Elastic knots

(elastic beam under finite rotation and self-contact)

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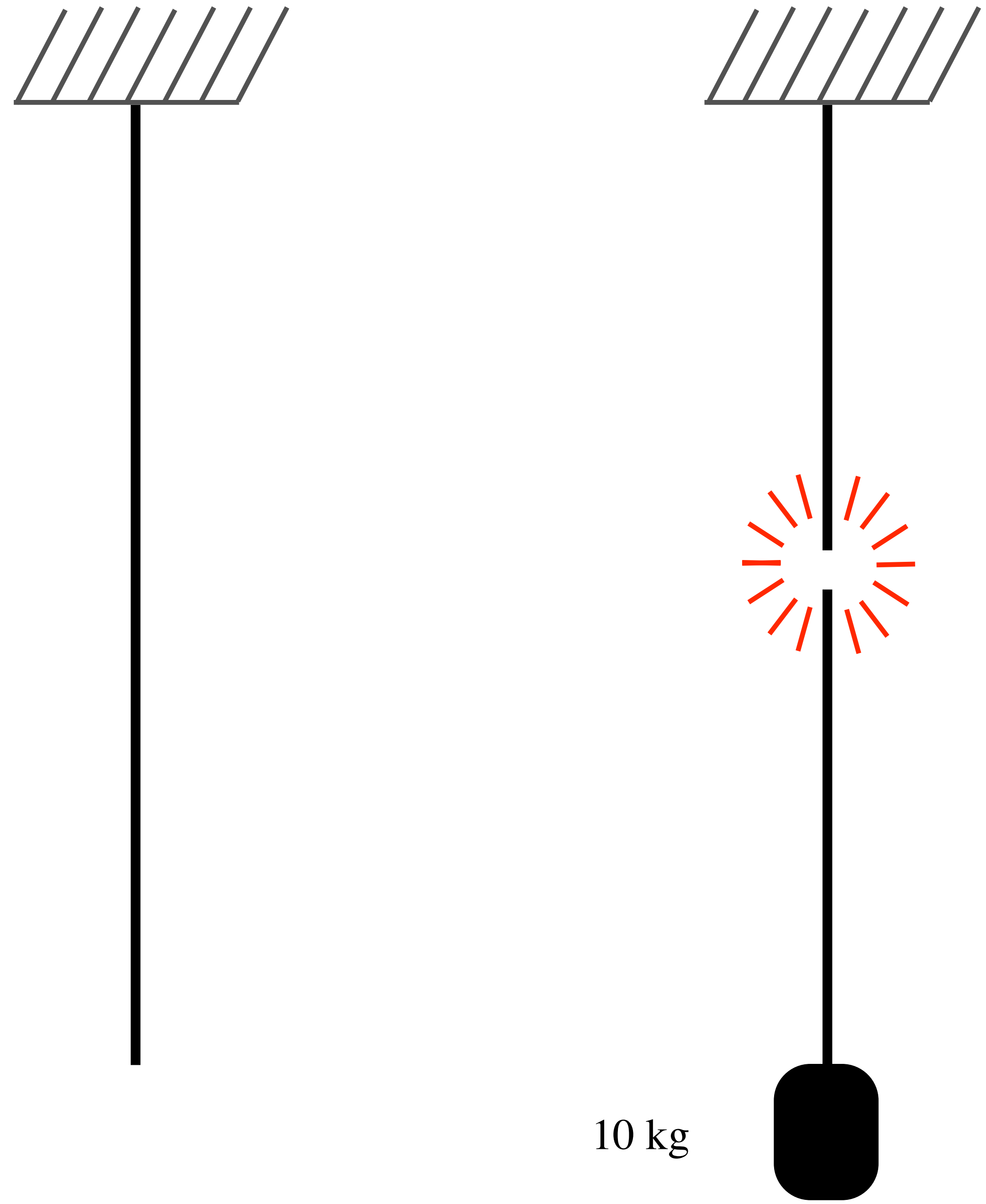
joint work with:
Nicolas Clauvelin (PhD work)
Basile Audoly

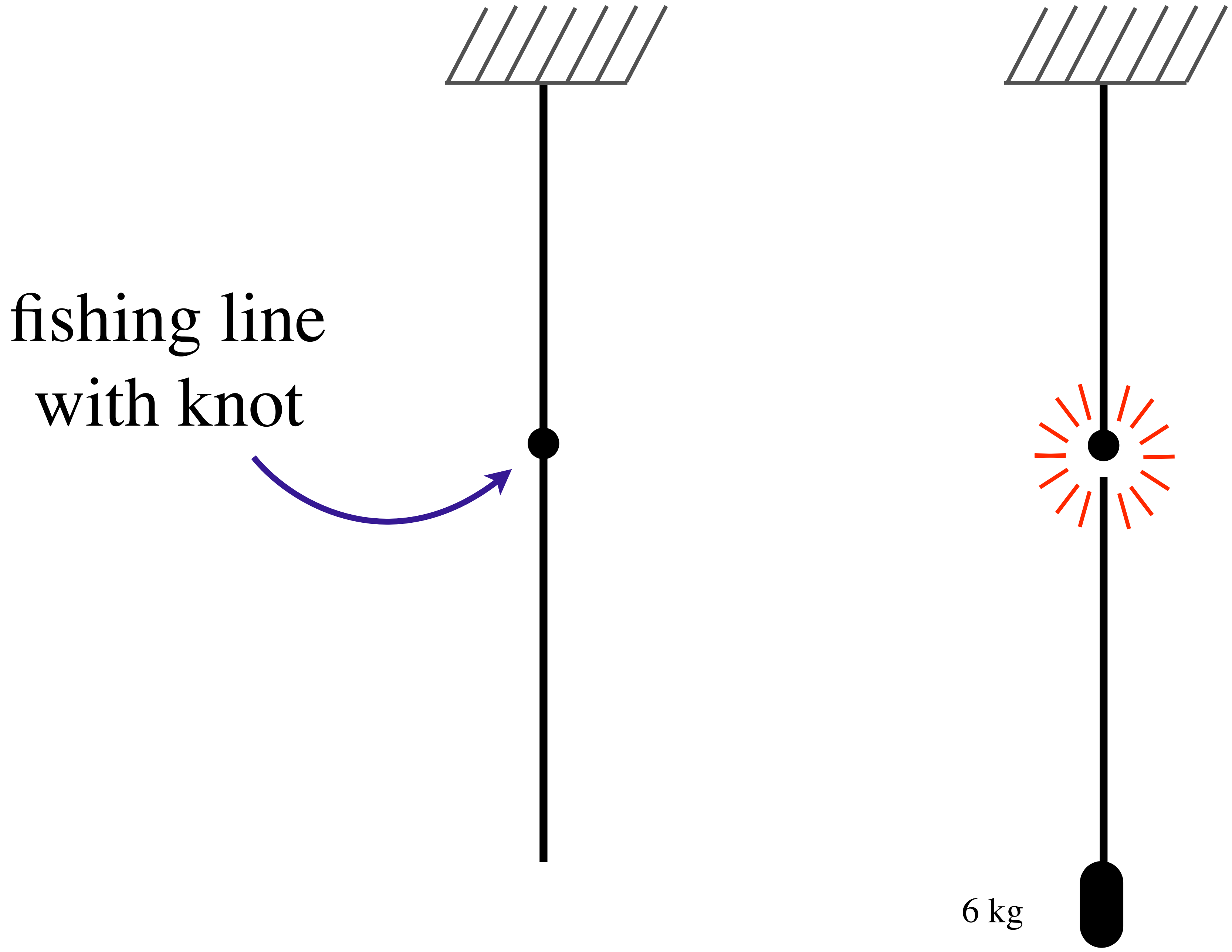
Tensile strength of a wire

fishing line



Stasiak et al, *Science* (1999)

Tensile strength of a wire



Stasiak et al, *Science* (1999)

Knots are everywhere

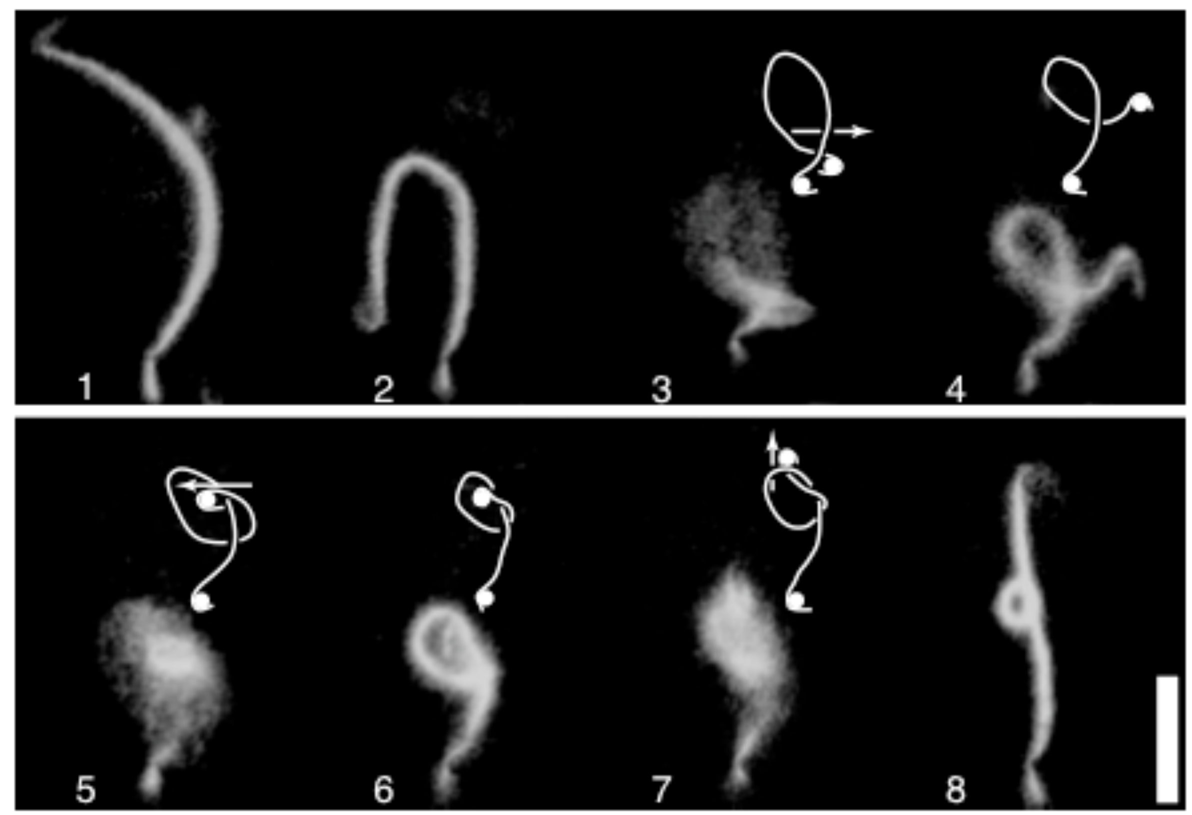
Long enough polymers are (almost) certainly knotted

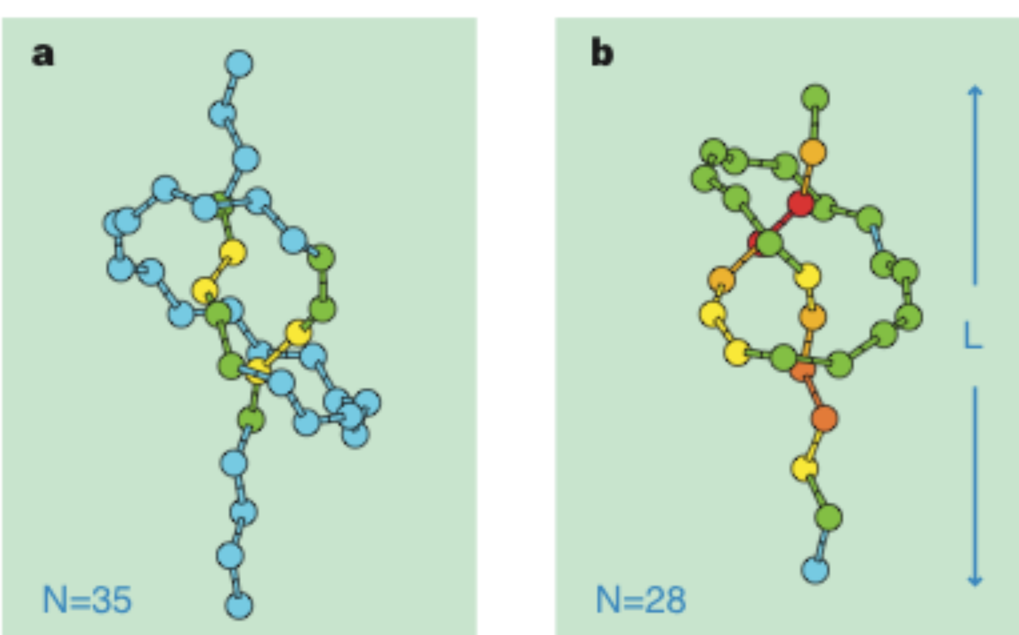
Sumners+Whittington, J. Phys. A : Math. Gen. 1988

273 knotted proteins in the ProteinDataBank (1%)

Single molecule experiment with knotted F-Actin filaments

Arai et al, *Nature* (1999)

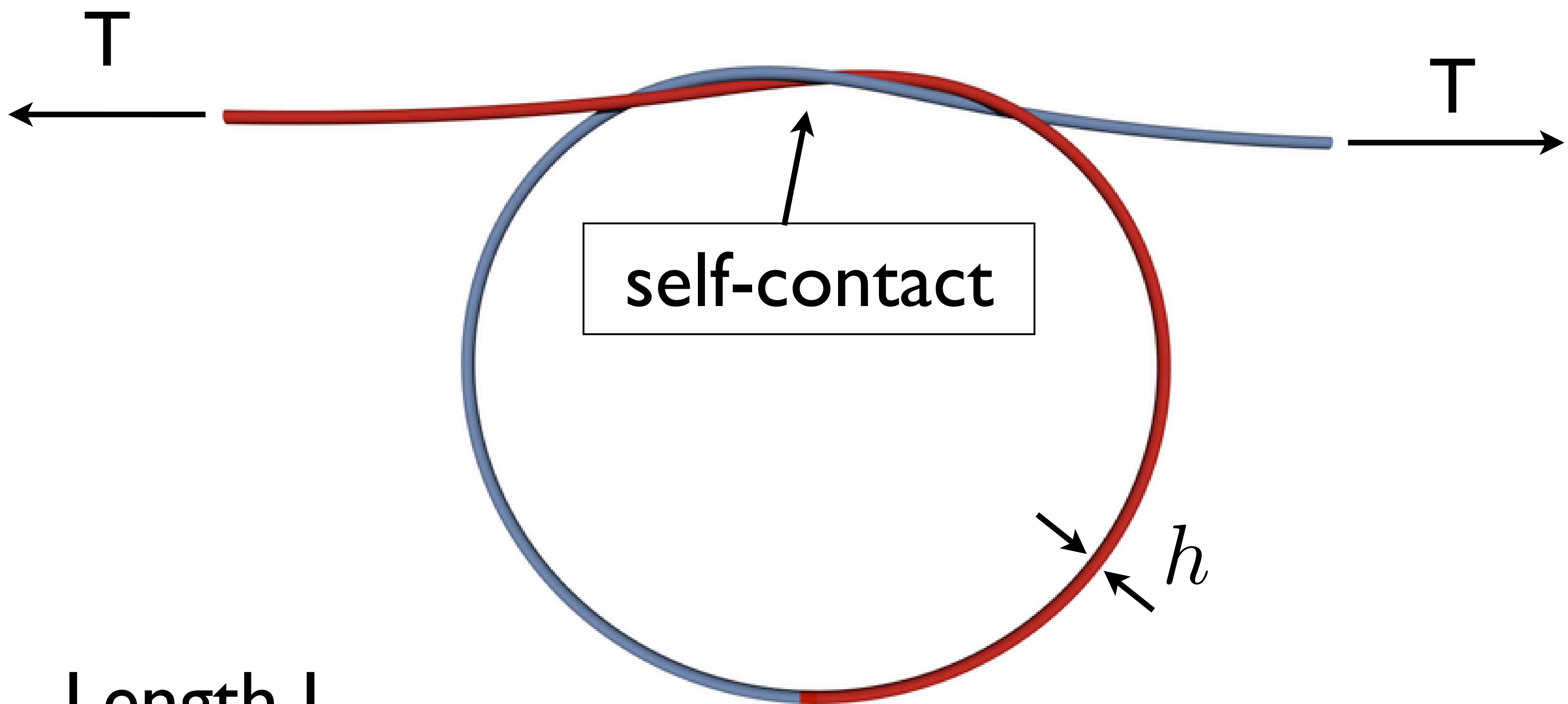




Ab-initio molecular simulations for alcane molecule (C10H22)

Saitta et al, *Nature* (1999)

