Elastic knots

(elastic beam under finite rotation and self-contact)

Sébastien Neukirch

CNRS & Univ Paris 6 (France)

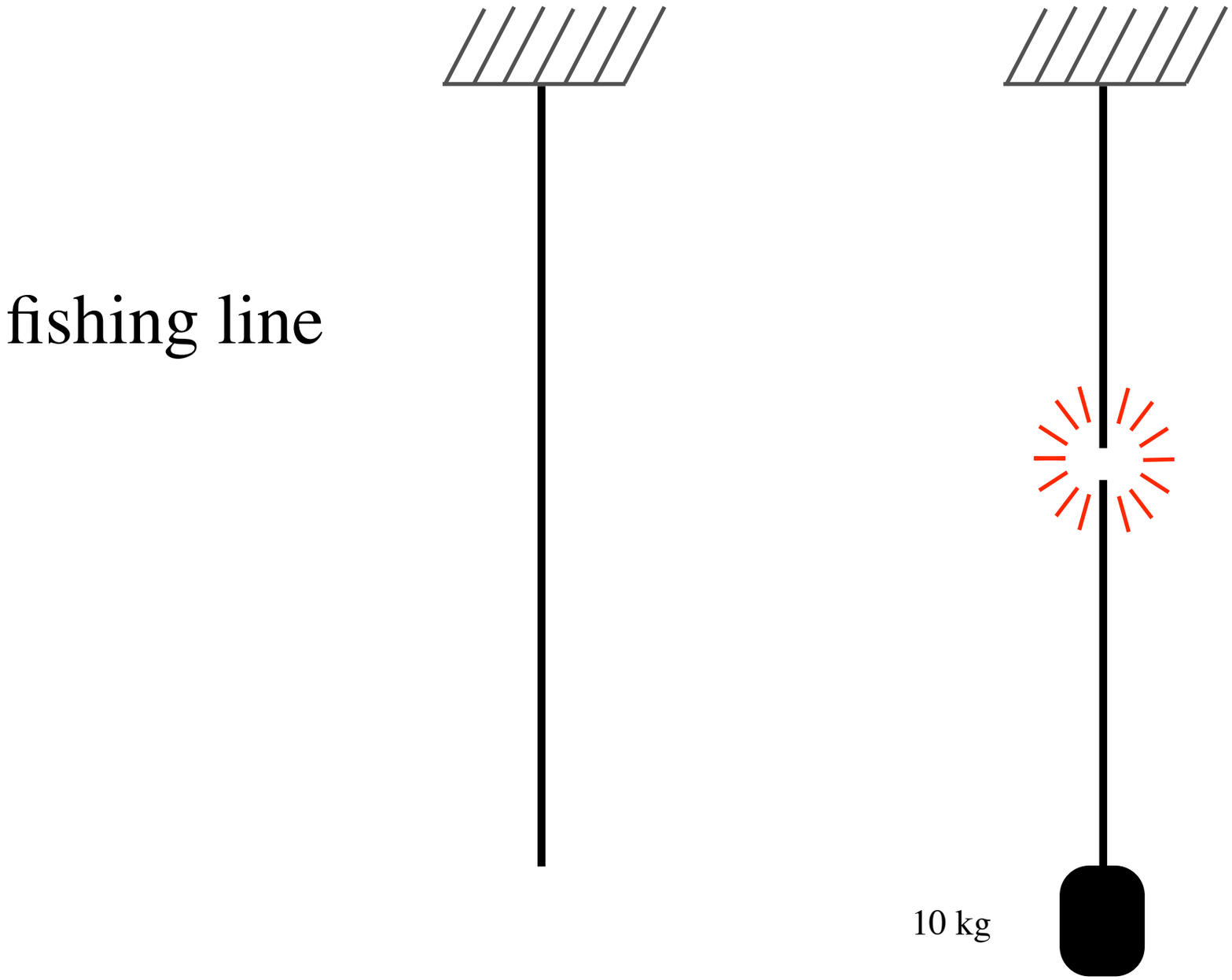
d'Alembert Institute for Mechanics

joint work with:

Nicolas Clauvelin (PhD work)

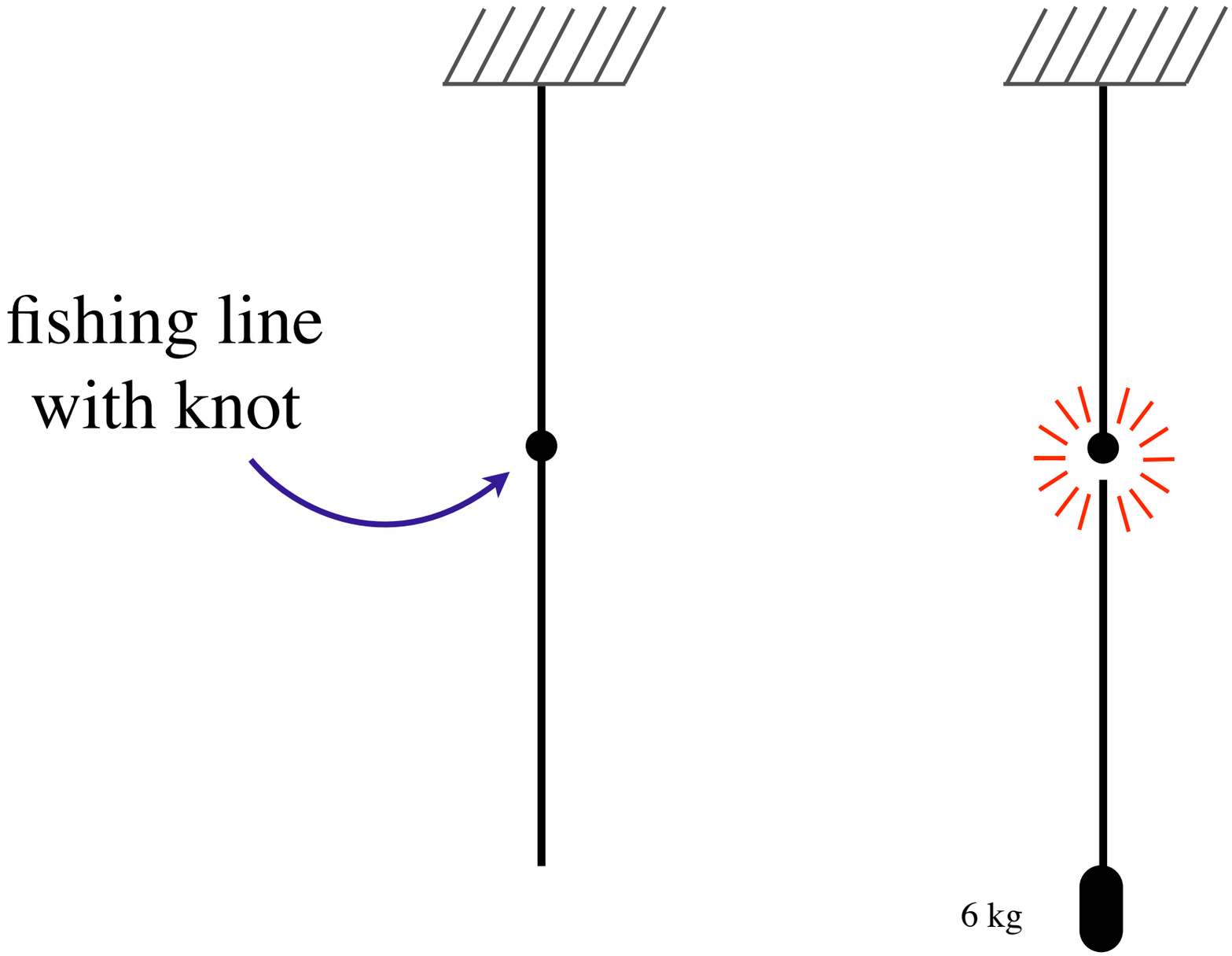
Basile Audoly

Tensile strength of a wire



Stasiak et al, *Science* (1999)

Tensile strength of a wire



Stasiak et al, *Science* (1999)

Knots are everywhere

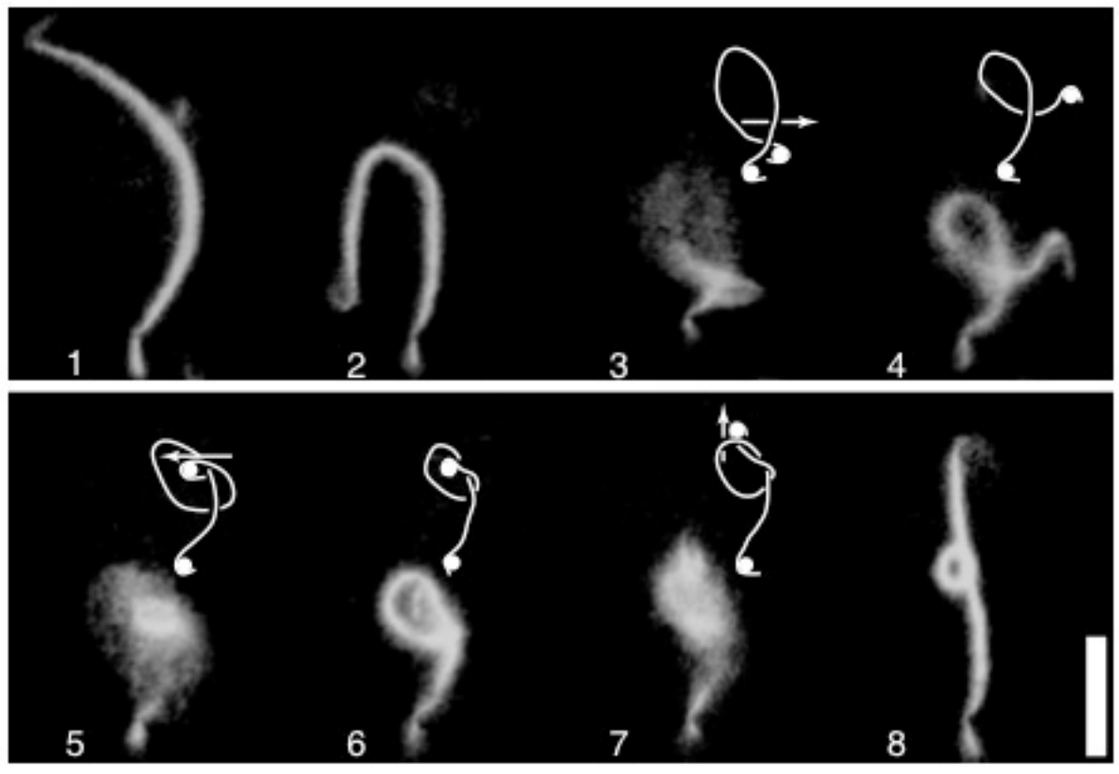
Long enough polymers are (almost) certainly knotted

