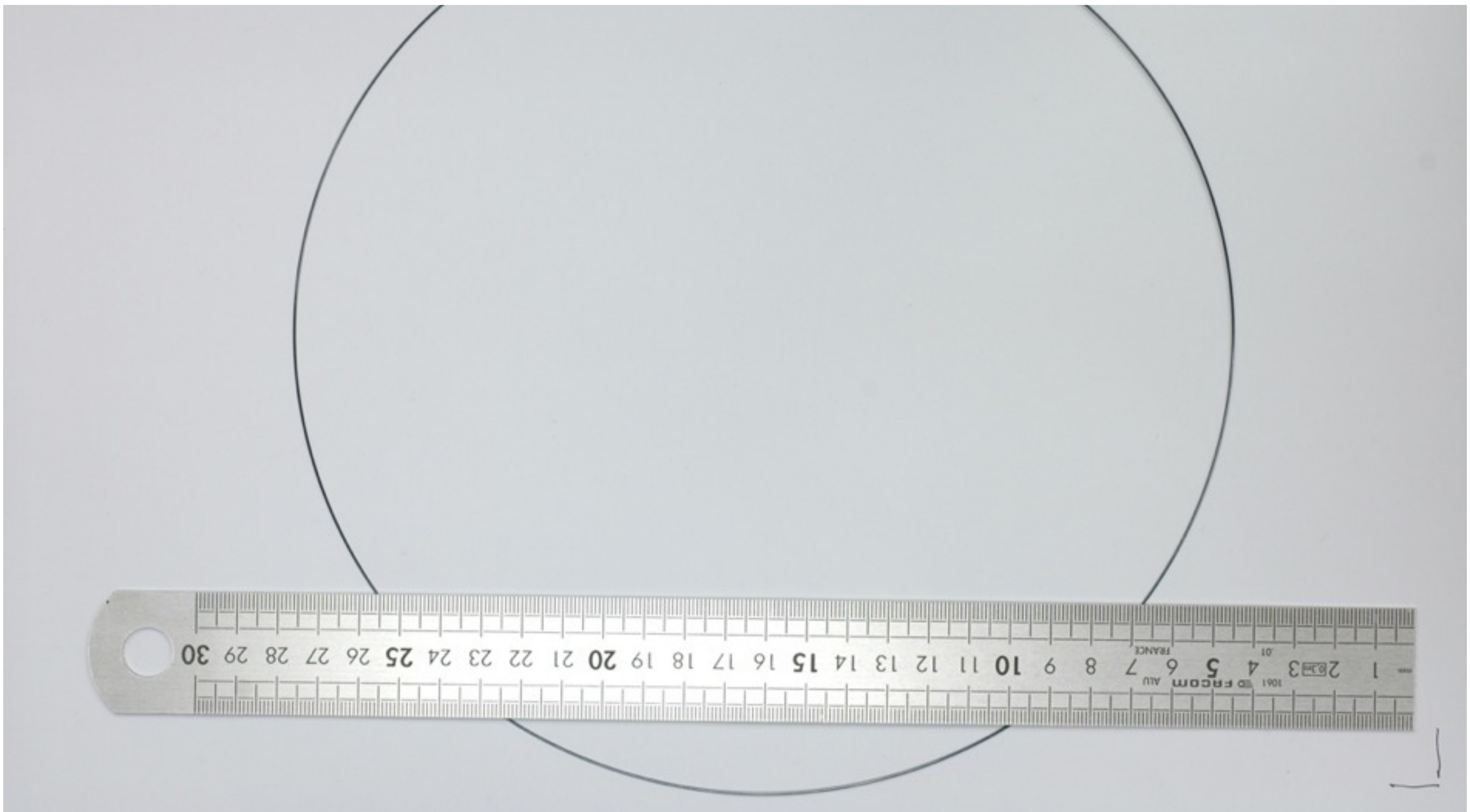
inter-strand distance



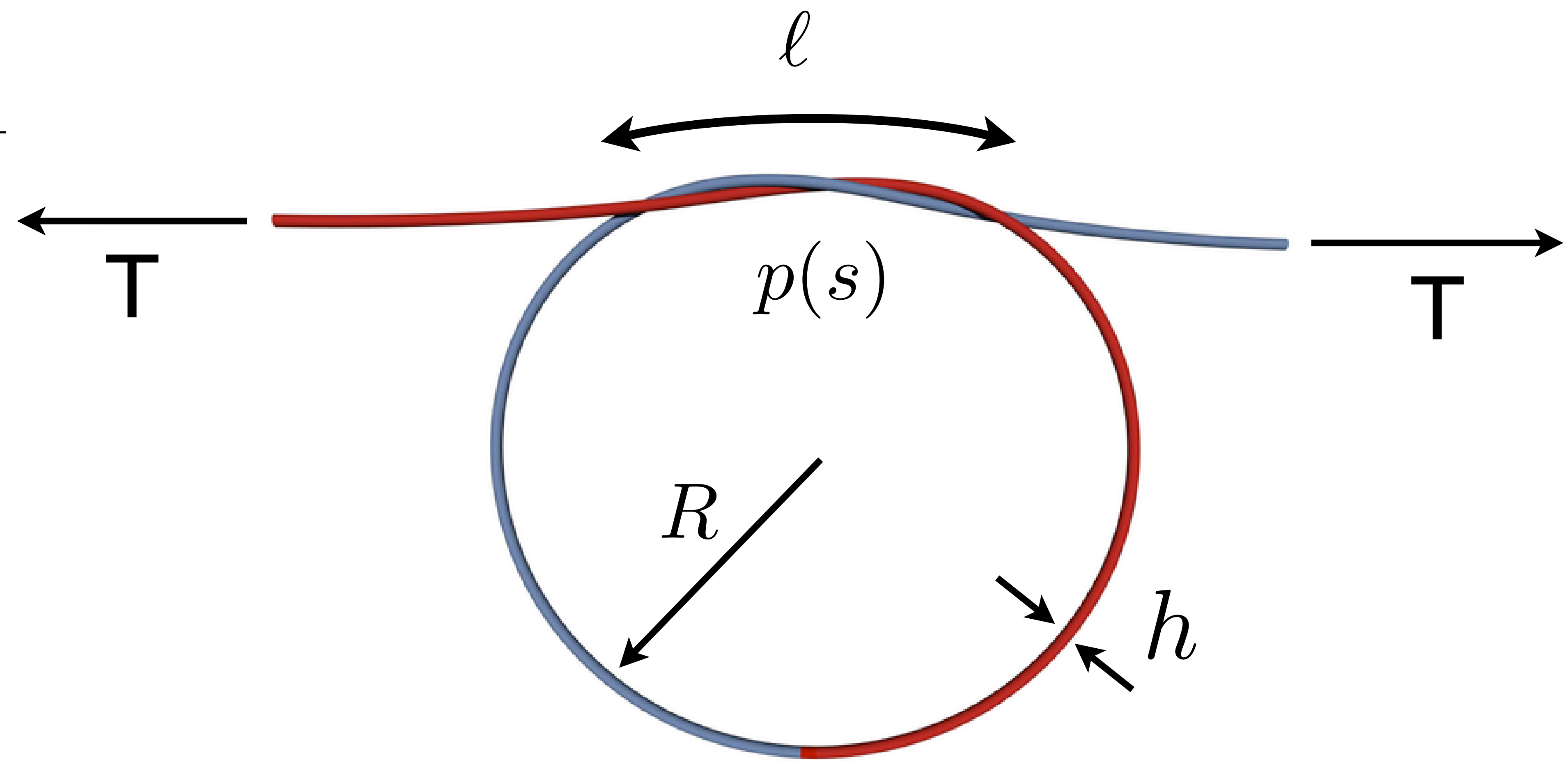
Braid : contact topology



Braid : contact topology



Results



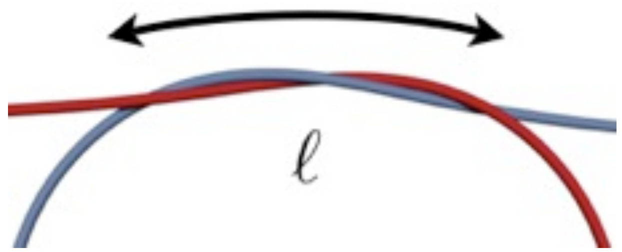
$$R = \sqrt{\frac{EI}{2T}}$$

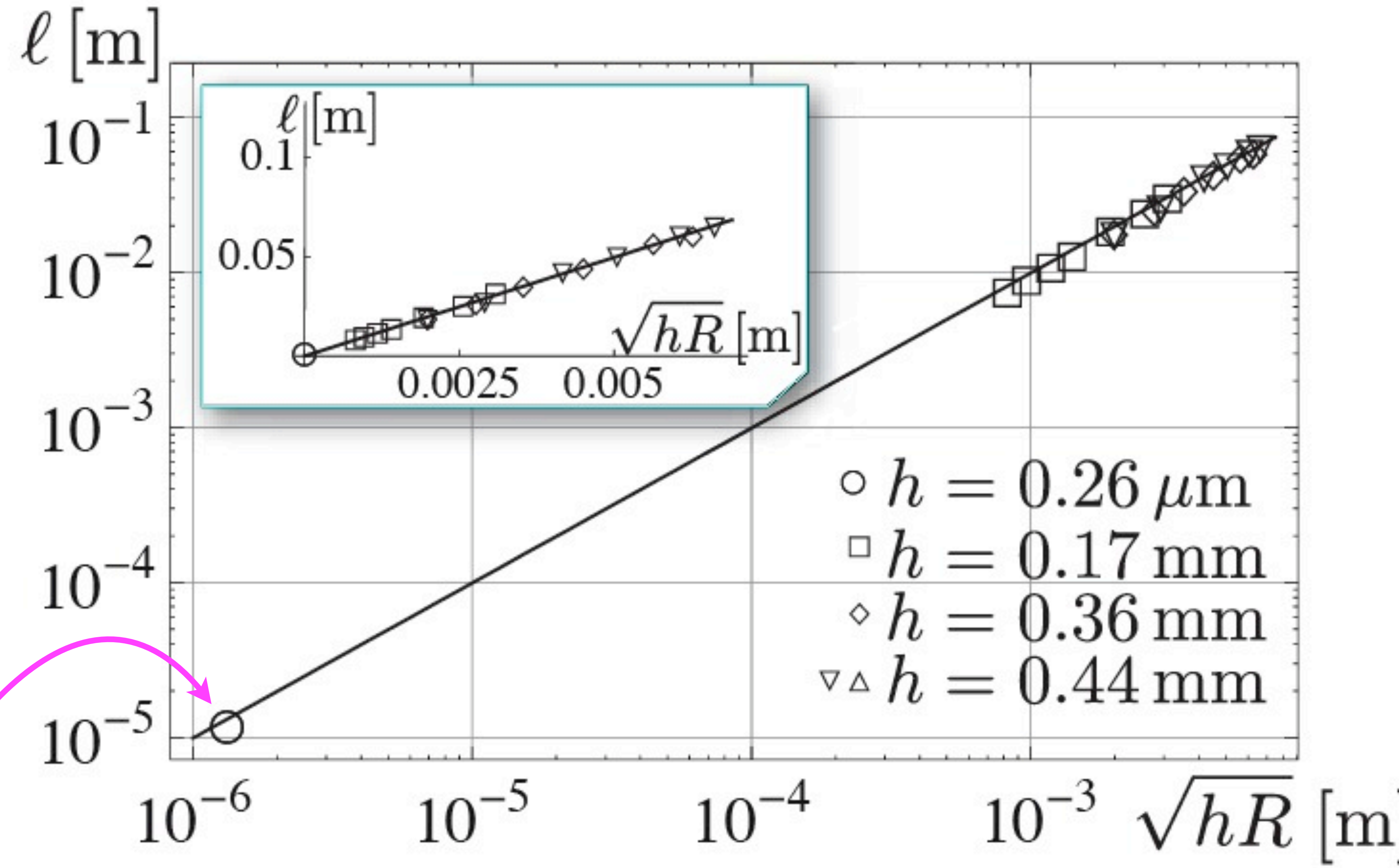
$$\ell = 9.91\, h^{1/2}\ (EI)^{1/4}\ T^{-1/4}$$