Elastic knots



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

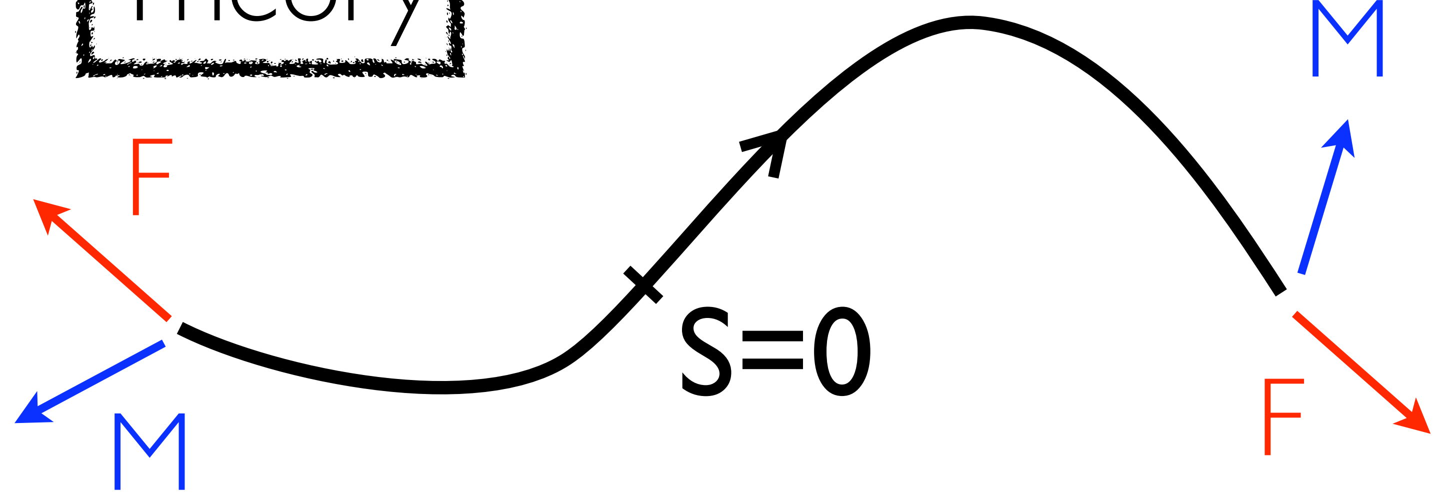
$$I = \frac{\pi h^4}{4}$$

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

E : Young's modulus G : shear modulus

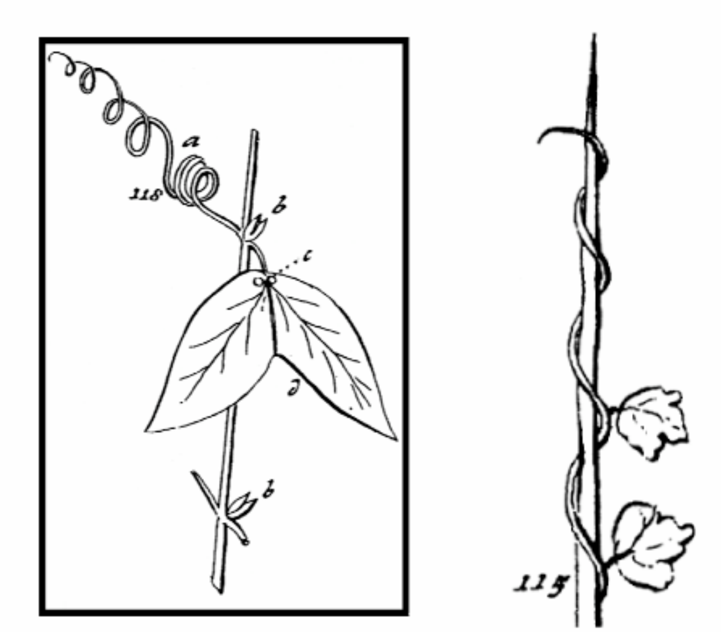
Elastic filaments

Theory

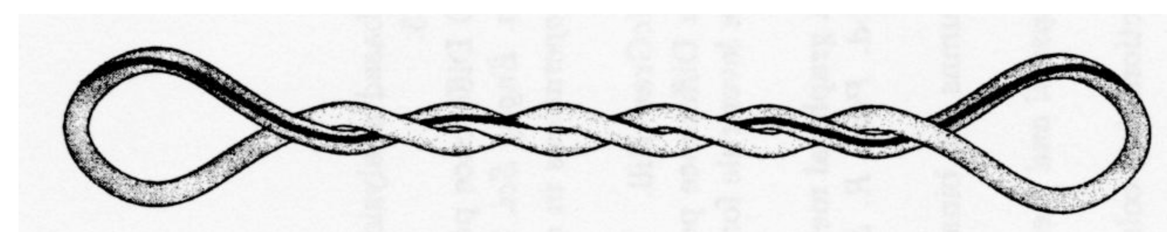


Applications

climbing plants

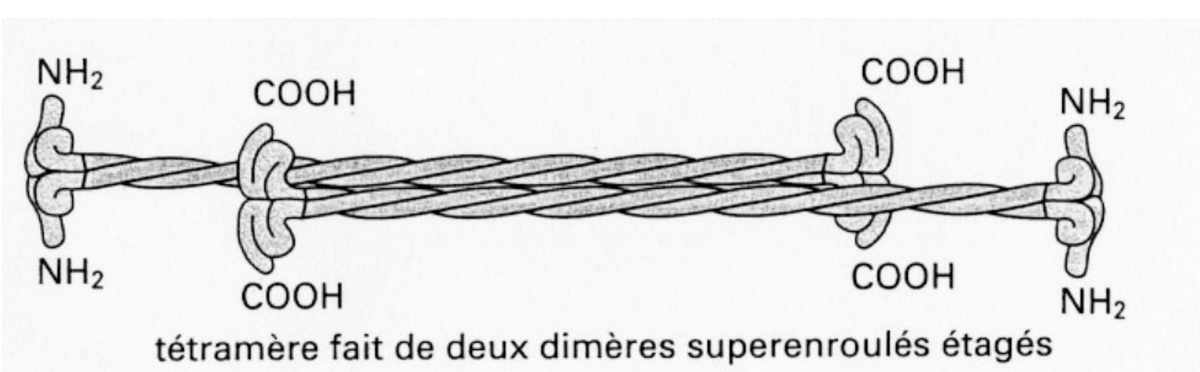


DNA supercoiling

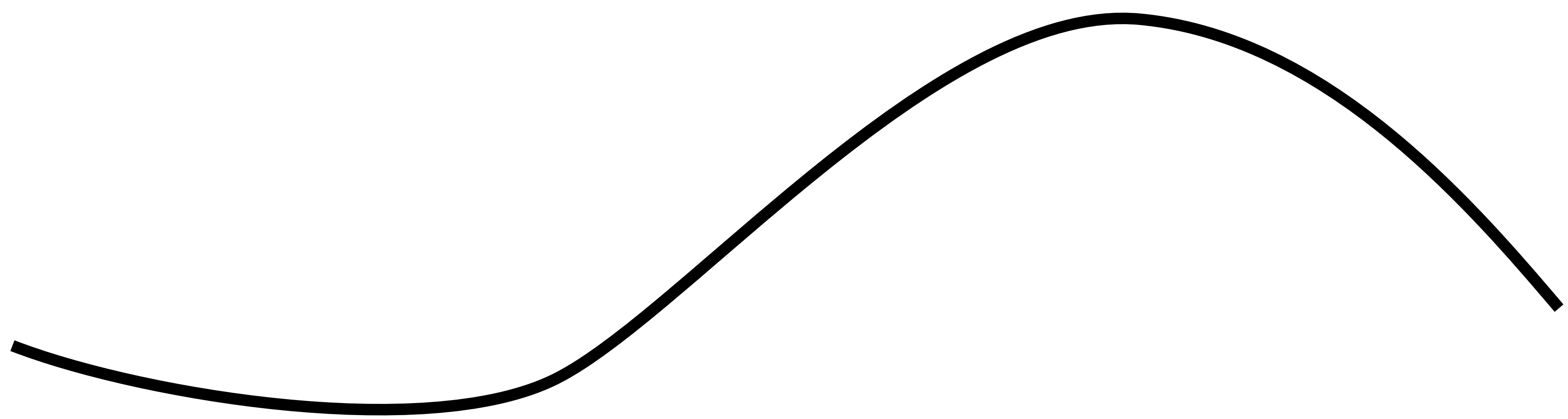


cables

fibrous proteins

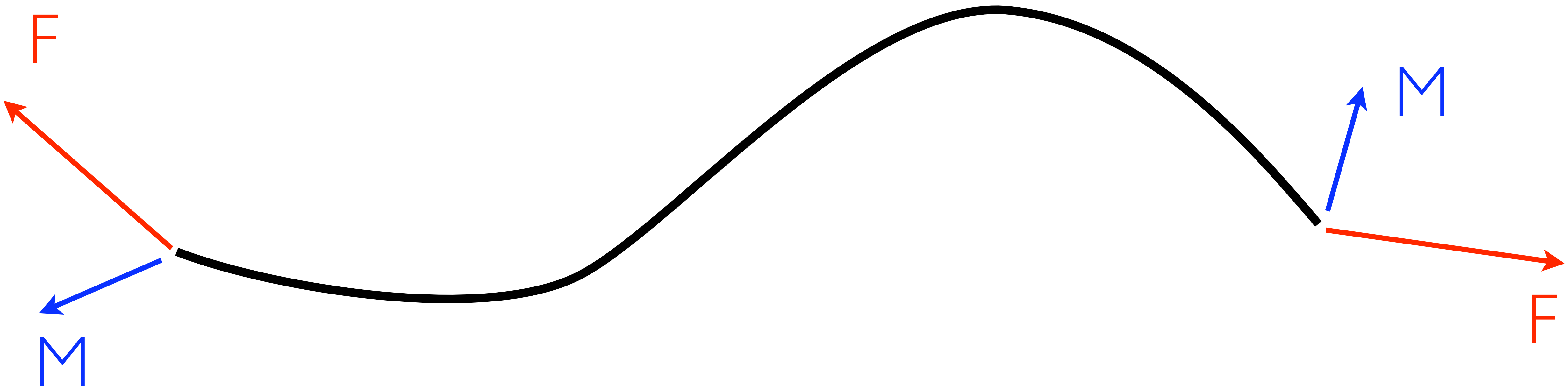


Kirchhoff equations

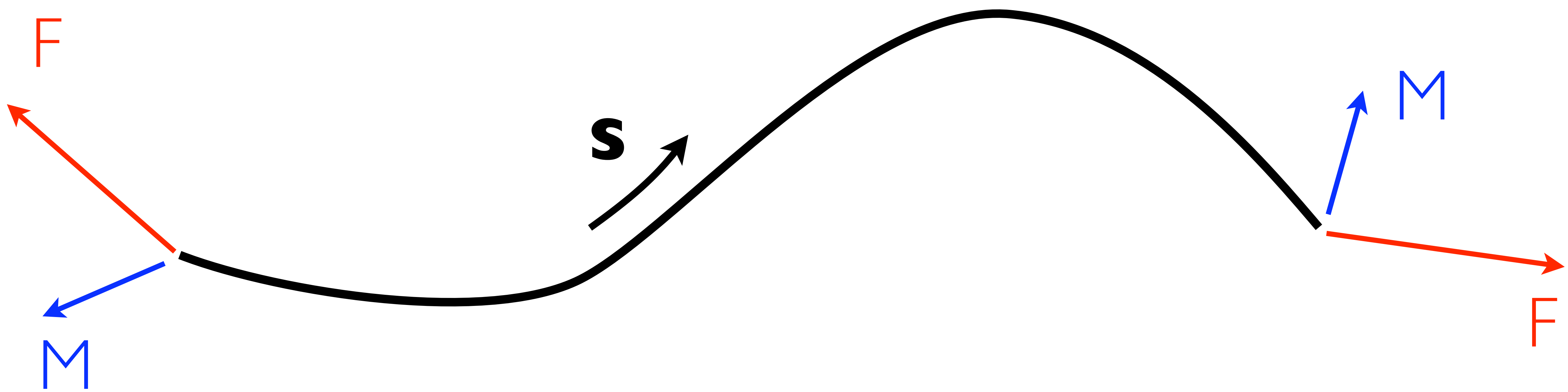


apply to :
- slender bodies
- not too bent

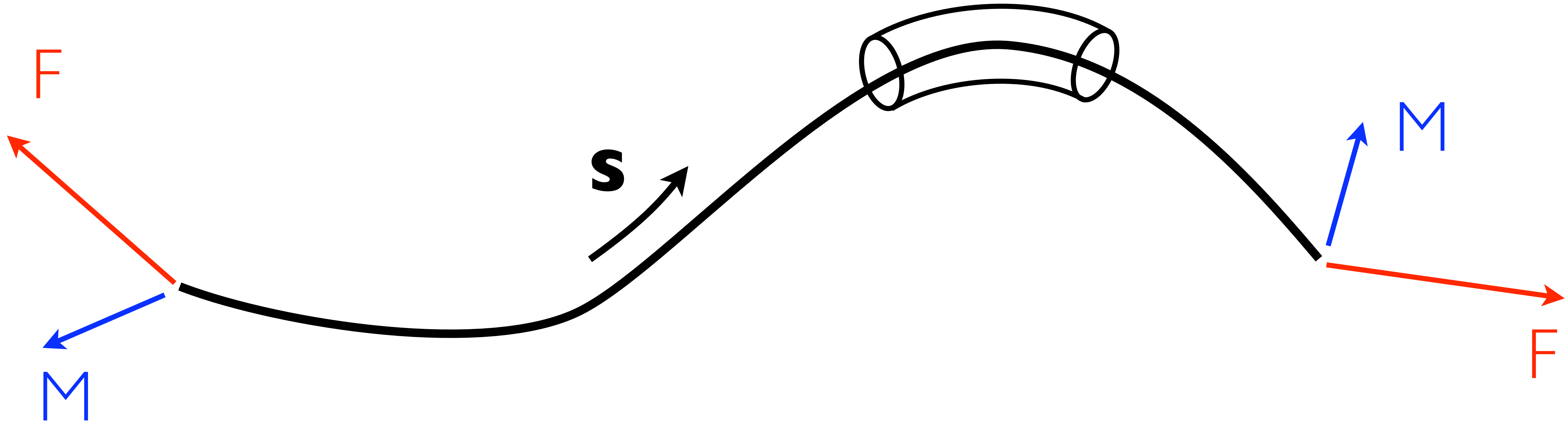
Kirchhoff equations



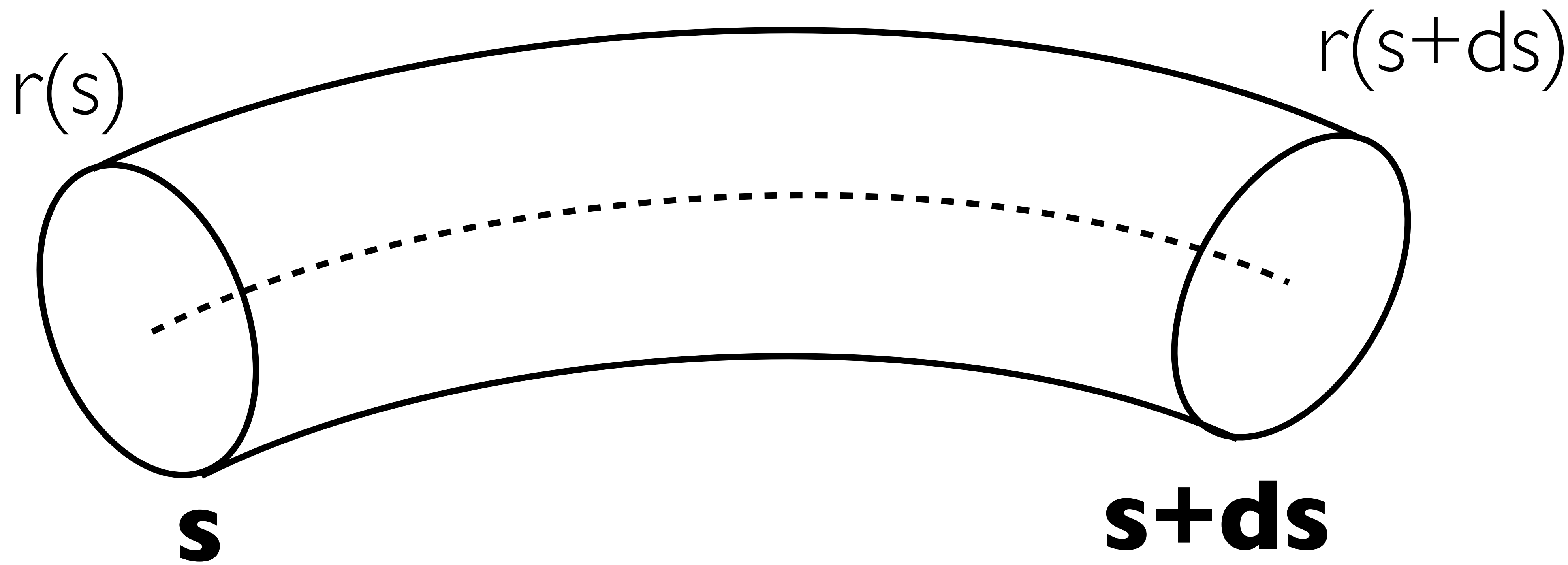
Kirchhoff equations



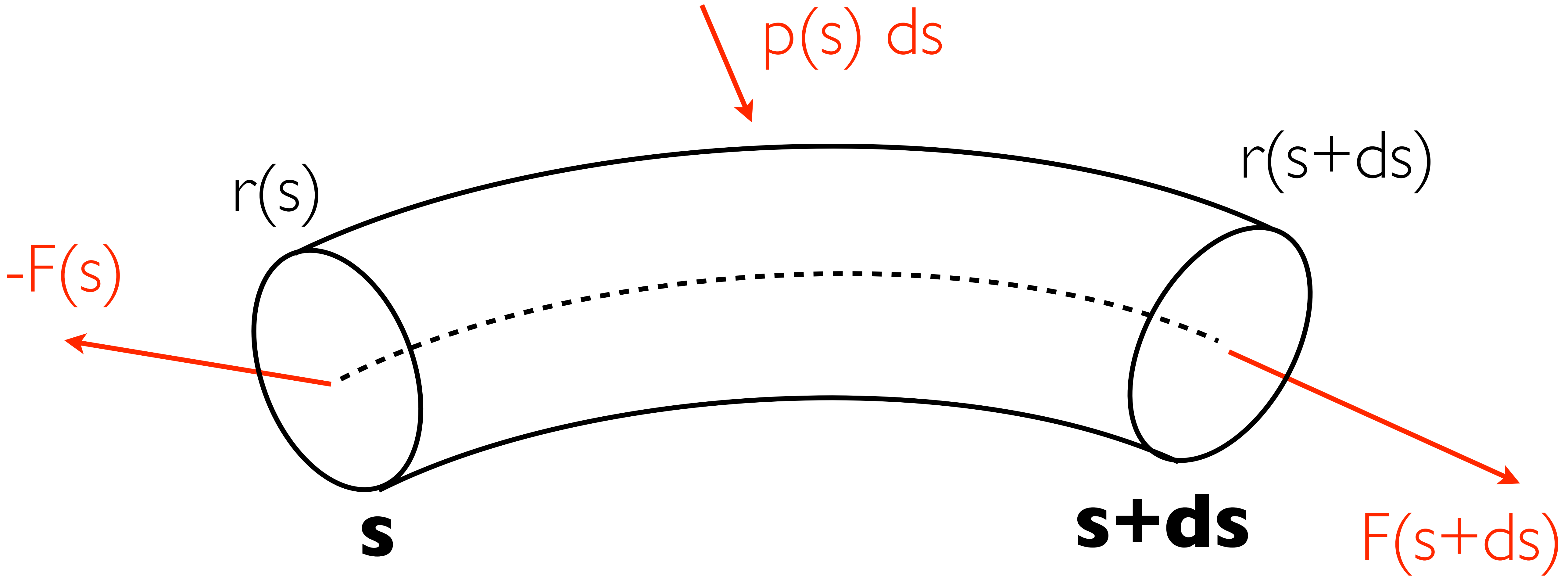
Kirchhoff equations



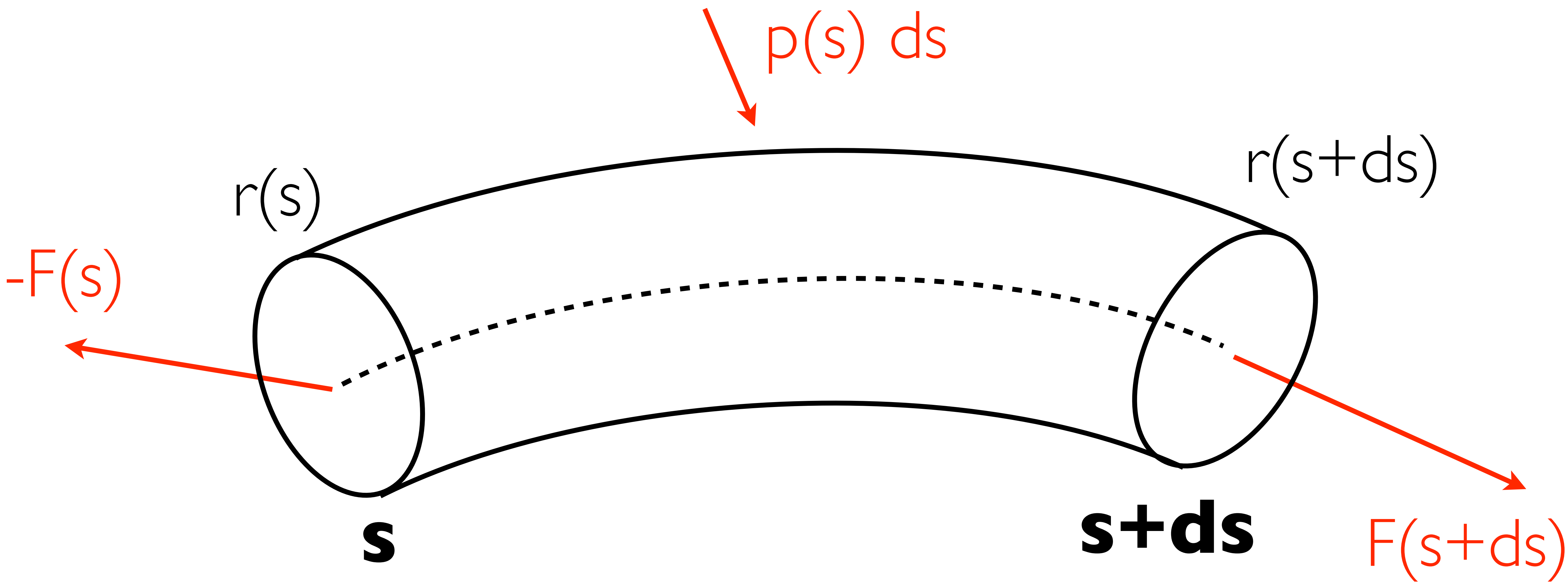
Kirchhoff equations



Kirchhoff equations



Kirchhoff equations

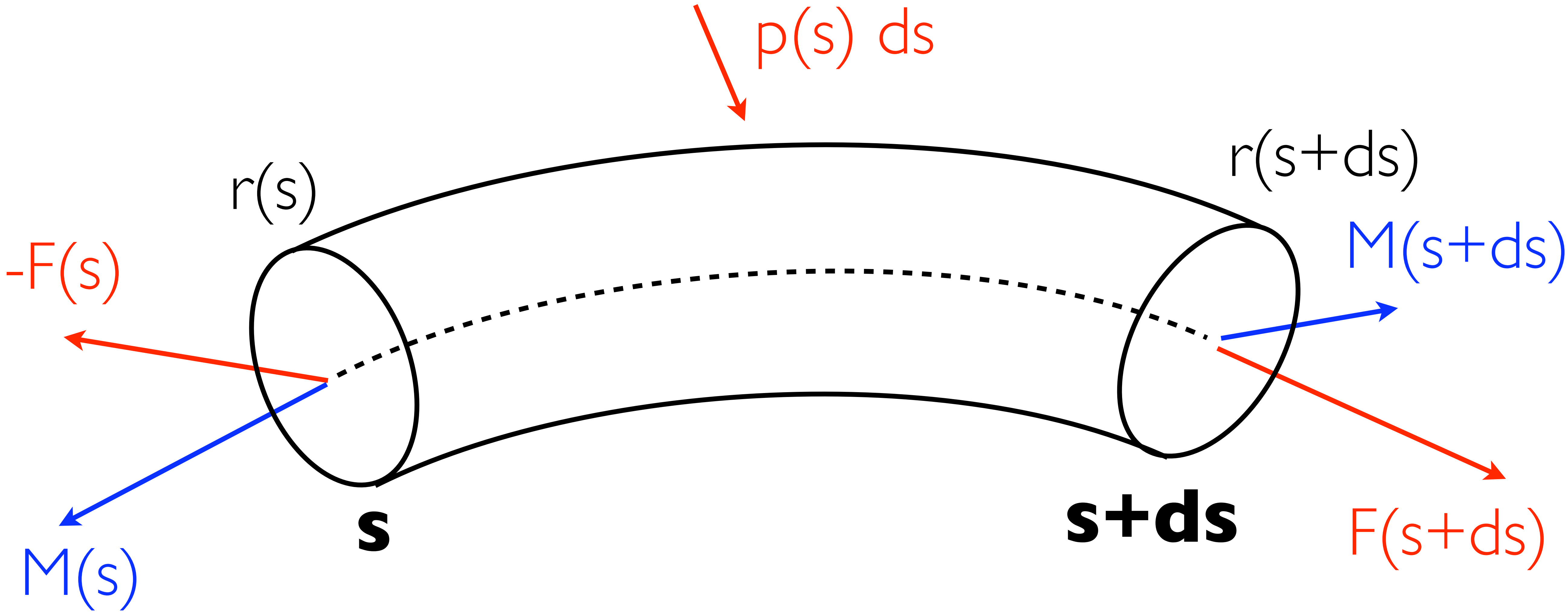


$$F(s+ds) - F(s) + p(s)\, ds = 0$$

Equilibrium

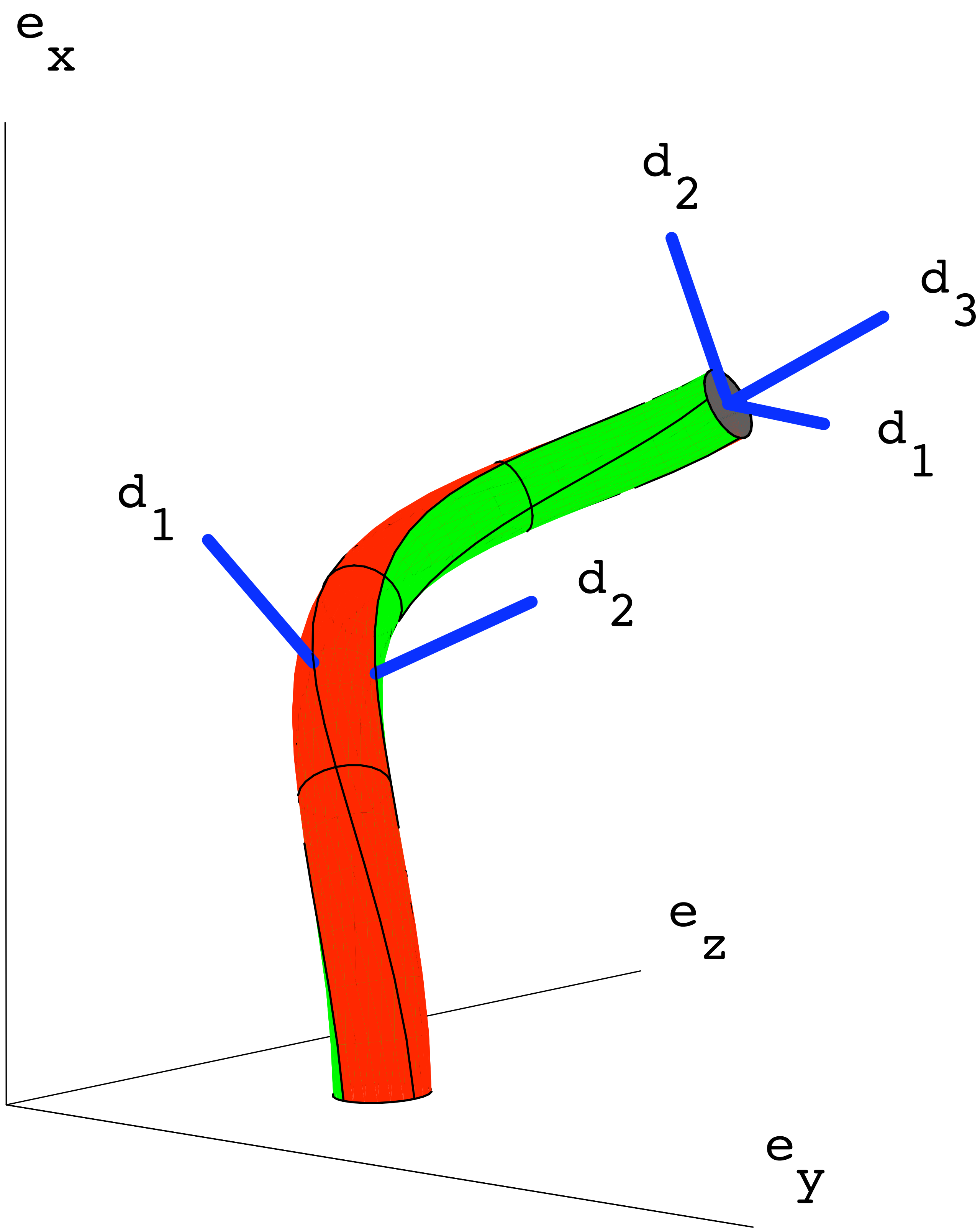
$$F'(s) + p(s) = 0$$

Kirchhoff equations



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

Kirchhoff equations



Cosserat frame

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

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

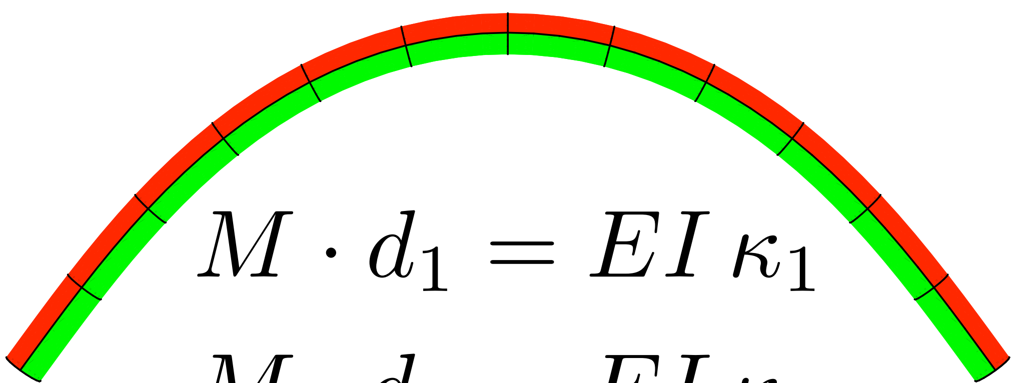