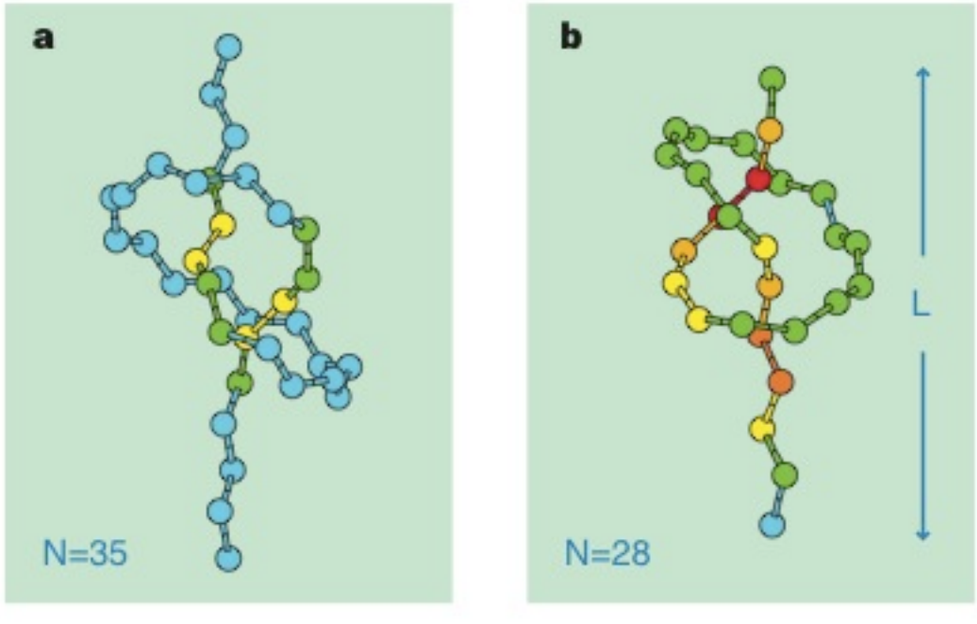
Sumners+Whittington, J. Phys. A : Math. Gen. 1988

273 knotted proteins in the ProteinDataBank (1%)

Single molecule experiment
with knotted F-Actin filaments

Arai et al, *Nature* (1999)

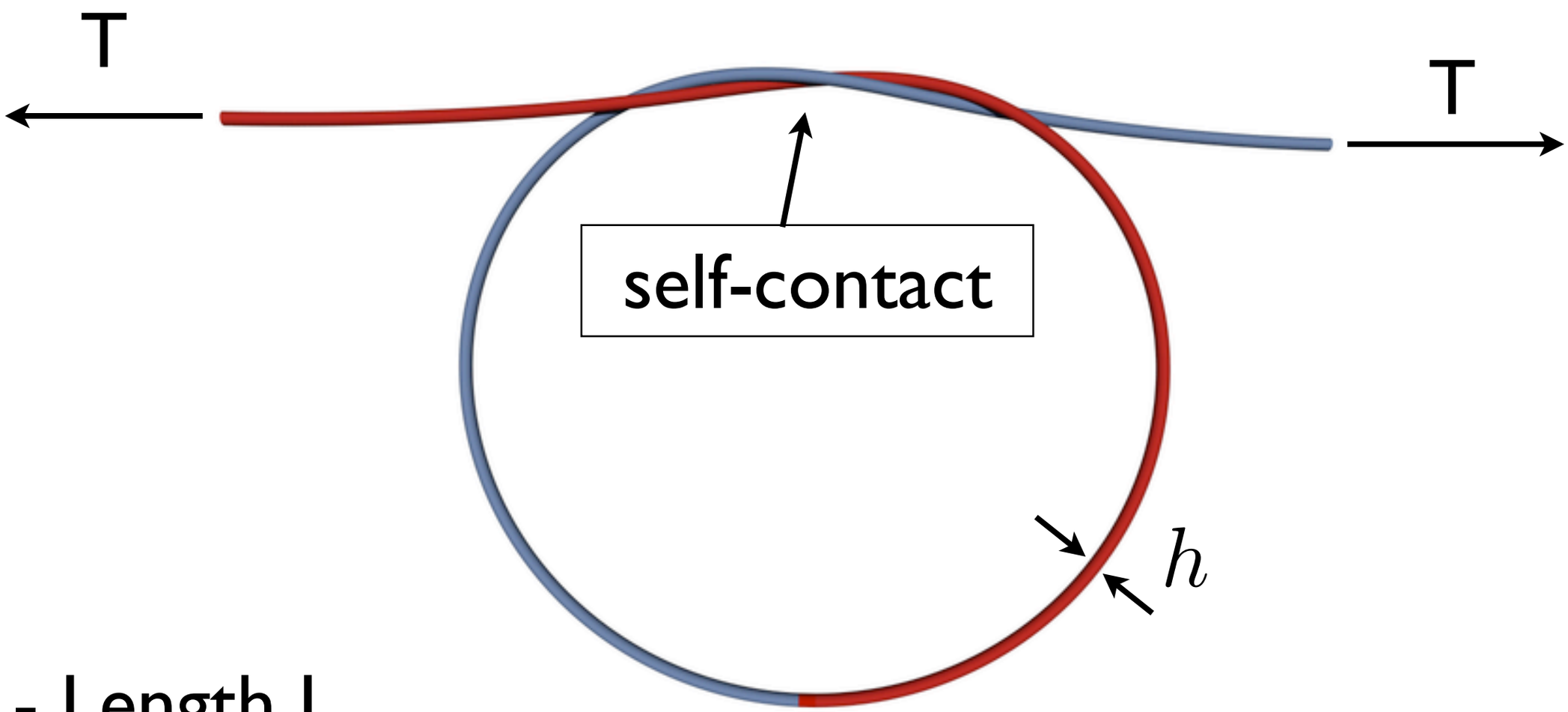




Ab-initio molecular simulations
for alcane molecule (C10H22)

Saitta et al, *Nature* (1999)

Elastic knots



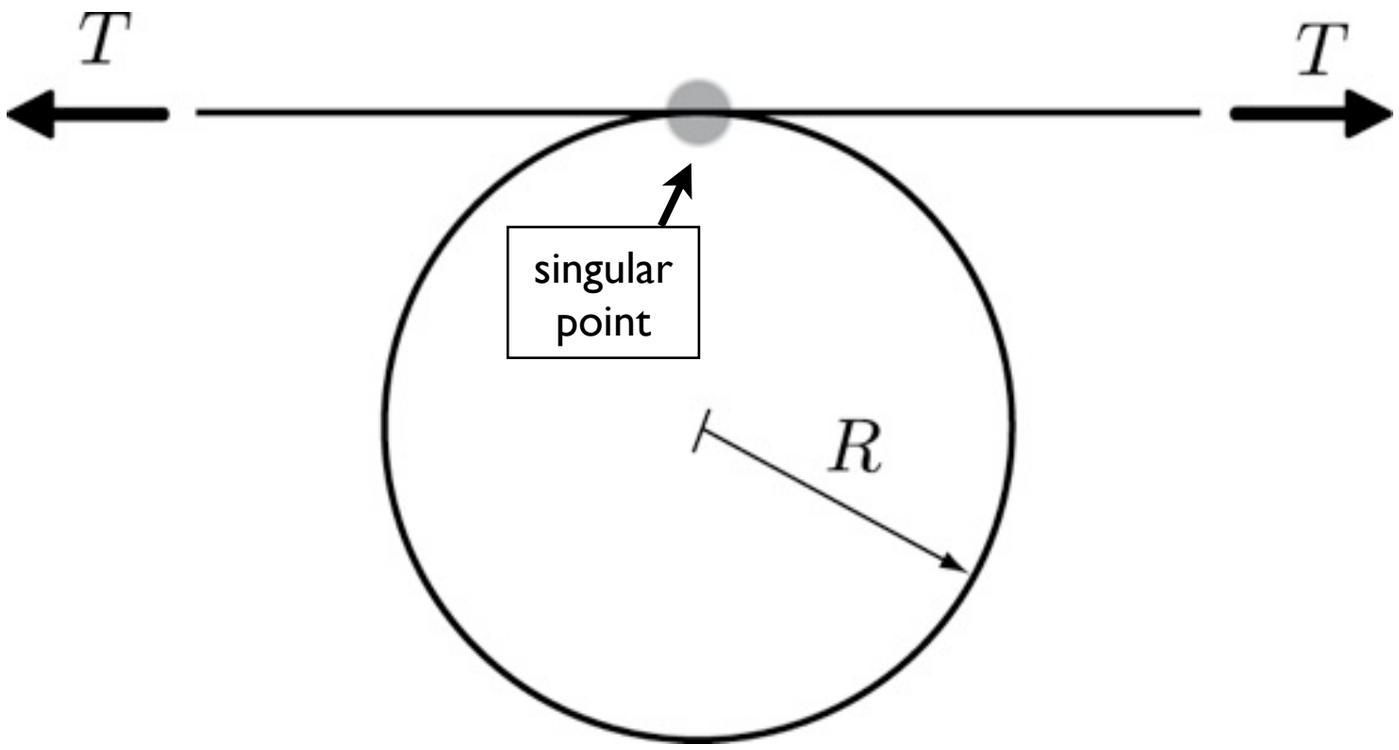
- Length L
- Circular cross-section: radius h
- Bending rigidity : E I
- Twist rigidity : G J

