Soft Motors: molecular to macroscopic perspectives

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Outline: microscopic

- What is a Motor?

- Molecular Motors 1. Anomalous Photoalignment
  - ideas of Landauer, Prost & Astumian

- Molecular Motors 2. Yokoyama - Tabe Experiment
  - Lehman effect

- Molecular Motors 3. ATP synthase
  - Boyer & Walker

- Molecular Motors 4. Myosin and Actin
  - muscles

- Molecular Motors 5. LC elastomers
  - elongation/contraction

- Broken symmetry
  - broken symmetry drives motors

Outline: macroscopic

- molecular & macroscopic length scales
- shape change
- motors based on elongation
- motors based on bend
- summary

what is a motor?

Motor

- what is a motor?
  - anything that produces or imparts motion *(dictionary.com)*

  - a machine that supplies motive power for a vehicle or other device *(O.E.D.)*

Motor

- what is a motor?
  - a device which uses energy (but not momentum!) to cause motion
- how does motion come about?
- car convinces the road to exert a force on it, and push it forward

Motor

- what is a motor?
  - a device which uses energy (but not momentum!) to cause motion

- motor causes one part of a system to exert a force/torque on another, causing motion

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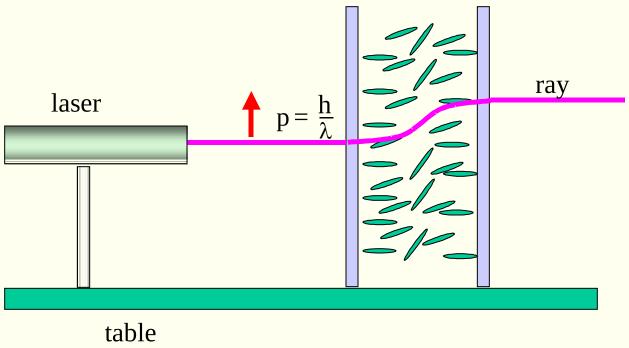
Molecular Motors 1. Anomalous Photoalignment

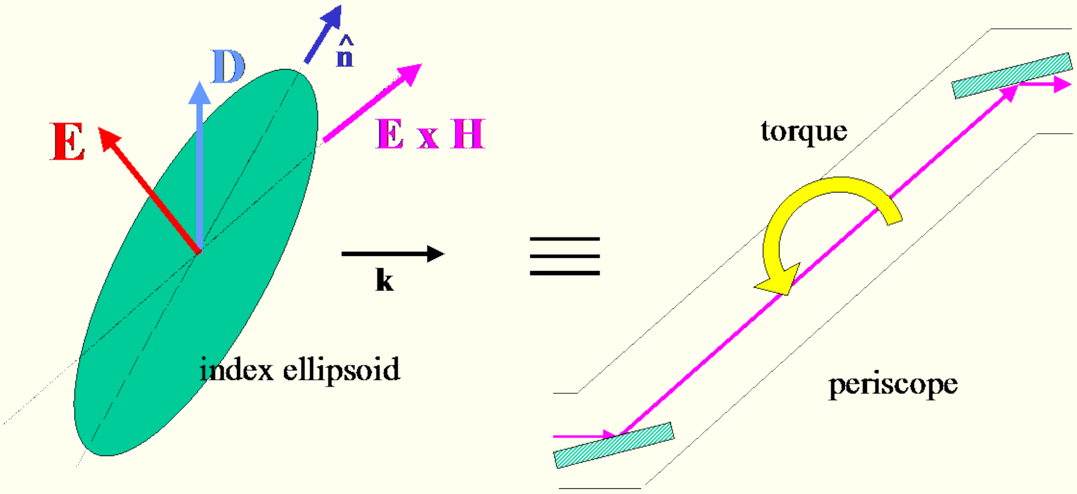
Direct optical torque



$$\tau_{vol}^{opt} = \mathbf{D} \times \mathbf{E}$$

$$\tau_{vol}^{el} + \tau_{vol}^{opt} = 0$$

angular momentum transfer:

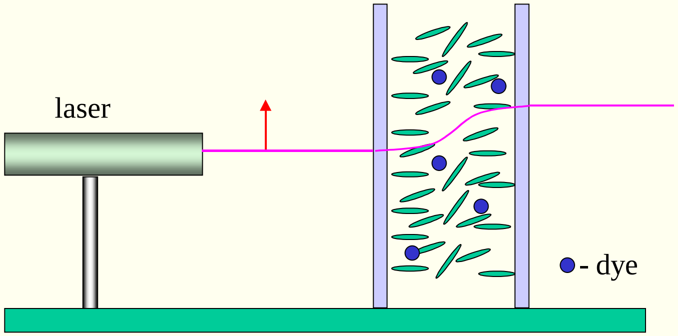


torque results from change in extrinsic angular momentum of light.