curvatures

twist

Kirchhoff equations

constitutive relations

curvature



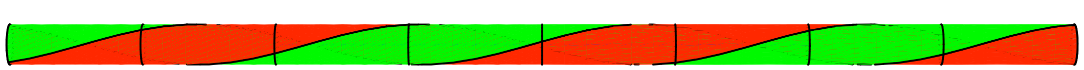
$$M \cdot d_1 = EI\,\kappa_1$$

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

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

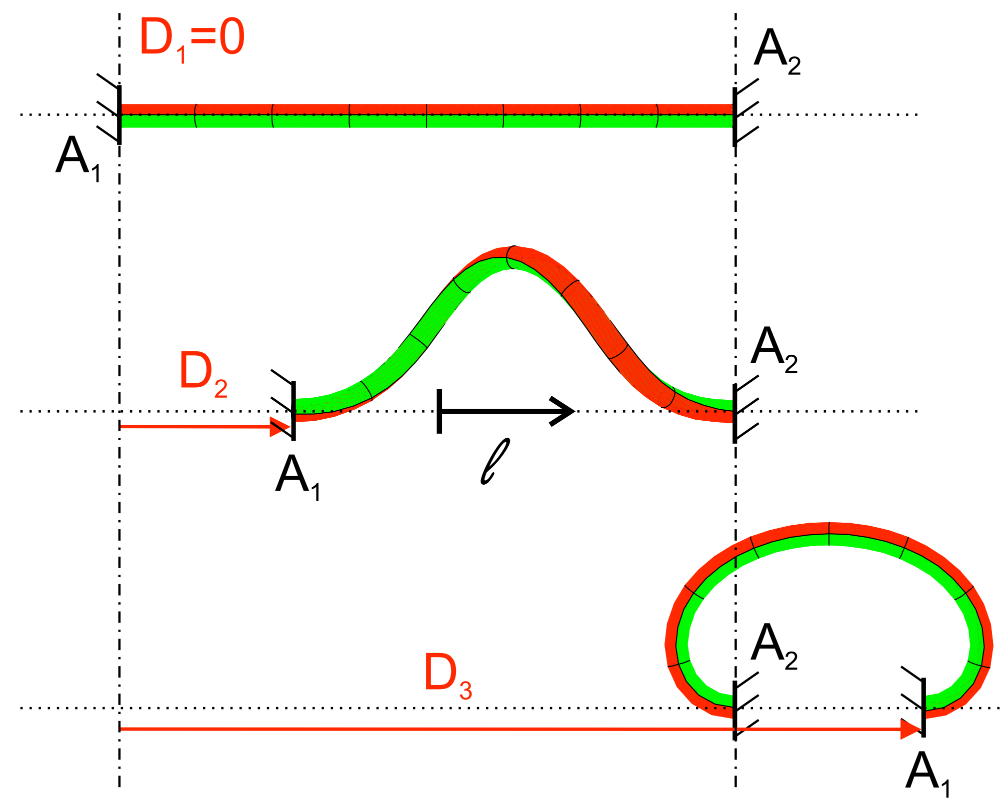
21 unknowns

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

$i=1,2,3$

boundary conditions

- how the rod is held
- few solutions are admissibles

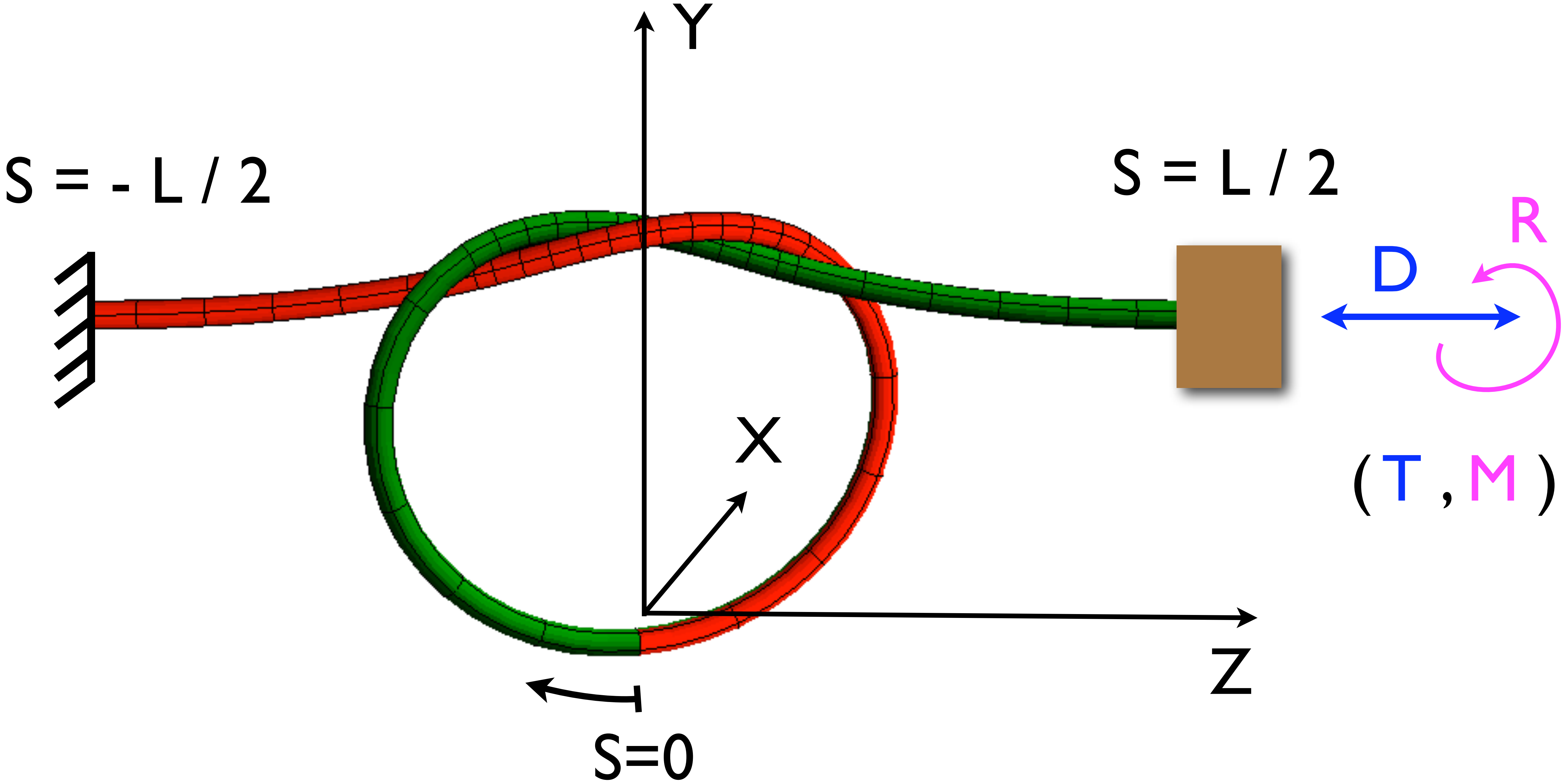


$$\vec{d}_3(A_1)=\vec{d}_3(A_2)$$

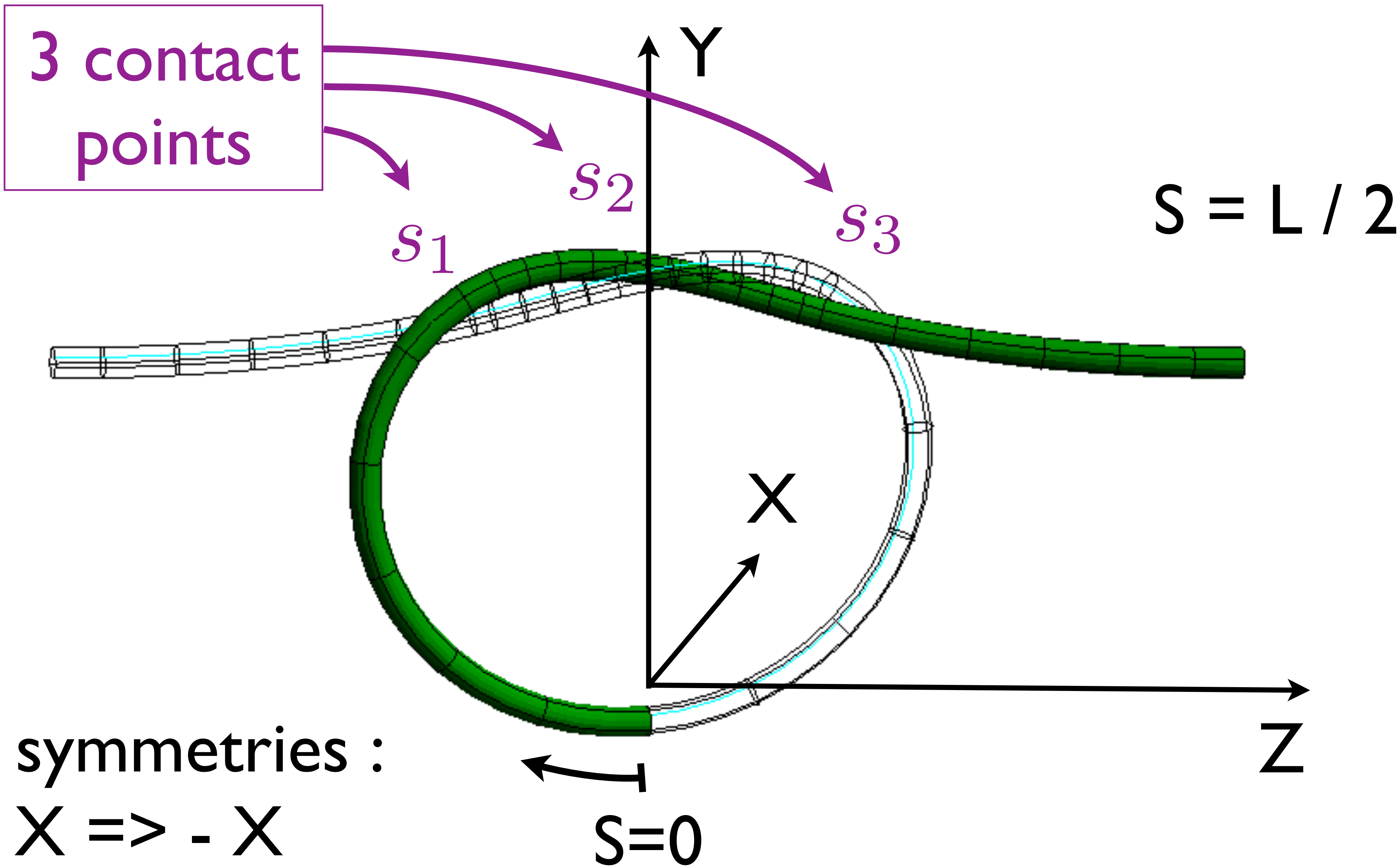
$$\vec{r}(A_2)-\vec{r}(A_1)=k\,\vec{d}_3(A_2)$$

$$(D=L-k)$$

Boundary value problem



Boundary value problem



symmetries :

X => - X

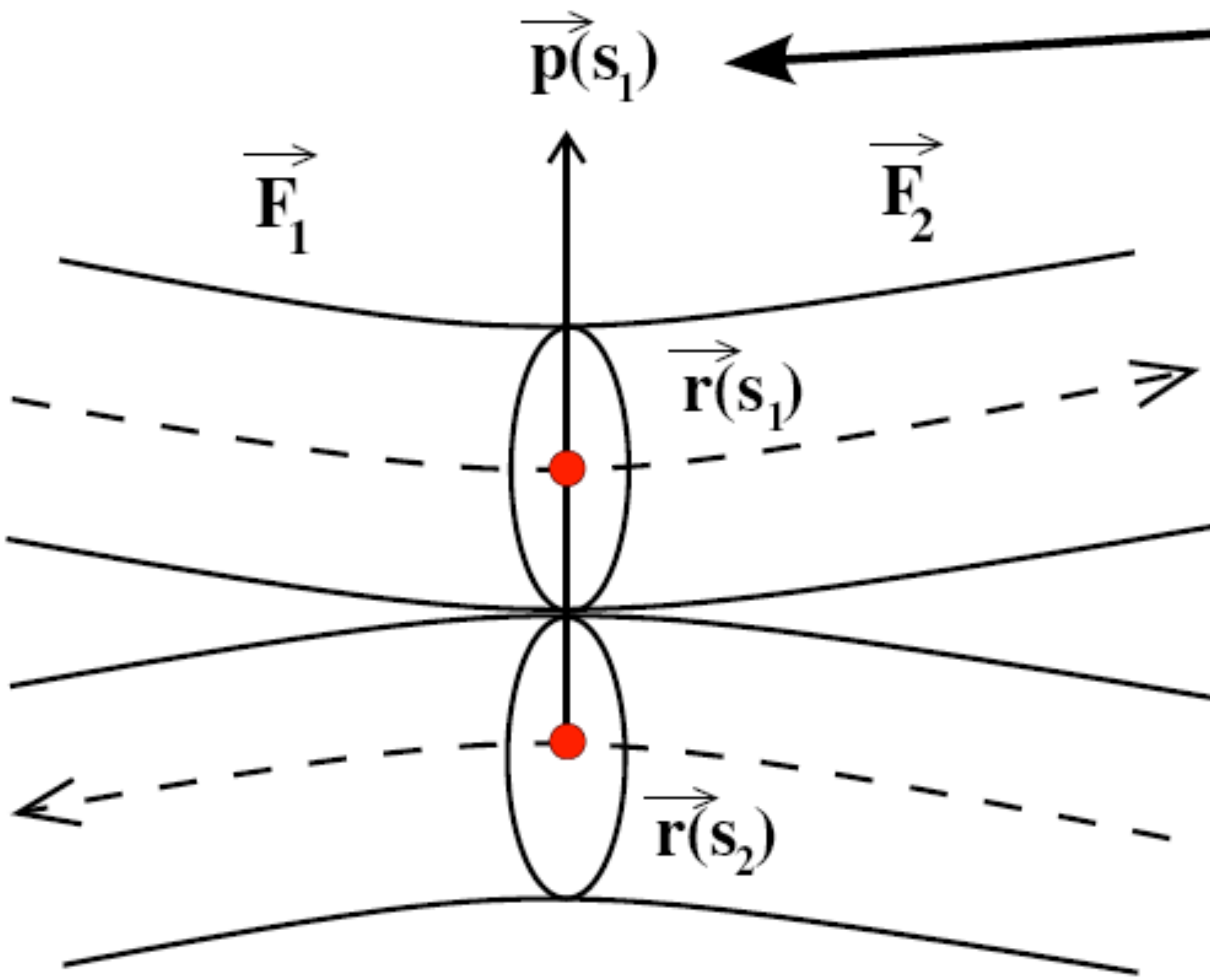
Y => Y

Z => - Z

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

Hard-wall contact, no friction

force from strand at s_2 acting on strand at s_1



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

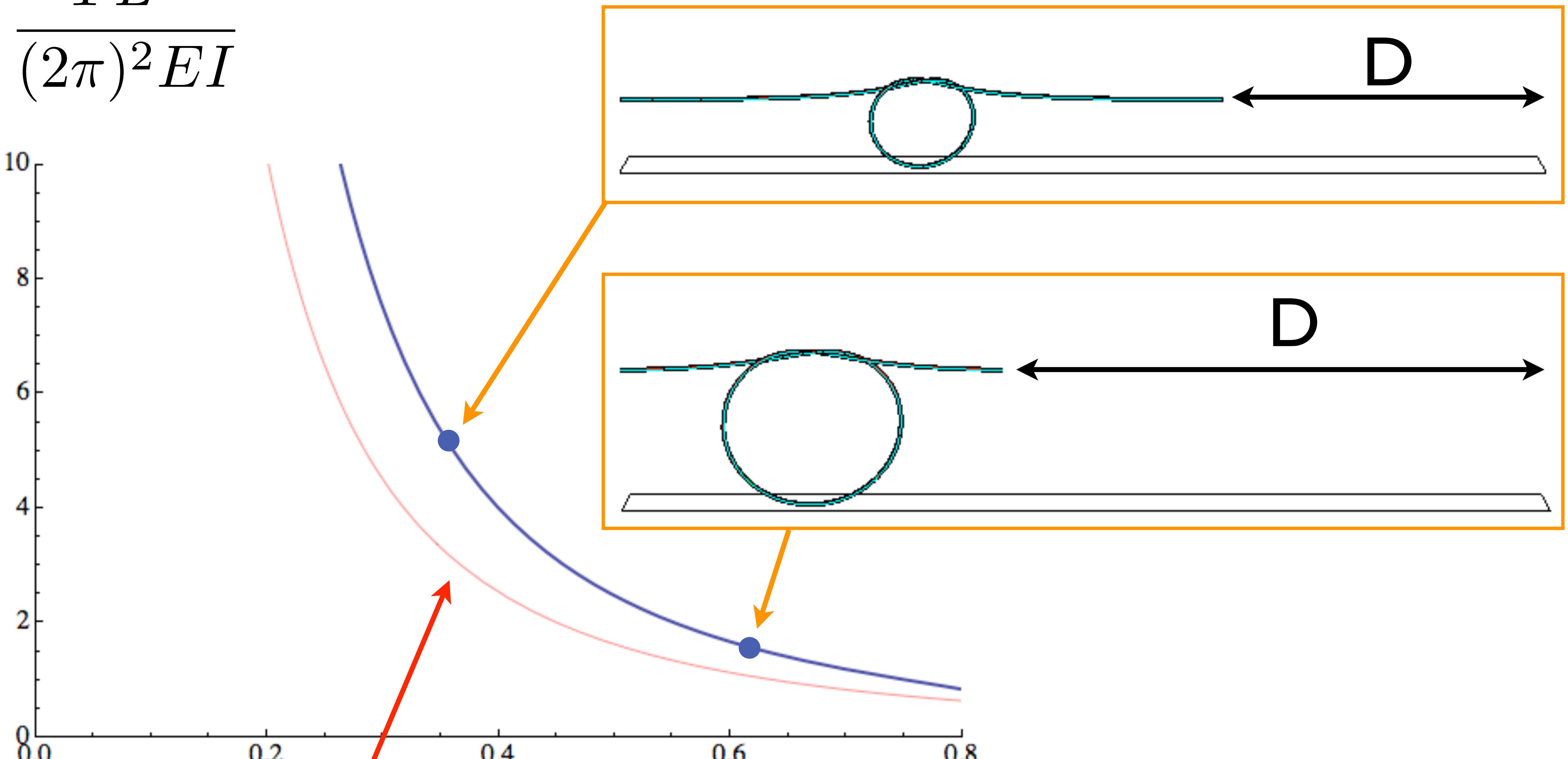
$$\vec{p} = p \frac{\vec{r}(s_1) - \vec{r}(s_2)}{|\vec{r}(s_1) - \vec{r}(s_2)|}$$

touching conditions :

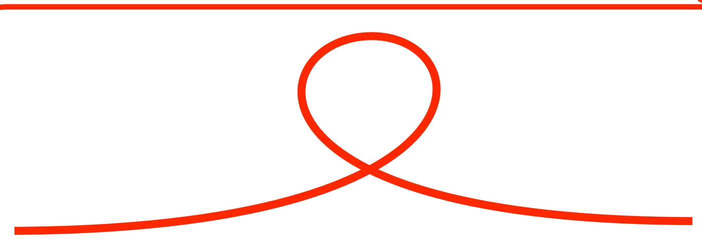
$$\begin{cases} |\vec{r}(s_1) - \vec{r}(s_2)| = \text{thickness} \\ (\vec{r}(s_1) - \vec{r}(s_2)) \perp \vec{d}_3(s_1) \\ (\vec{r}(s_1) - \vec{r}(s_2)) \perp \vec{d}_3(s_2) \end{cases}$$