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

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

E : Young's modulus G : shear modulus

Zero thickness case

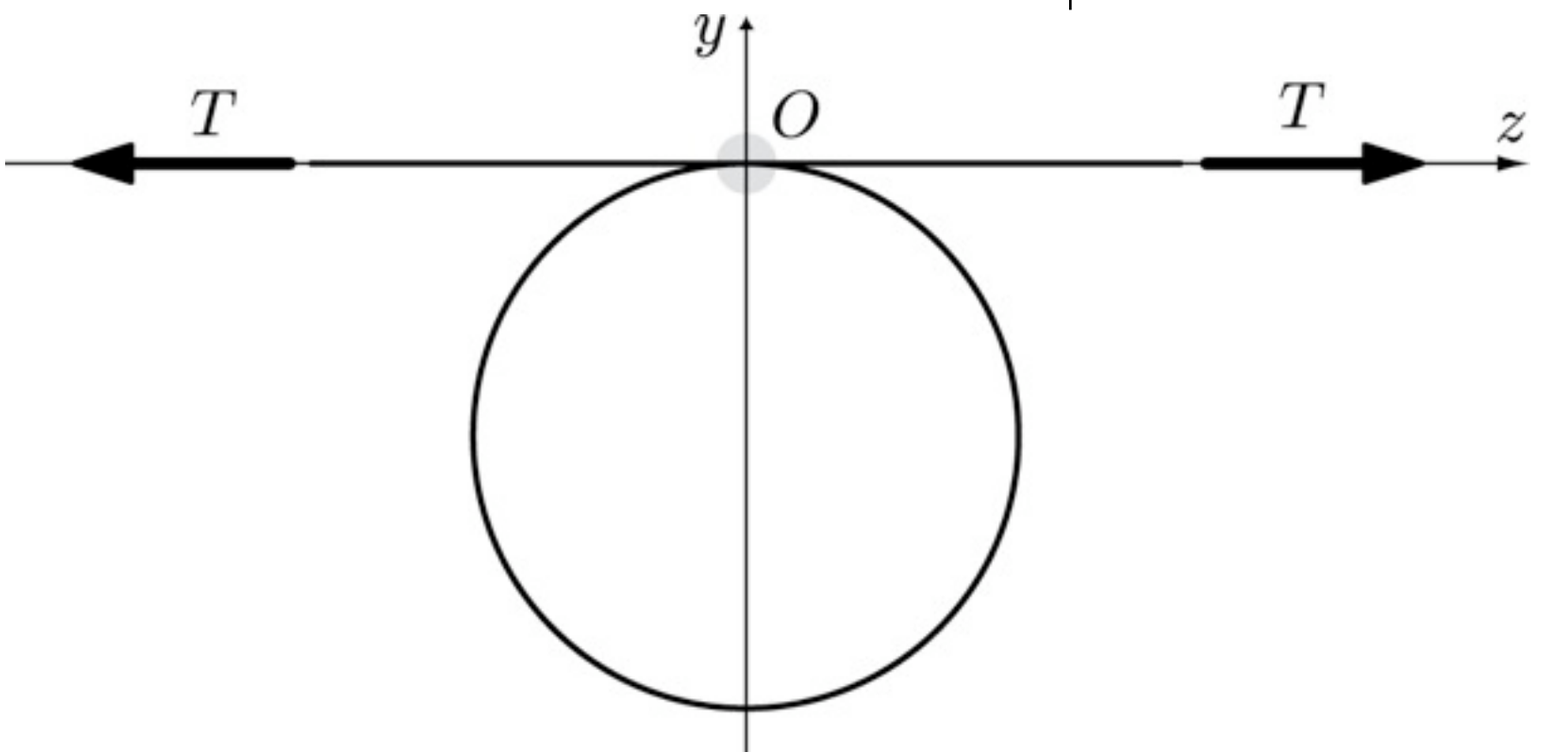


equilibrium : $T = \dfrac{EI}{2R^2}$

tension T —(singular point)→ curvature $\dfrac{1}{R}$

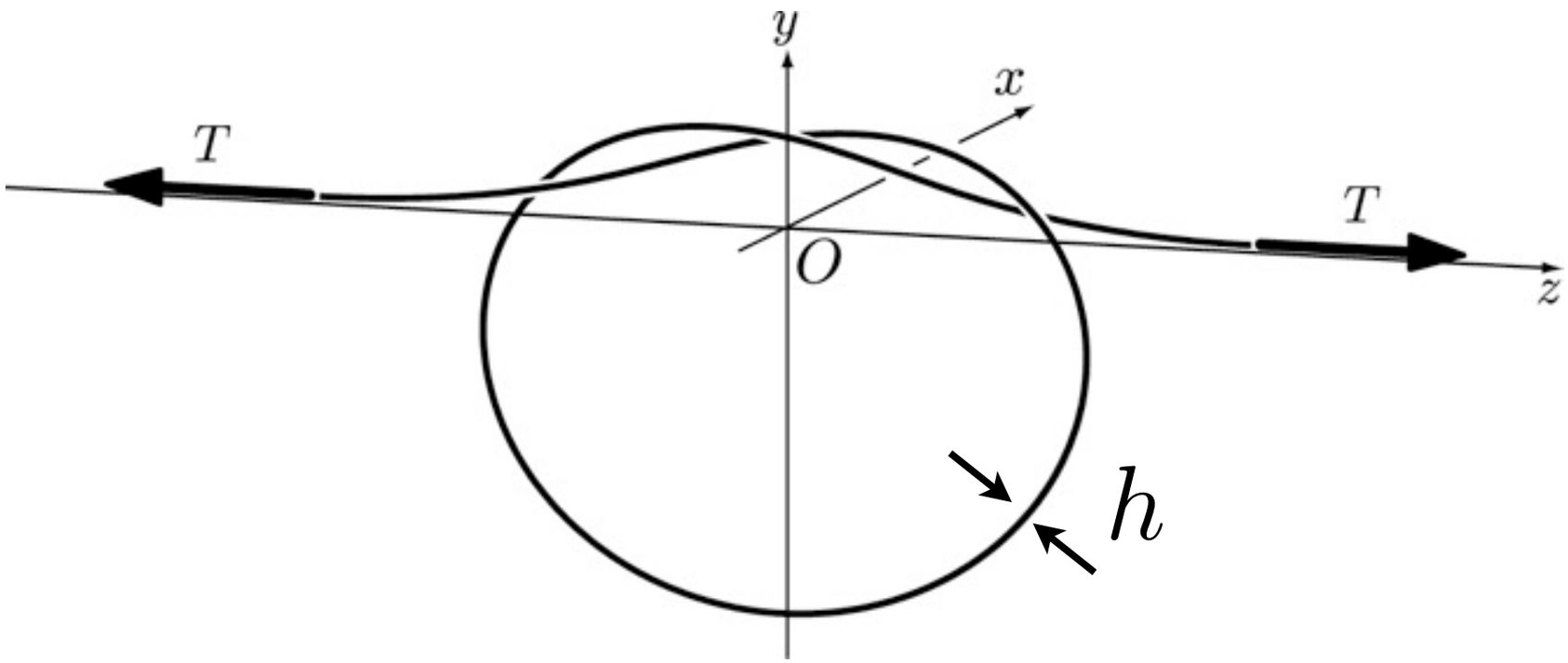
Perturbative problem

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

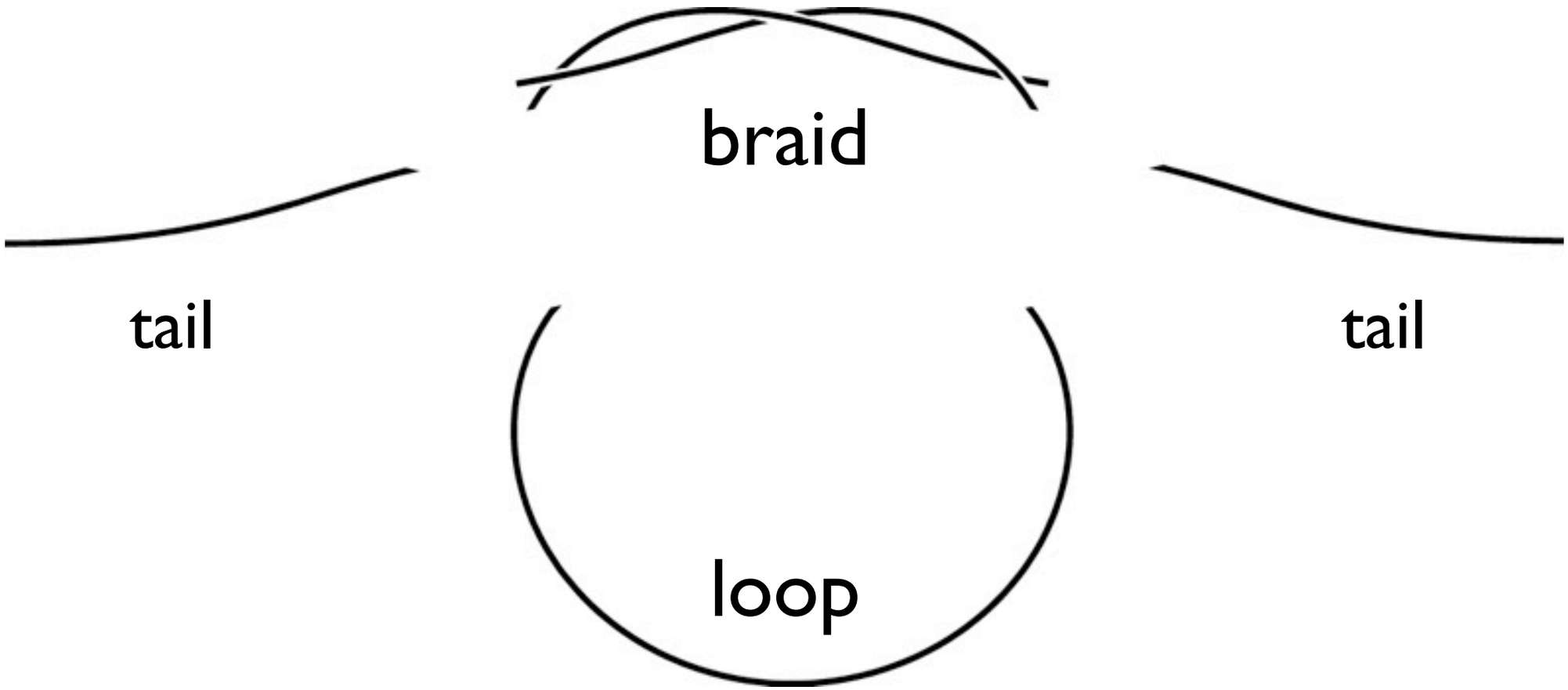


small parameter

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



Matched asymptotic expansions



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

Kirchhoff Equations

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

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

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