Indirect optical torque

addition of 1% of anthroquinone dye

$\Rightarrow$ reduction of threshold intensity[1] by $\sim\times 100$!



without dye: $\tau_{vol}^{el} + \tau_{vol}^{opt} = 0$

with dye: $\tau_{vol}^{el} + \frac{1}{100}\tau_{el}^{opt} + ?? = 0$

Torque on nematic causing elastic deformation CANNOT come from light! Source of torque??

1. I. Janossy, A.DD. Lloyd and B.S. Wherret, *Mol. Cryst.Liq. Cryst*. **179**, 1, 1990.
   I. Janossy, *Phys. Rev. E* **49**, 2957, 1994.

Puzzle 1:

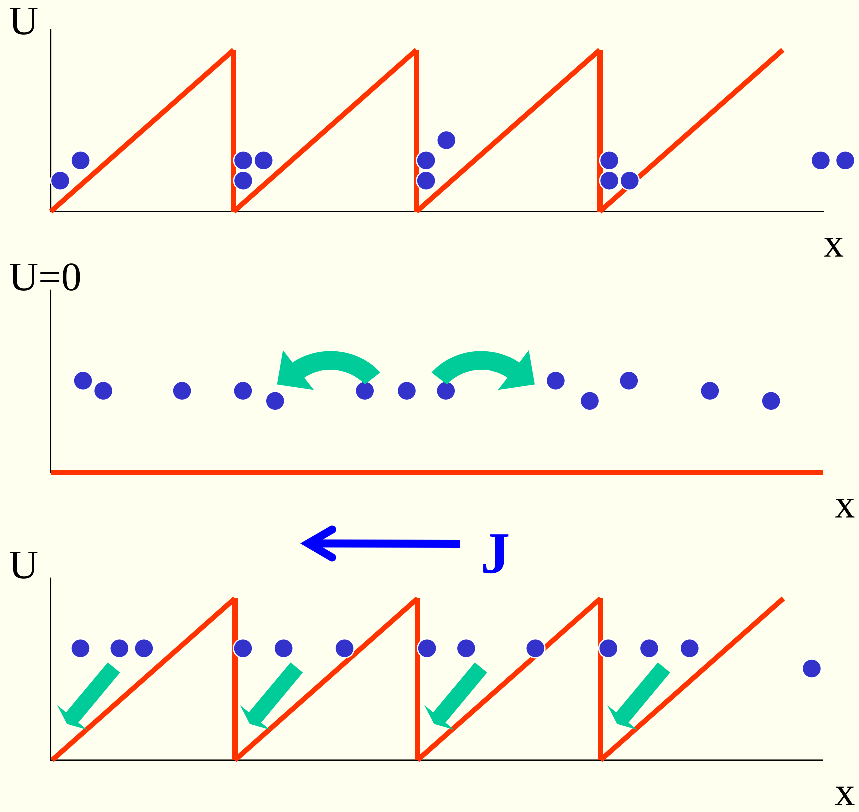
- light causes the director to reorient, against a restoring elastic torque, essentially without the transfer of angular momentum.

- light causes rotation without exerting a torque!

???