Numerical Path Following : Results

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



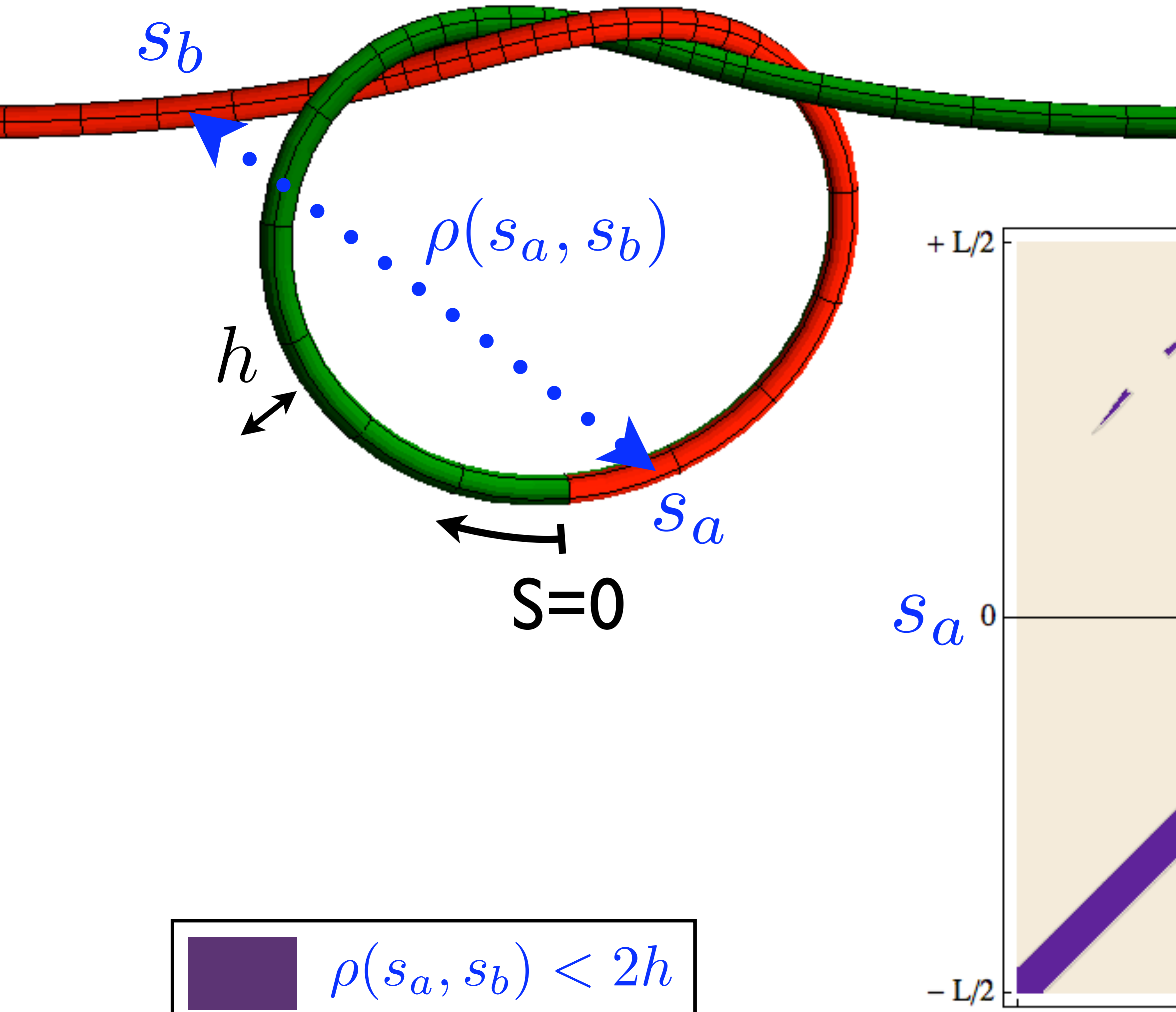
$$d = \frac{D}{L}$$

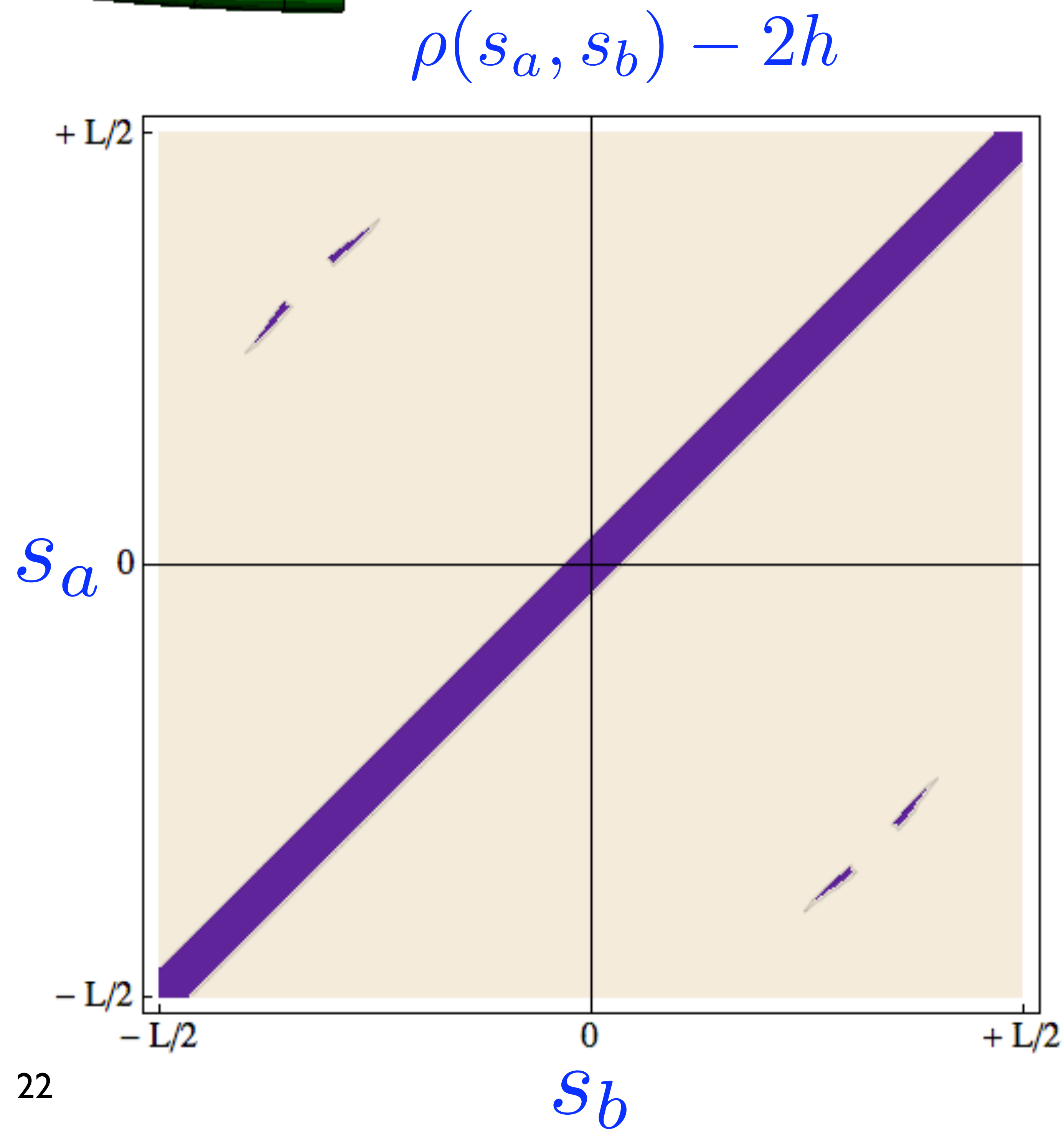


Planar Elastica

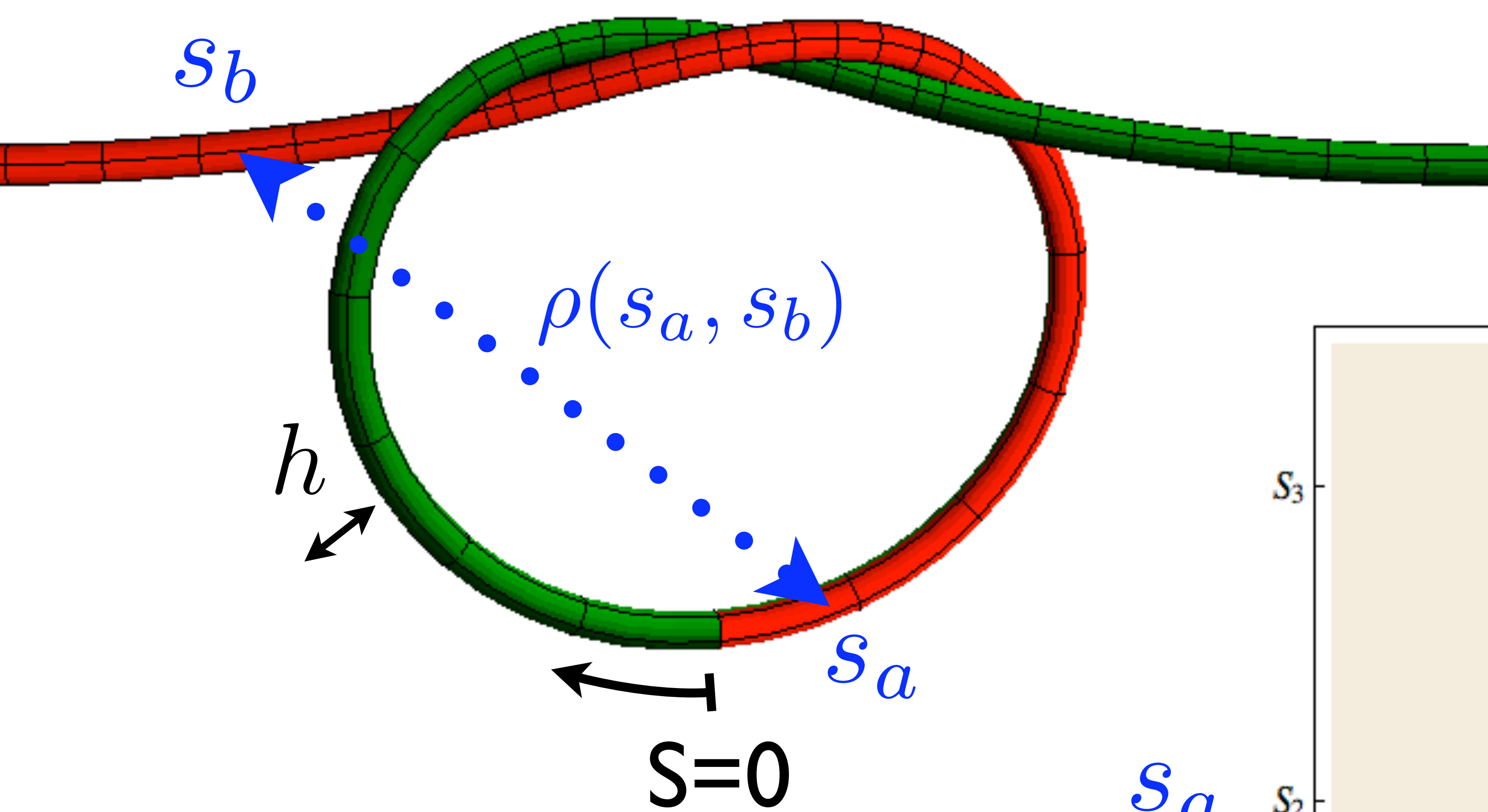
$$t = \left(\frac{2/\pi}{d}\right)^2$$

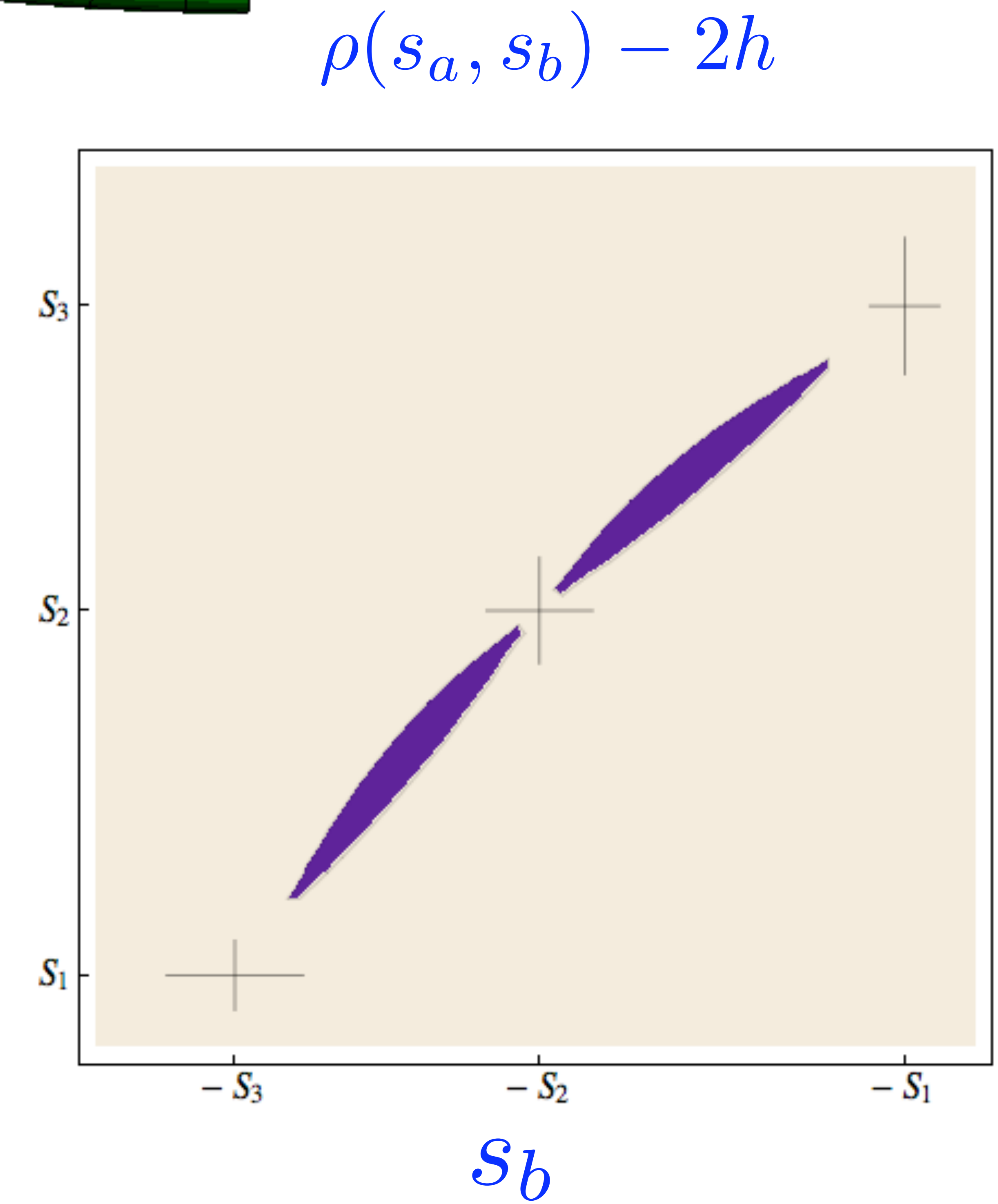
Distance of self-approach





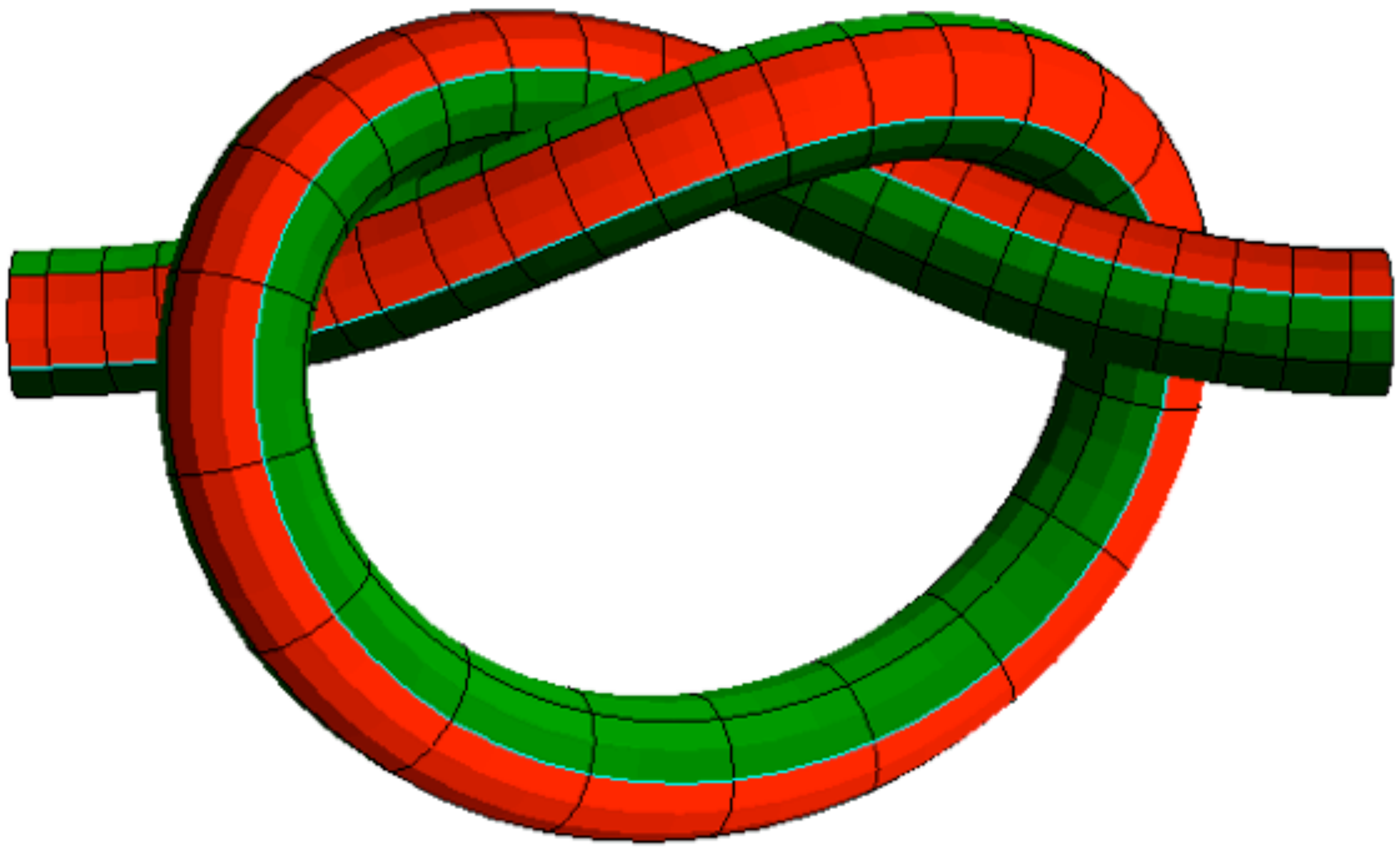
Distance of self-approach



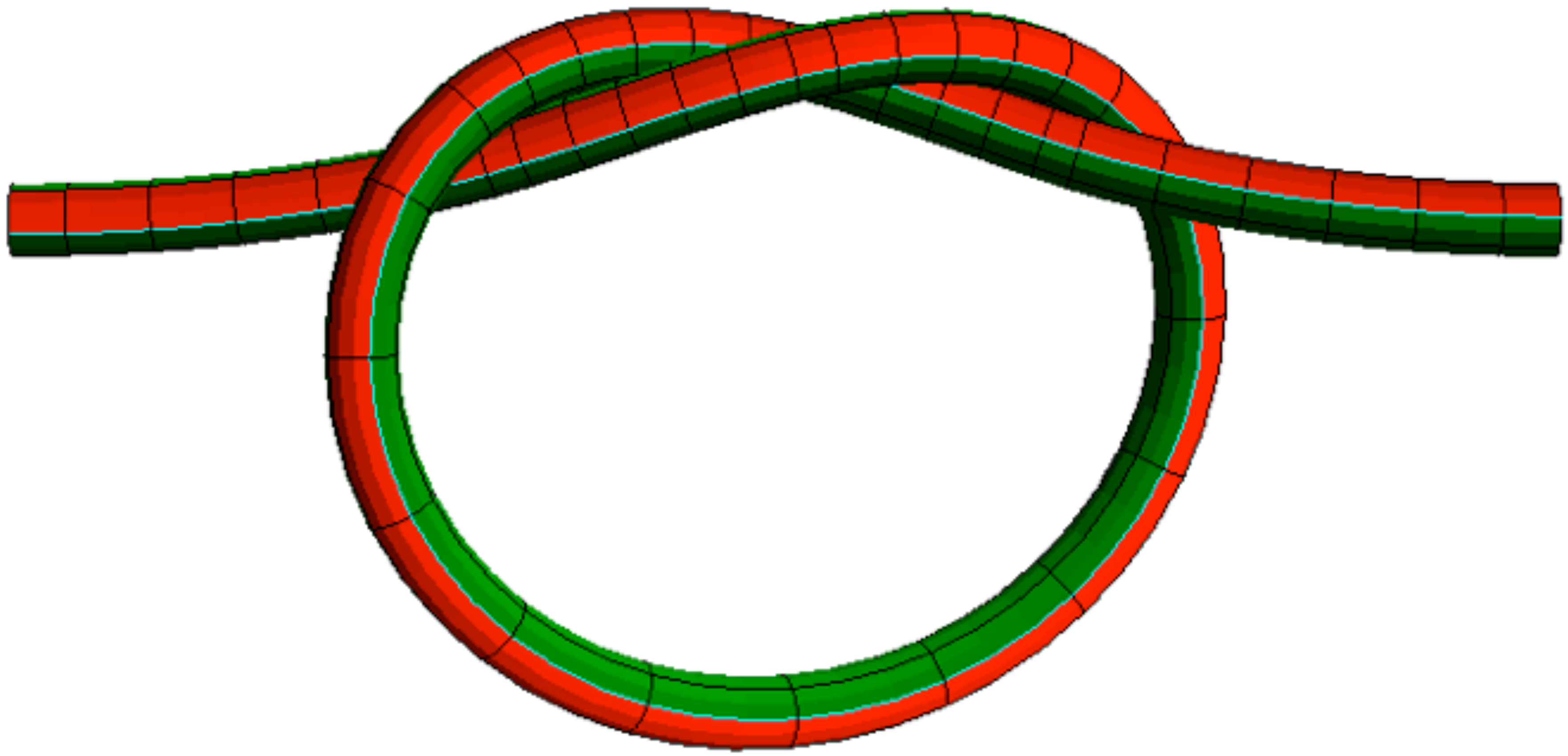


$\rho(s_a, s_b) < 2h$

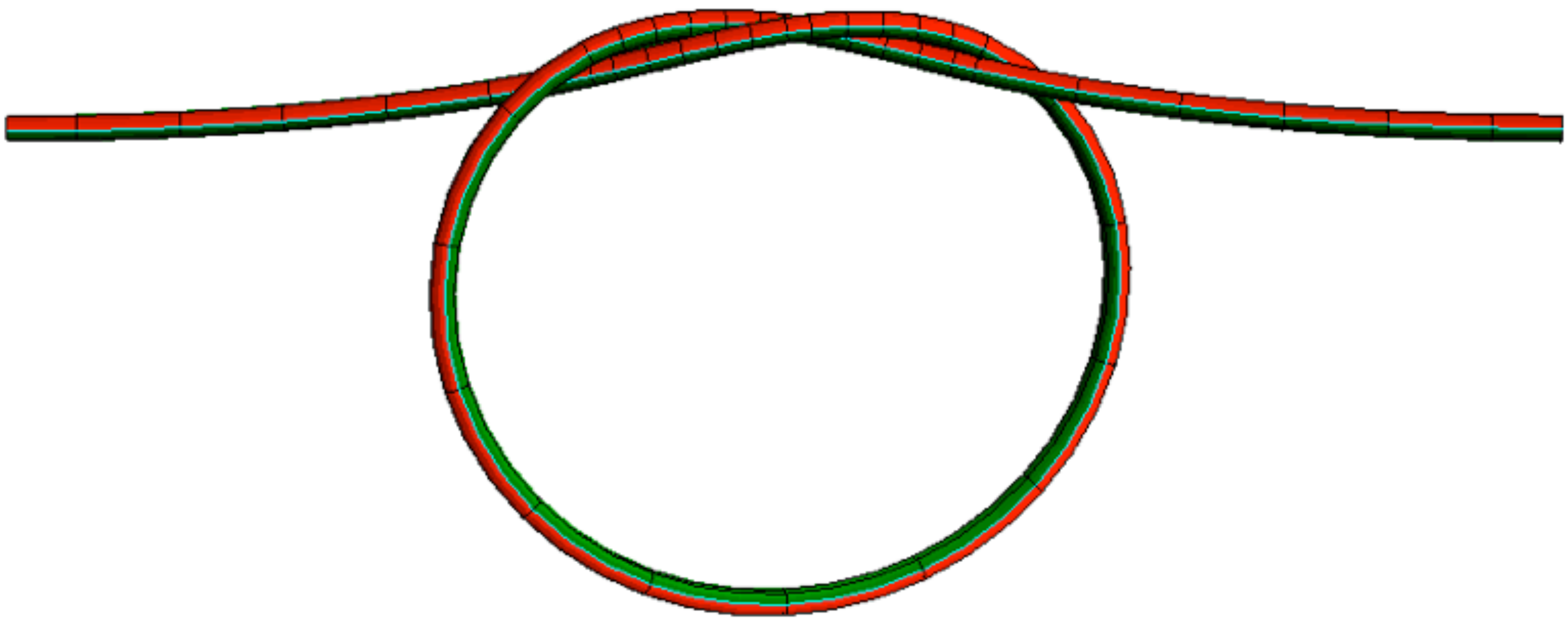
Making the rod thinner



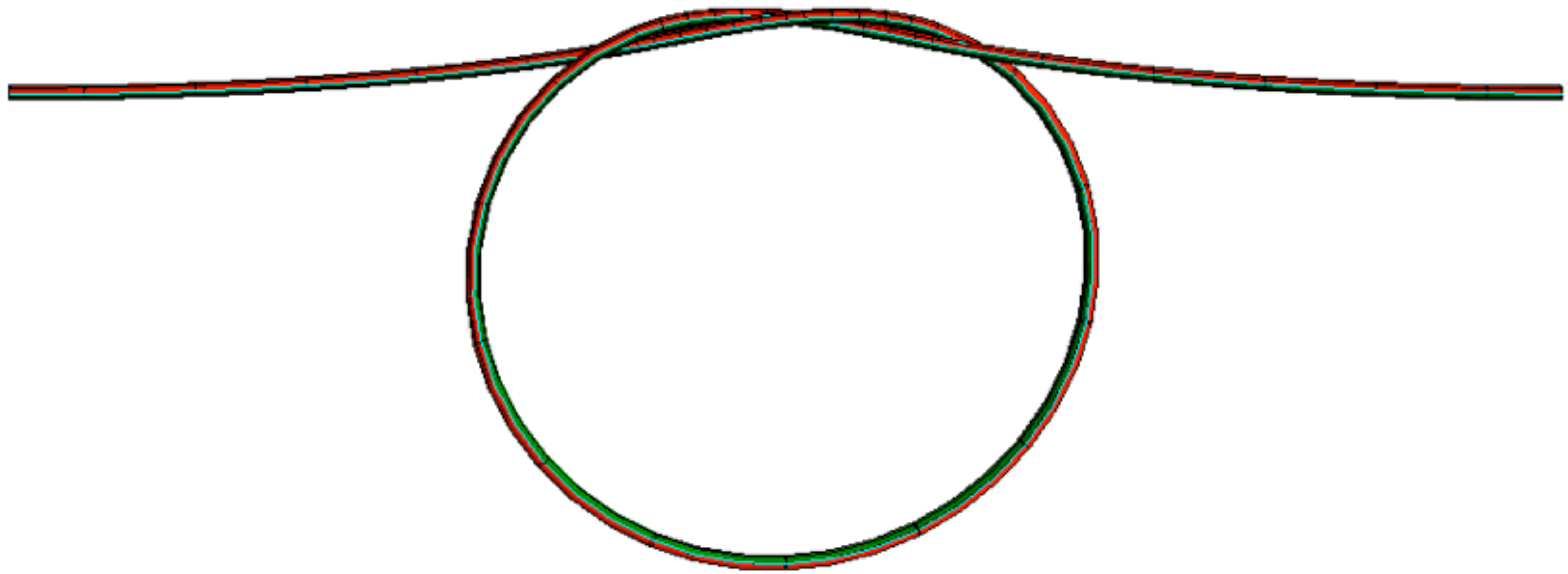
Making the rod thinner



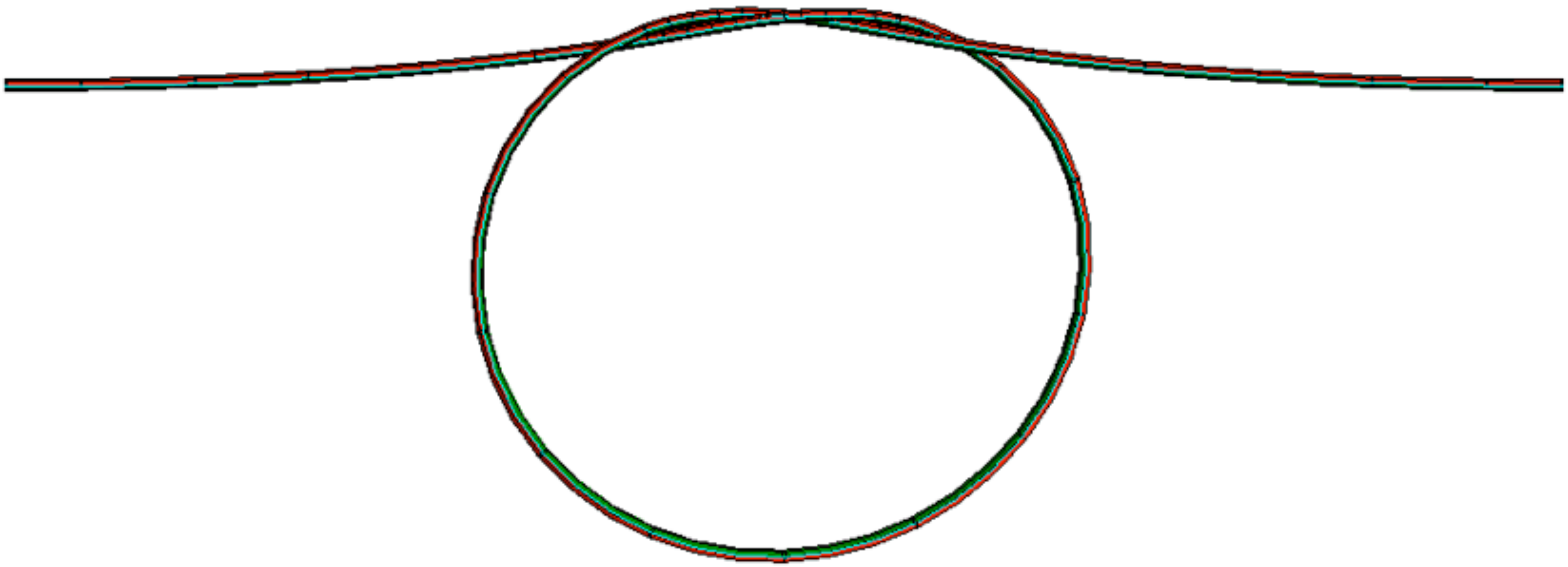
Making the rod thinner



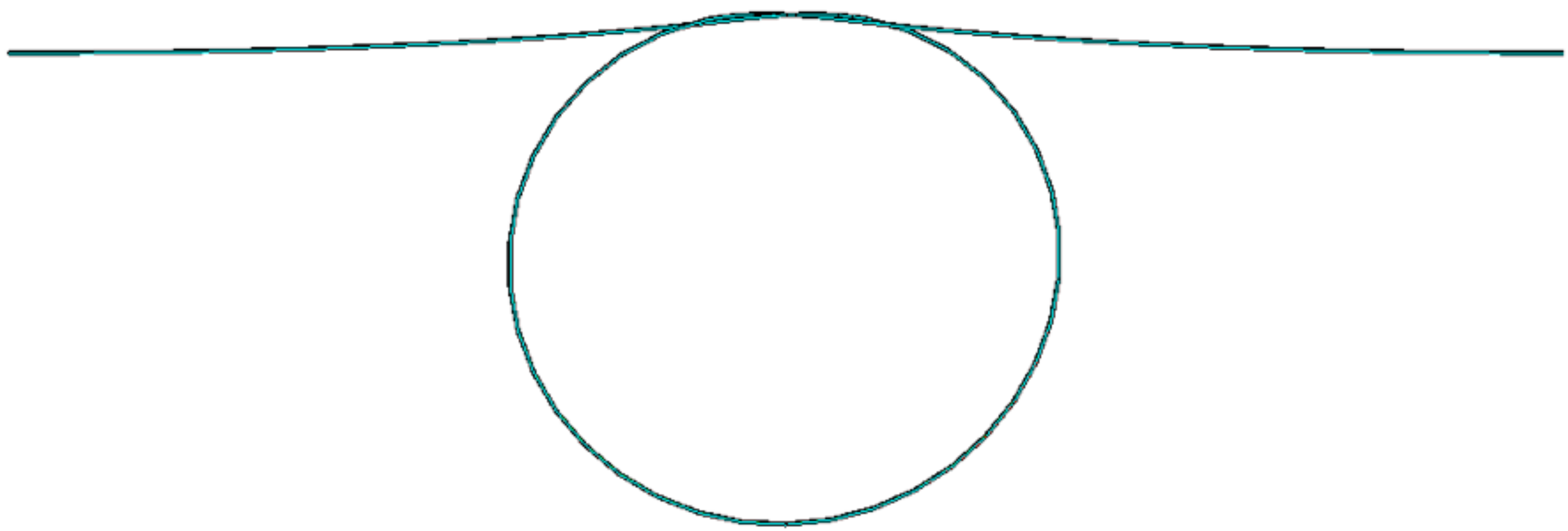
Making the rod thinner



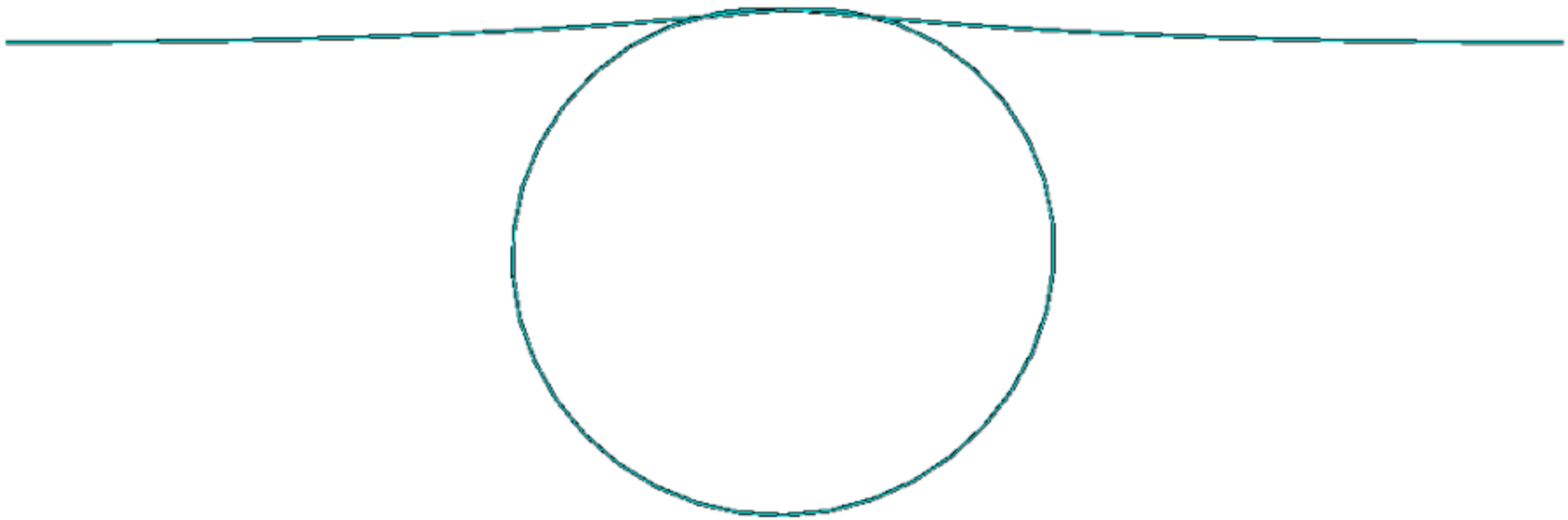
Making the rod thinner



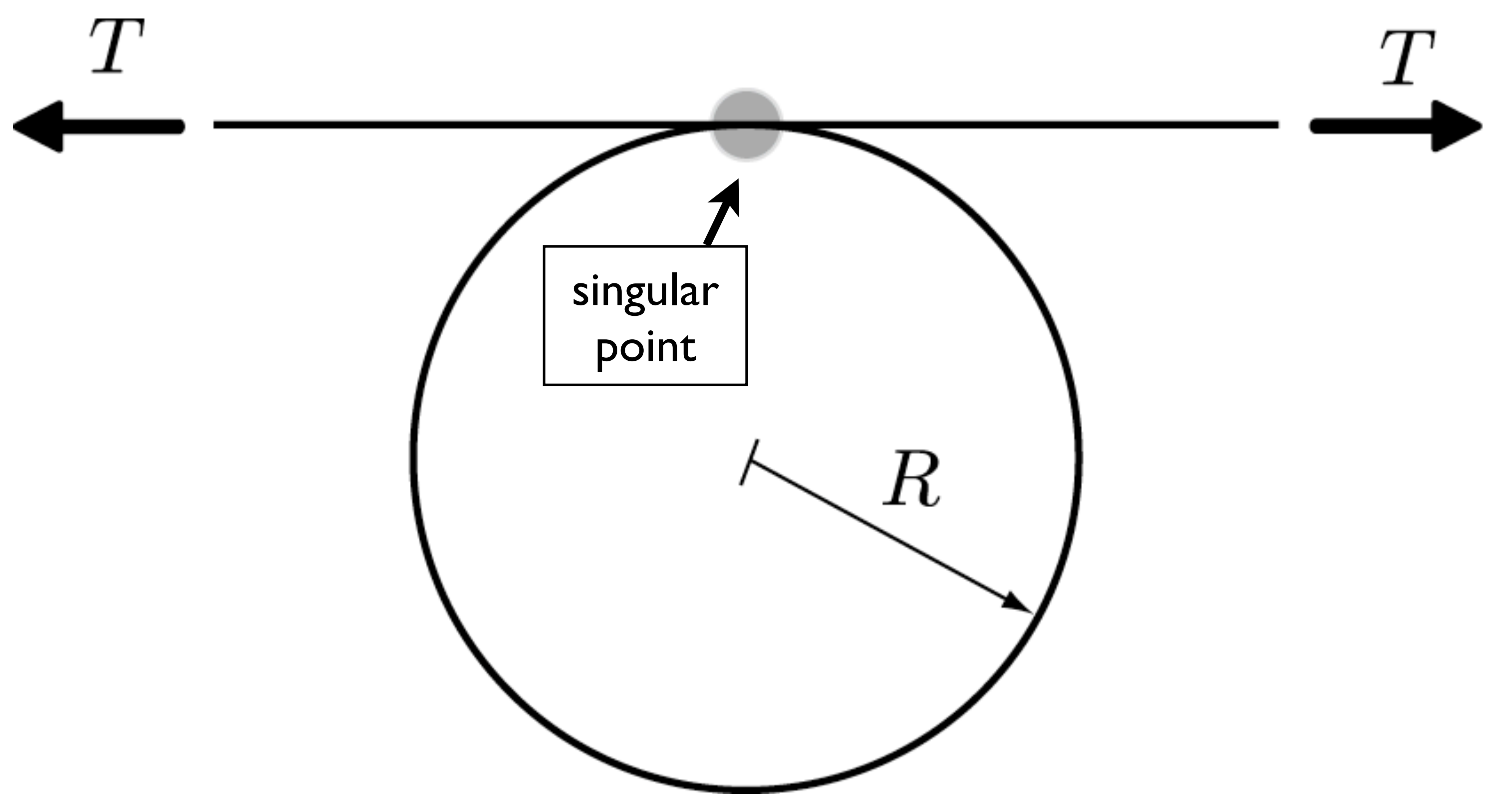
Making the rod thinner



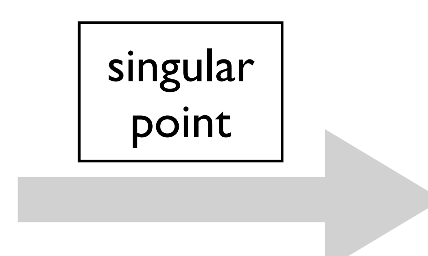
Making the rod thinner



Zero thickness limit

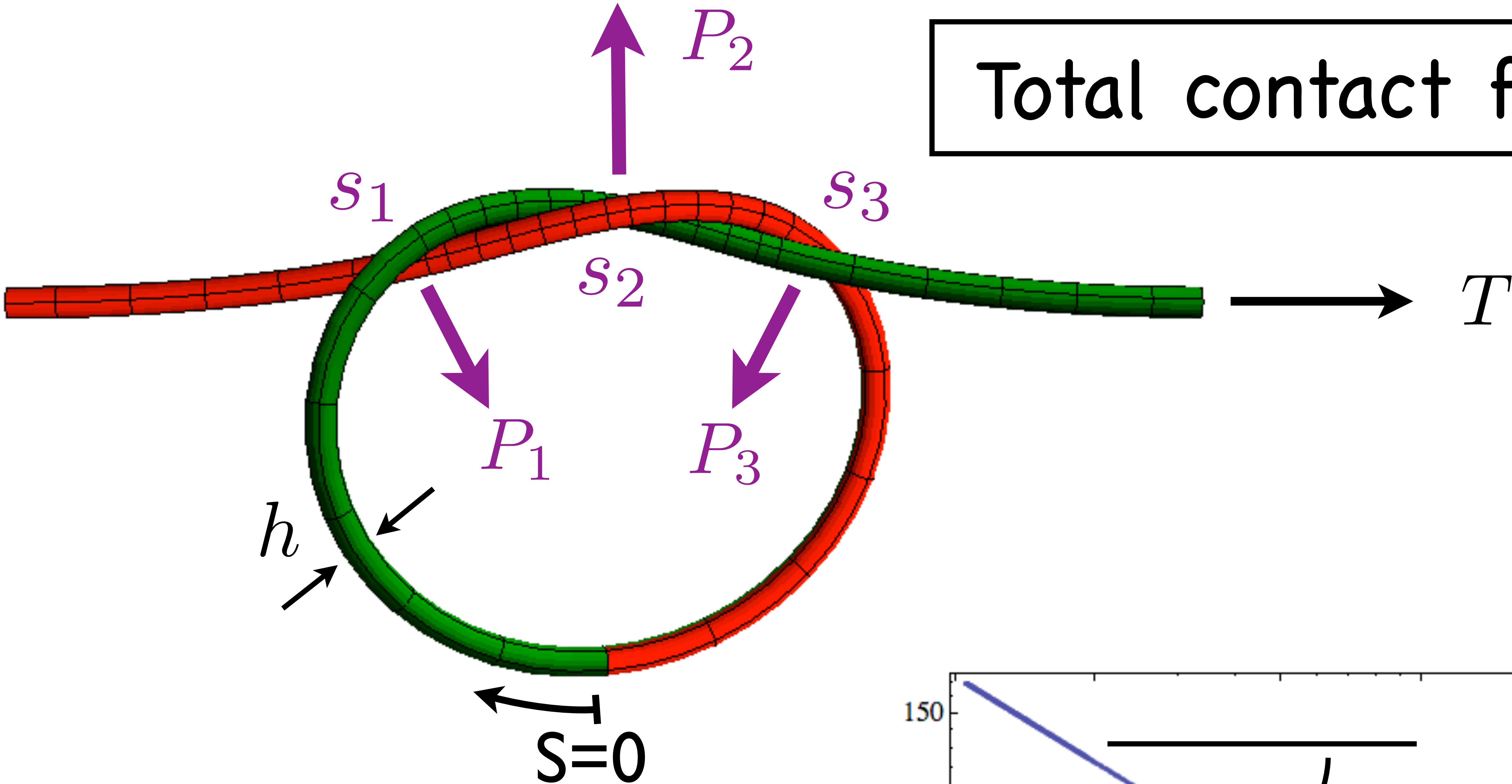


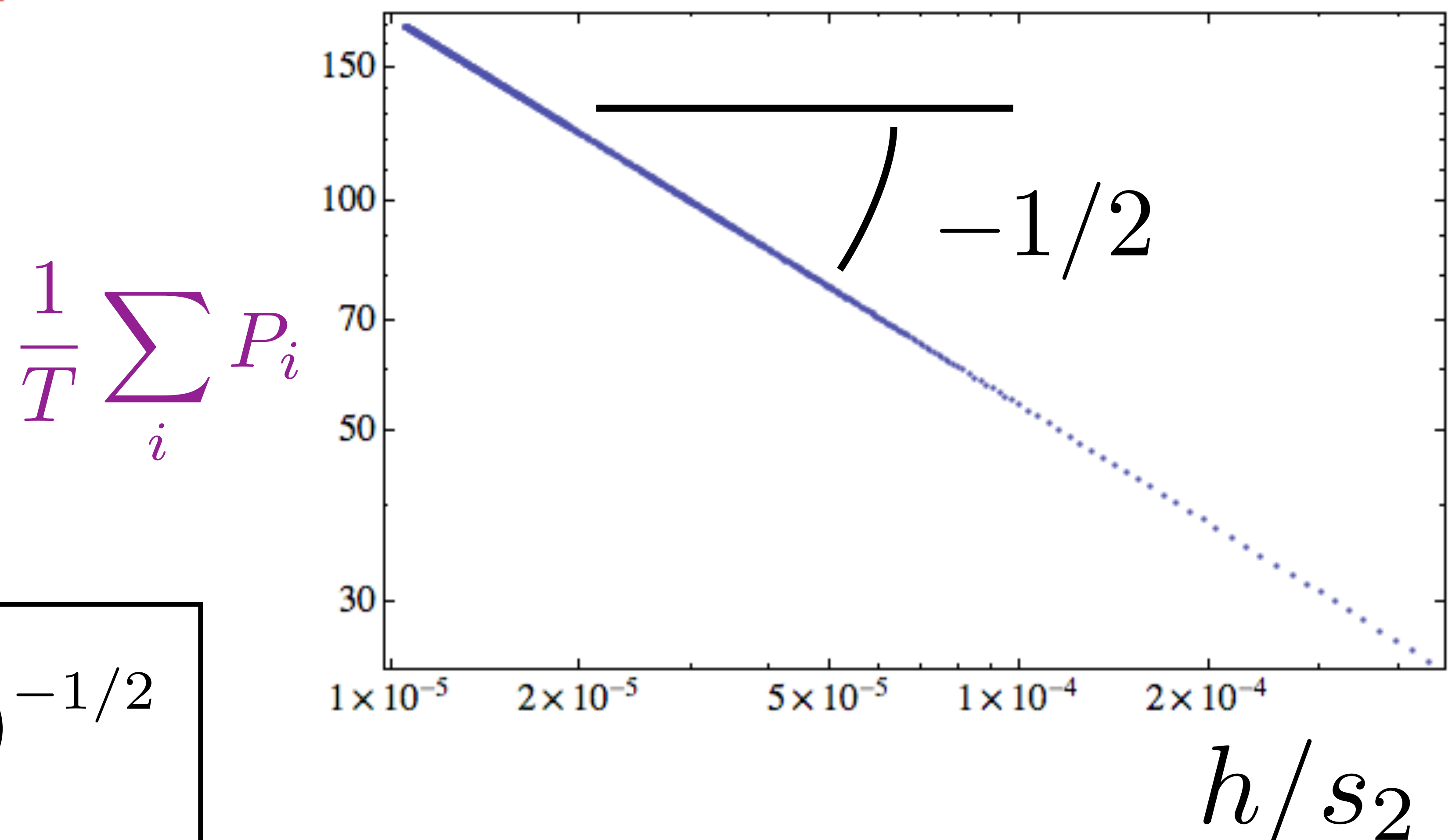
equilibrium : $T = \dfrac{EI}{2R^2}$ Arai et al (1999)



tensile force T → 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

$$\left\{\begin{array}{rcl}\vec{F}' & = & -\vec{p} \\ \vec{M}' & = & \vec{F}\times\vec{t} \\ \vec{t}' & = & \dfrac{1}{EI}\,\vec{M}\times\vec{t} \\ \vec{R}' & = & \vec{t}\end{array}\right.$$