Contact pressure $p(s)$

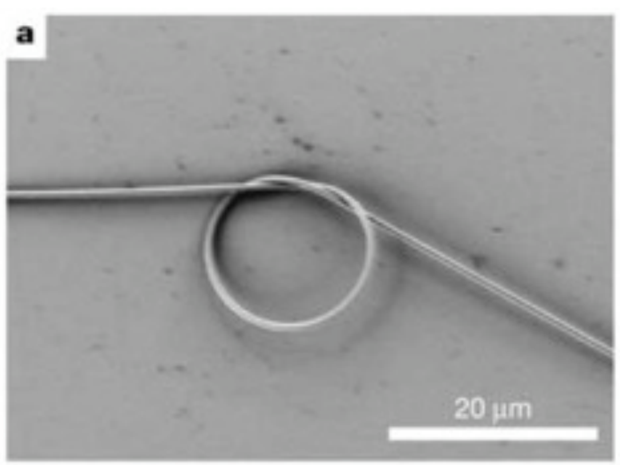
Total contact force $P = \int_0^\ell p(s) ds = 0.82\, h^{-1/2}\ (EI)^{1/4}\ T^{3/4}$

Experiments



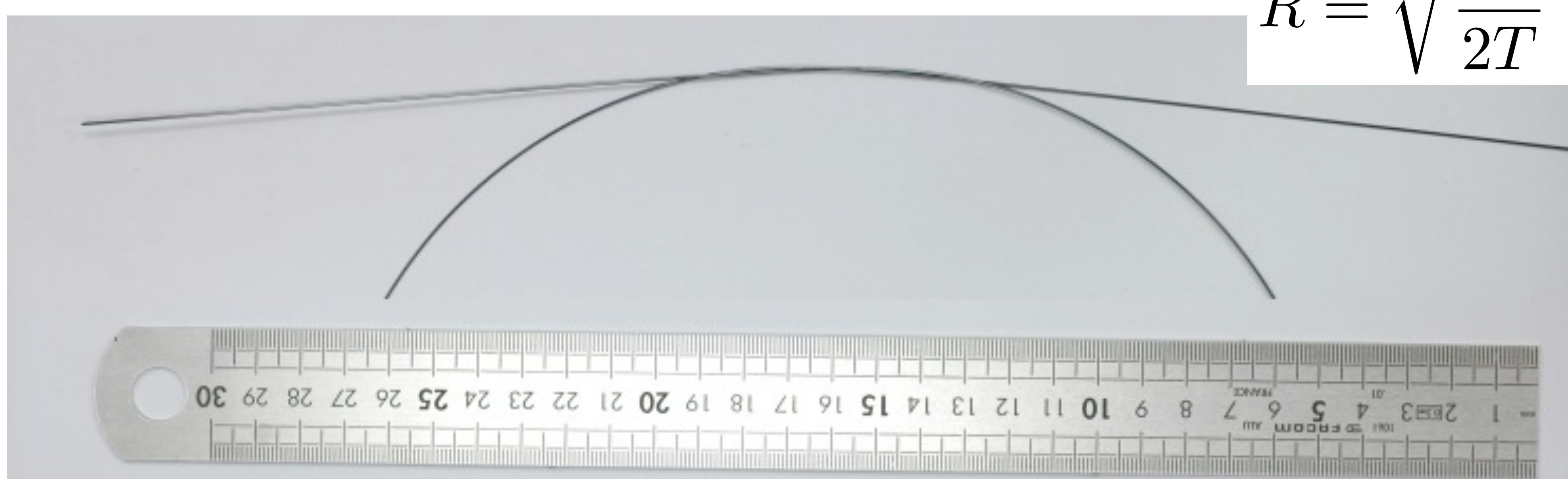


Tong et al., Nature 2003

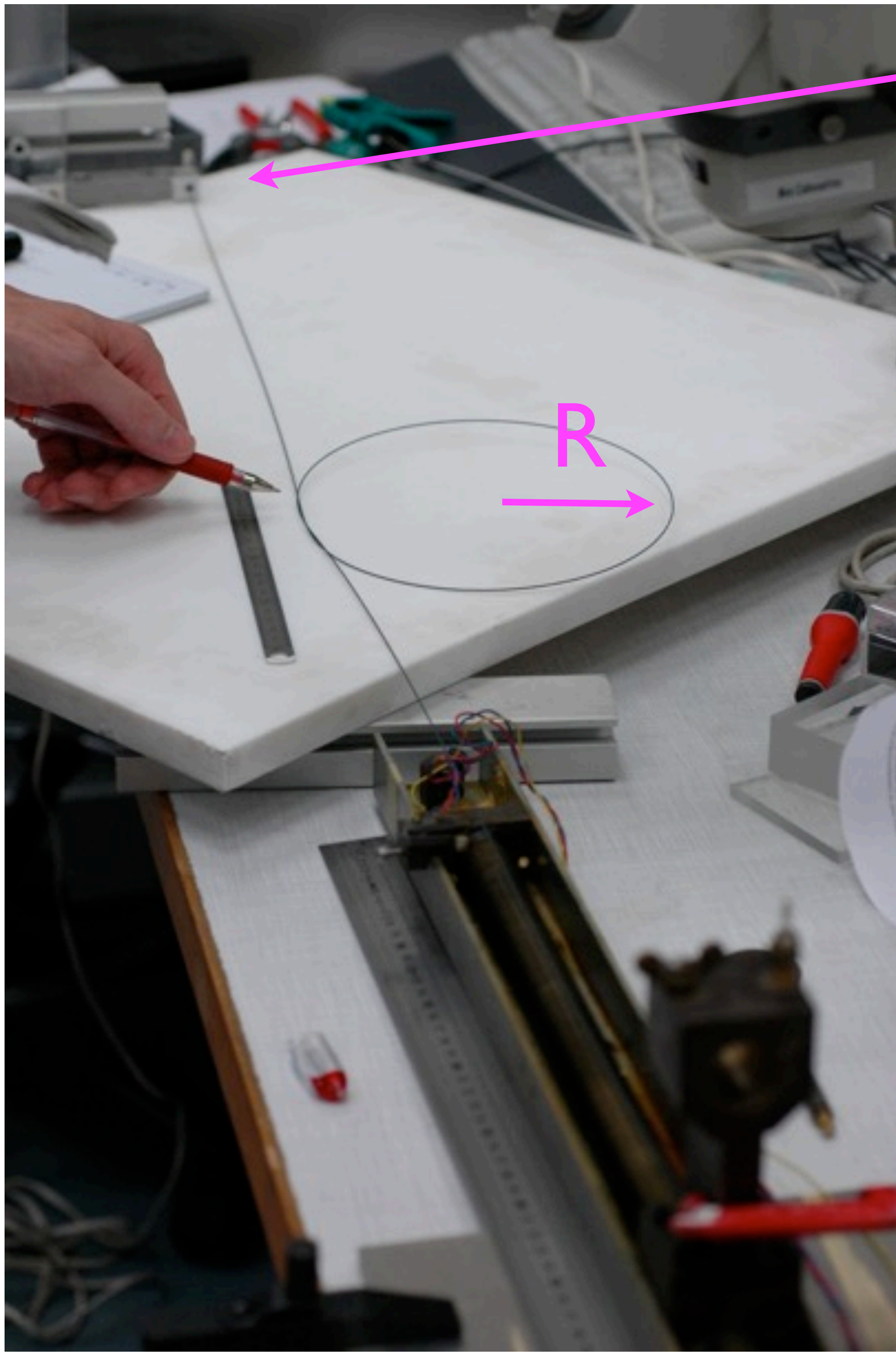


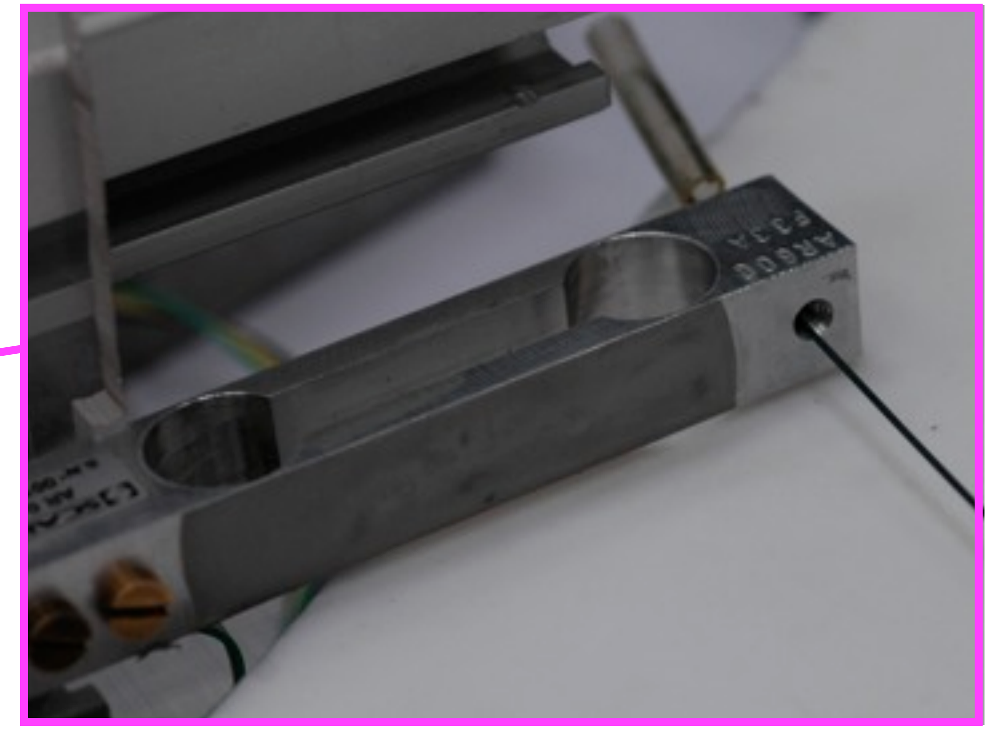
silica wire
h = 1/2 micron

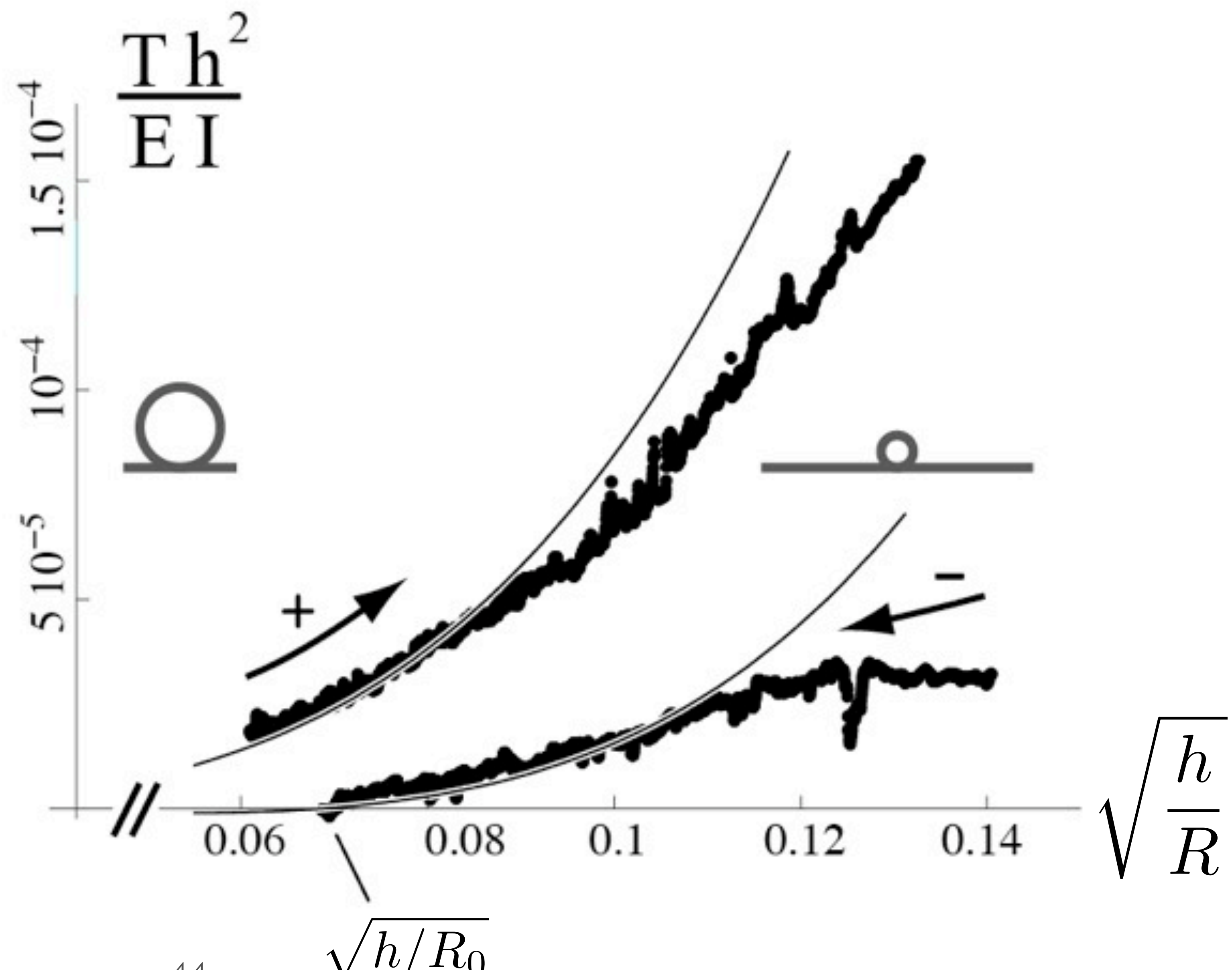
$$R = \sqrt{\frac{EI}{2T}}$$



Experiments