Prost, Astumian

The translational ratchet*



Particles in asymmetric periodic potential:

When potential is turned OFF, particles diffuse, no net current

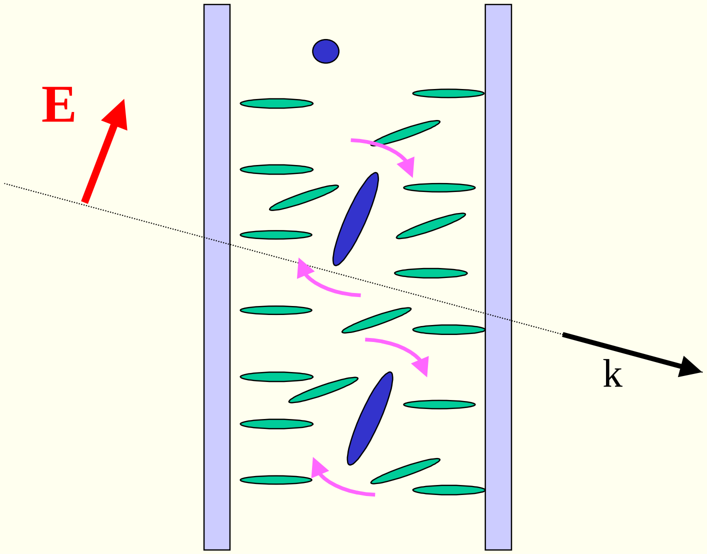
When potential is turned ON, particles move towards minimum, giving rise to current.

* R.D. Astumian et al: *Phys.Rev.Lett.* **72**, 1766, 1994.
J. Prost et al: *Phys. Rev. Lett.* **72**, 2652, 1994.

Simple model:

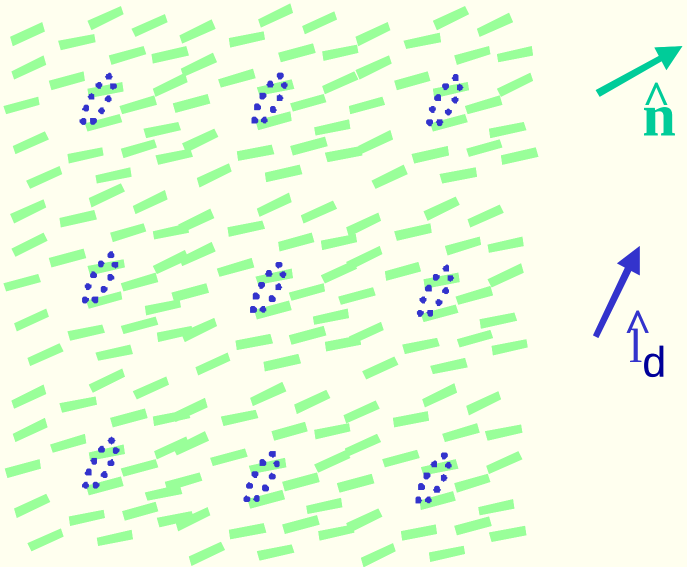
- dye
    - anisotropic molecule with orientation $\hat{l}_d$
    - in ground state does not interact with nematic
    - in excited state becomes 'nematic' molecule
    - probability of excitation depends on $(\hat{l}_d \cdot \mathbf{E})^2$
    - lifetime of excited state is t_o

- optical field
    - transfers energy, but no momentum to the sample



Torque on liquid crystal:

Average orientation of excited dye molecule is NOT along nematic director

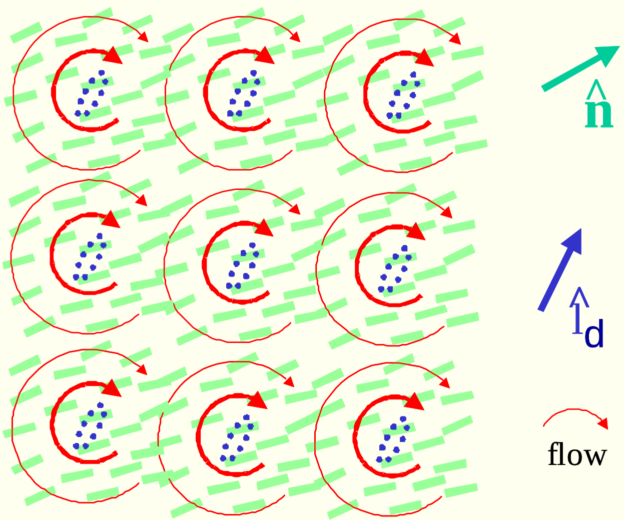


interaction between liquid crystal and excited dye gives rise to torque!