$\vec{R}(s)$ position

$\vec{t}(s)$ tangent

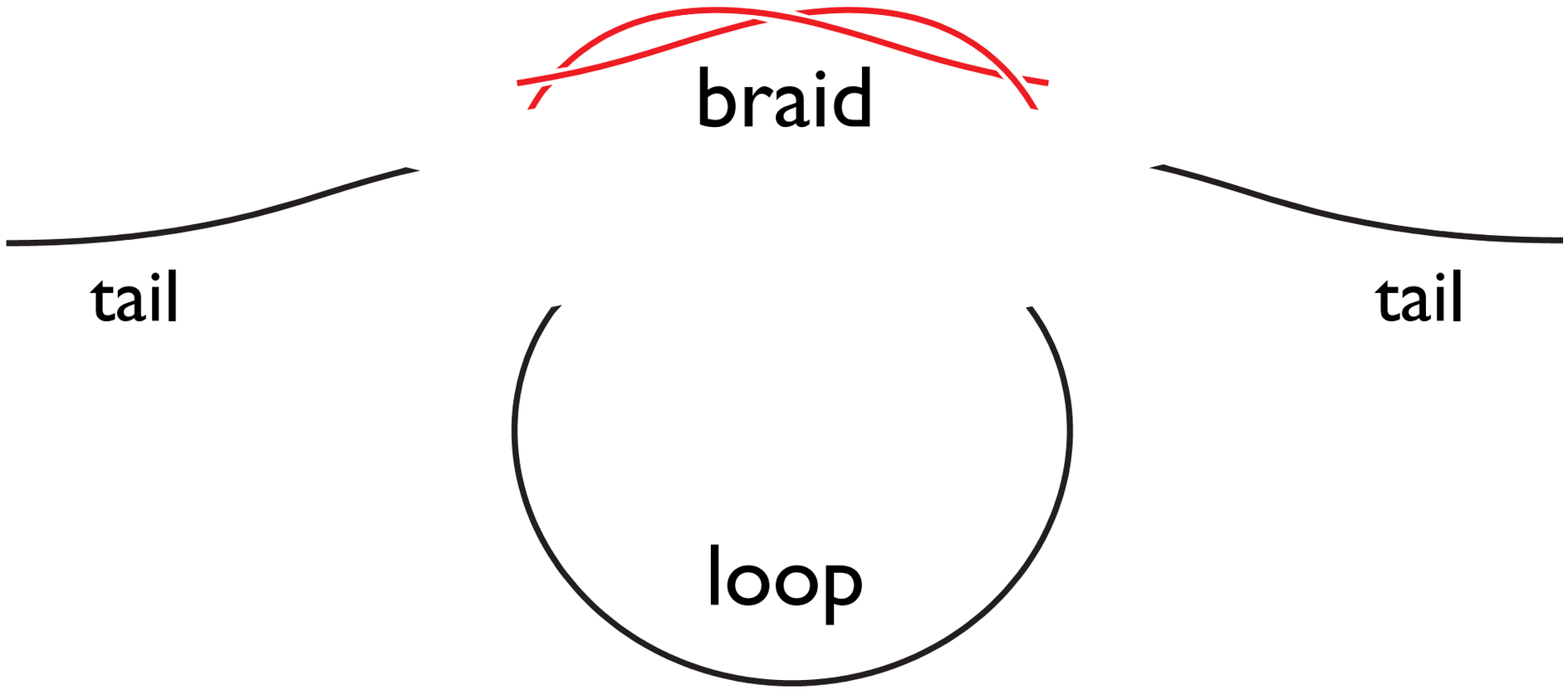
$$' \equiv \frac{d}{ds}$$

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

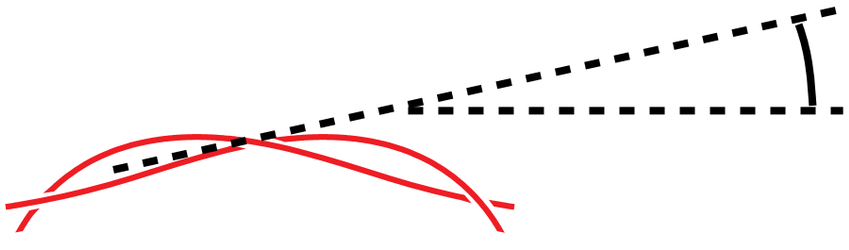
constitutive equations:

$$\begin{aligned} M_\kappa &= EI\,\kappa && \text{curvature } \kappa \\ M_\tau &= GJ\,\tau && \text{twist } \tau \end{aligned}$$

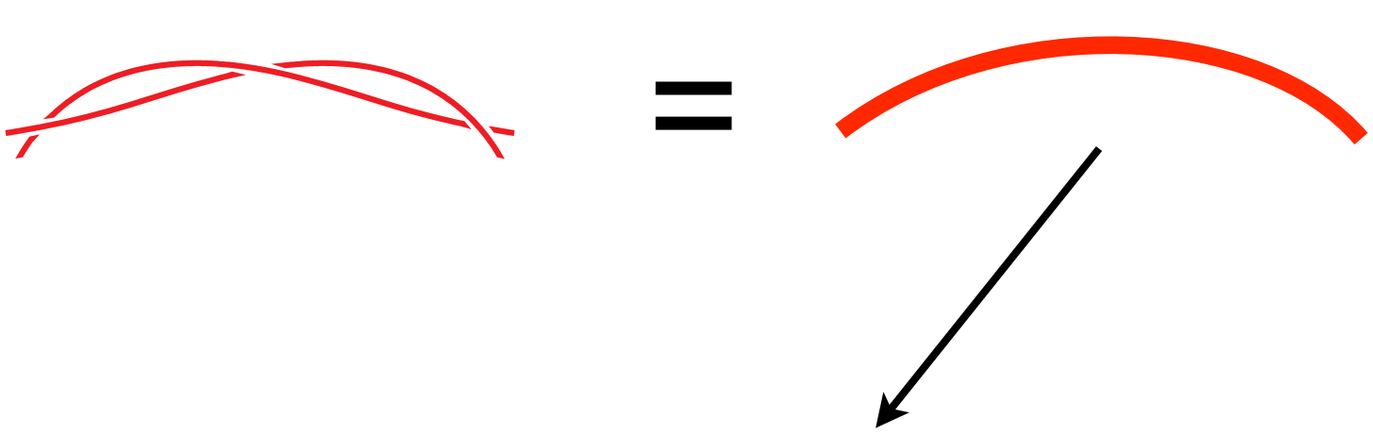
Braid : self-contact zone



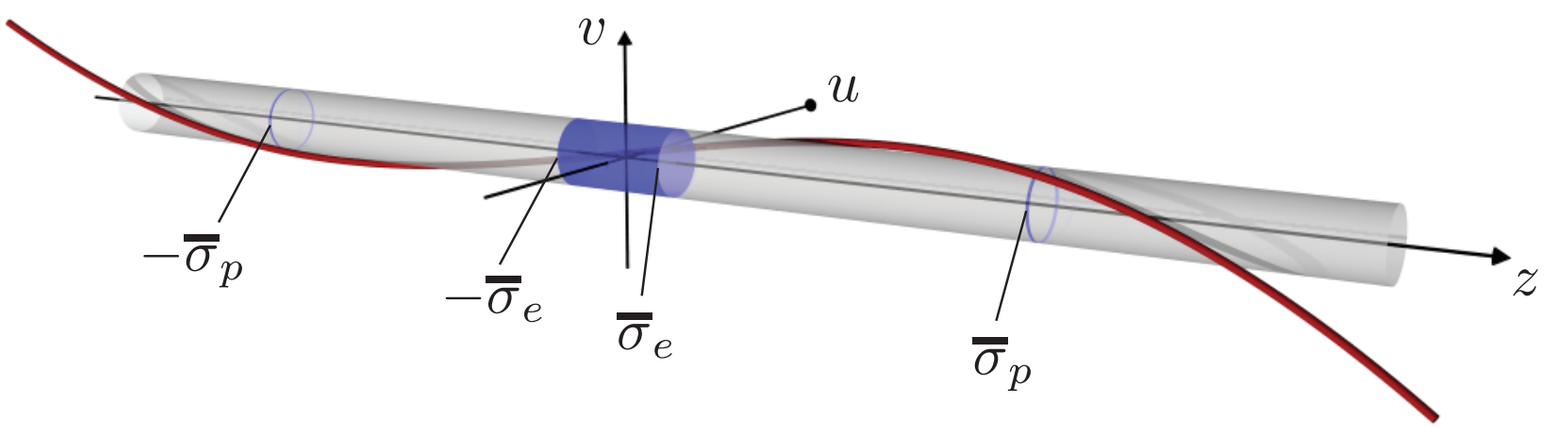
Braid : linear superposition



small deflections => linear problem



Braid : variational formulation



Kirchhoff equations => minimizing an energy

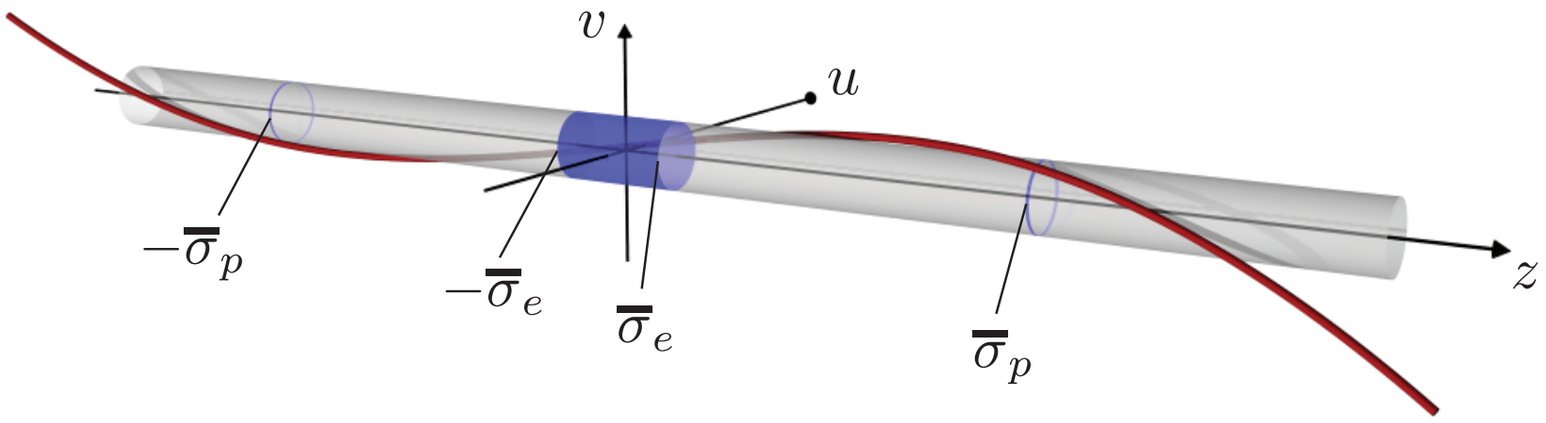
$$V = \frac{1}{2}\int_{-\infty}^{+\infty}\left(u''^2 + v''^2\right)d\sigma \; + \underbrace{v'(+\infty) + v'(-\infty)}$$