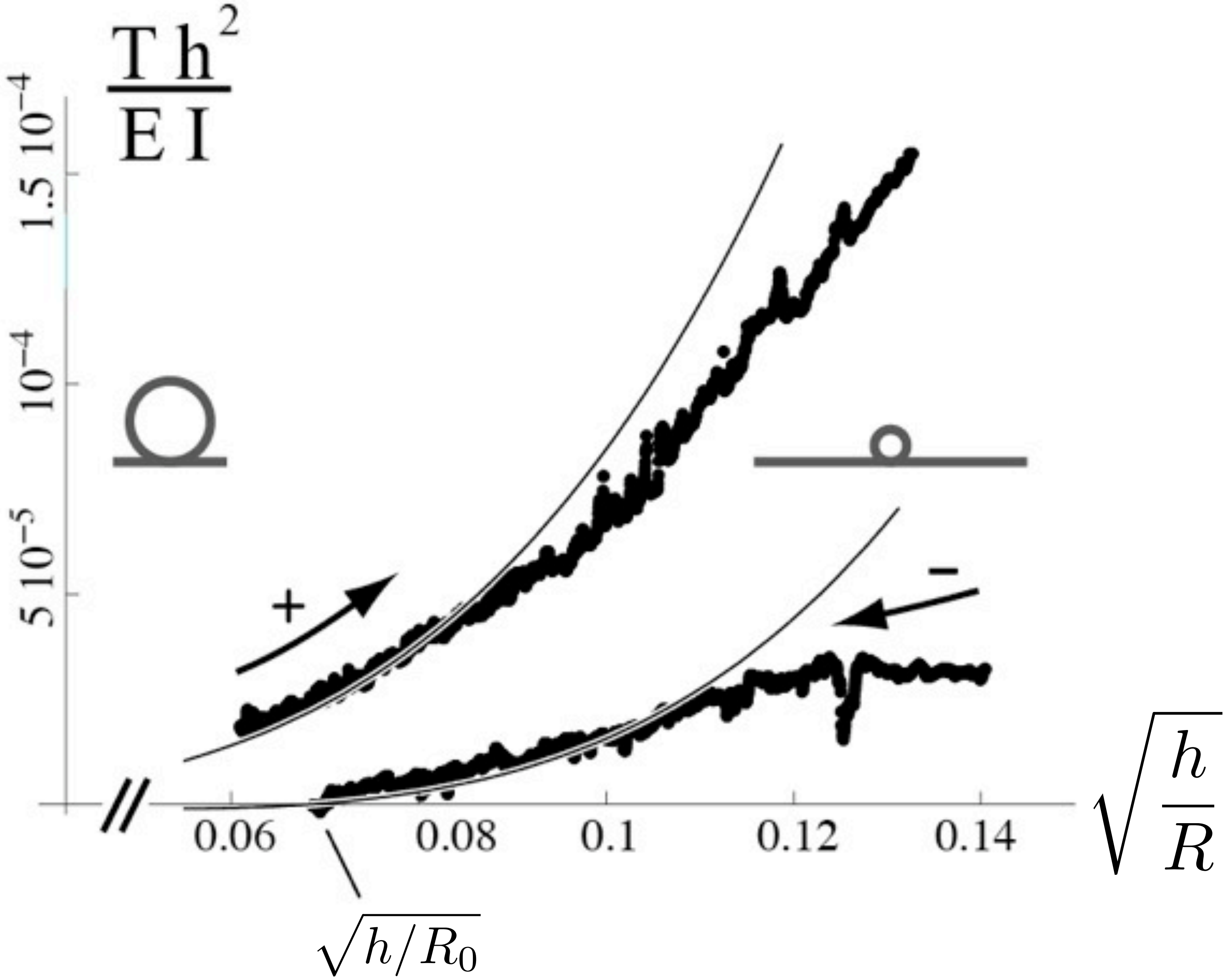


Expériences

sans frottement

$$T = \frac{1}{2}\,\frac{EI}{R^2}$$

$$\Rightarrow \frac{Th^2}{EI} = \frac{1}{2}\,\frac{h^2}{R^2}$$



avec frottement $$\left|\frac{Th^2}{EI} - \frac{1}{2}\,\frac{h^2}{R^2}\right| \leq \mu\,P = 0.49\,\mu\,\left(\frac{h}{R}\right)^{3/2}$$

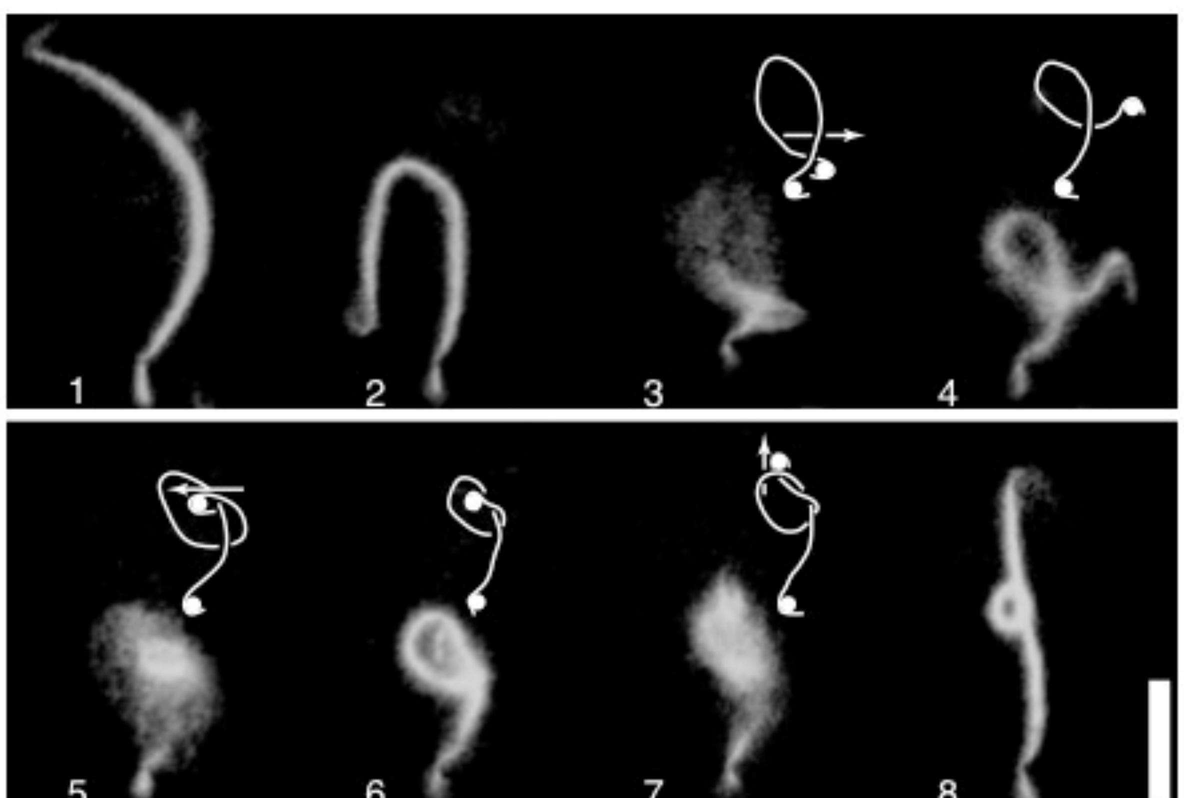
si $T = 0$: glissement jusqu'à $R = R_0$ tel que : $\mu = 1.02\sqrt{\frac{h}{R_0}}$