Rotating dye gives rise to shear flow

dye: - rotation $\Rightarrow$ source of vorticity

liquid crystal: - aligned by nematic field of dye



viscous shear carries angular momentum from cell walls to dye

angular momentum current: dye $\xrightarrow{\text{molecular}}$ nematic $\xrightarrow{\text{elastic}}$ cell walls $\xrightarrow{\text{shear}}$ dye

Summary of Puzzle 1

- Janossy effect[1] (source provides energy but not torque yet causes rotation) $\Rightarrow$ orientational ratchet[2]
- dye is light-driven rotor with continuous rotation
- energy from optical field drives shear flow
- viscous stress carries angular momentum from dye to cell walls

1. T. Kosa and I. Janossy, *Opt.Lett.* **17**, 1183, 1992; *Opt. Lett.* **20**, 1231, 1995.
2. W. E and P. Palffy-Muhoray, *Mol.Cryst.Liq.Cryst.* **320**, 193, 1998

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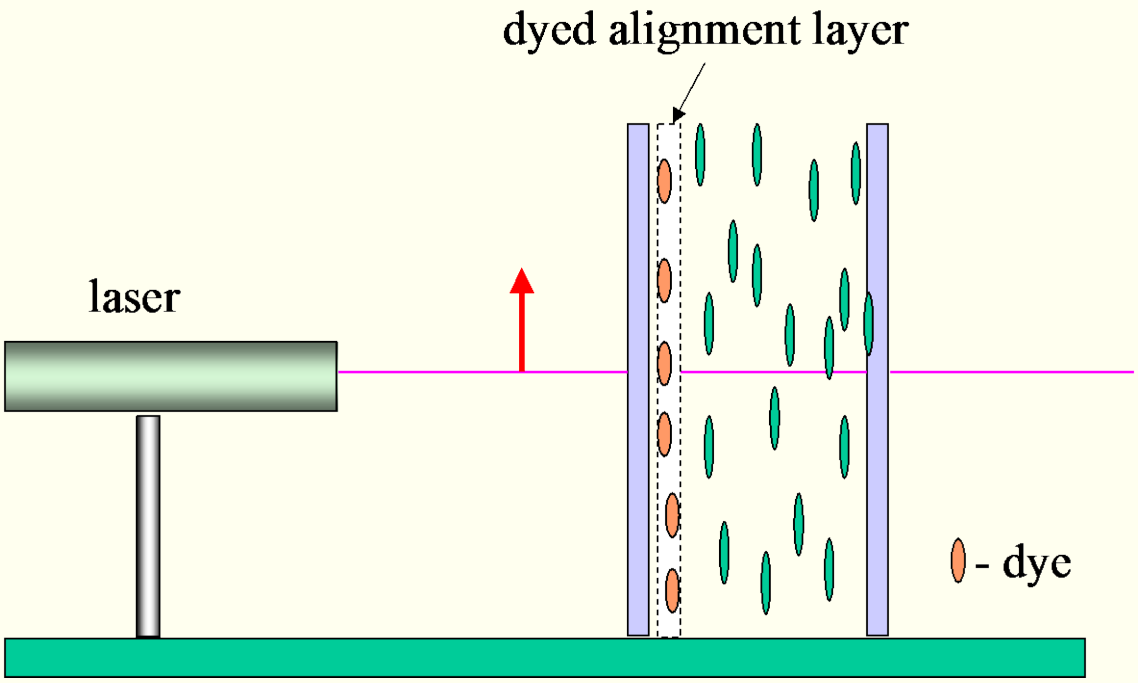
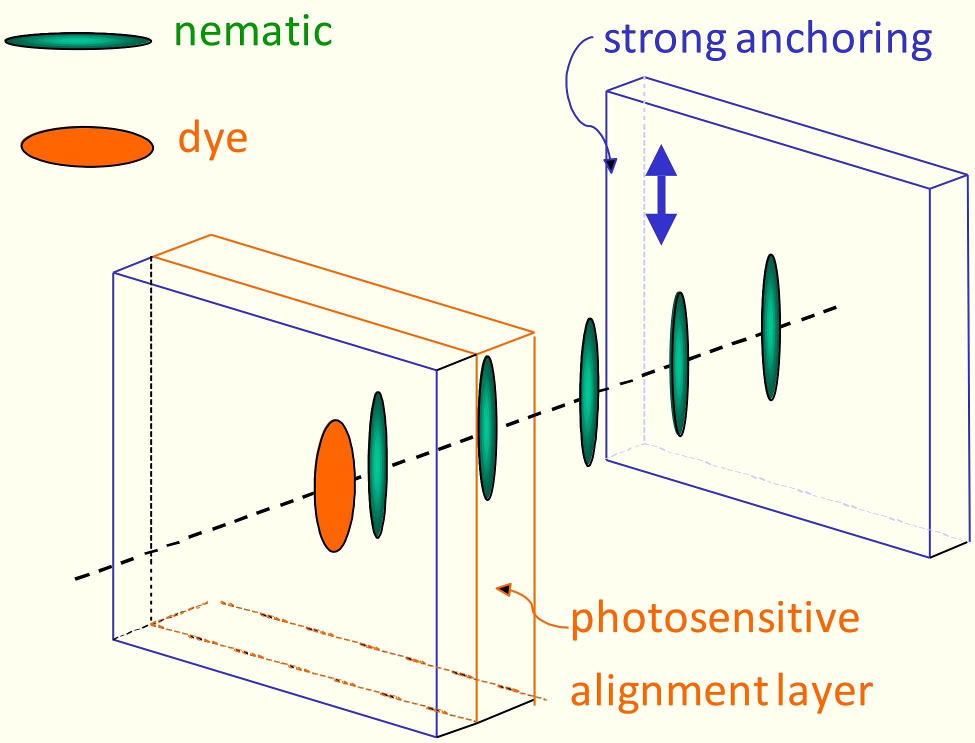
Puzzle 2. Photoinduced Twist