work of external applied moments

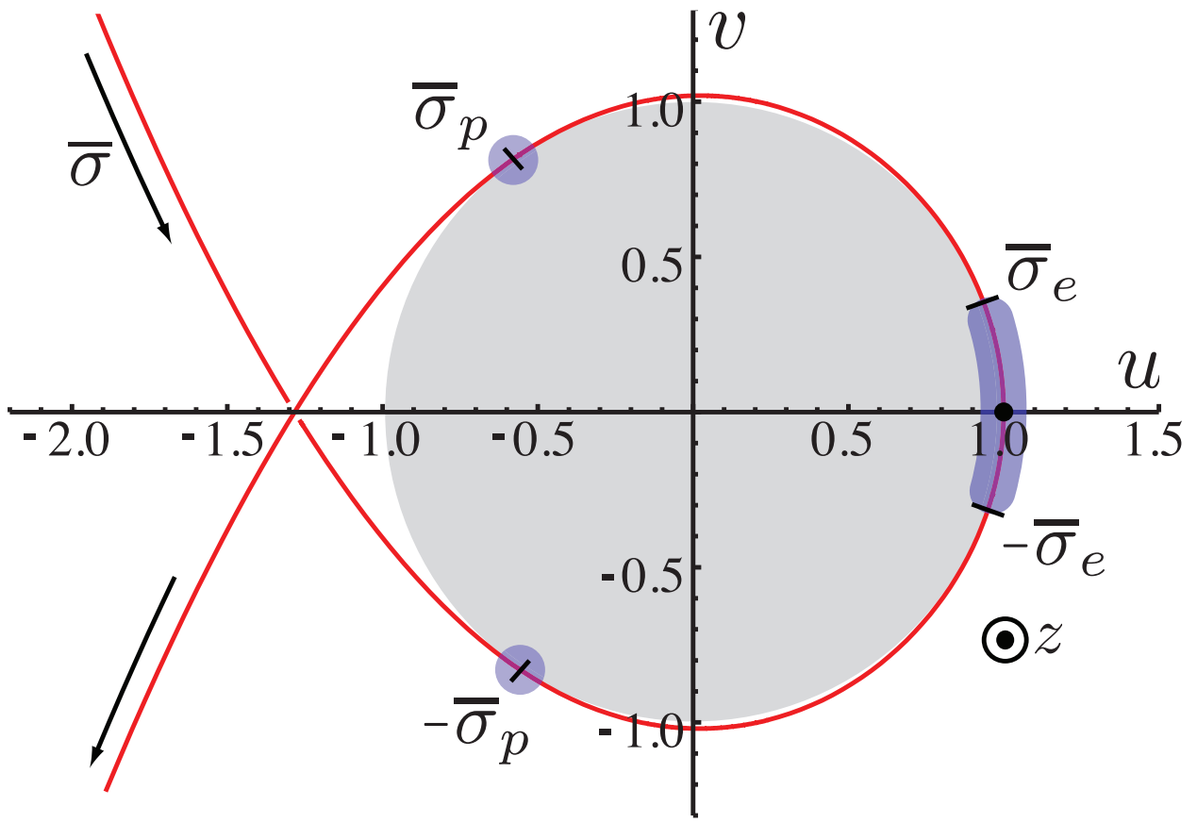
with constraint:

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

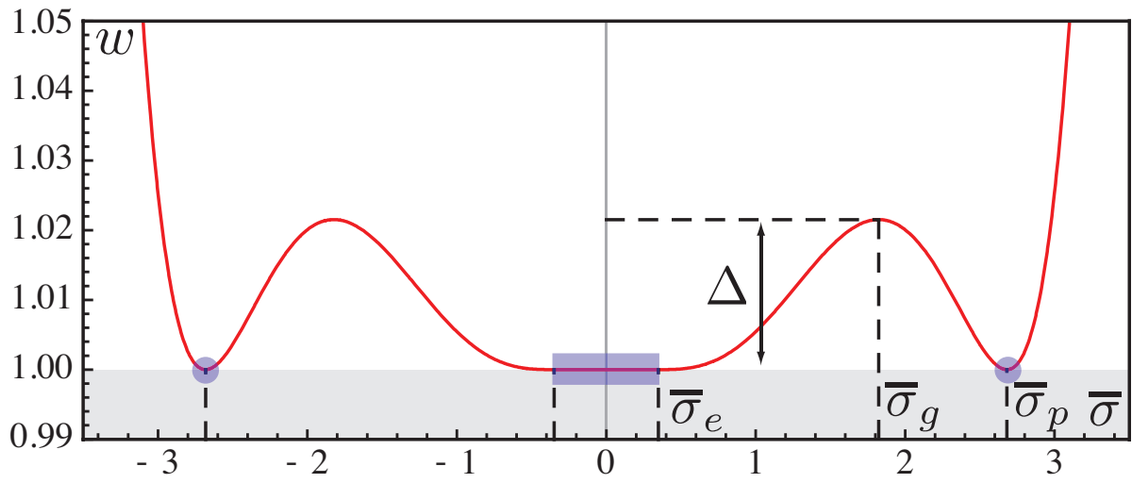
Braid : contact topology



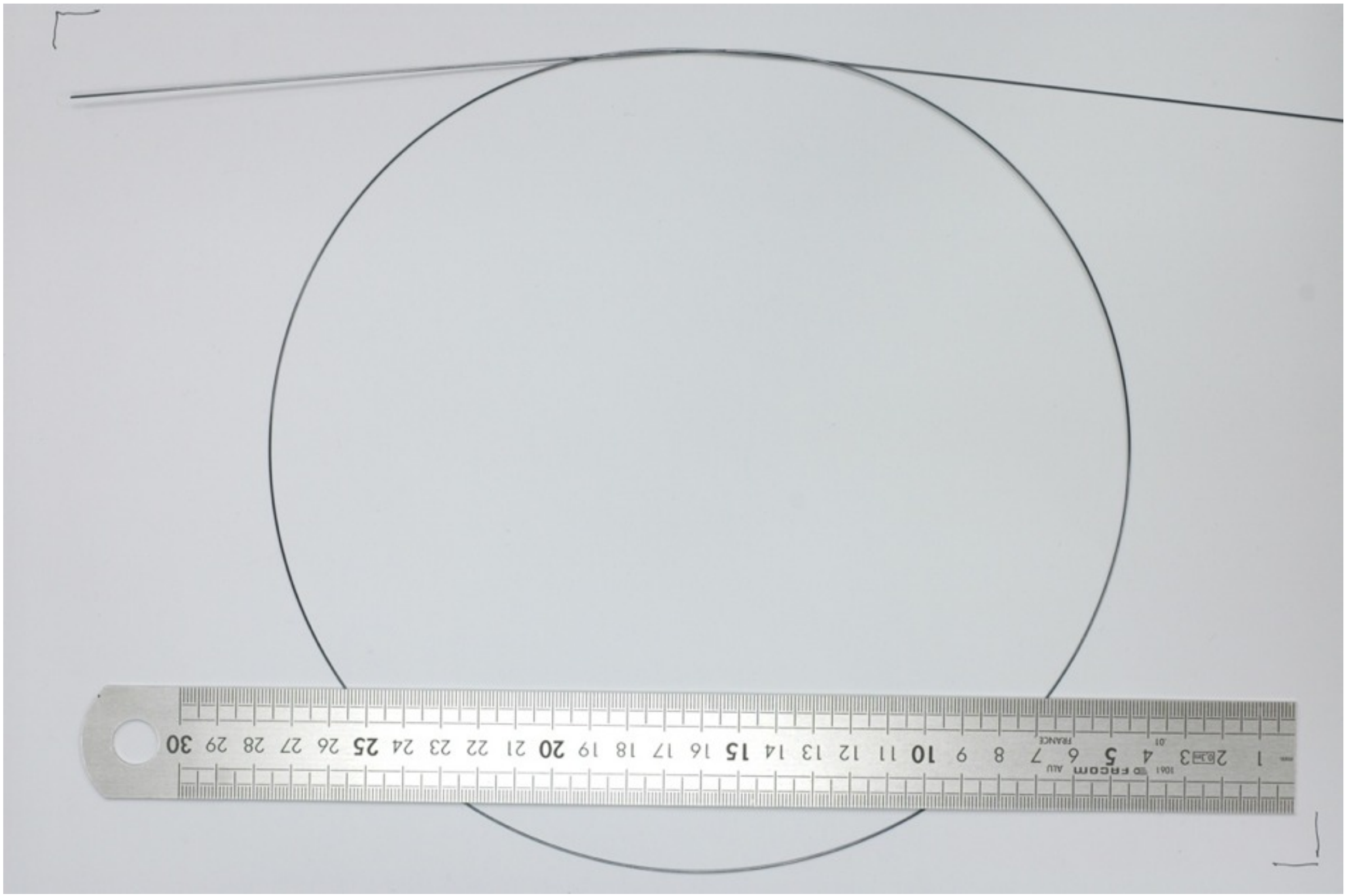
side view



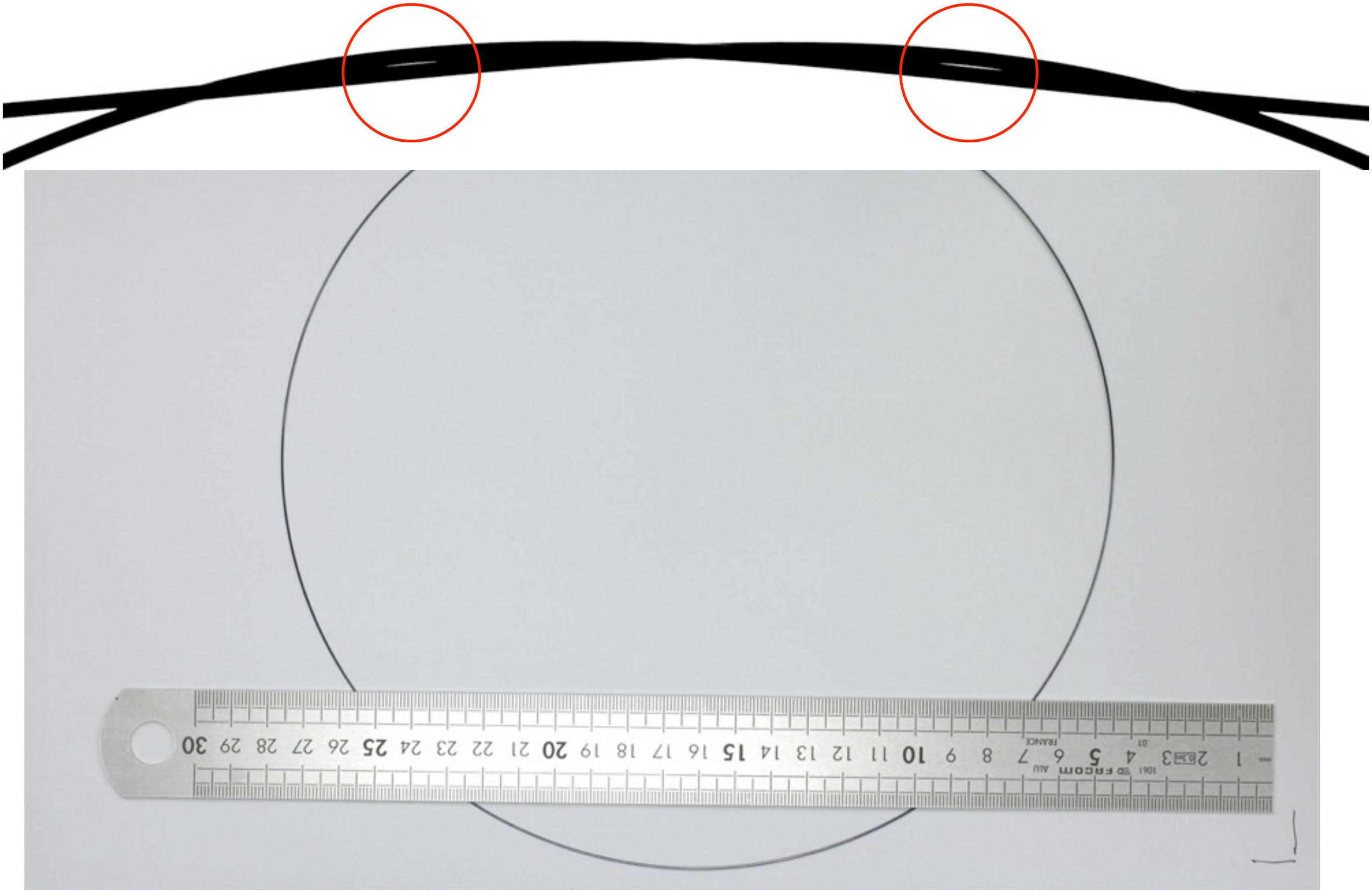
inter-strand distance



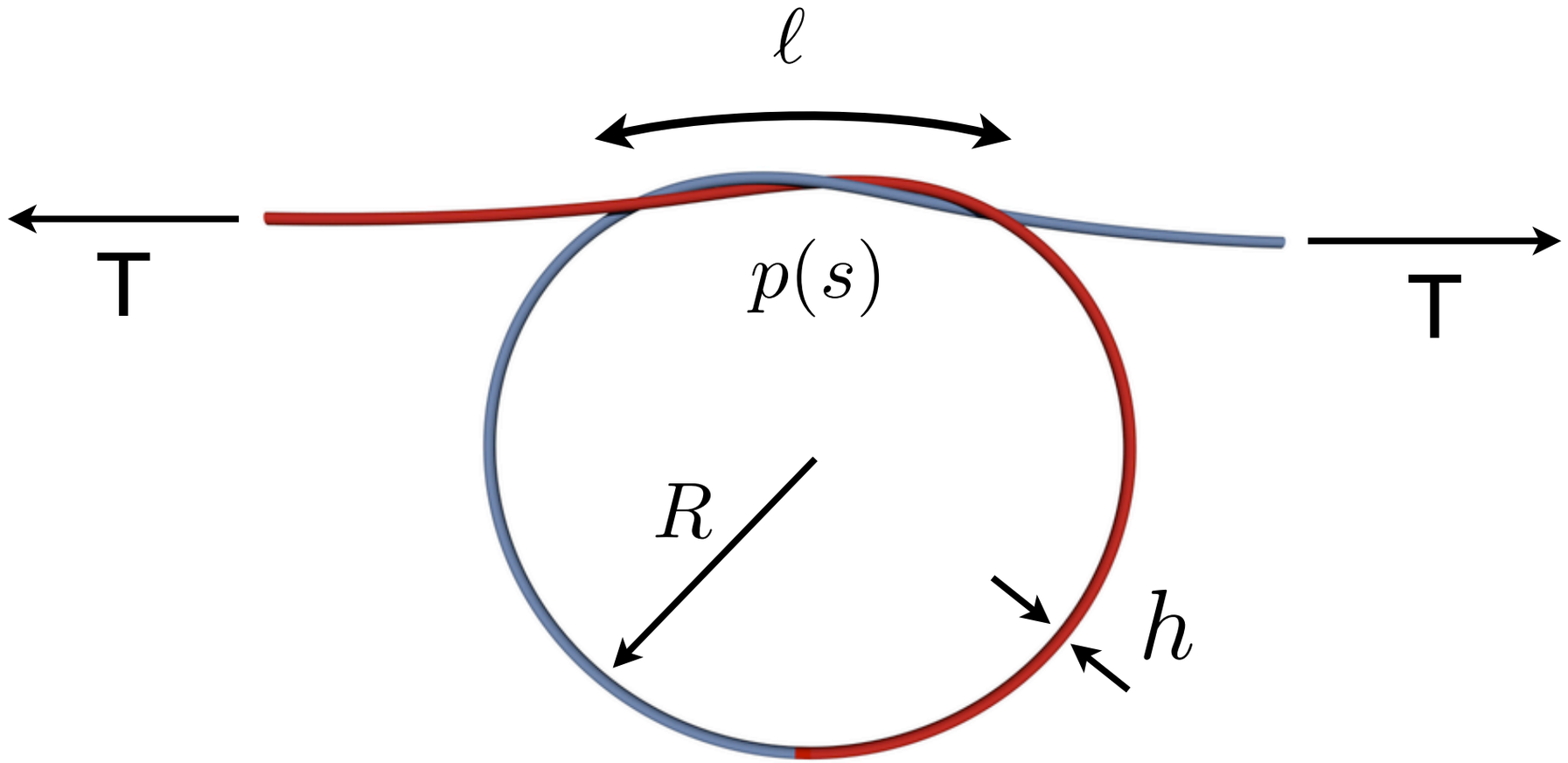
Braid : contact topology



Braid : contact topology



Results



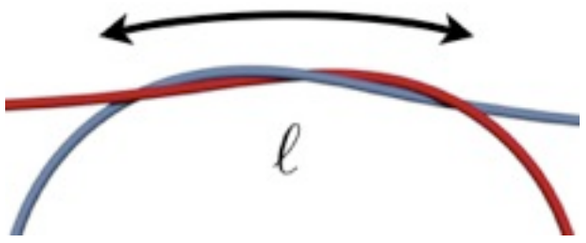
$$R = \sqrt{\frac{EI}{2T}}$$

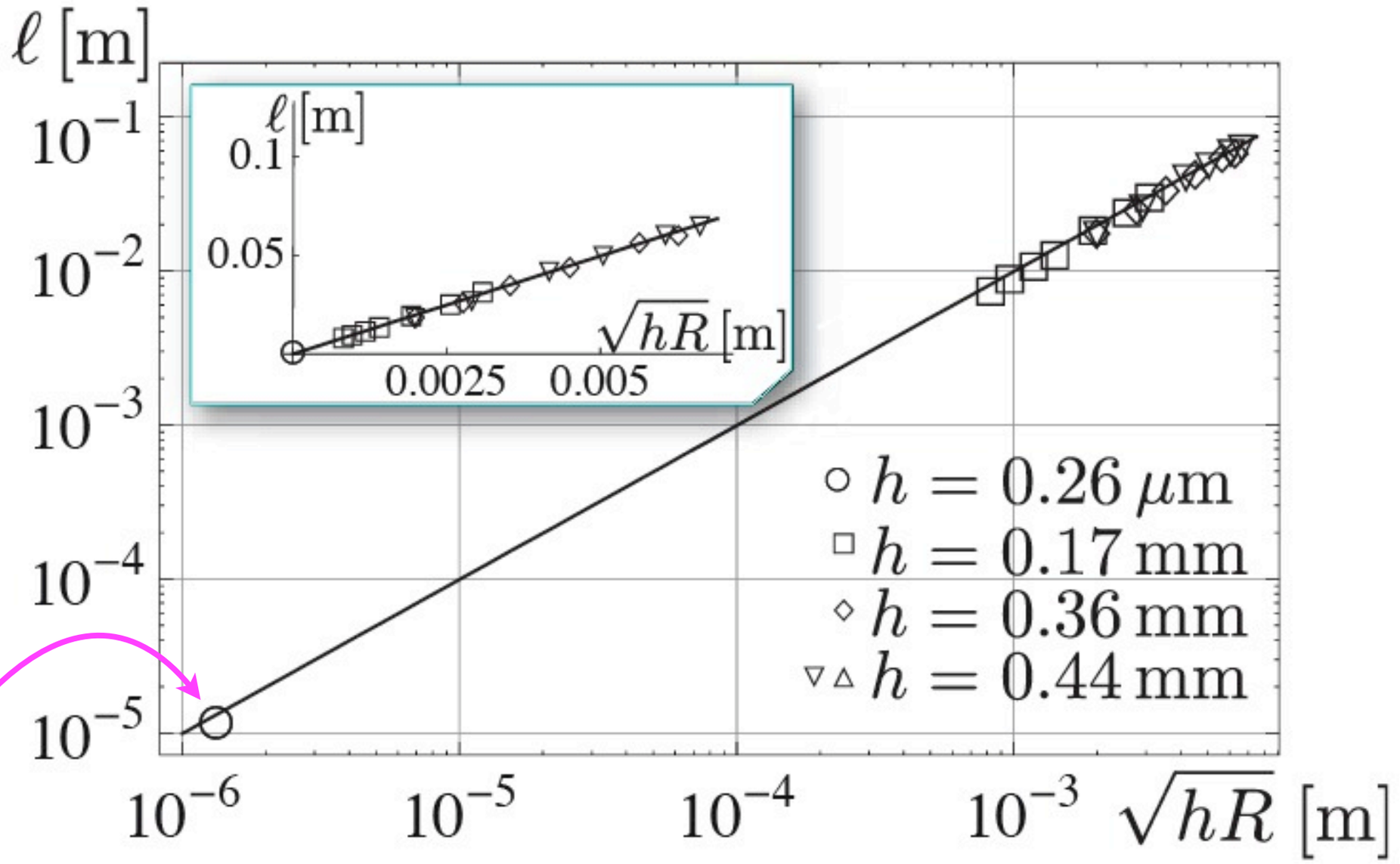
$$\ell = 9.91\, h^{1/2}\, (EI)^{1/4}\, T^{-1/4}$$