forces equil.

moments equil.

kinematics

tangent def.

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

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

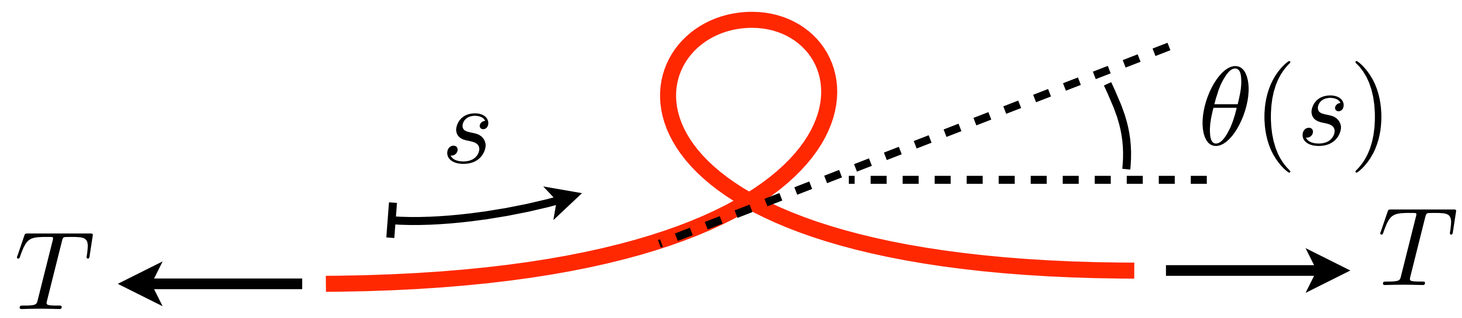
$\vec{M}(s)$ internal moment

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

$\vec{R}(s)$ position

$\vec{t}(s)$ tangent

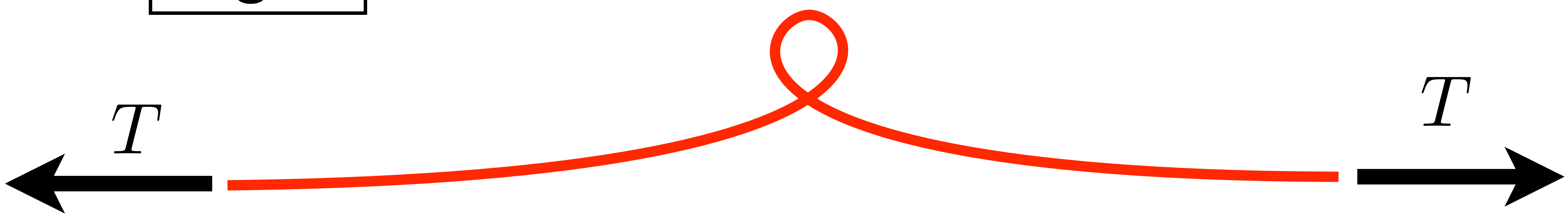
Planar Elastica



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

Planar Elastica

large T

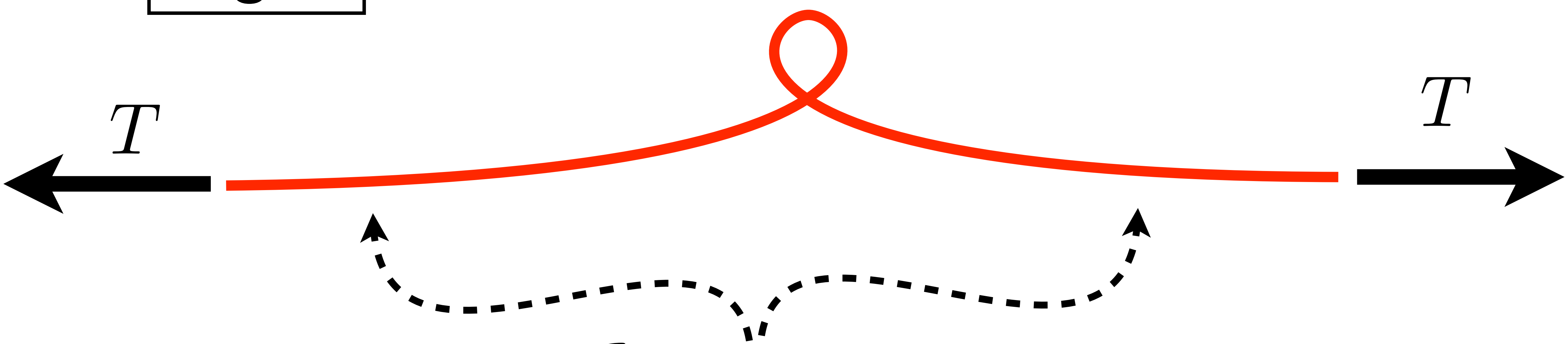


$$\frac{EI}{T}\,\theta'' = \sin\theta$$

singular perturbation

Planar Elastica

large T

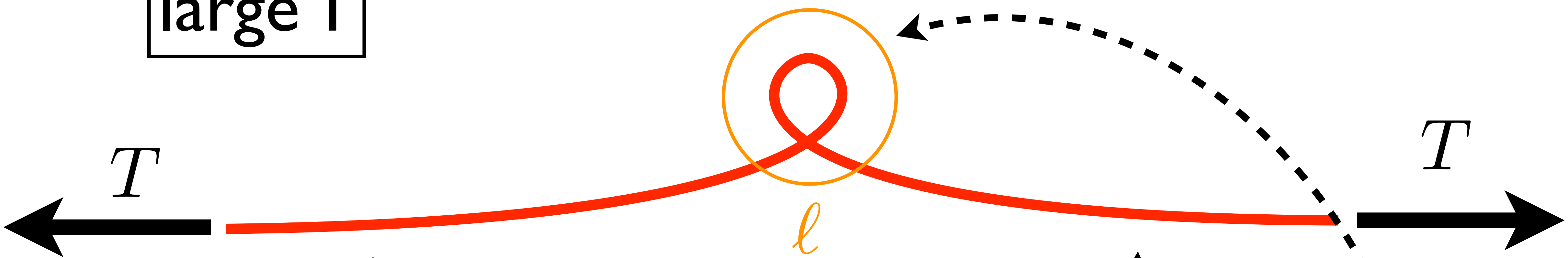


$$\frac{EI}{T}\theta'' = \sin\theta \quad \left\{ \begin{array}{l} \sin\theta \approx 0 \Rightarrow \theta(s) \approx 0 \\ \\ \end{array} \right.$$

singular perturbation

Planar Elastica

large T

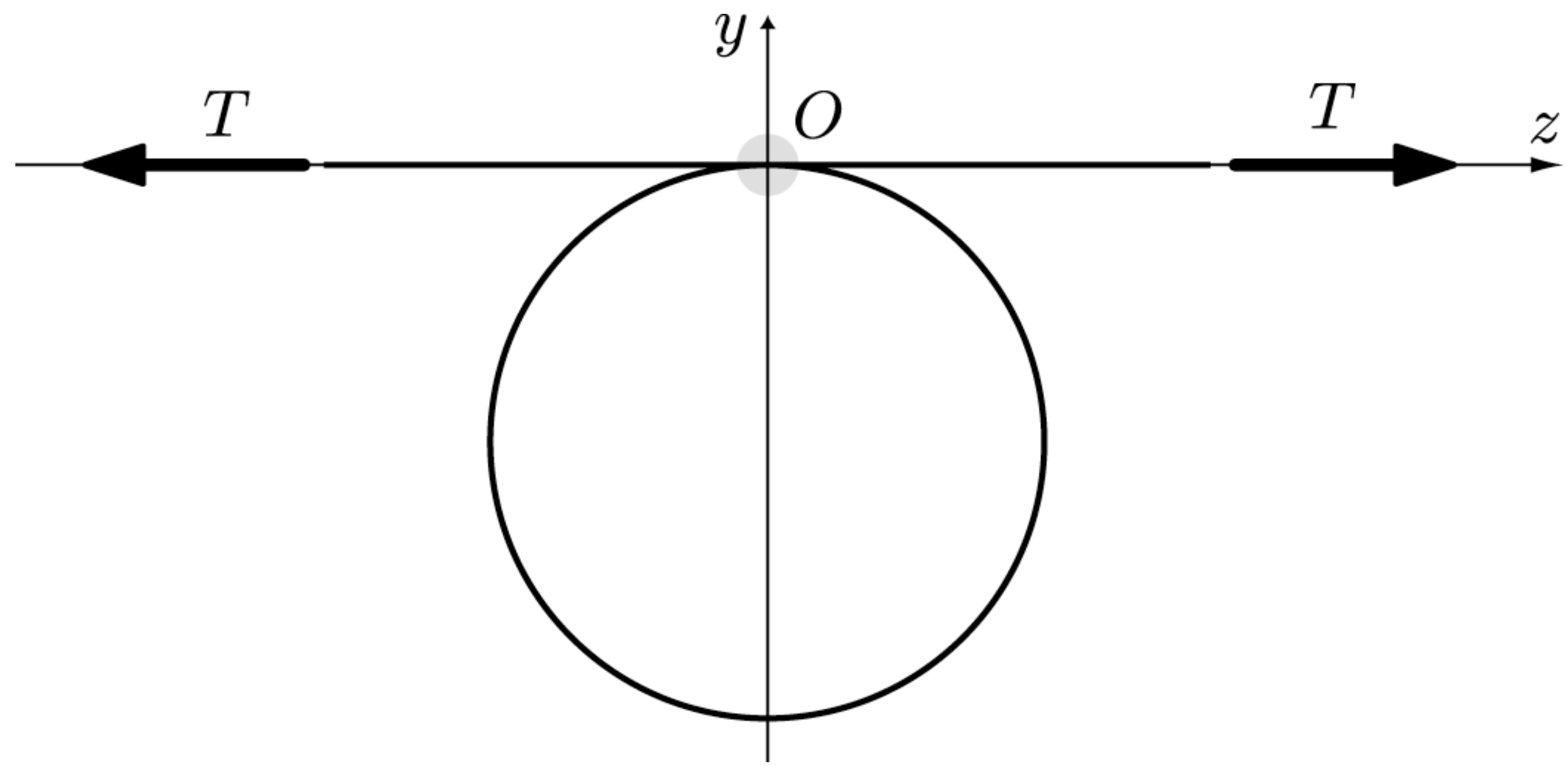


$$\frac{EI}{T}\theta'' = \sin\theta \quad \begin{cases} \sin\theta \approx 0 \Rightarrow \theta(s) \approx 0 \\ \theta(s) \ \text{ rapidly varying} \end{cases}$$

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

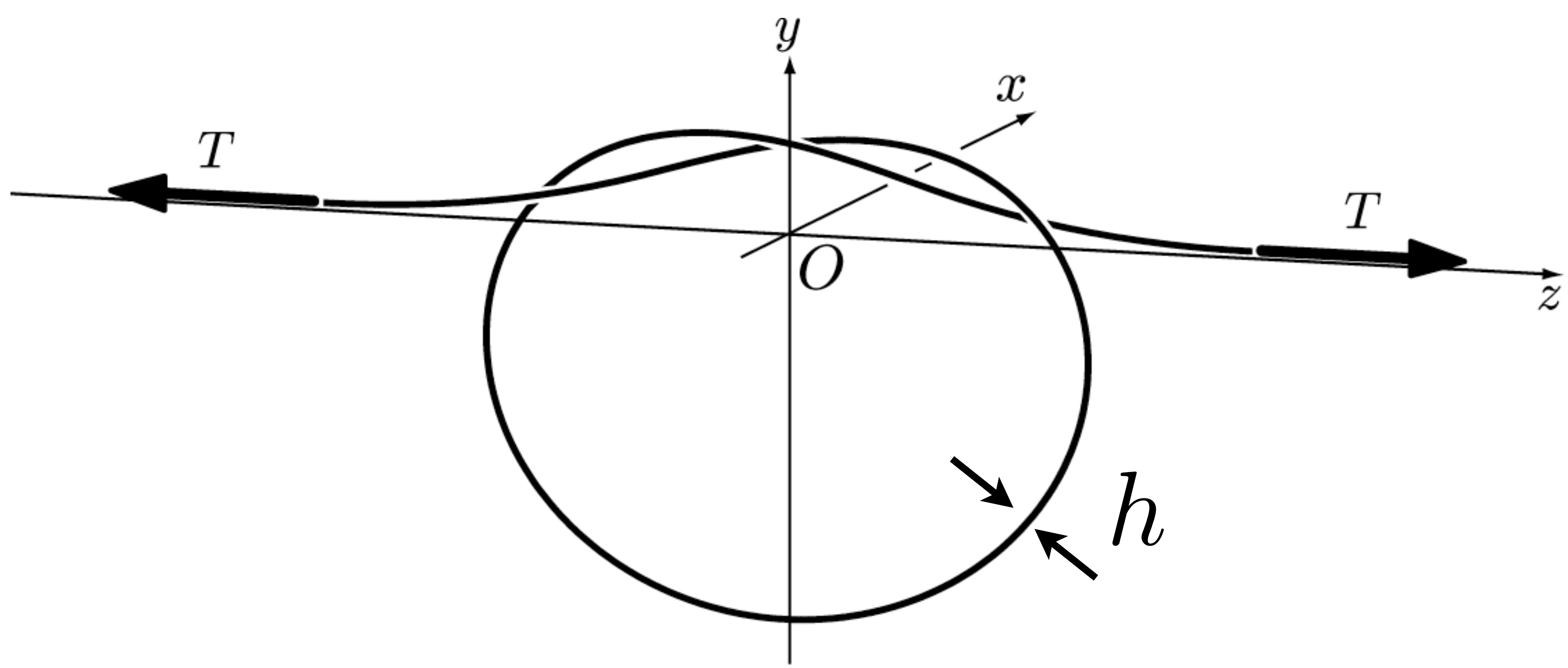
singular perturbation → inner layer

Perturbative problem



$\epsilon = 0$

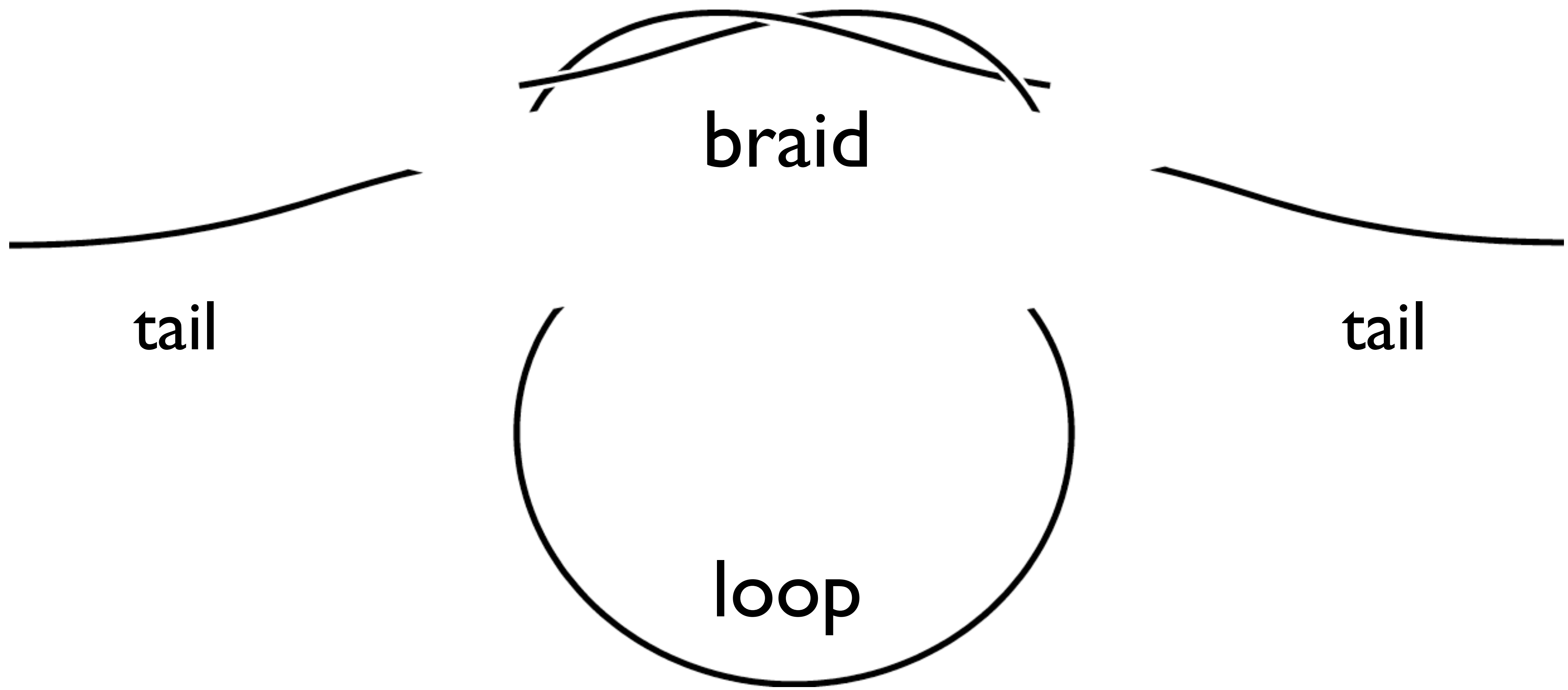
$(h = 0)$



small parameter

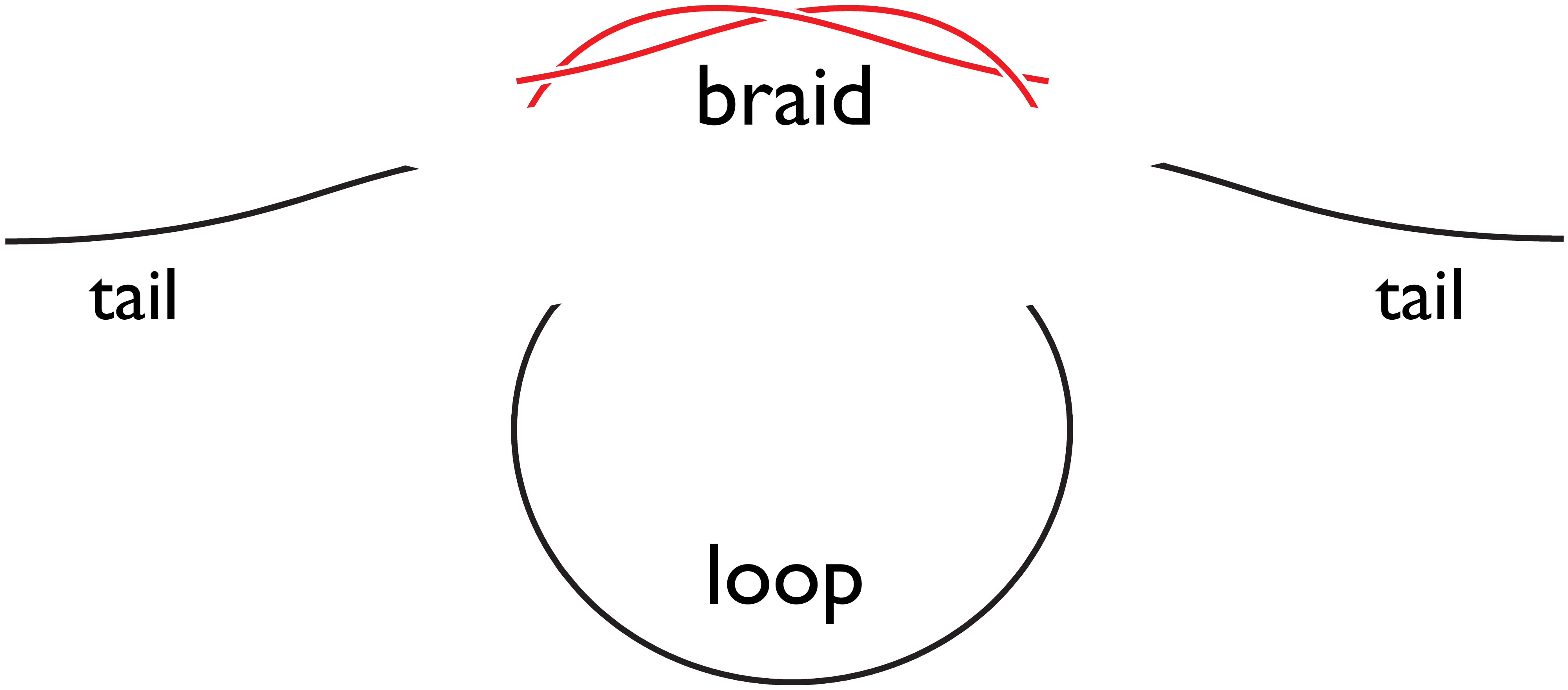
$$\epsilon = \left(\frac{2h^2 T}{EI}\right)^{1/4} \ll 1$$