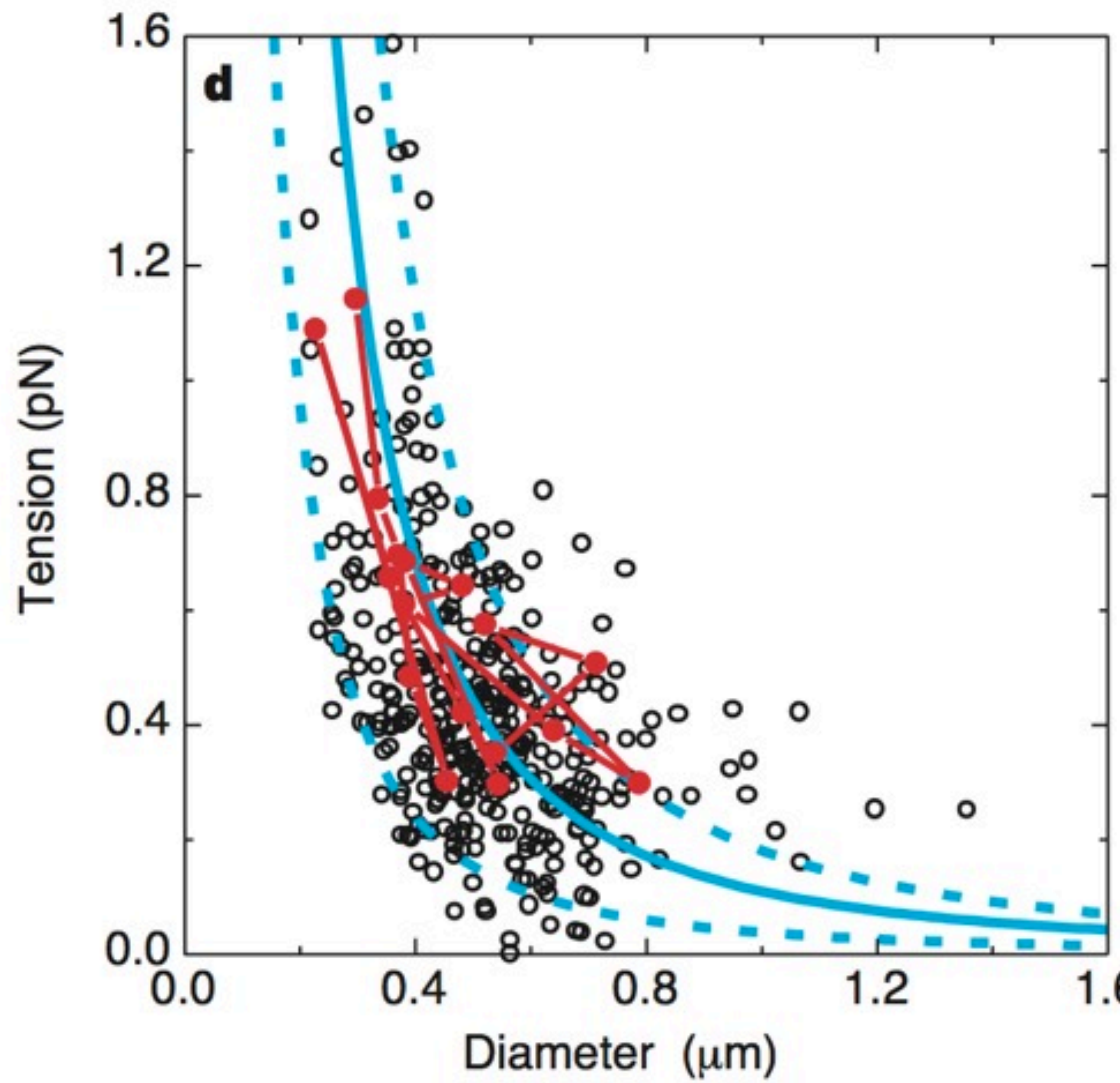
F-Actin

Cytoskelton filament
Active network
Locomotion

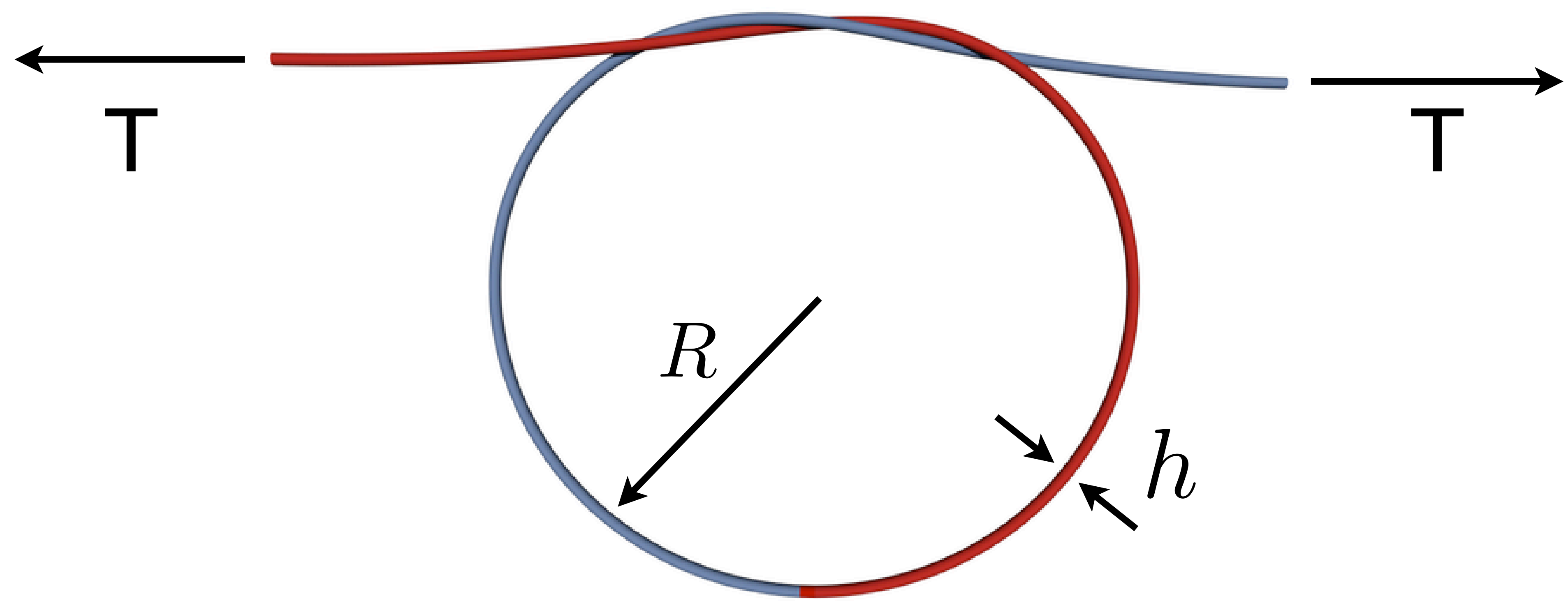
Single molecule experiment with knotted F-Actin filaments

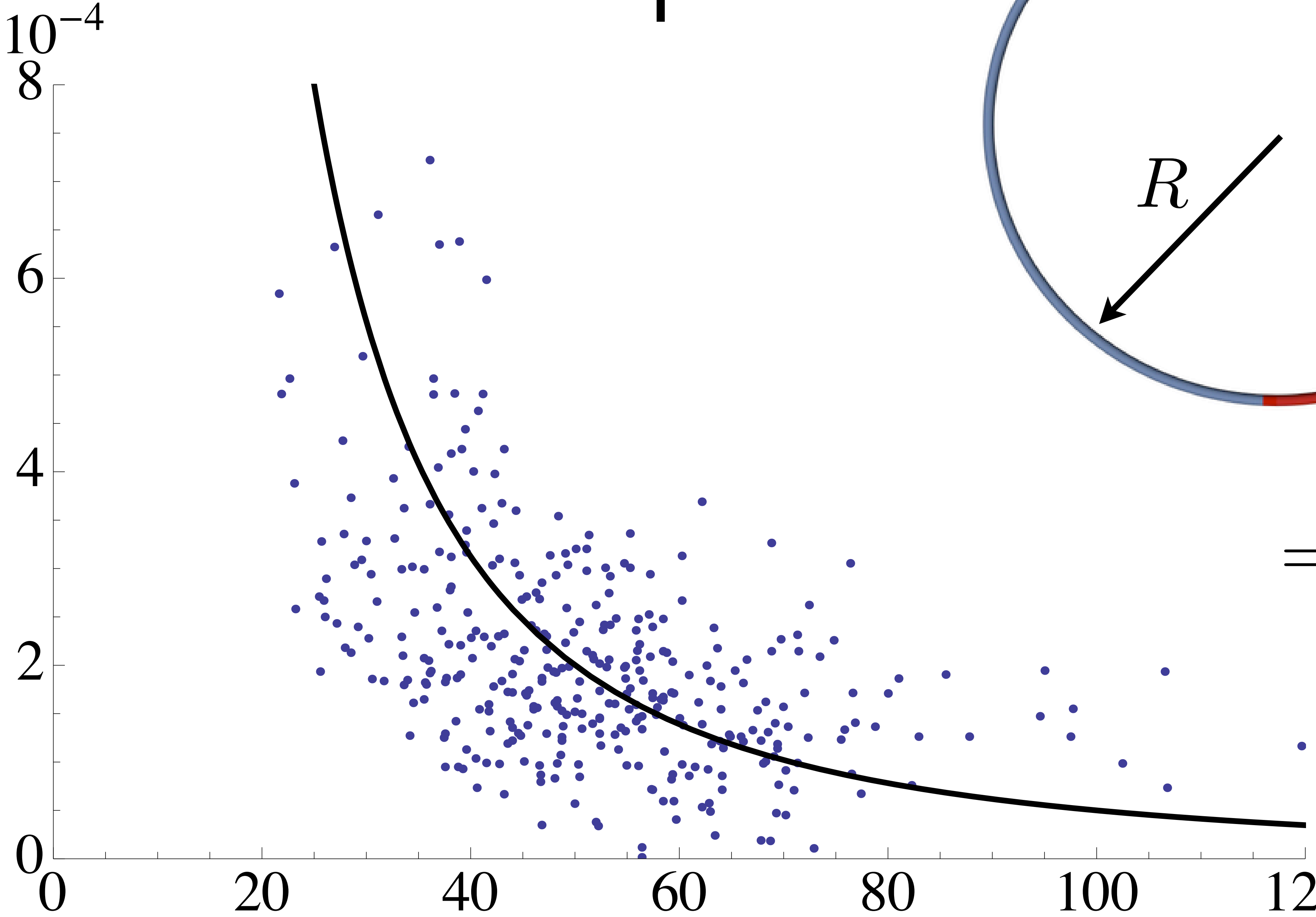
Arai et al, *Nature* (1999)





F-Actin : bending rigidity





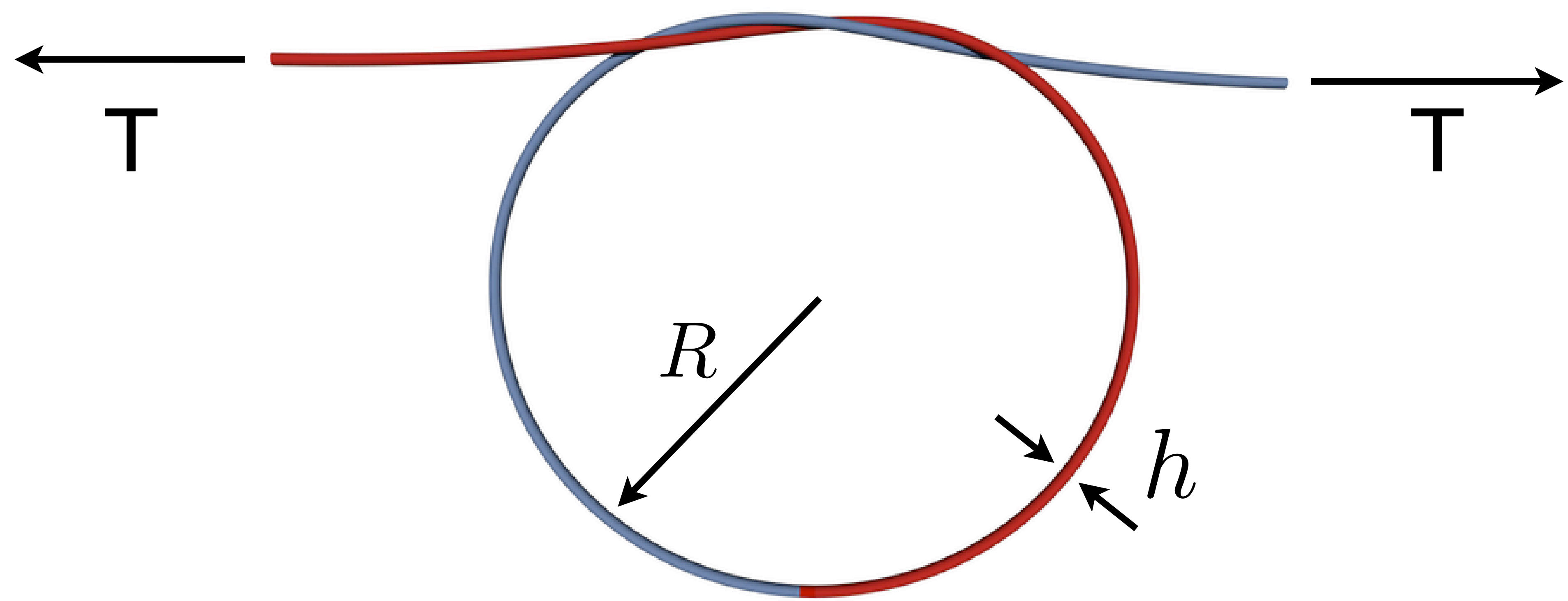
$\Rightarrow EI = 1300\,\mu\text{m}\,kT$