Contact pressure $p(s)$

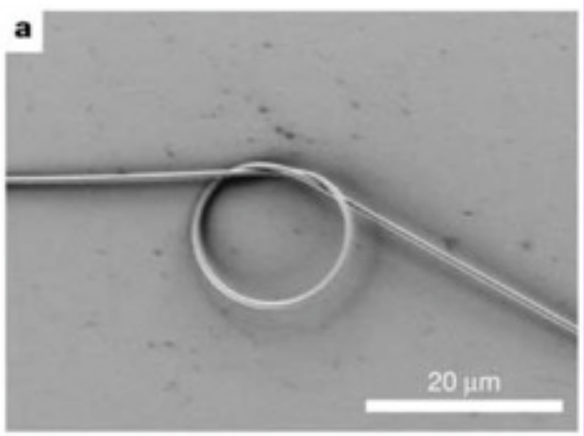
Total contact force $P = \int_0^\ell p(s)ds = 0.82\, h^{-1/2}\, (EI)^{1/4}\, T^{3/4}$

Experiments



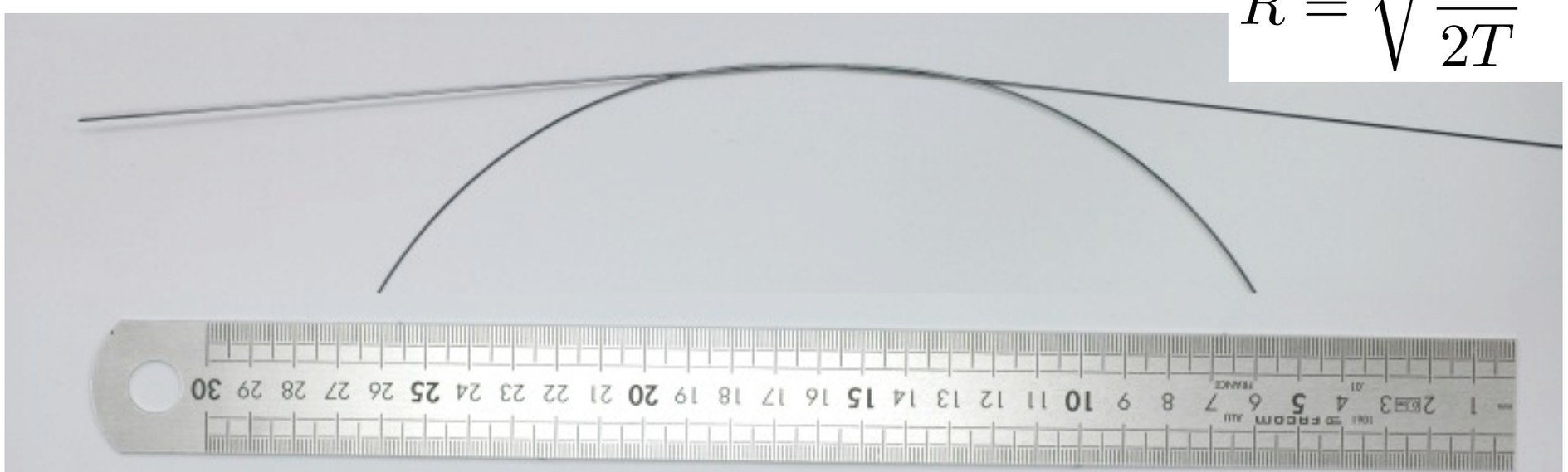


Tong et al., Nature 2003

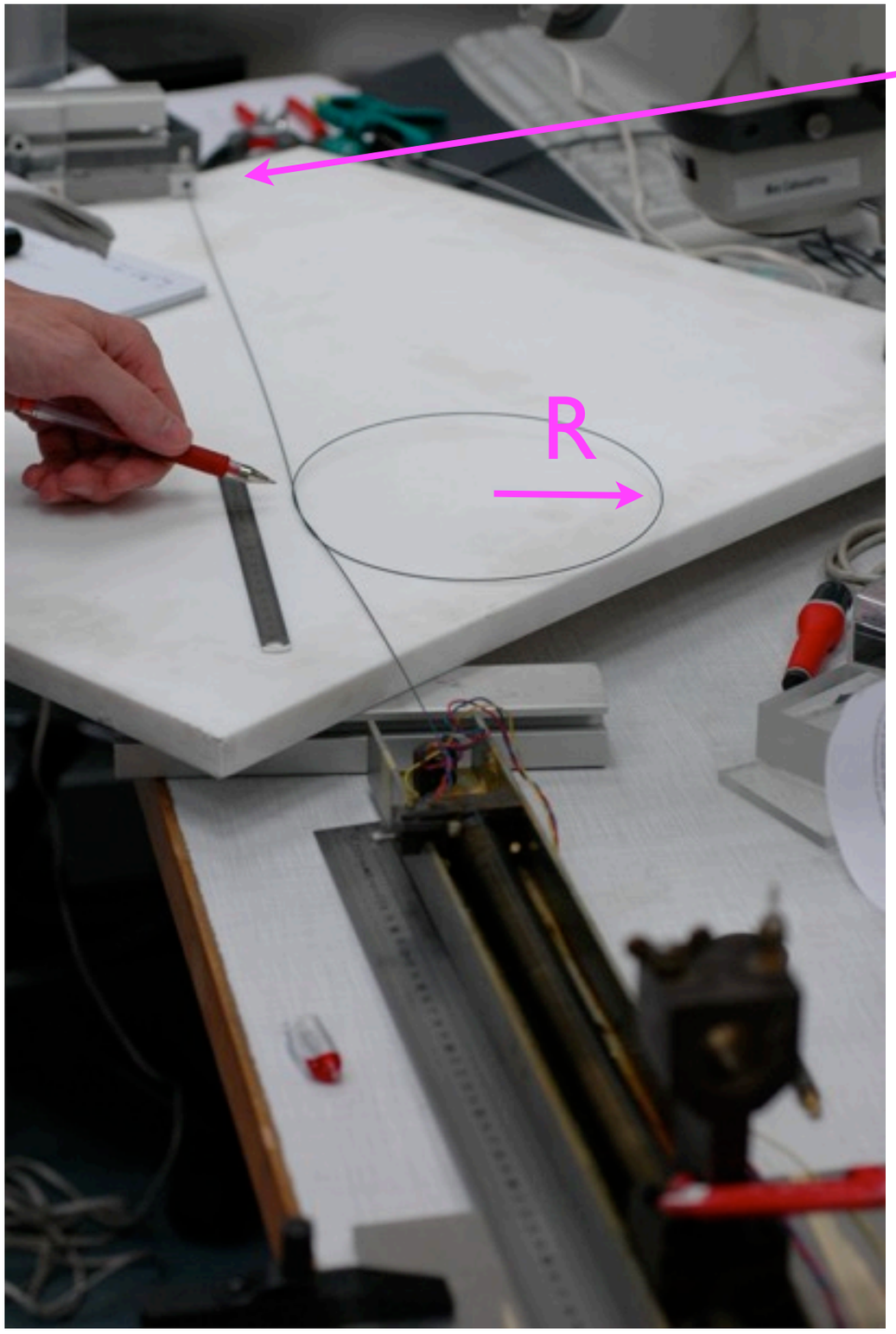


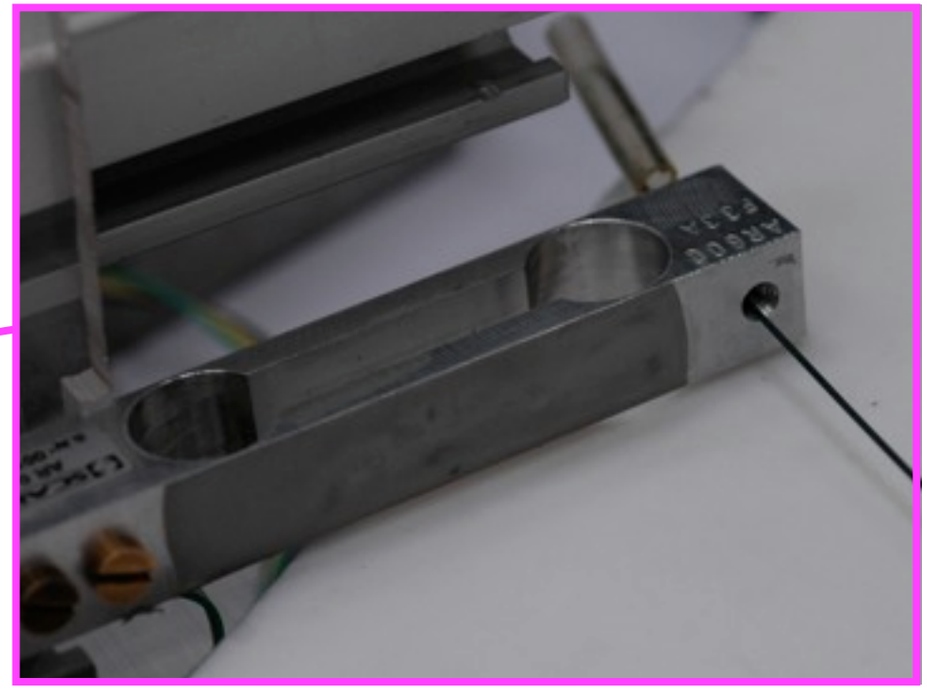