Matched asymptotic expansions

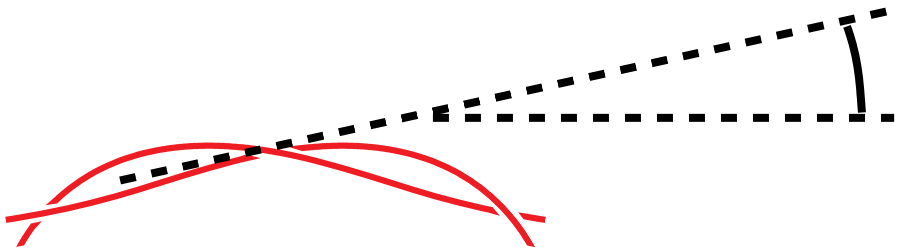


small parameter : $\epsilon = \left(\frac{2h^2 T}{EI} \right)^{1/4} \ll 1$

Braid : self-contact zone



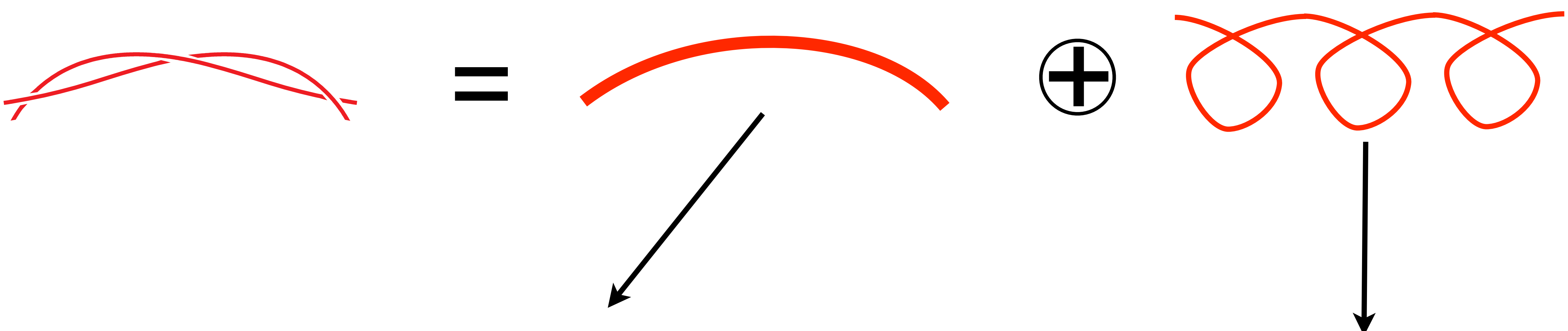
Braid : linear superposition



$\theta \ll 1$

small deflections => linear problem

$x^A \, , \, x^B$ = $x^B + x^A$ $\oplus$ $x^B - x^A$



twice more rigid

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

self-contact

=>

contact with obstacle

Kirchhoff Equations

$$
\left\{
\begin{array}{rcl}
\vec{F}' & = & -\vec{p} \\
\vec{M}' & = & \vec{F} \times \vec{t} \\
\vec{t}' & = & \dfrac{1}{EI}\,\vec{M} \times \vec{t} \\
\vec{R}' & = & \vec{t}
\end{array}
\right.
$$

forces equil.

moments equil.

kinematics

tangent def.

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

constitutive relations:

$$M_\kappa = EI\,\kappa$$ curvature κ

$$M_\tau = GJ\,\tau$$ twist τ

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

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

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

$\vec{R}(s)$ position

$\vec{t}(s)$ tangent

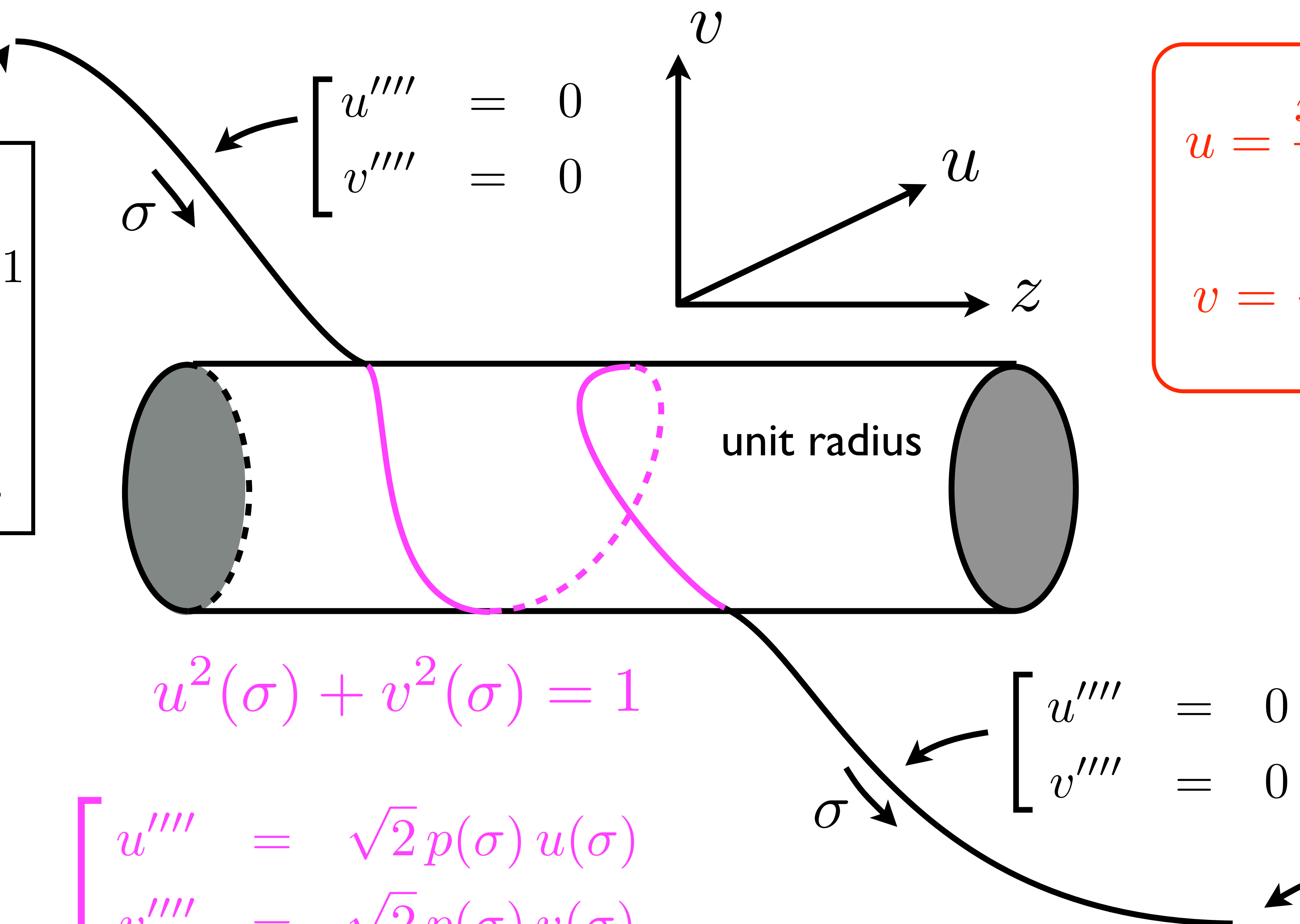
Braid : boundary value problem (BVP)

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

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

boundary conditions

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



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

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

$$p(\sigma) = ?$$

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

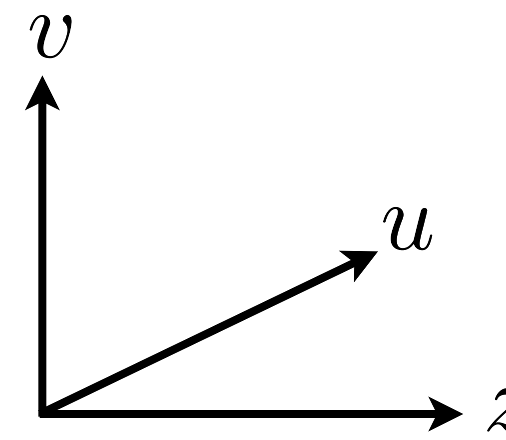
moments

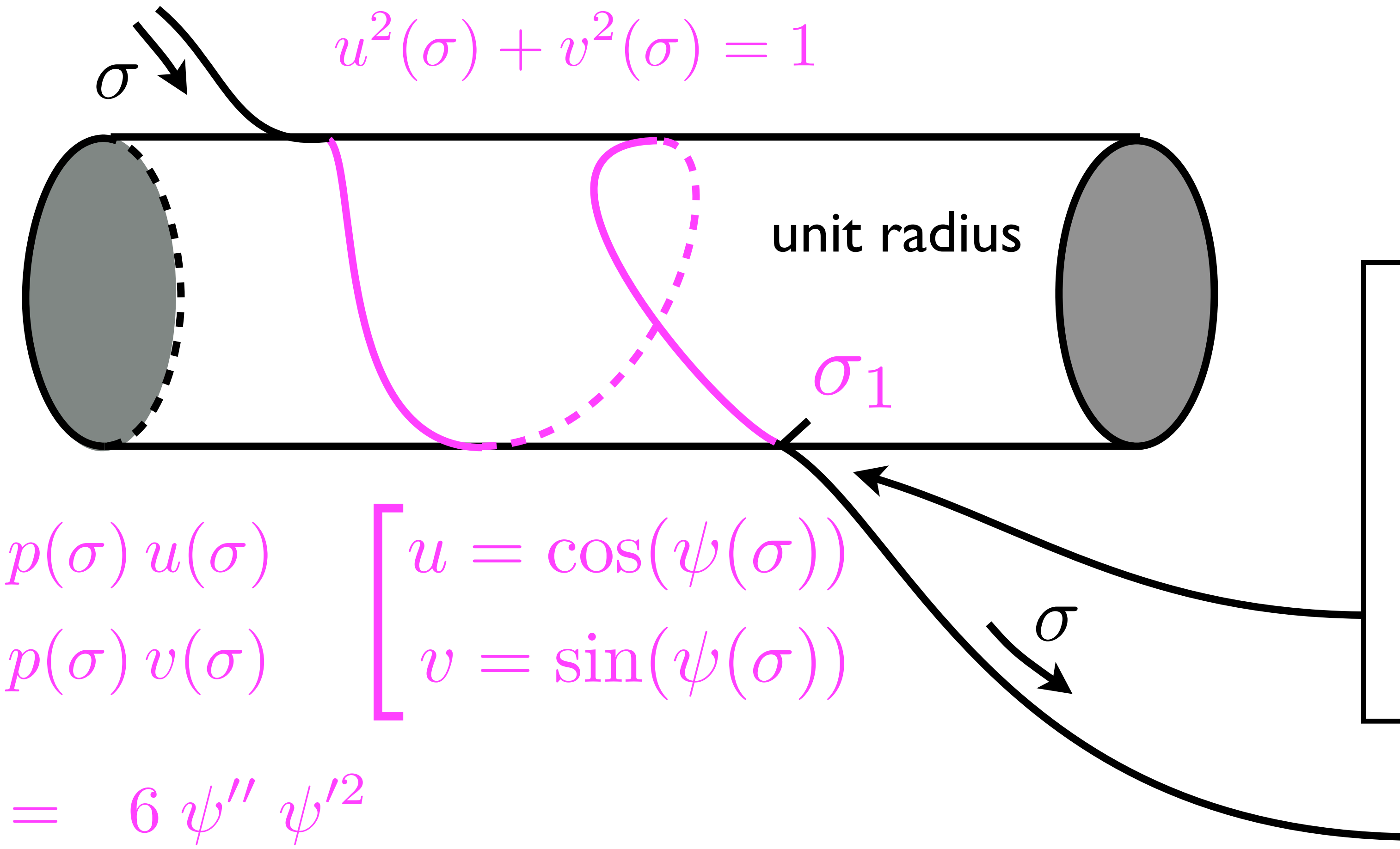
$$\begin{aligned} u''(+\infty) &= 0 \\ v''(+\infty) &= -1 \\ u'''(+\infty) &= 0 \\ v'''(+\infty) &= 0 \end{aligned}$$

forces

boundary conditions

Braid : first kind of solutions





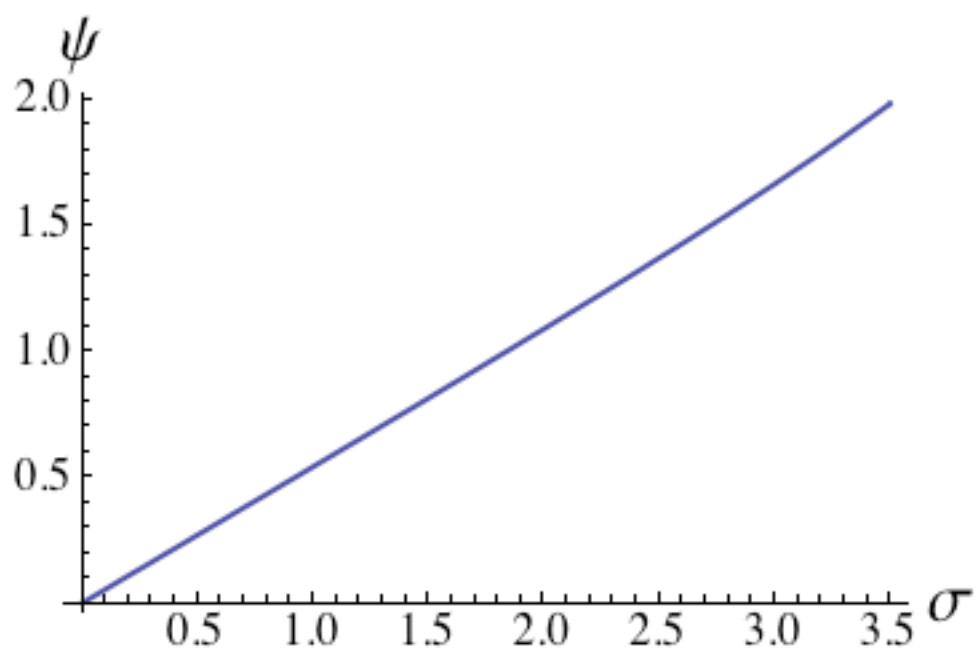
boundary conditions

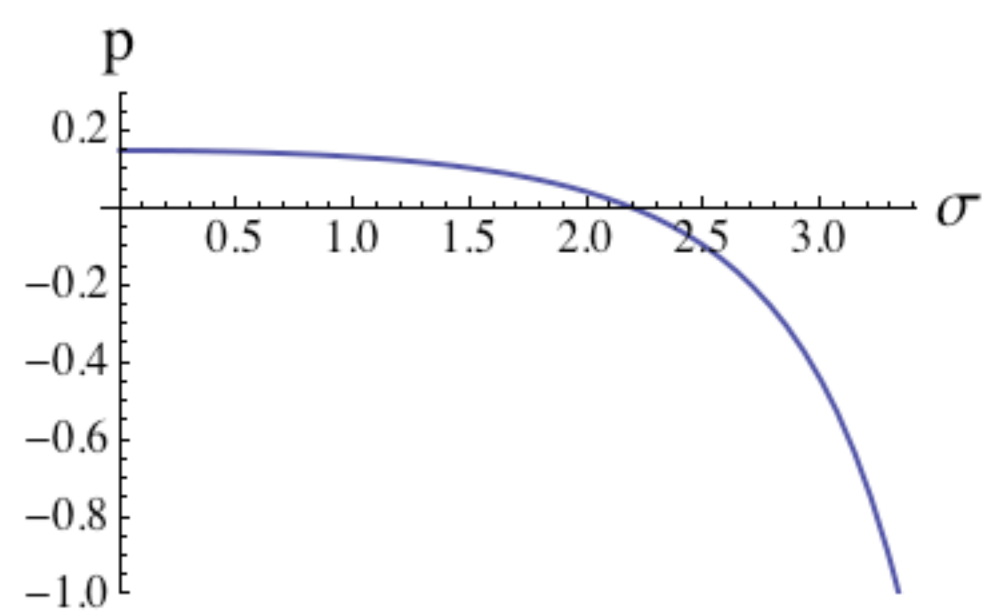
$$
\begin{aligned}
u''(\sigma_1) &= 0 \\
v''(\sigma_1) &= -1 \\
u'''(\sigma_1) &= 0 \\
v'''(\sigma_1) &= 0
\end{aligned}
$$

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

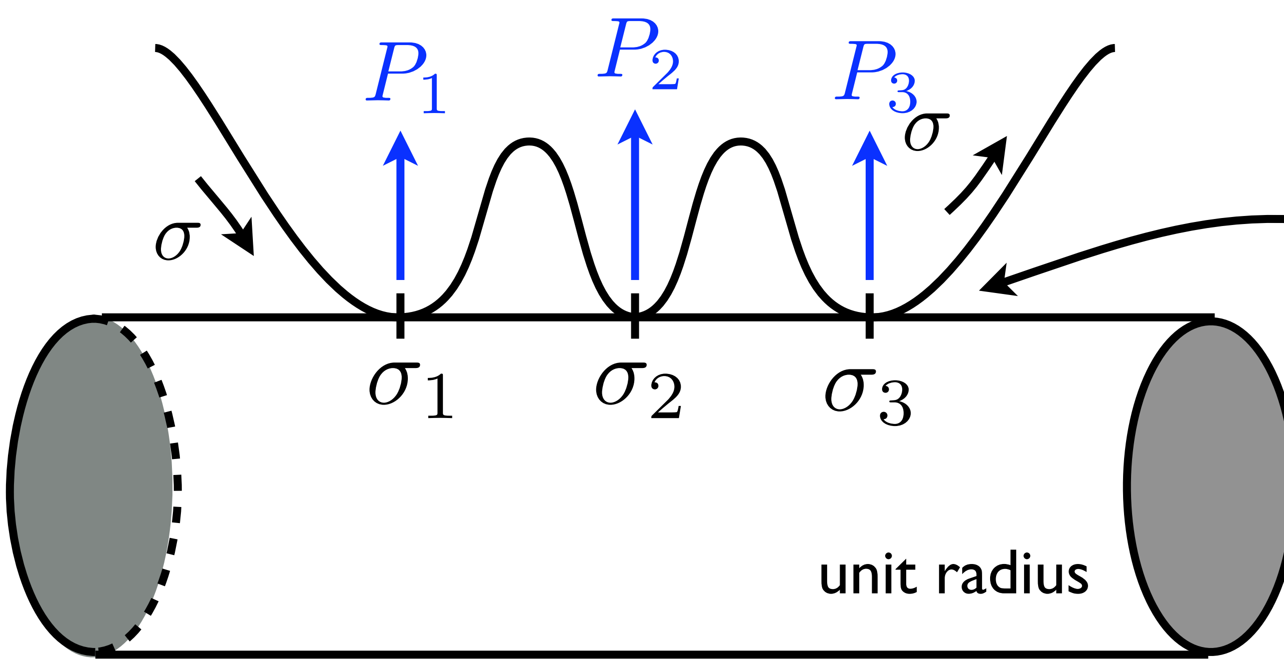
$$
\to \left\{\begin{aligned}
\psi'''' &= 6\, \psi''\, \psi'^2 \\
p(\sigma) &= \left(\psi'^4 - 3\psi''^2 - 4\psi'\psi'''\right)/\sqrt{2}
\end{aligned}\right.
$$

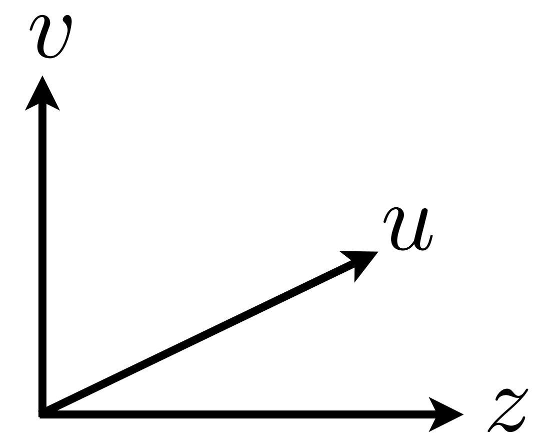
$$
\begin{aligned}
\psi(0) &= 0 \\
\psi'(0) &= 0.54 \\
\psi''(0) &= 0 \\
\psi'''(0) &= 0.004 \\
\sigma_1 &= 3.50
\end{aligned}
$$





Braid : second kind of solutions





boundary conditions

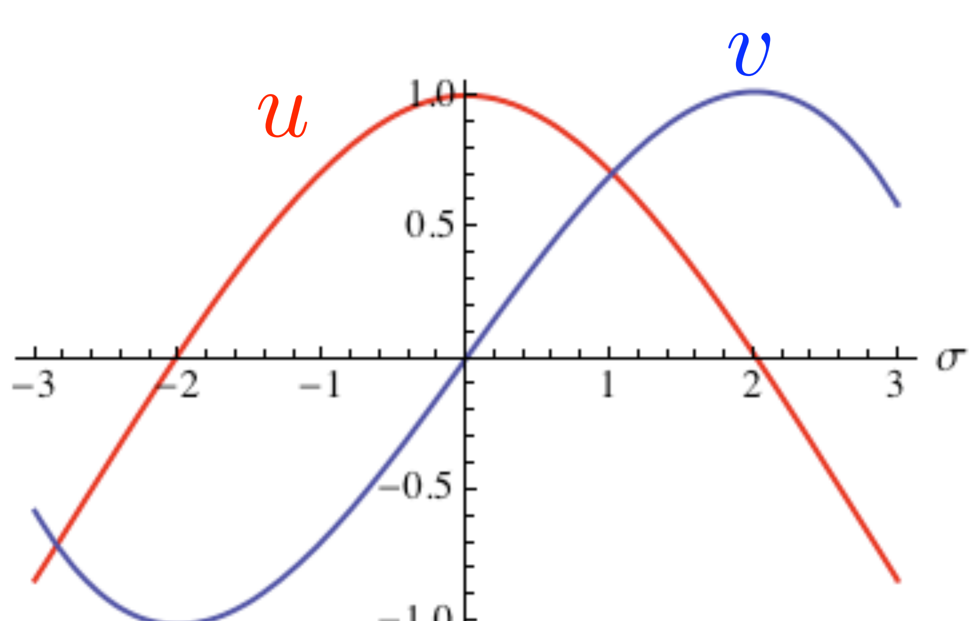
$$
\begin{aligned}
u''(+\sigma_3) &= 0 \\
v''(+\sigma_3) &= -1 \\
u'''(+\sigma_3) &= 0 \\
v'''(+\sigma_3) &= 0
\end{aligned}
$$

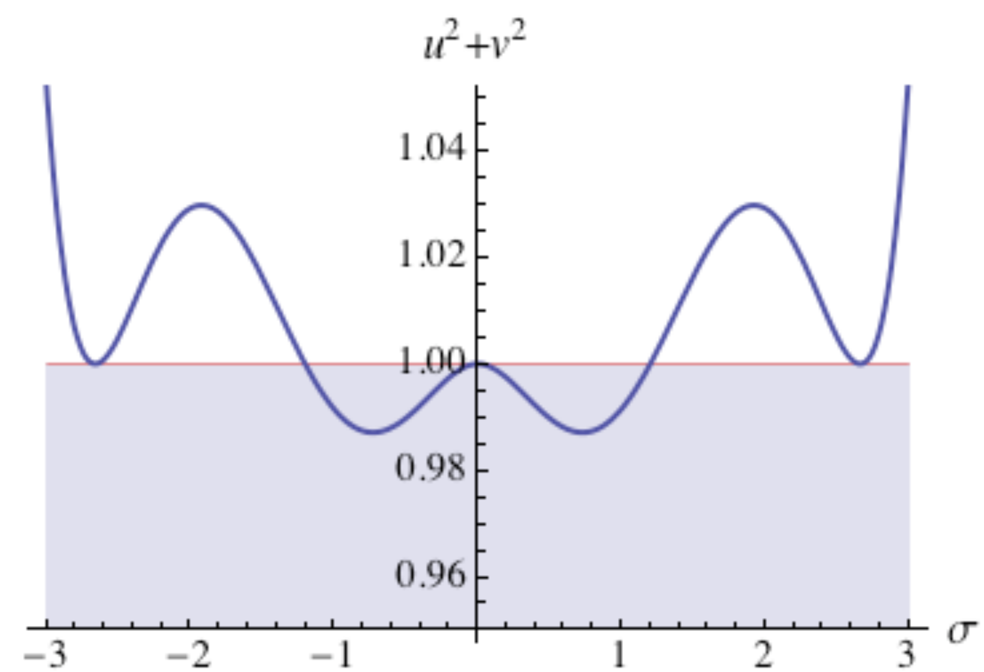
$$
\begin{cases}
u'''' = \sqrt{2}\, p(\sigma)\, u(\sigma) \\
v'''' = \sqrt{2}\, p(\sigma)\, v(\sigma)
\end{cases}
$$