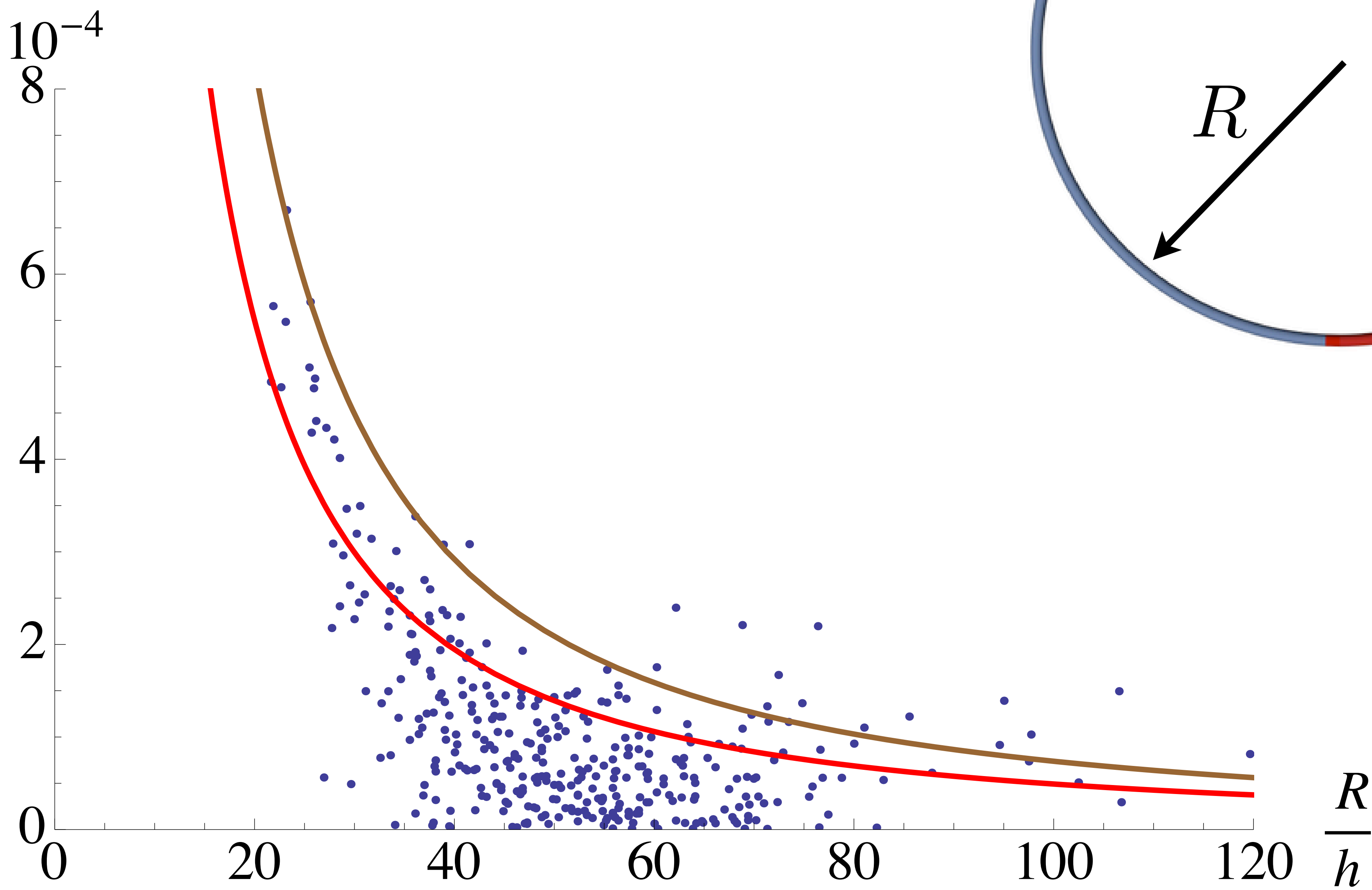
Arai et al, *Nature* (1999)

sans frottement $$\frac{Th^2}{EI} = \frac{1}{2}\,\frac{h^2}{R^2}$$

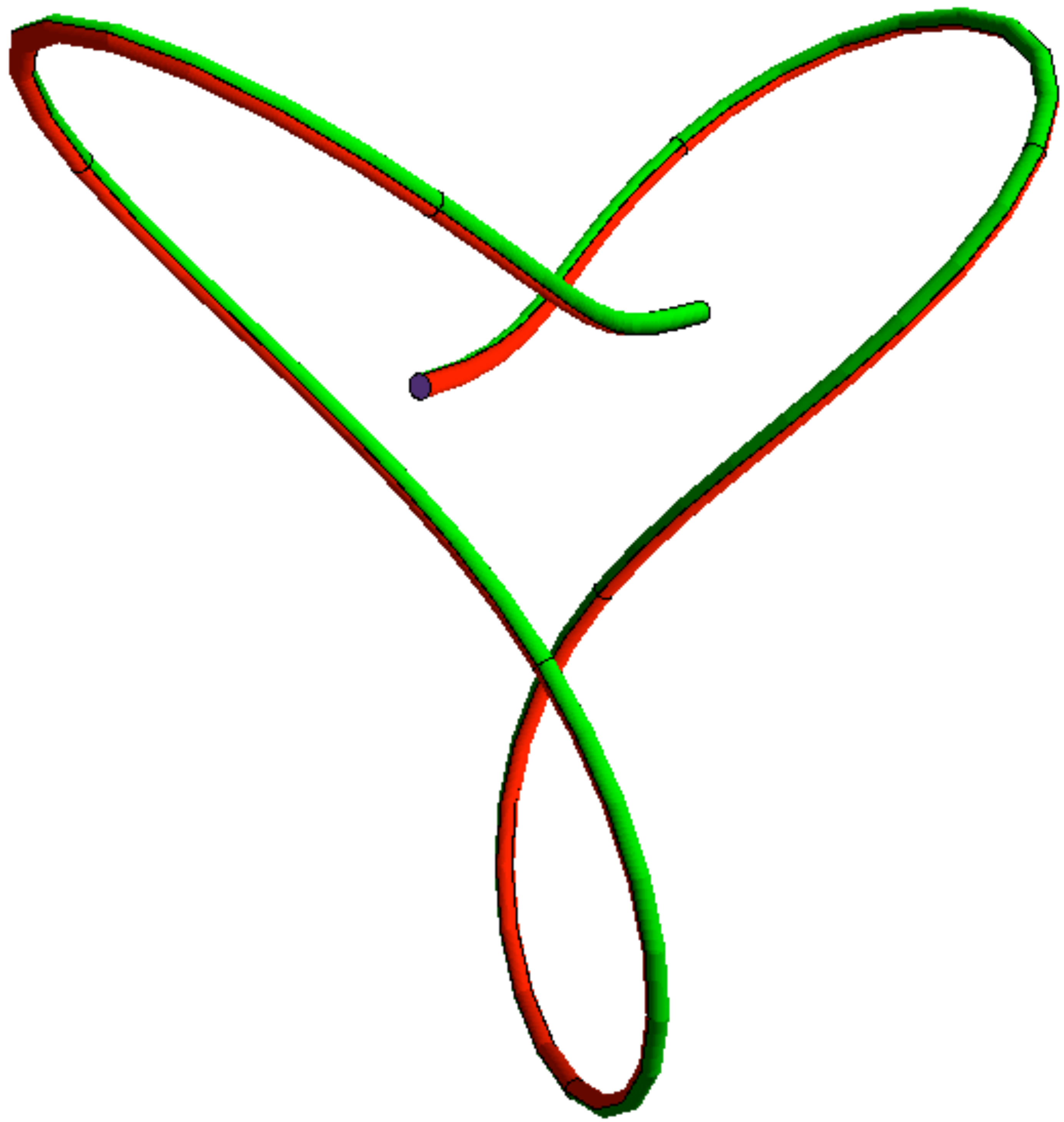
F-Actin :self- friction coefficient

$$\left| \frac{Th^2}{EI} - \frac{1}{2}\,\frac{h^2}{R^2} \right|$$





avec frottement $\left| \frac{Th^2}{EI} - \frac{1}{2}\,\frac{h^2}{R^2} \right| \leq \mu\, P = 0.49\,\mu\, \left(\frac{h}{R}\right)^{3/2}$



do stable open trefoil knotted configurations exist ?

Langer + & Singer (J. London Math. Soc) 1984 conjecture that no.
(for closed configurations though)

Fin

www.ida.upmc.fr/~neukirch

B. Audoly, N. Clauvelin, and S. Neukirch. *Physical Review Letters*, 99 (2007) 164301.

N. Clauvelin, B. Audoly, and S. Neukirch. *Journal of the Mechanics and Physics of Solids*, 57 (2009) 1623–1656.

H. O. Kirchner and S. Neukirch. *Journal of the Mechanical Behavior of Biomedical Materials*, 3 (2010) 121–123.

Variational formulation

$$E = \int_{-\infty}^{+\infty} \left(\frac{B}{2}\kappa^2 + \frac{C}{2}\tau^2 \right) ds + TD_\infty - UR_\infty,$$

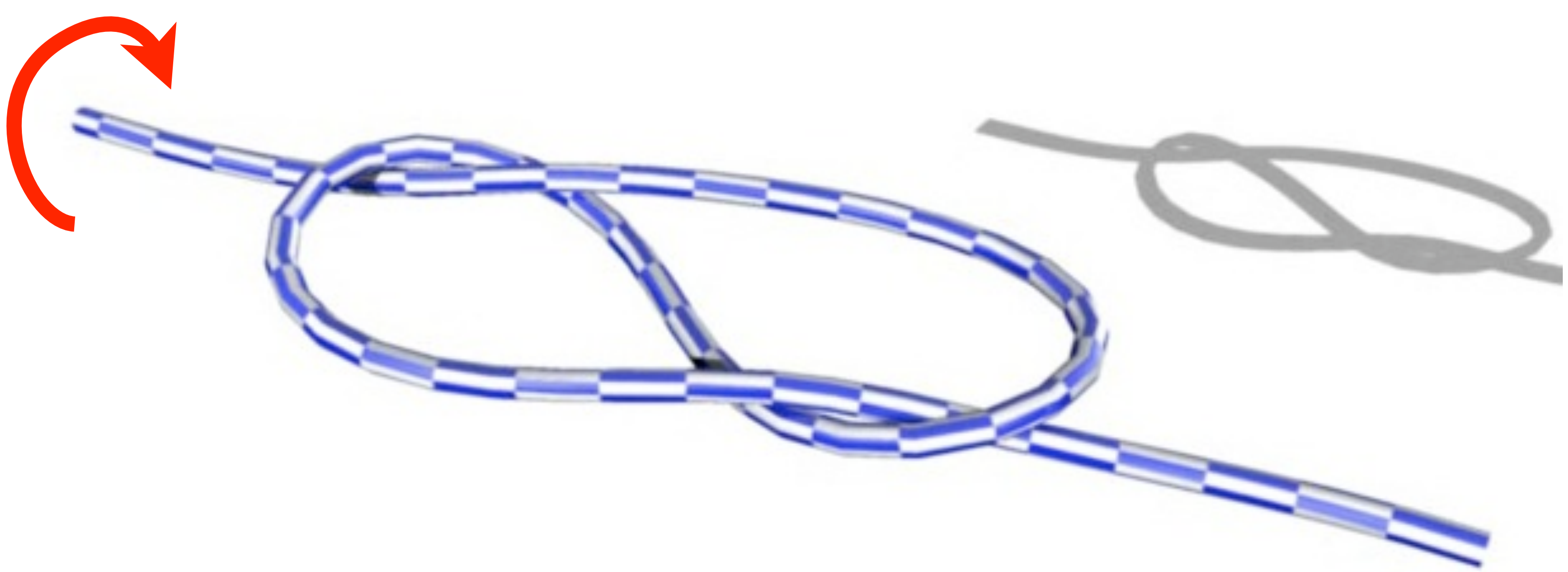
where κ and τ stand for the curvature and the twist of the rod.

$$\kappa = |\mathbf{t}'(s)|.$$

$$|\mathbf{r}(s_1) - \mathbf{r}(s_2)| \geq 2h,$$

for any s_1 and s_2 such that $|s_1 - s_2| > 4h$.