silica wire
h = 1/2 micron

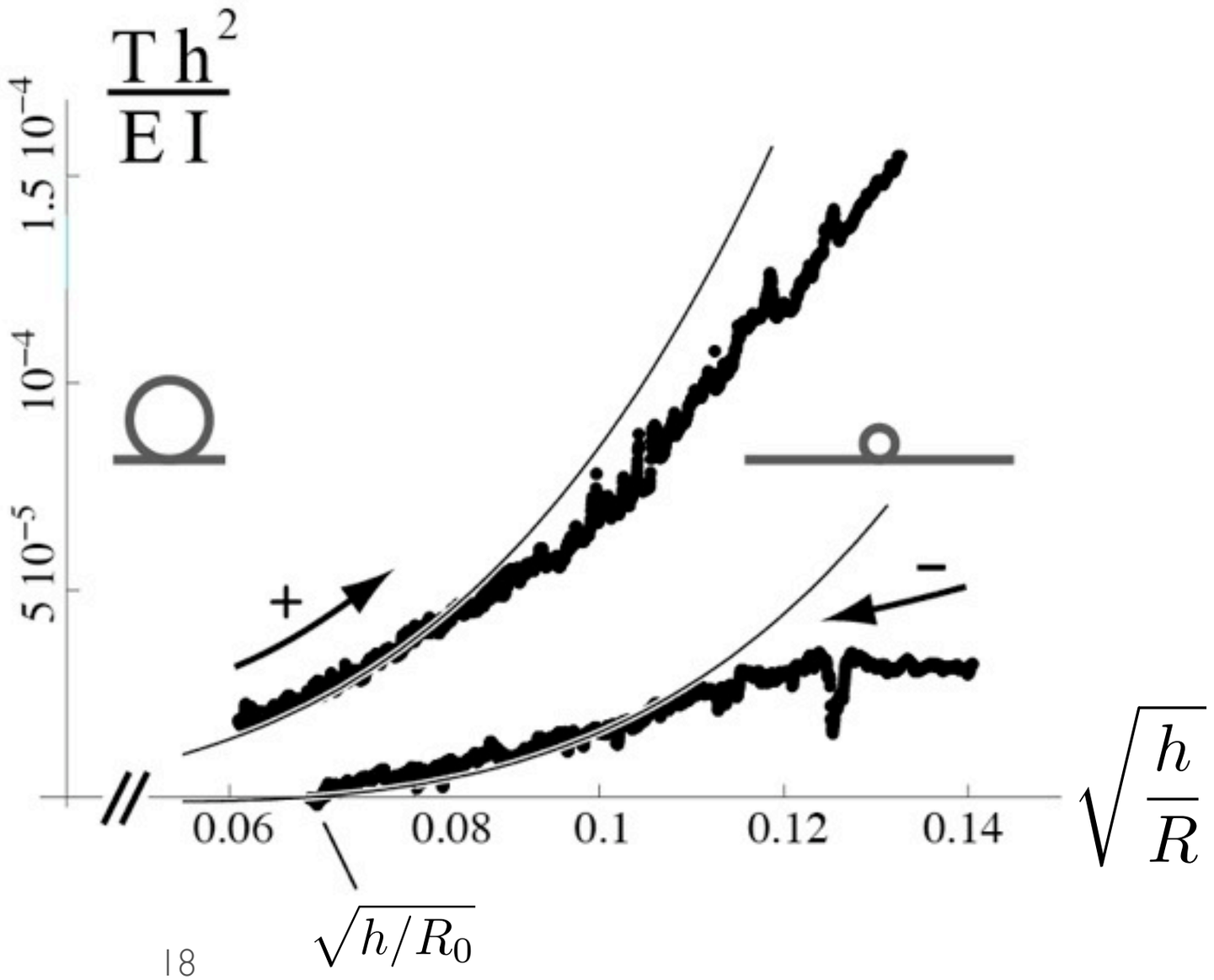
$$R = \sqrt{\frac{EI}{2T}}$$



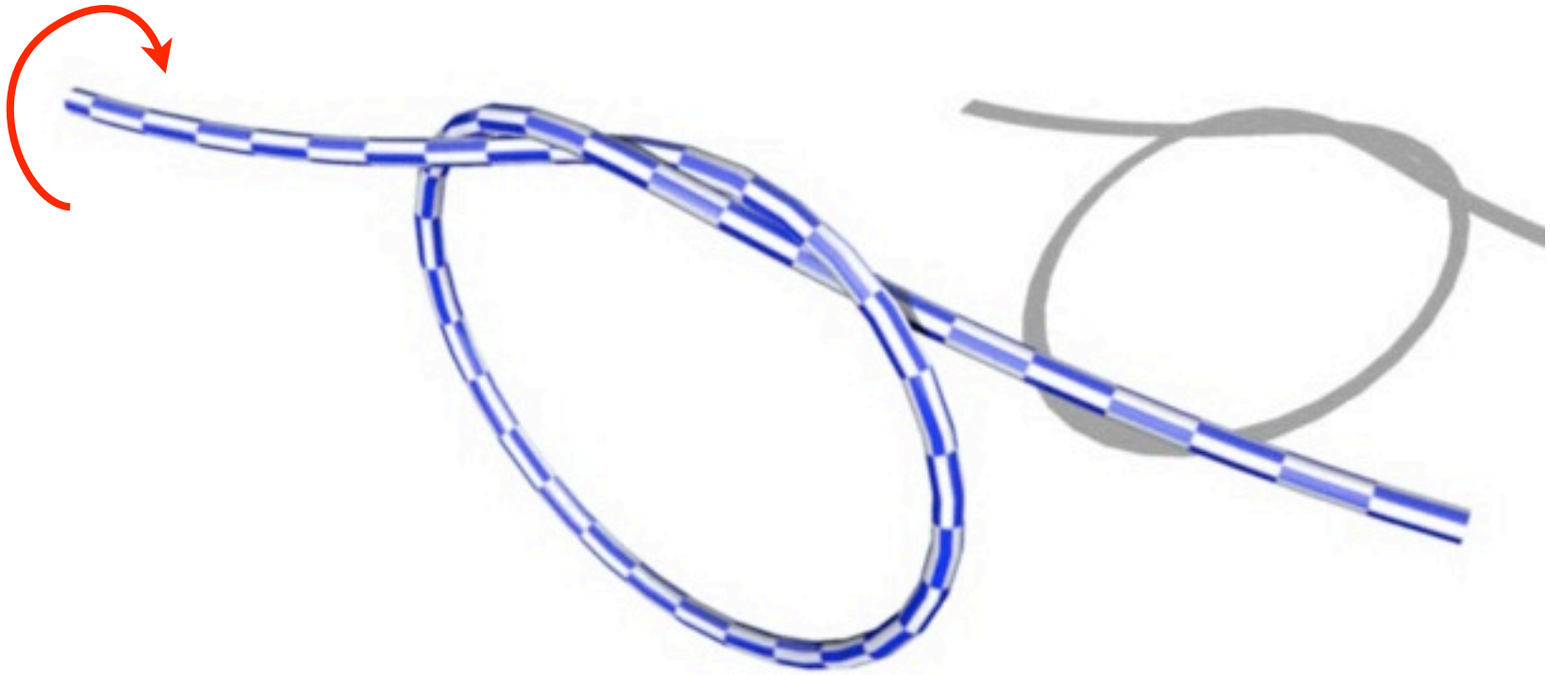
Experiments

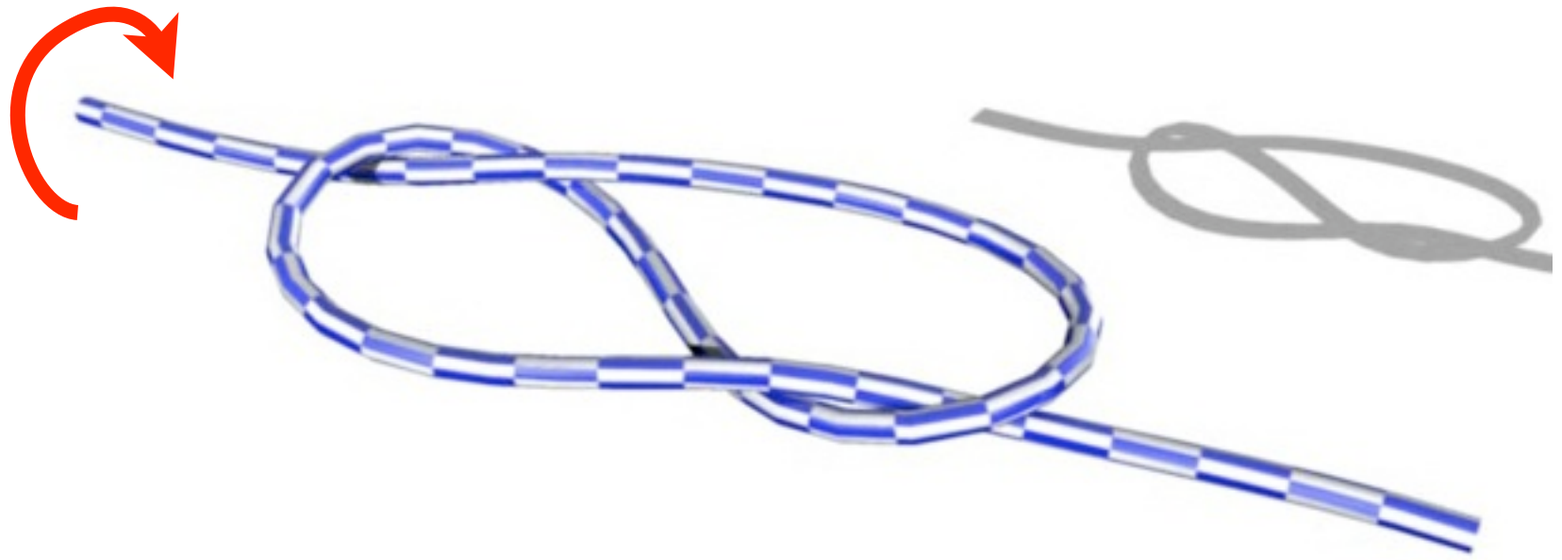






Twist Instability





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

ACM Transactions on Graphics (SIGGRAPH), 2008