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

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

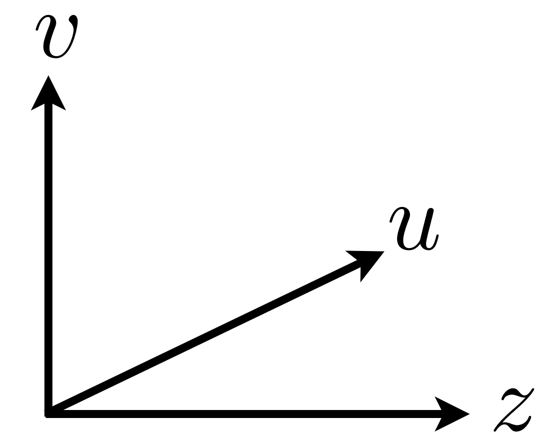
$$
\begin{aligned}
v(0) &= 0 \\
v'(0) &= 0.76 \\
v''(0) &= 0 \\
v'''(0) &= -0.38
\end{aligned}
$$

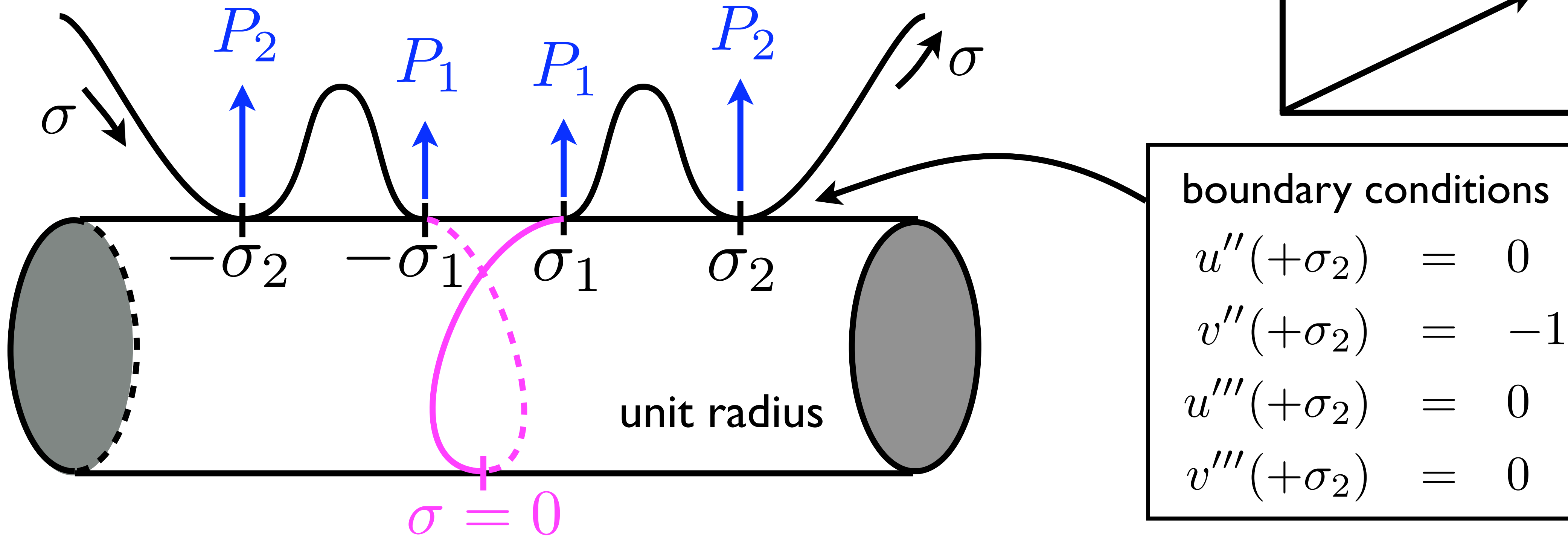




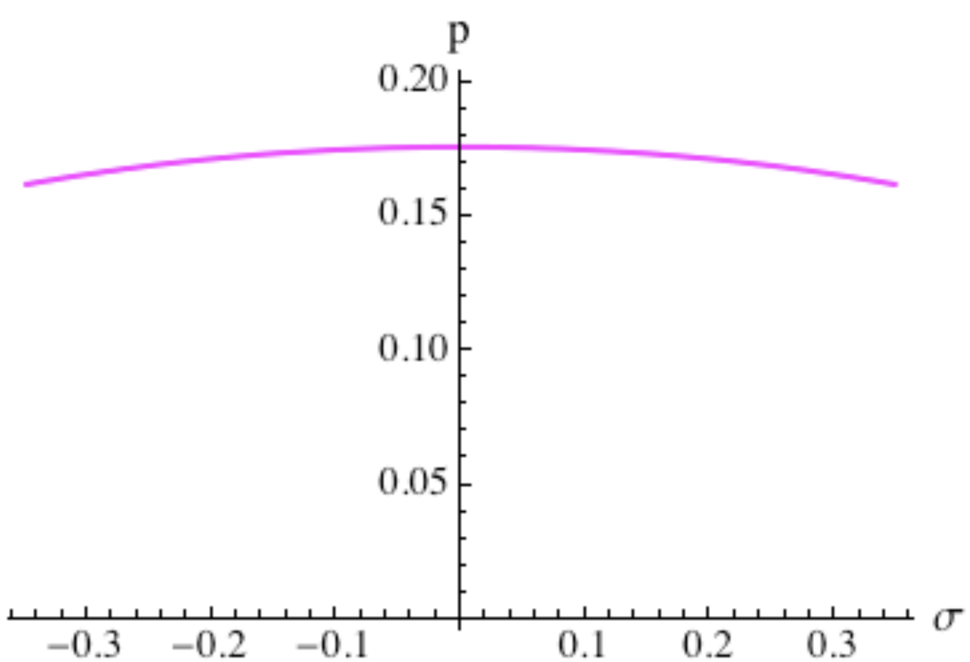
$\sigma_3 = -\sigma_1 = 2.66$; $\sigma_2 = 0$; $P_1 = P_3 = 0.32$; $P_2 = 0.35$

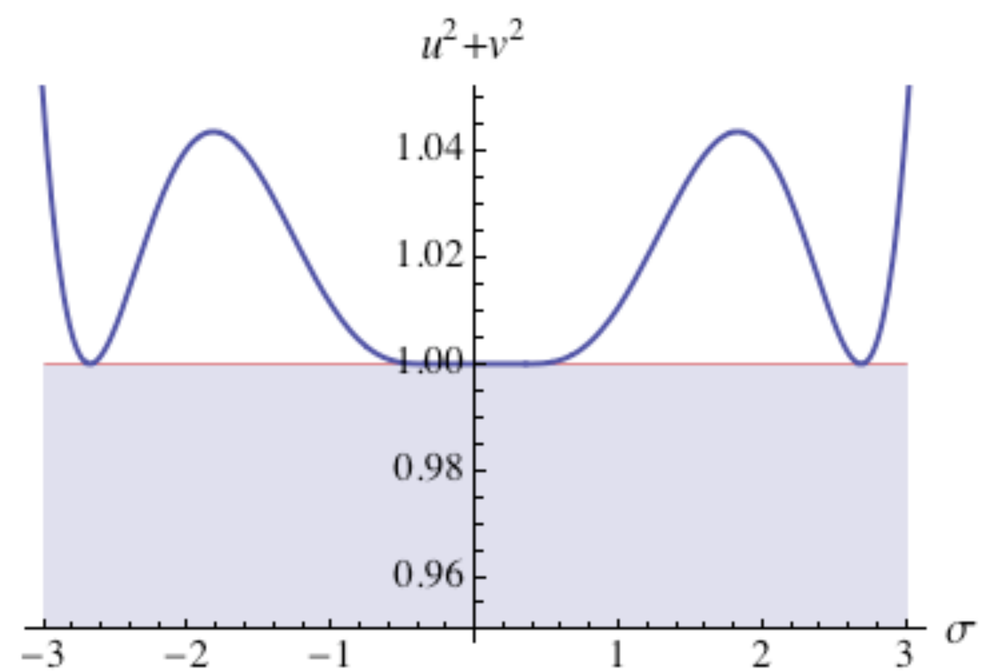
Braid : third kind of solutions



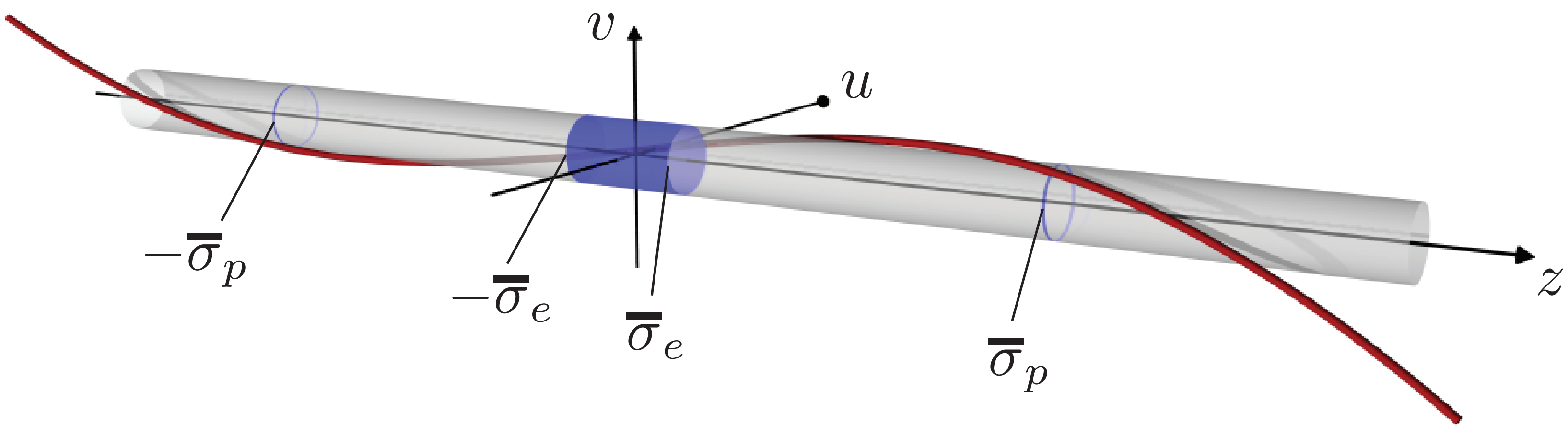


$$
\begin{aligned}
\sigma_1 &= 0.35\\
\sigma_2 &= 2.68\\
P_1 &= 0.12\\
P_2 &= 0.31
\end{aligned}
$$