Twist Instability

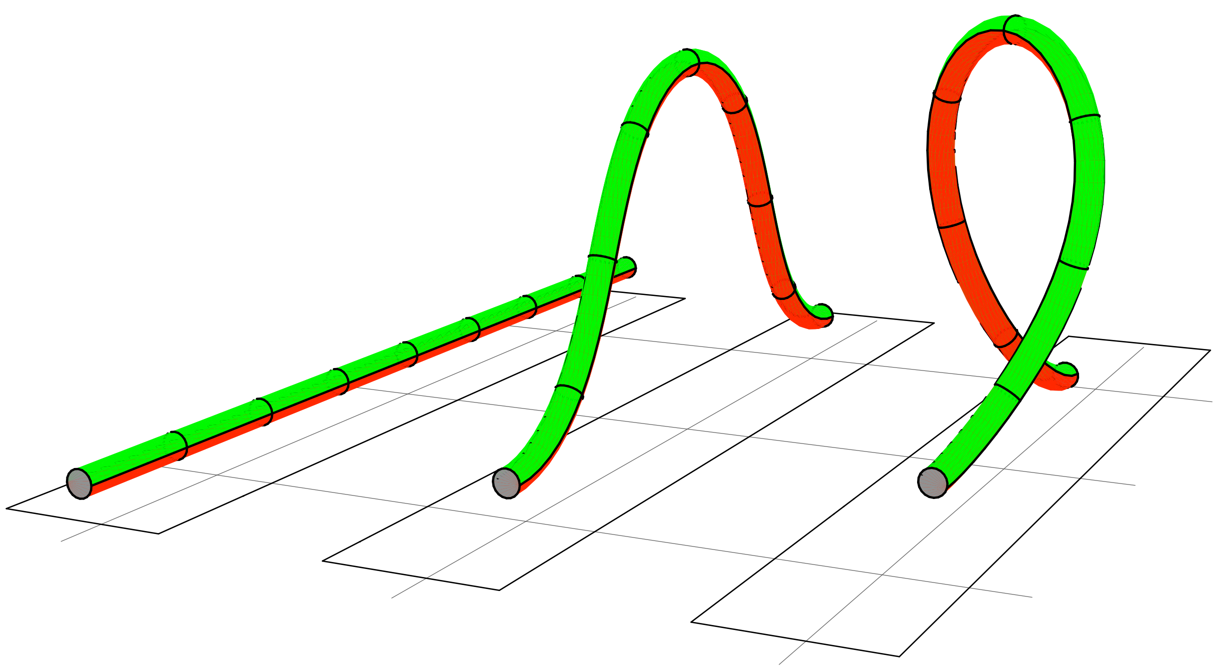


numerical simulations : M. Bergou, M. Wardetzky, S. Robinson, B. Audoly, and E. Grinspun.

ACM Transactions on Graphics (SIGGRAPH), 2008

Twisted rods : the ideal case

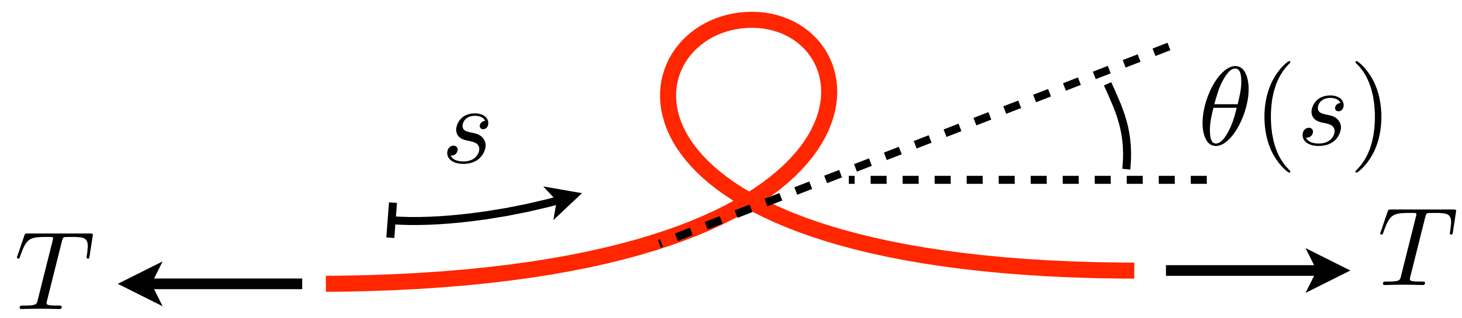
if rod is uniform, isotropic, naturally straight



system reduction
21 D => 6D

$$
\begin{aligned}
r' &= d_3 \\
d_3' &= (F \times r + M_0) \times d_3
\end{aligned}
$$

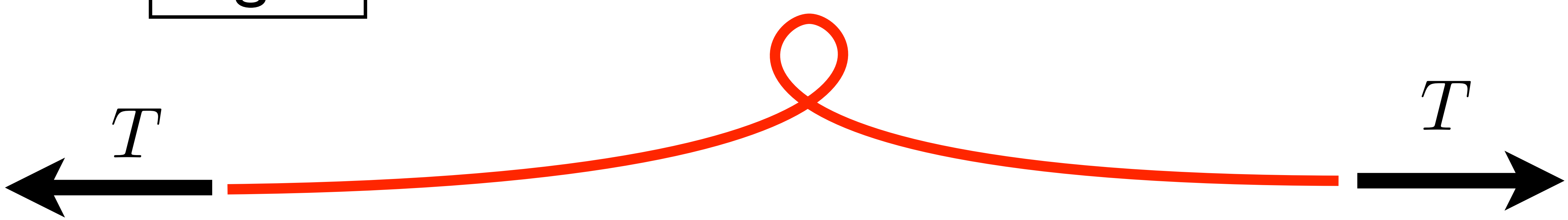
Planar Elastica



$$EI\theta'' = T \sin\theta$$

Planar Elastica

large T

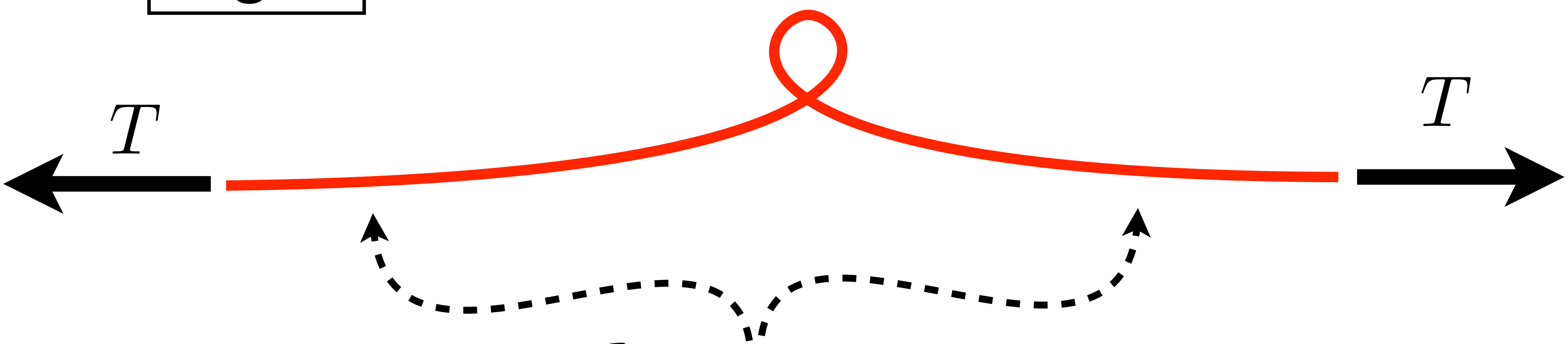


$$\frac{EI}{T}\,\theta'' = \sin\theta$$

singular perturbation

Planar Elastica

large T

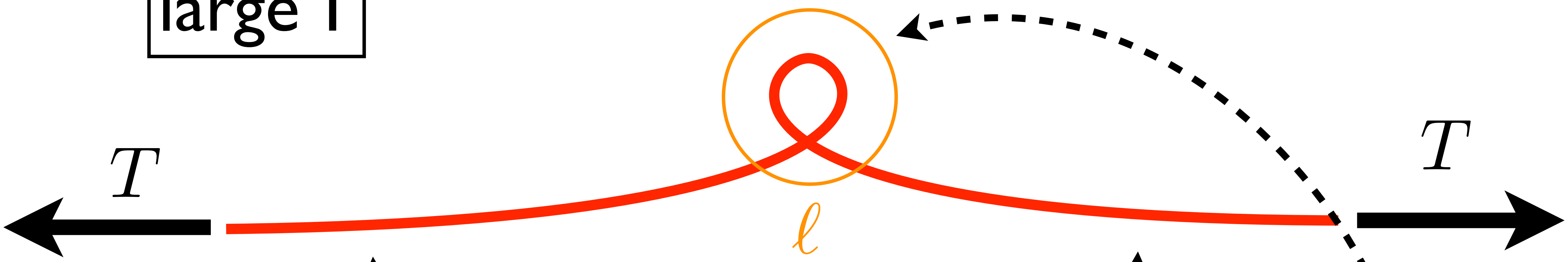


$$\frac{EI}{T}\,\theta'' = \sin\theta \quad \left\{ \begin{array}{l} \sin\theta \approx 0 \Rightarrow \theta(s) \approx 0 \\ \\ \end{array} \right.$$

singular perturbation

Planar Elastica

large T



$$\frac{EI}{T}\,\theta'' = \sin\theta \quad \begin{cases} \sin\theta \approx 0 \Rightarrow \theta(s) \approx 0 \\ \theta(s) \ \text{rapidly varying} \end{cases}$$

region size : $\ell \sim \sqrt{\frac{EI}{T}}$

singular perturbation → inner layer

Kirchhoff Equations

$$\begin{cases} \vec{F}' = -\vec{p} & \text{forces equil.} \\ \vec{M}' = \vec{F} \times \vec{t} & \text{moments equil.} \\ \vec{t}' = \frac{1}{EI}\, \vec{M} \times \vec{t} & \text{kinematics} \\ \vec{R}' = \vec{t} & \text{tangent def.} \end{cases}$$

$$' \equiv \frac{d}{ds}$$

constitutive relations:

$$M_\kappa = EI\,\kappa \qquad \text{curvature } \kappa$$

$$M_\tau = GJ\,\tau \qquad \text{twist } \tau$$

$\vec{p}(s)$ ext. pressure

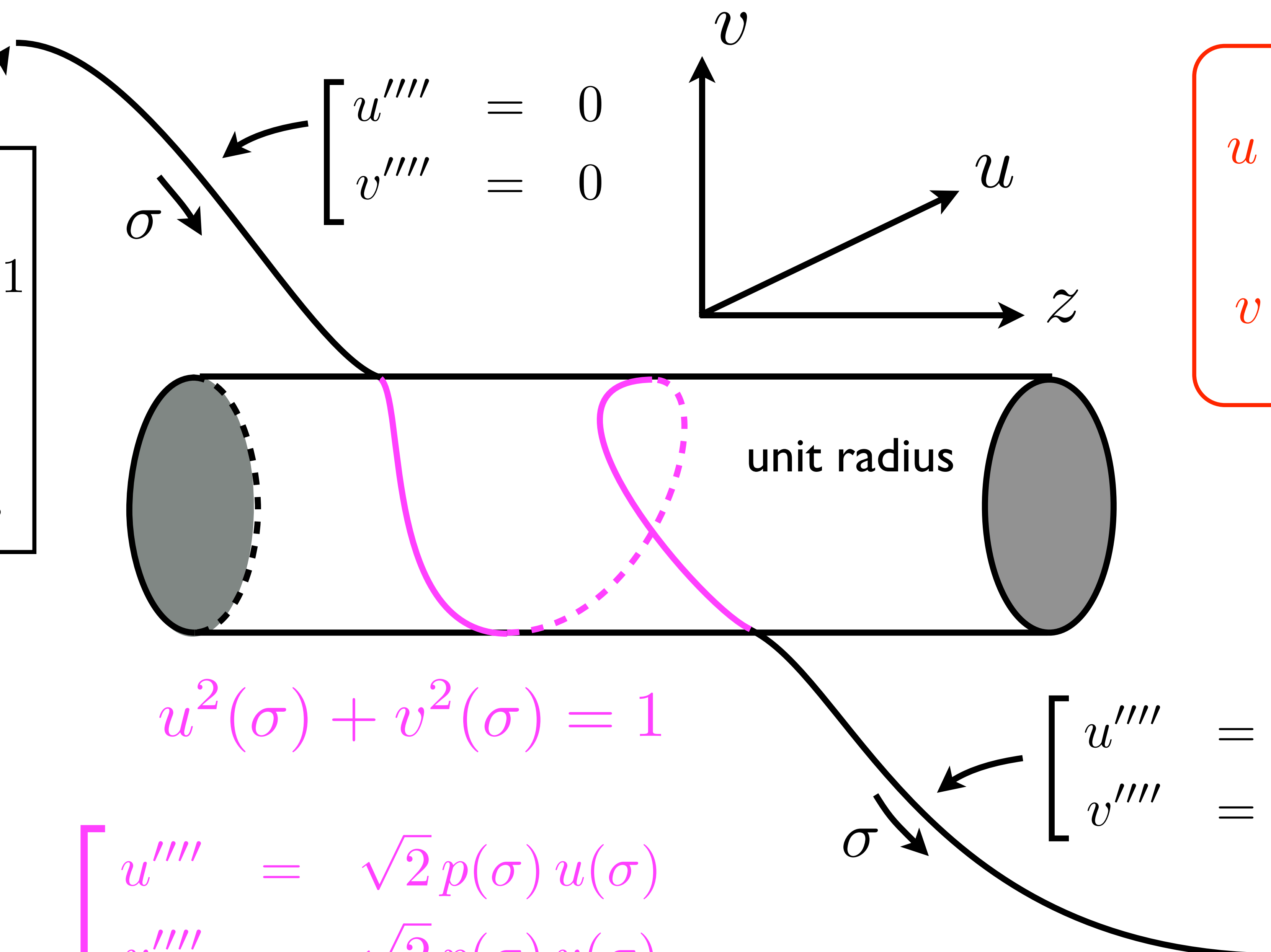
$\vec{M}(s)$ internal moment

$\vec{F}(s)$ internal force

$\vec{R}(s)$ position

$\vec{t}(s)$ tangent

Braid : boundary value problem (BVP)