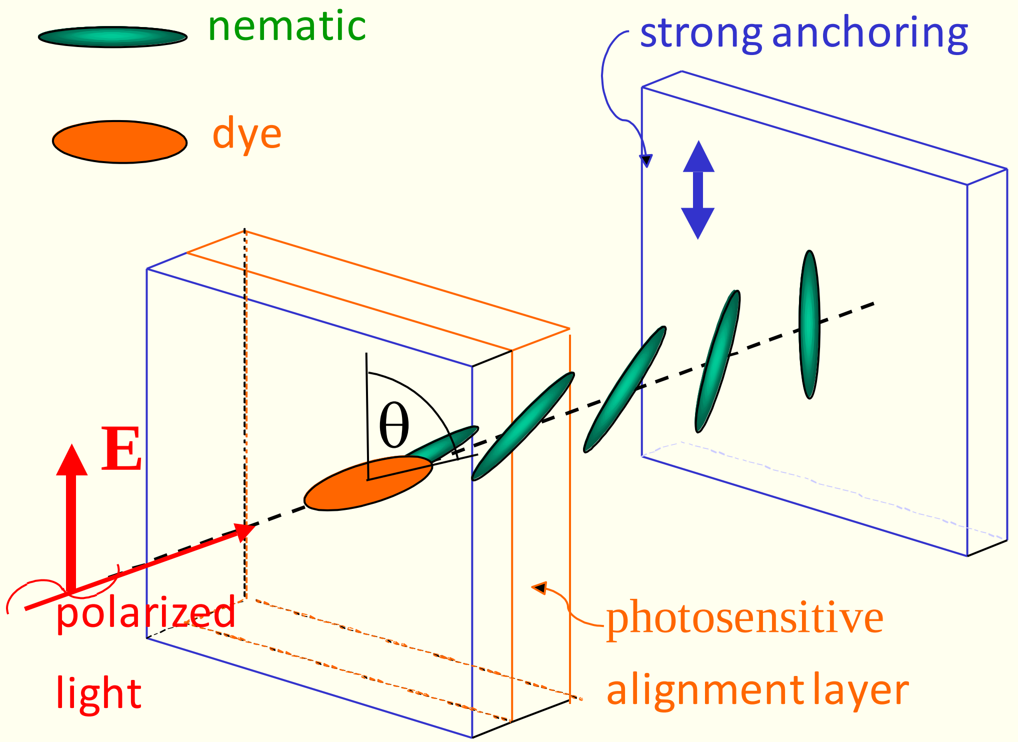
Photoinduced Twist

laser OFF



Photoinduced Twist

laser ON

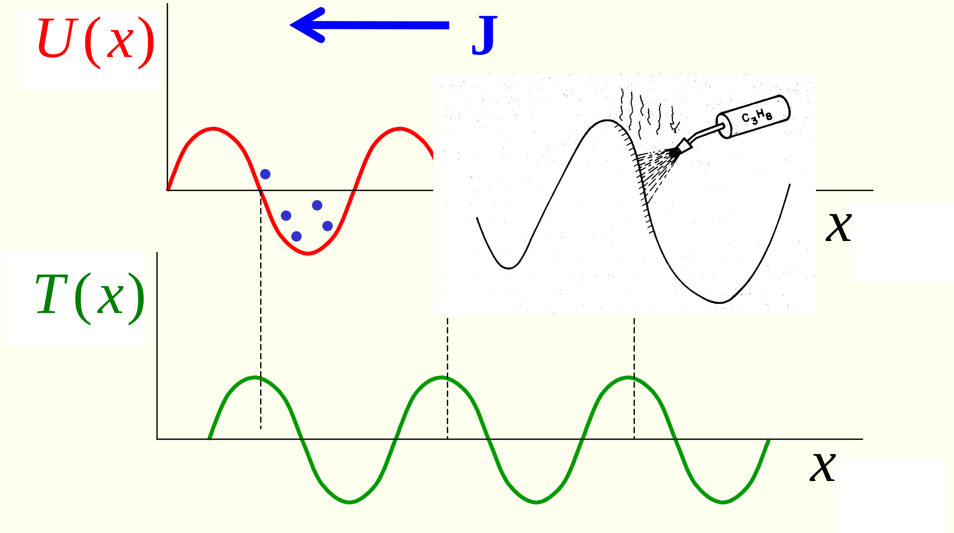


Origin of torque

- before deformation takes place, polarization is parallel to the director, hence optical torque **D** x **E** = 0.
- optical field *stabilizes* configuration!
- source of torque?

Landauer

Landauer's Blowtorch



particles in periodic potential