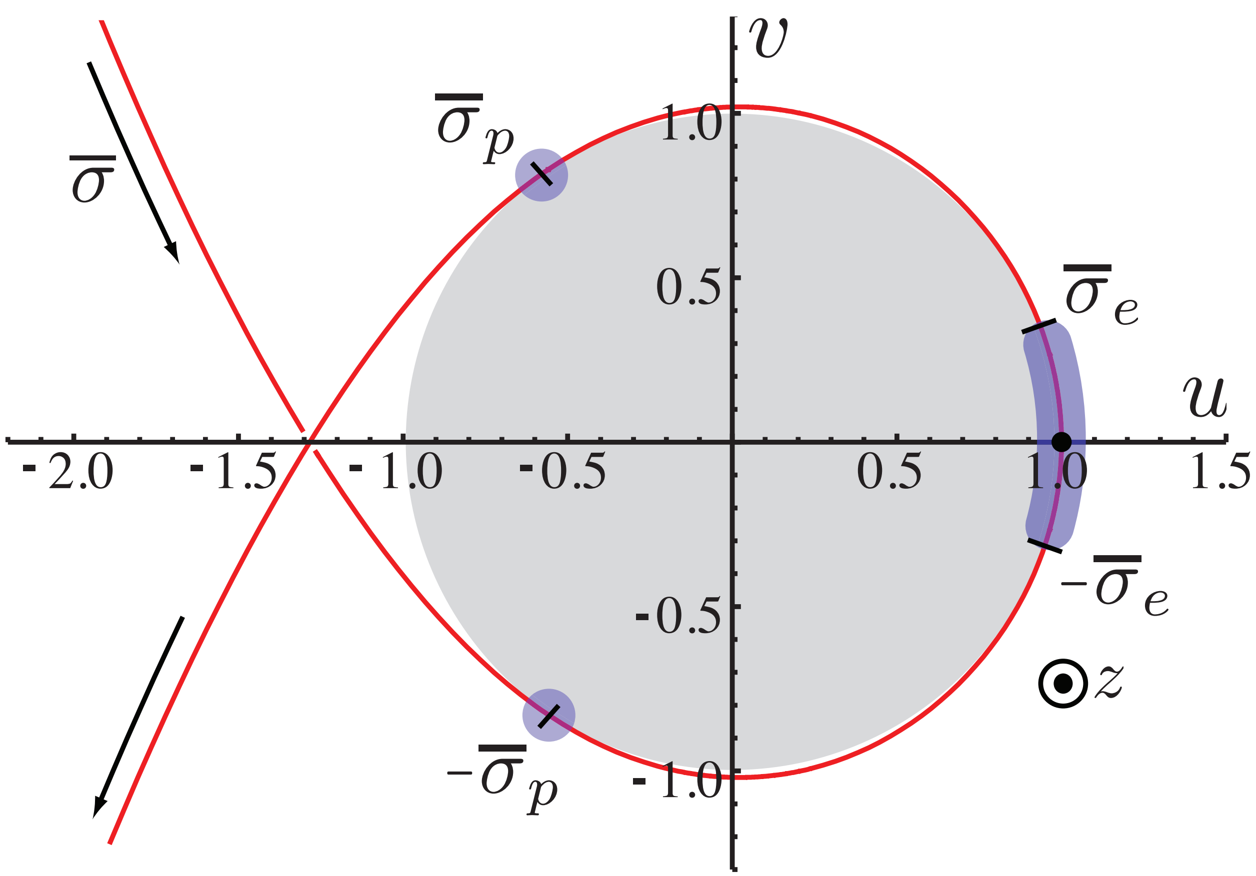




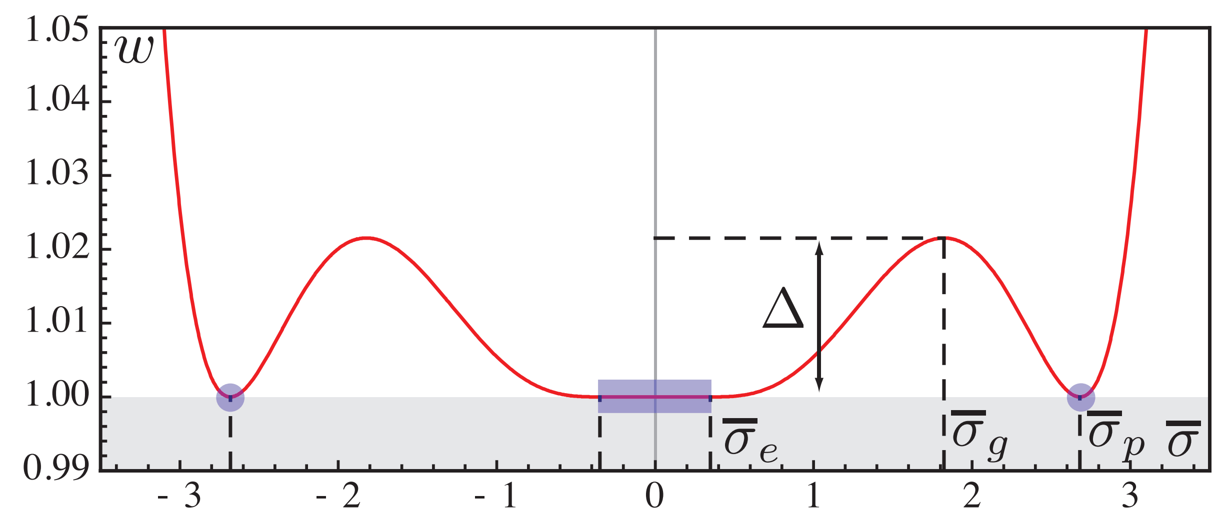
Braid : contact topology



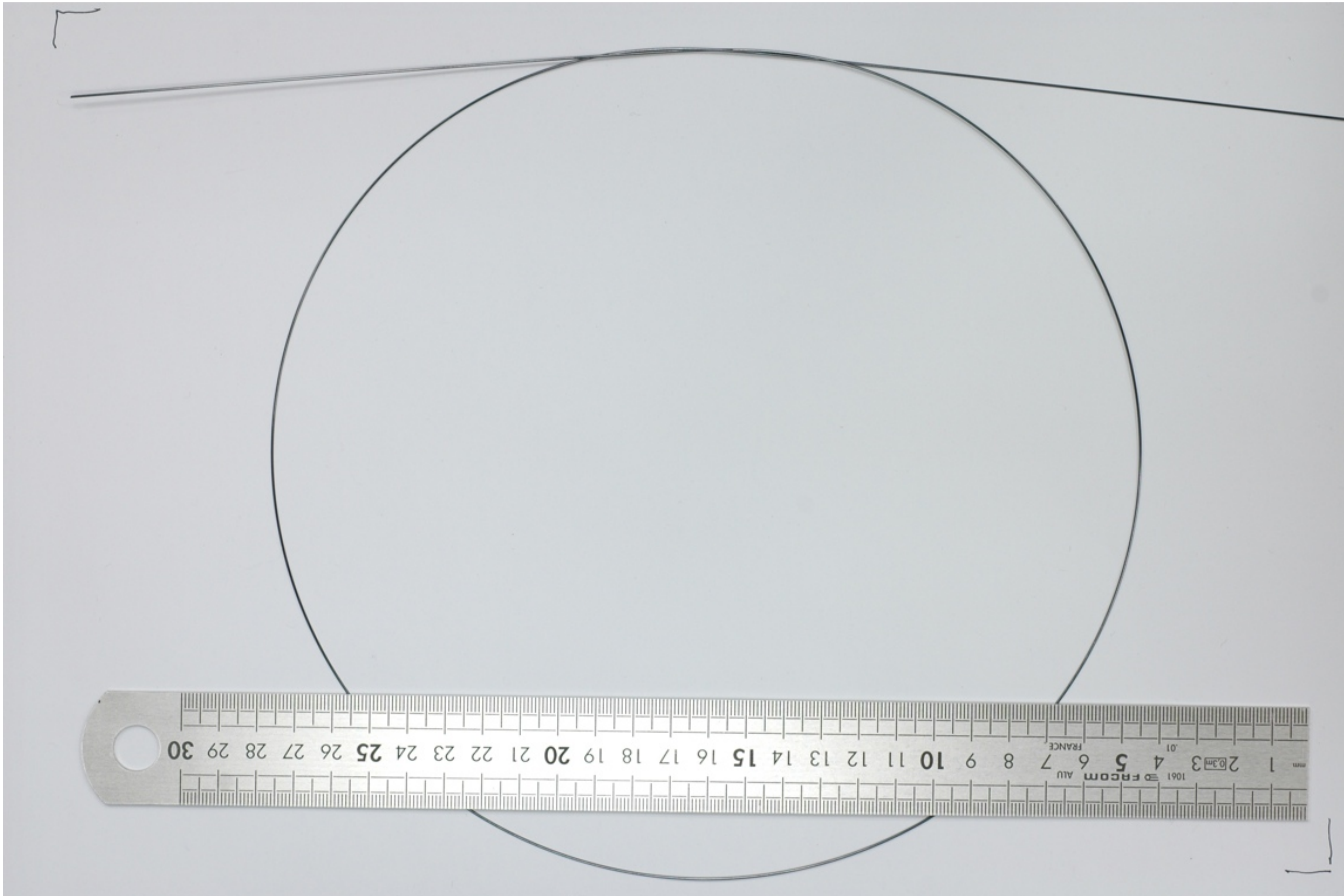
side view



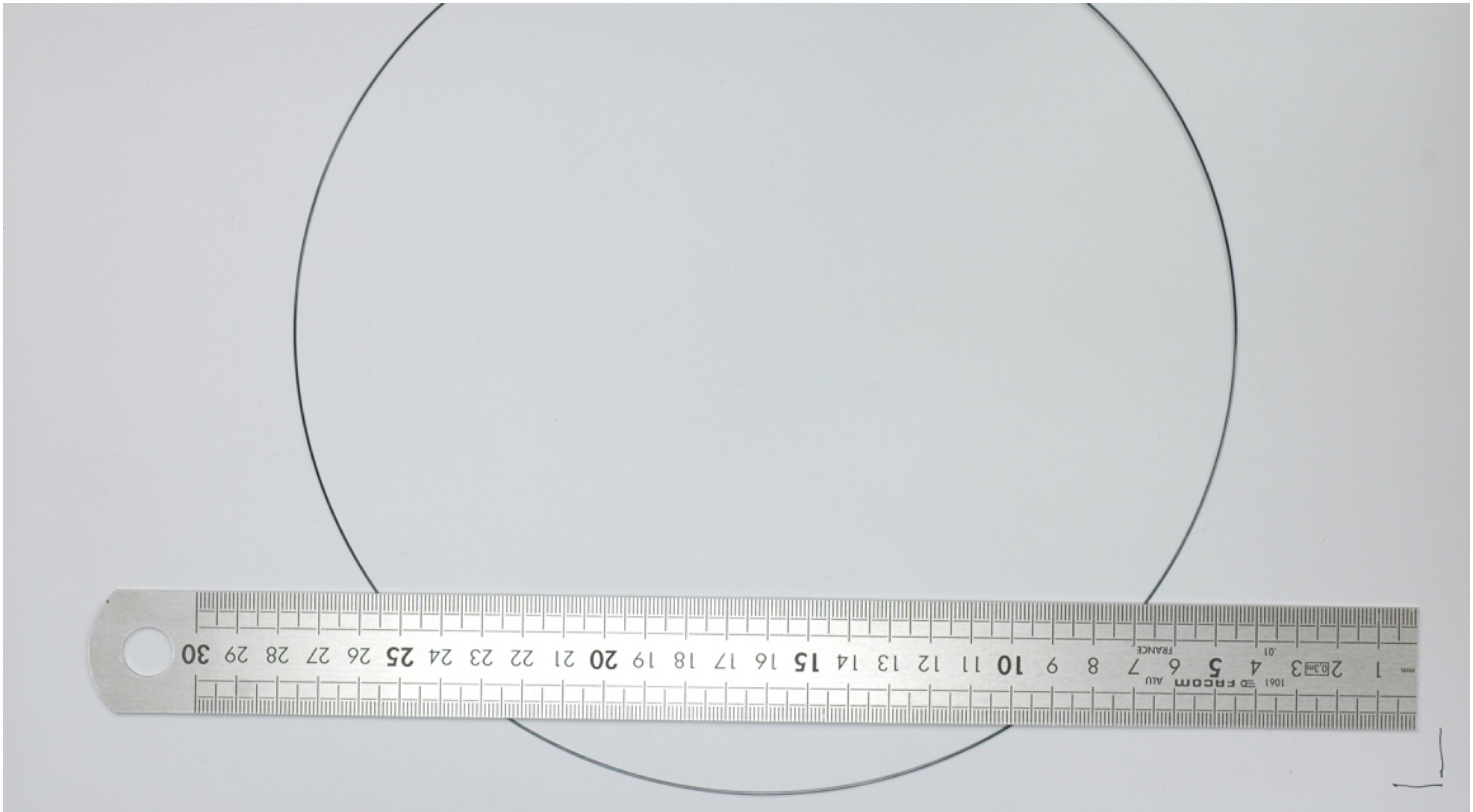
inter-strand distance



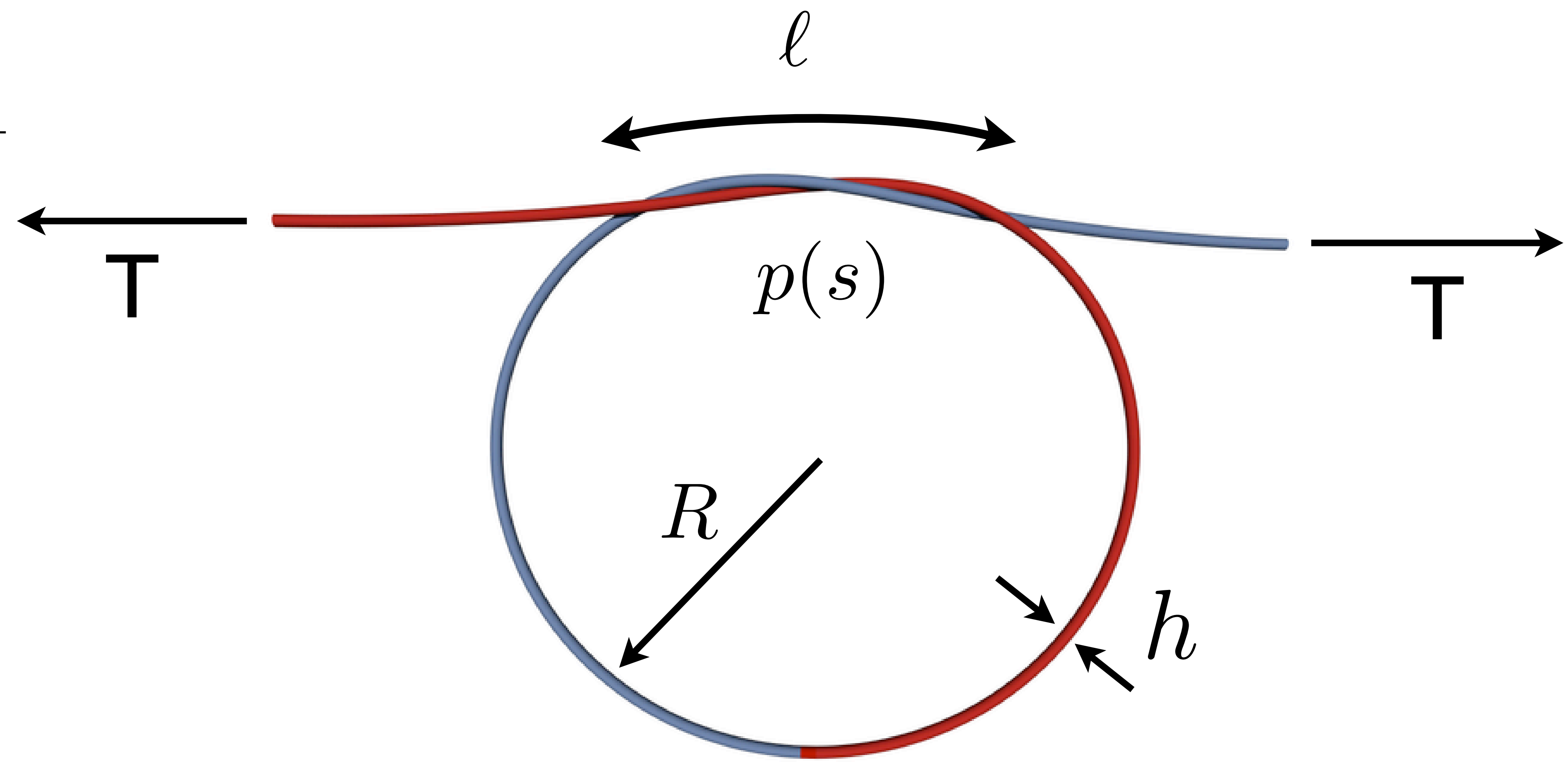
Braid : contact topology



Braid : contact topology



Results



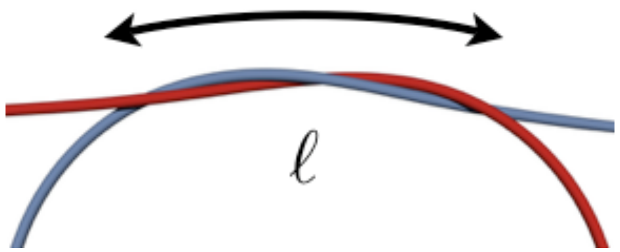
$$R = \sqrt{\frac{EI}{2T}}$$

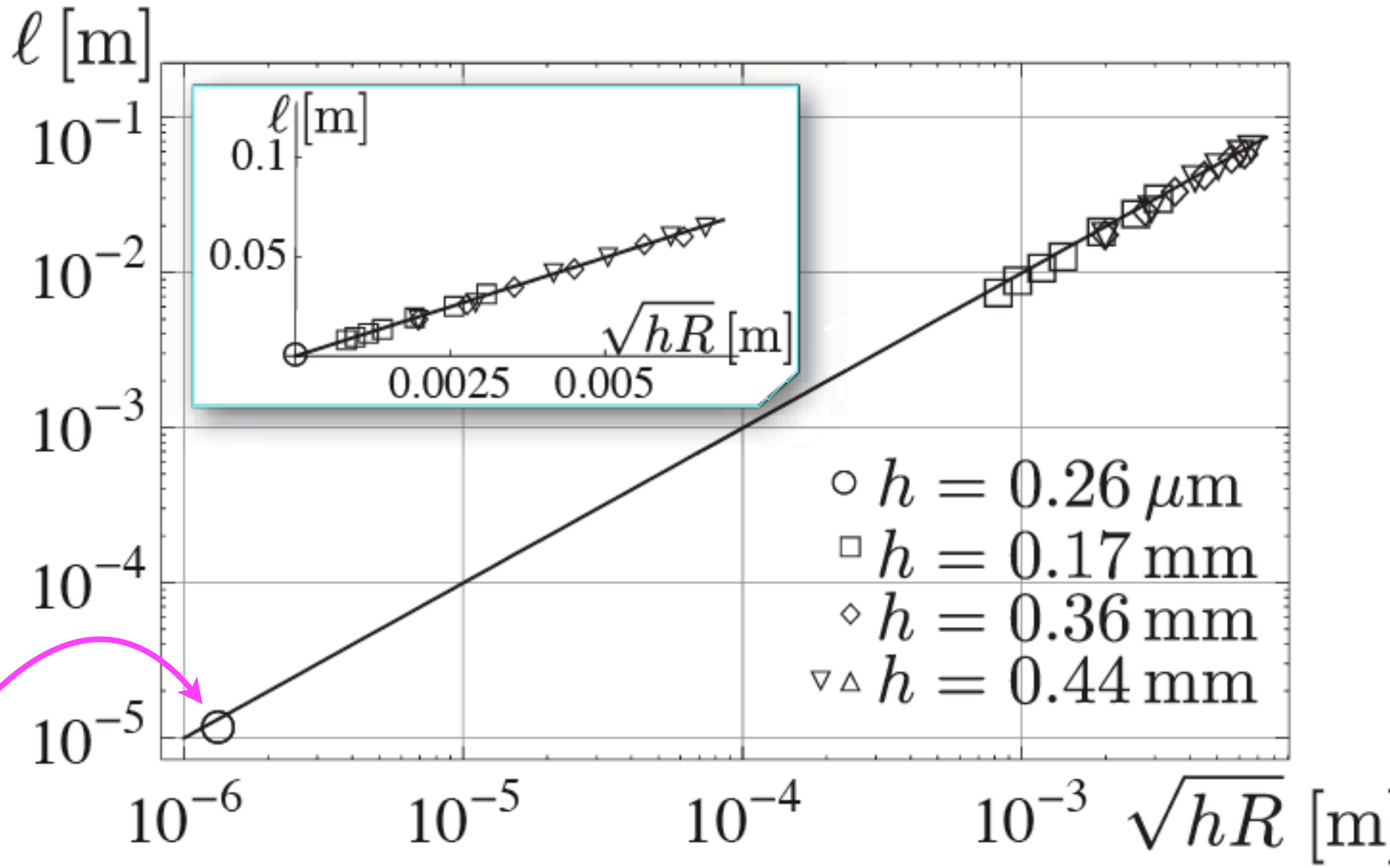
$$\ell = 9.91\, h^{1/2}\ (EI)^{1/4}\ T^{-1/4}$$

Contact pressure $p(s)$

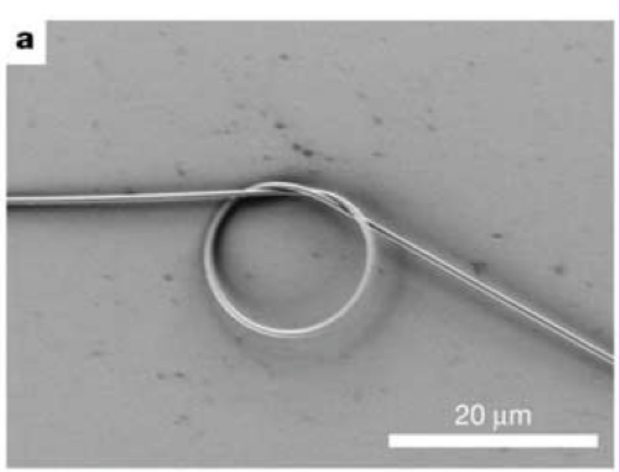
Total contact force $P = \int_0^{\ell} p(s) ds = 0.82\, h^{-1/2}\ (EI)^{1/4}\ T^{3/4}$

Experiments



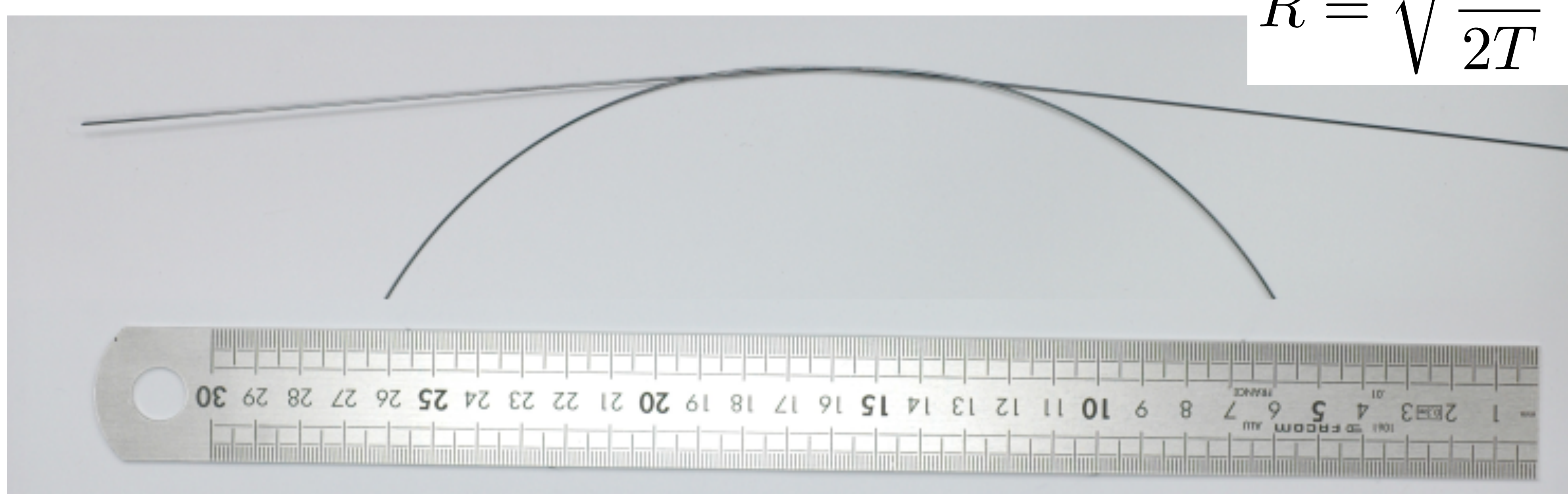


Tong et al., Nature 2003

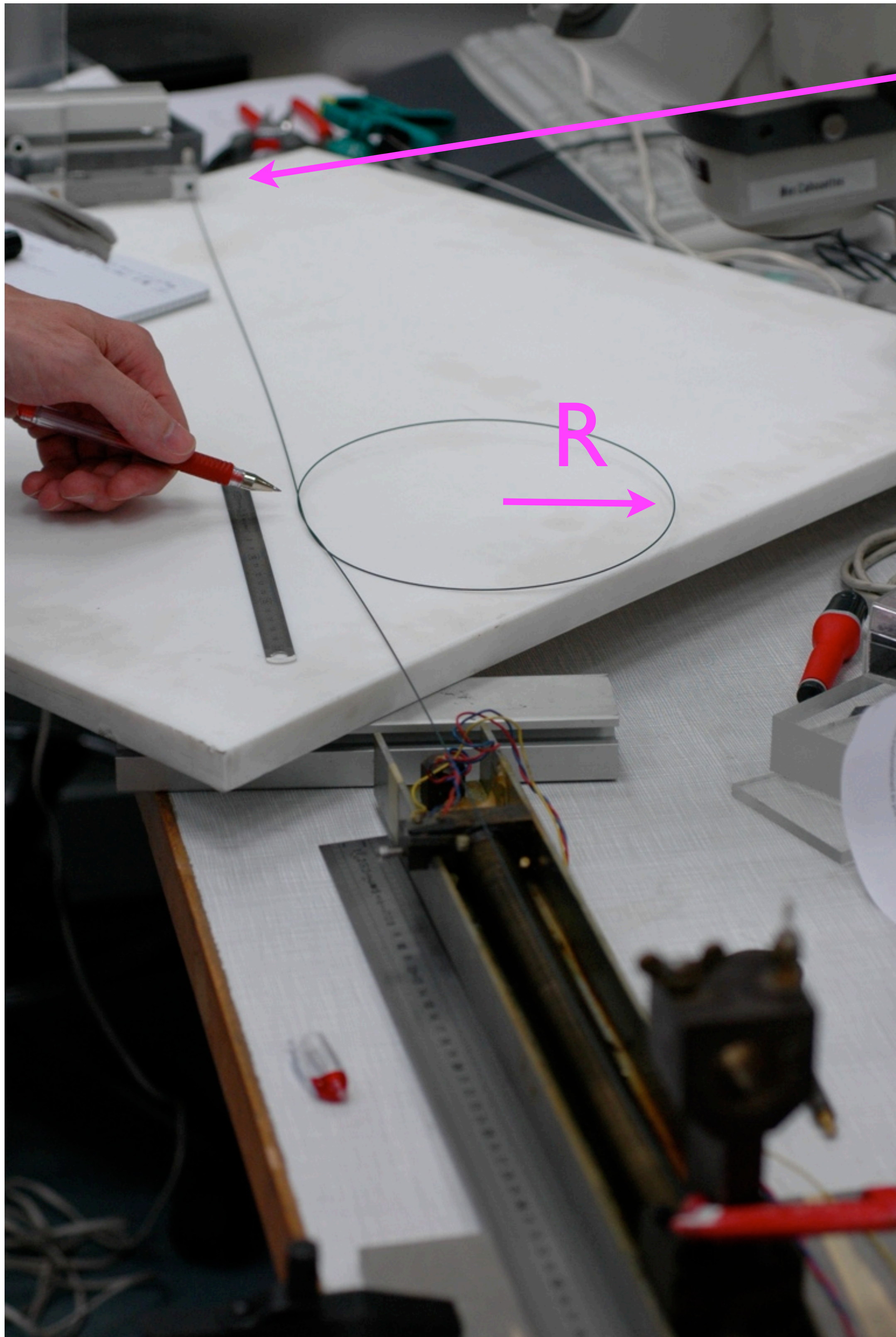


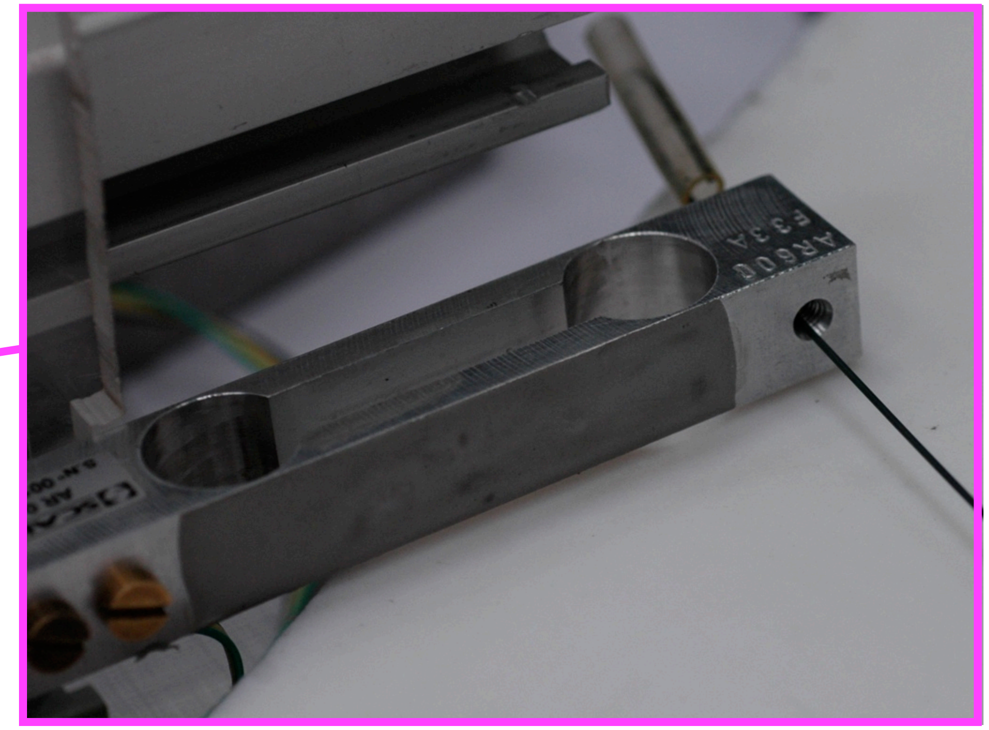
silica wire
h = 1/2 micron

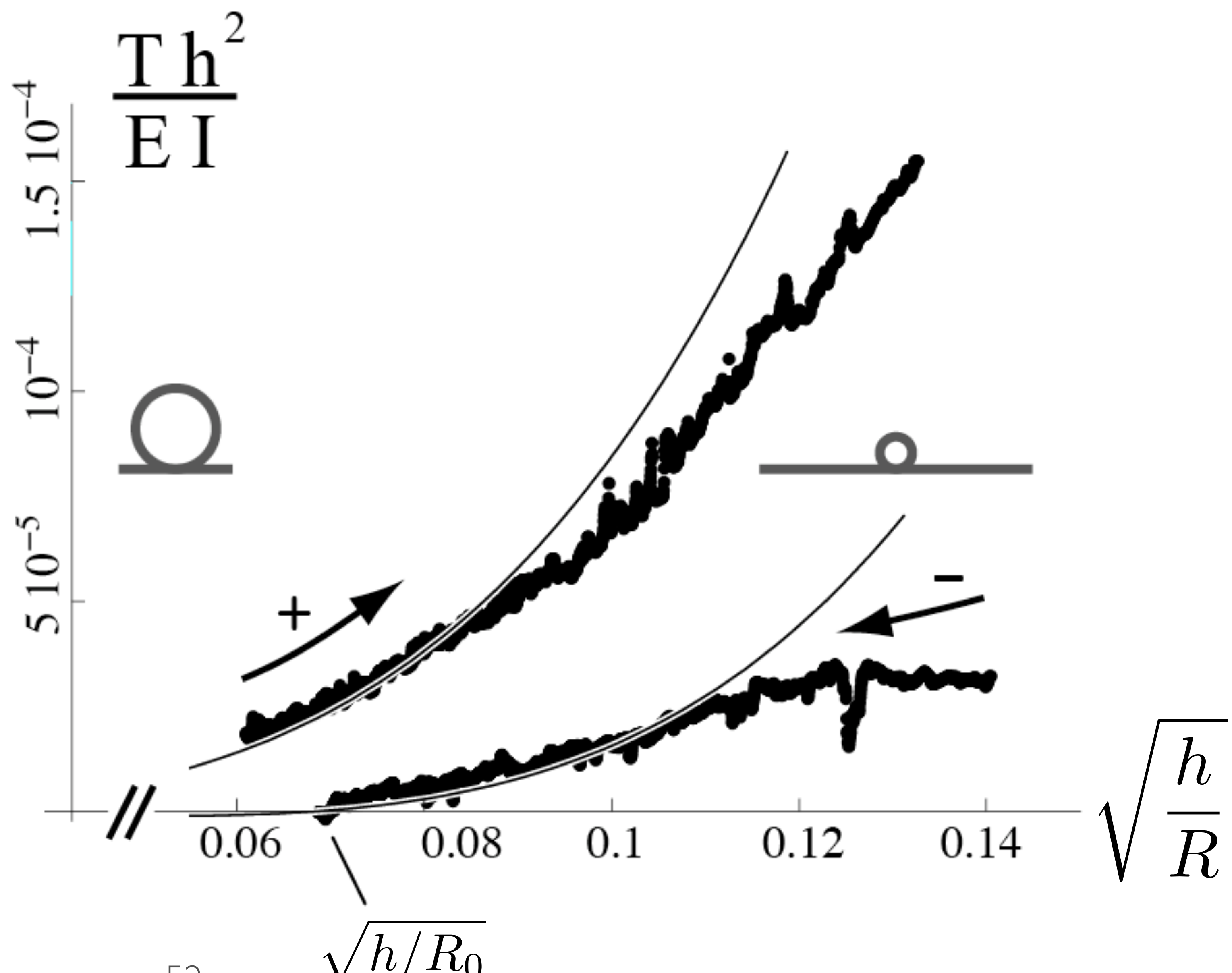
$$R = \sqrt{\frac{EI}{2T}}$$



Experiments

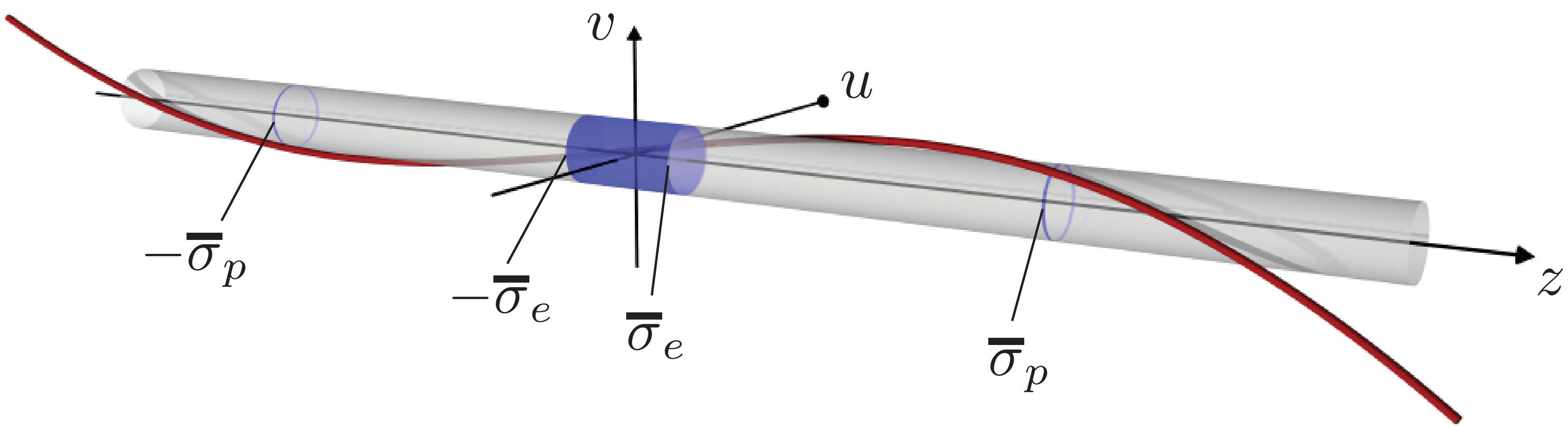






Fin

Braid : variational formulation



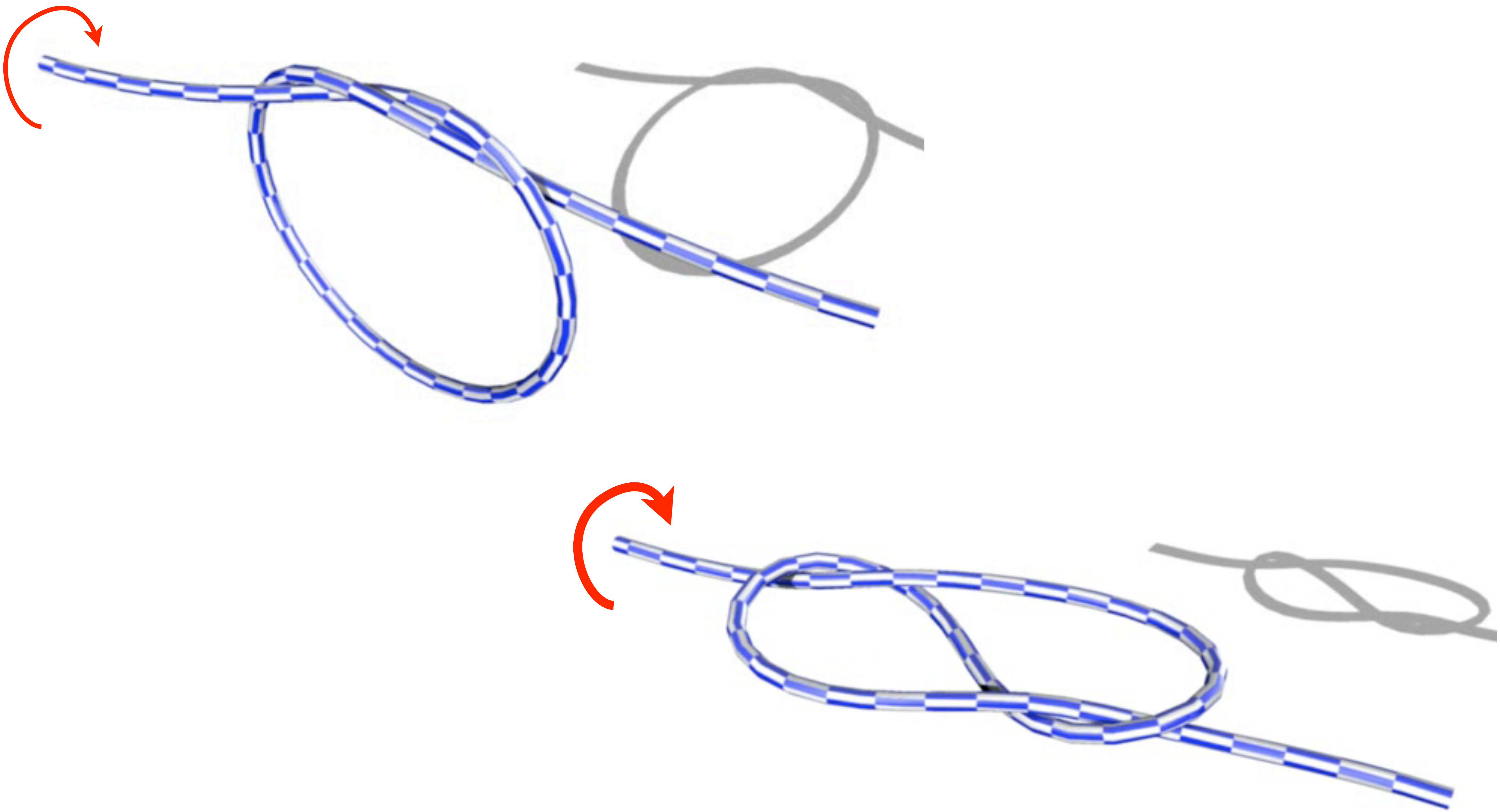
Kirchhoff equations => minimizing an energy

$$V = \frac{1}{2} \int_{-\infty}^{+\infty} \left(u''^2 + v''^2 \right) d\sigma \; + \underbrace{v'(+\infty) + v'(-\infty)}$$

work of external applied moments

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

Twist Instability

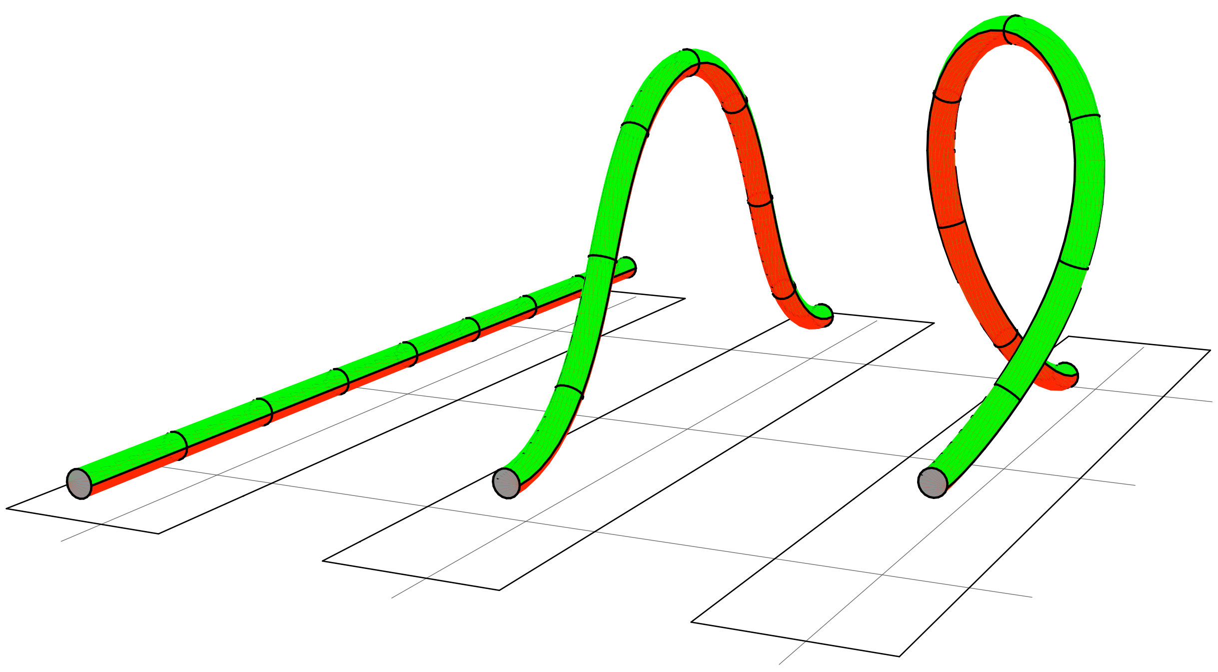


numerical simulations : M. Bergou, M. Wardetzky, S. Robinson, B. Audoly, and E. Grinspun.

ACM Transactions on Graphics (SIGGRAPH), 2008

Twisted rods : the ideal case

if rod is uniform, isotropic, naturally straight



system reduction
21 D => 6D

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