$$\begin{aligned} u''(-\infty) &= 0 \\ v''(-\infty) &= +1 \\ u'''(-\infty) &= 0 \\ v'''(-\infty) &= 0 \end{aligned}$$

boundary conditions

$$\left[\begin{aligned} u'''' &= 0 \\ v'''' &= 0 \end{aligned}\right.$$

$$u = \frac{x^B - x^A}{\sqrt{2}}$$
$$v = \frac{y^B - y^A}{\sqrt{2}}$$

$$u^2(\sigma) + v^2(\sigma) = 1$$

$$\left[\begin{aligned} u'''' &= \sqrt{2}\, p(\sigma)\, u(\sigma) \\ v'''' &= \sqrt{2}\, p(\sigma)\, v(\sigma) \end{aligned}\right.$$

$$p(\sigma) = ?$$

$$\left[\begin{aligned} u'''' &= 0 \\ v'''' &= 0 \end{aligned}\right.$$

moments

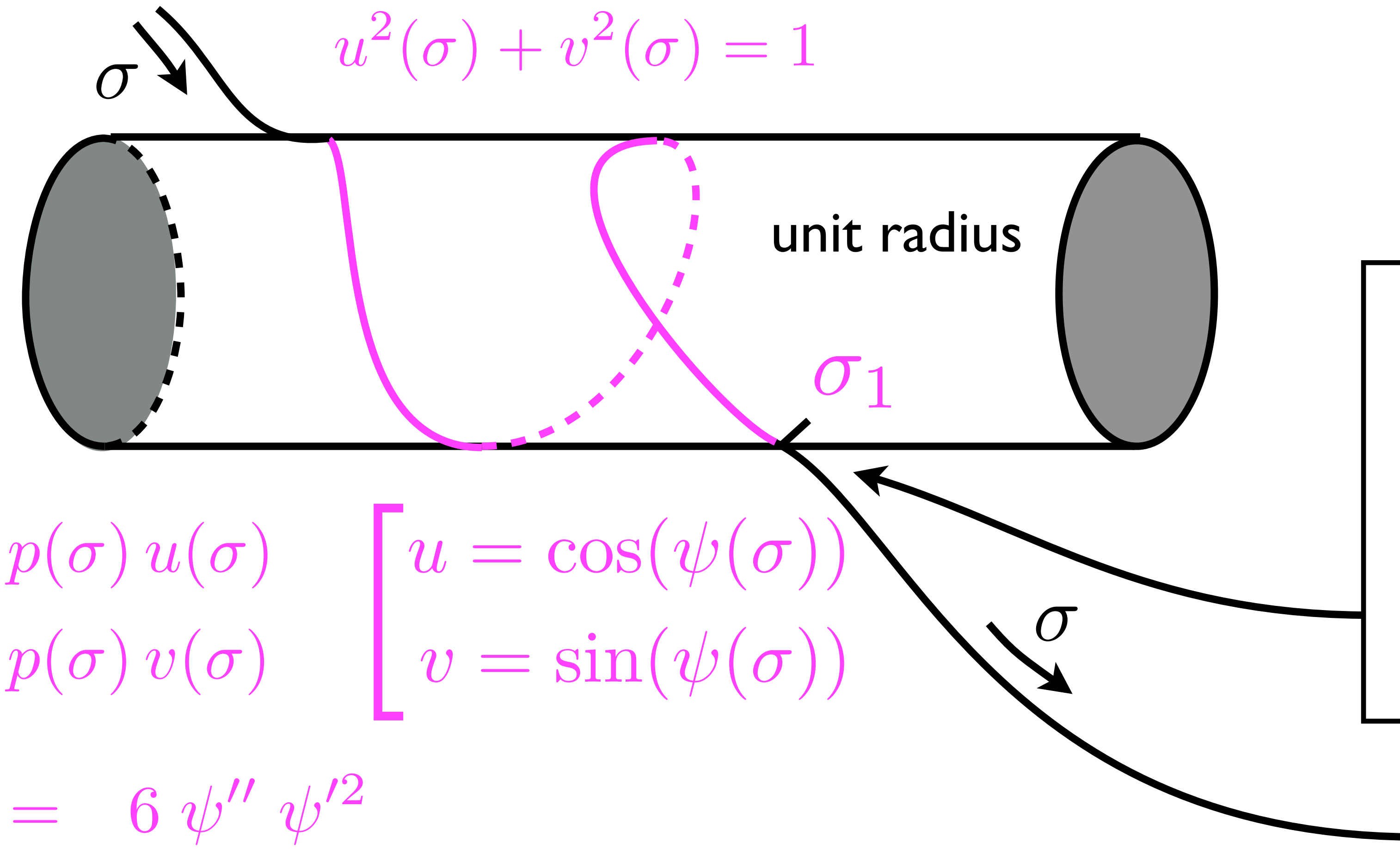
$$\begin{aligned} u''(+\infty) &= 0 \\ v''(+\infty) &= -1 \end{aligned}$$

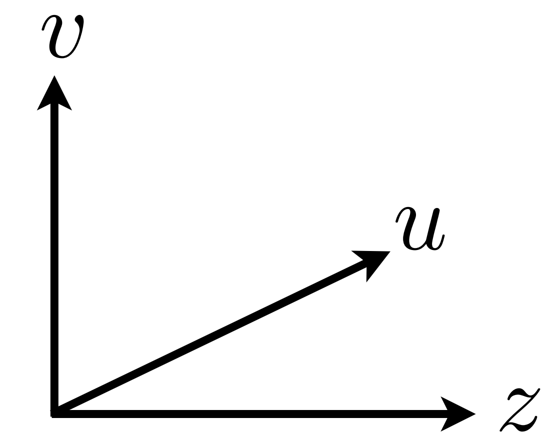
forces

$$\begin{aligned} u'''(+\infty) &= 0 \\ v'''(+\infty) &= 0 \end{aligned}$$

boundary conditions

Braid : first kind of solutions





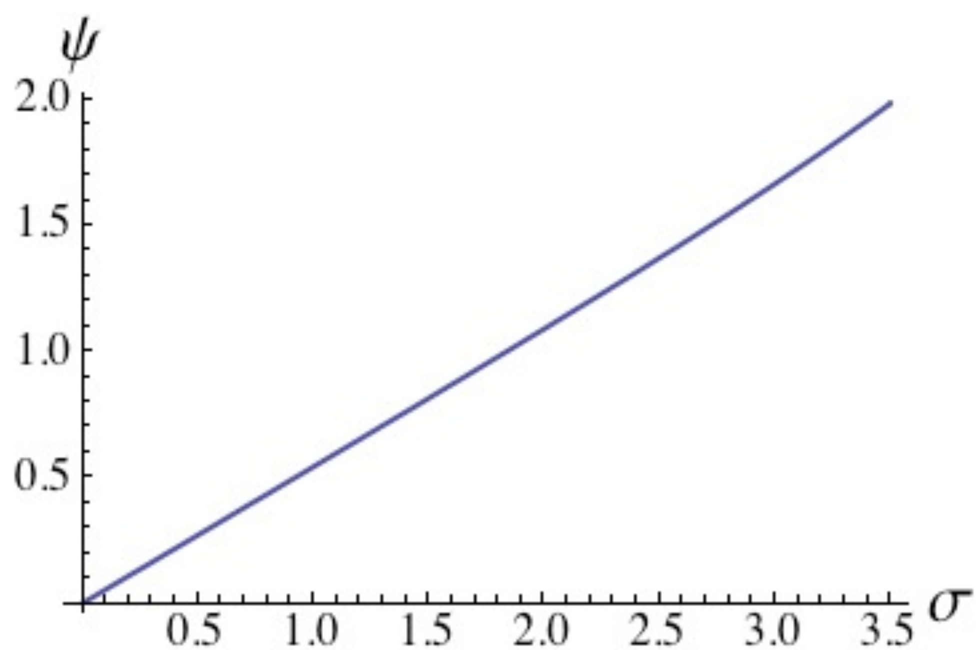
boundary conditions

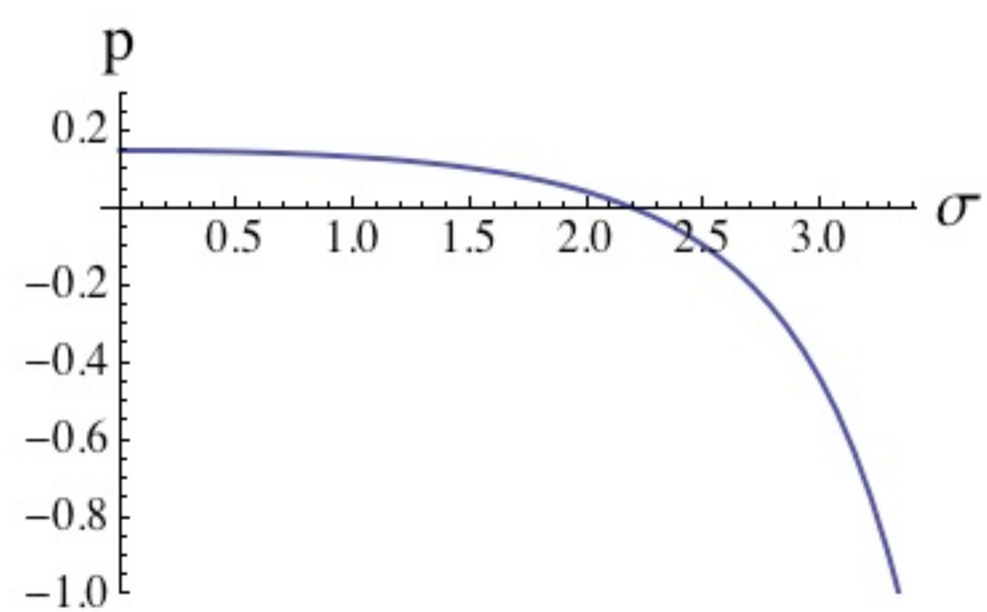
$$
\begin{aligned}
u''(\sigma_1) &= 0\\
v''(\sigma_1) &= -1\\
u'''(\sigma_1) &= 0\\
v'''(\sigma_1) &= 0
\end{aligned}
$$

$$
\left[\begin{aligned}
u'''' &= \sqrt{2}\,p(\sigma)\,u(\sigma)\\
v'''' &= \sqrt{2}\,p(\sigma)\,v(\sigma)
\end{aligned}\right.
\qquad
\left[\begin{aligned}
u &= \cos(\psi(\sigma))\\
v &= \sin(\psi(\sigma))
\end{aligned}\right.
$$

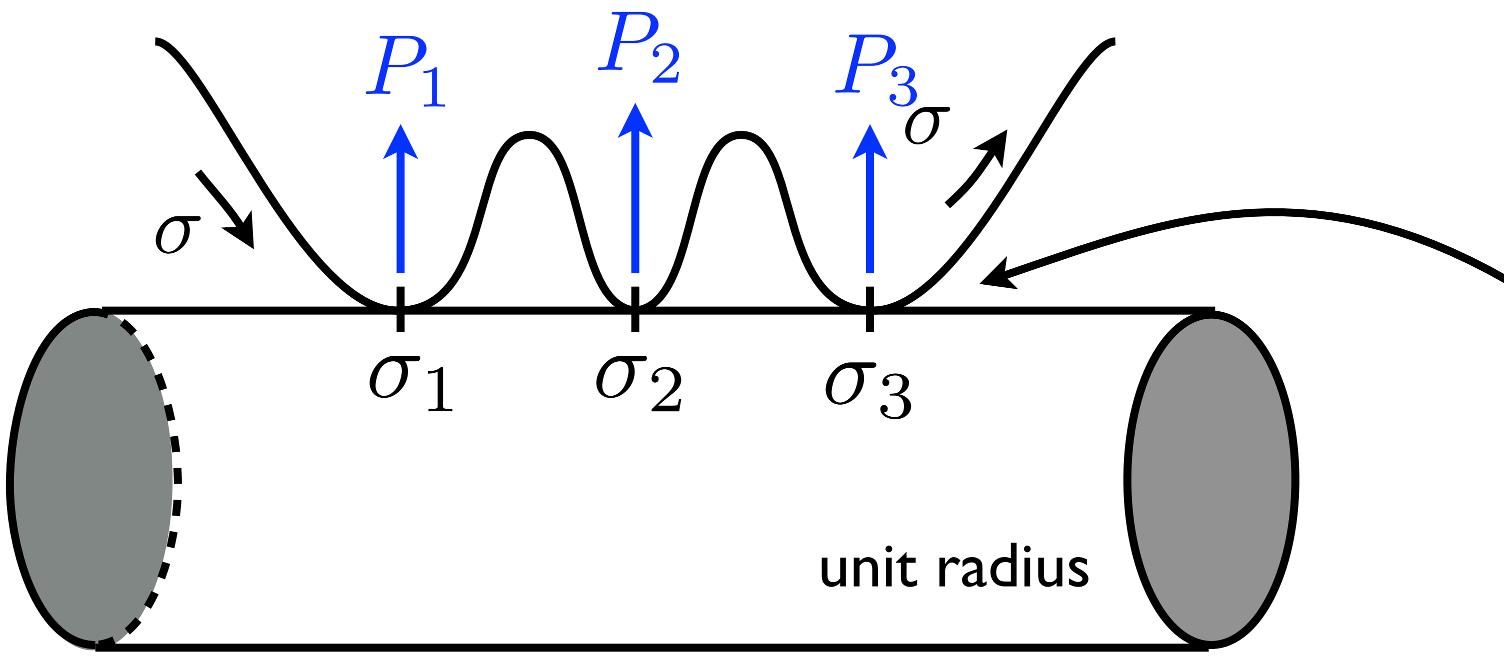
$$
\left\{\begin{aligned}
\psi'''' &= 6\,\psi''\,\psi'^2\\
p(\sigma) &= \left(\psi'^4 - 3\psi''^2 - 4\psi'\psi'''\right)/\sqrt{2}
\end{aligned}\right.
$$

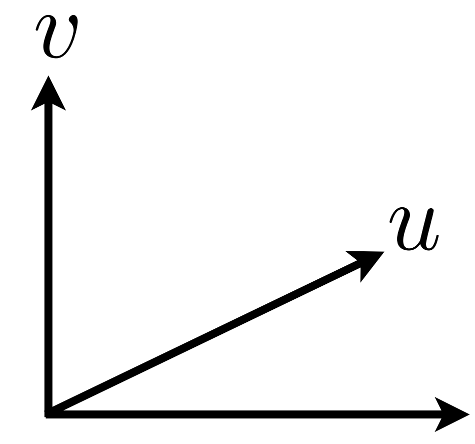
$$
\begin{aligned}
\psi(0) &= 0\\
\psi'(0) &= 0.54\\
\psi''(0) &= 0\\
\psi'''(0) &= 0.004\\
\sigma_1 &= 3.50
\end{aligned}
$$





Braid : second kind of solutions





boundary conditions

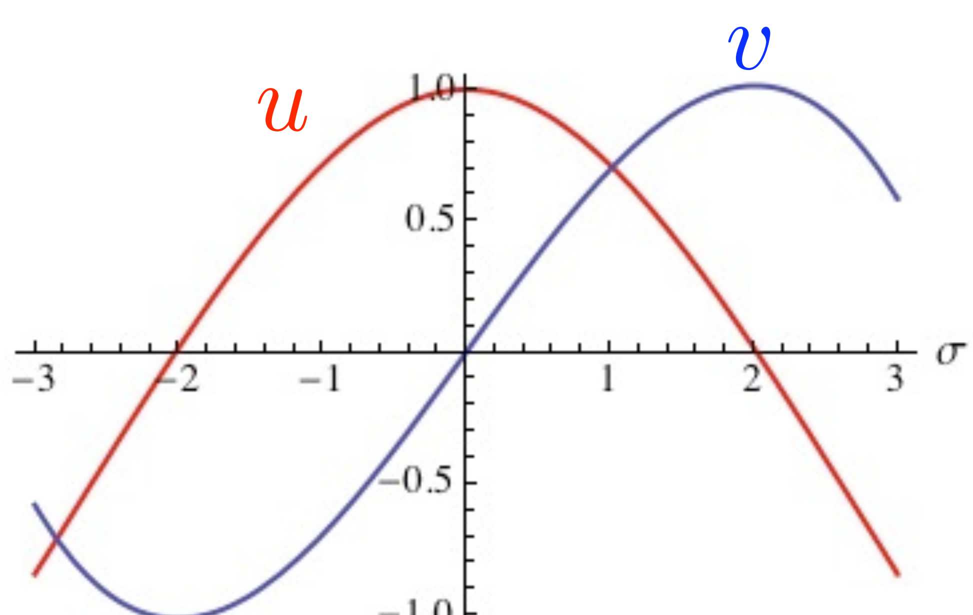
$$\begin{aligned} u''(+\sigma_3) &= 0 \\ v''(+\sigma_3) &= -1 \\ u'''(+\sigma_3) &= 0 \\ v'''(+\sigma_3) &= 0 \end{aligned}$$

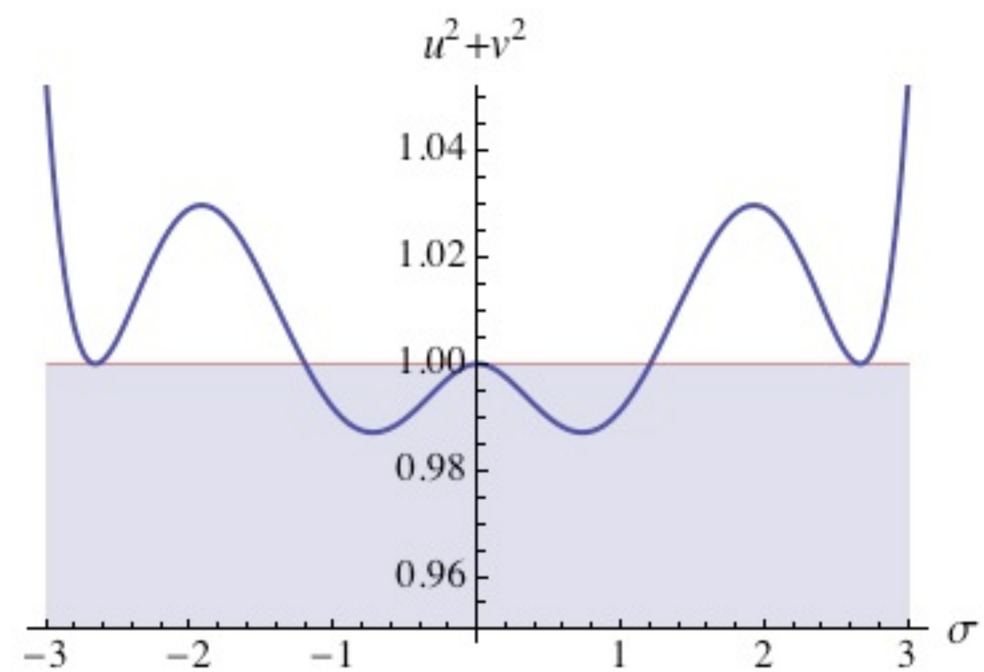
$$\begin{cases} u'''' &= \sqrt{2}\,p(\sigma)\,u(\sigma) \\ v'''' &= \sqrt{2}\,p(\sigma)\,v(\sigma) \end{cases}$$

avec $p(\sigma) = P_1\,\delta(\sigma-\sigma_1) + P_2\,\delta(\sigma-\sigma_2) + P_3\,\delta(\sigma-\sigma_3)$

$$\begin{aligned} u(0) &= 1 \\ u'(0) &= 0 \\ u''(0) &= -0.66 \\ u'''(0) &= 0.25 \end{aligned}$$

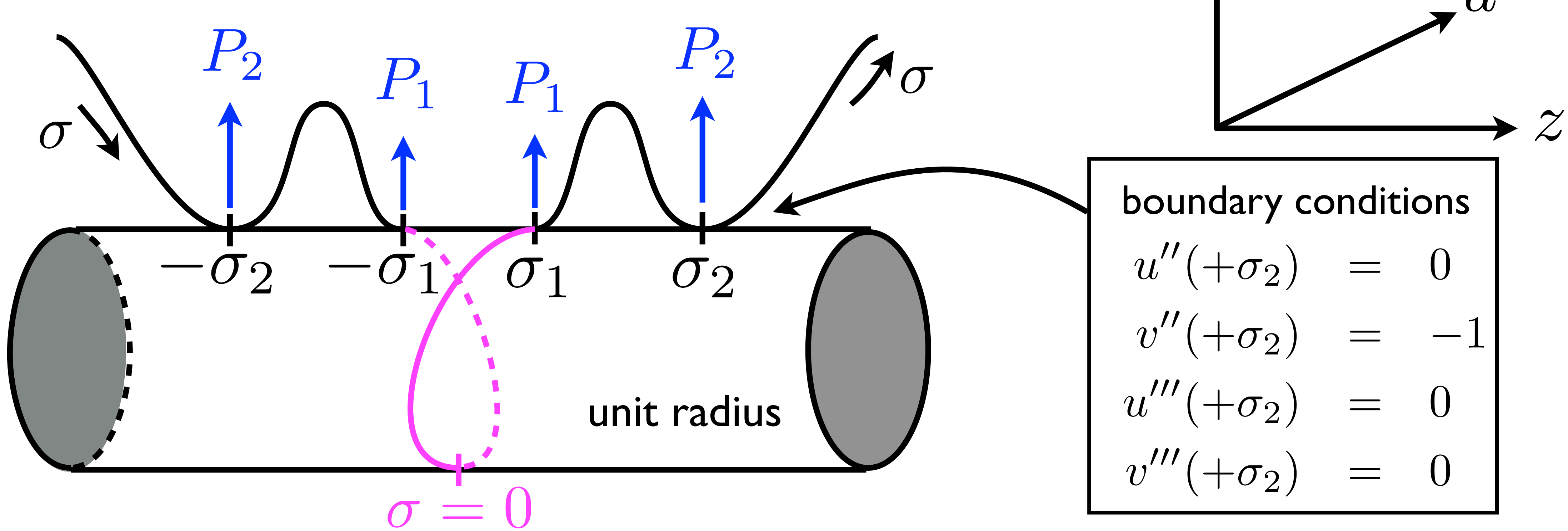
$$\begin{aligned} v(0) &= 0 \\ v'(0) &= 0.76 \\ v''(0) &= 0 \\ v'''(0) &= -0.38 \end{aligned}$$





$\sigma_3 = -\sigma_1 = 2.66$; $\sigma_2 = 0$; $P_1 = P_3 = 0.32$; $P_2 = 0.35$

Braid : third kind of solutions



$$\begin{aligned} \sigma_1 &= 0.35 \\ \sigma_2 &= 2.68 \\ P_1 &= 0.12 \\ P_2 &= 0.31 \end{aligned}$$