'hot' molecules are more excited
& diffuse over barrier

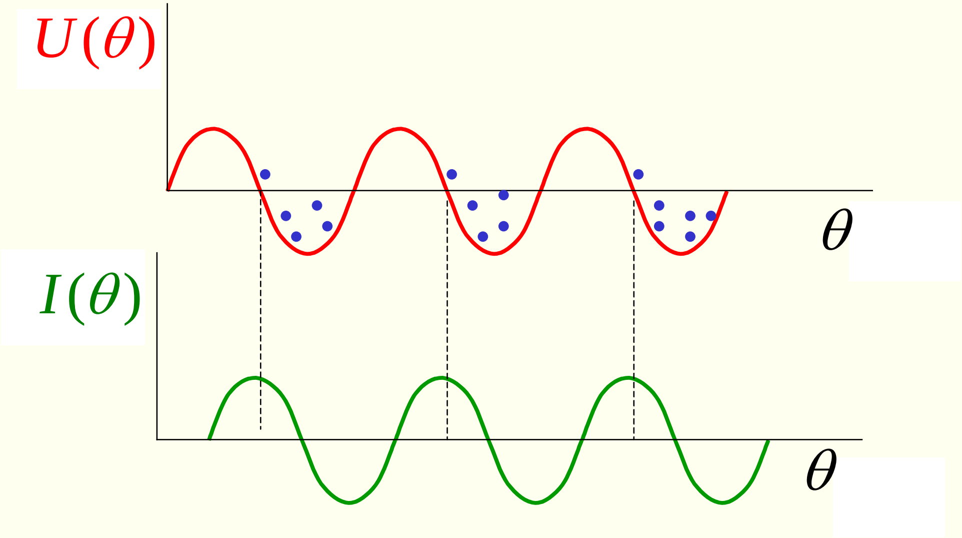
∴ steady current: system is molecular motor (pump)

one part of system pushes on other;
no momentum transfer from outside.

M. Büttiker, Z. Phys. B **68**, 161 (1987).

R. Landauer, *J. Stat. Phys*. **53**, 233 (1988)

Indirect optical torque: Brownian ratchet



dye molecules in nematic field

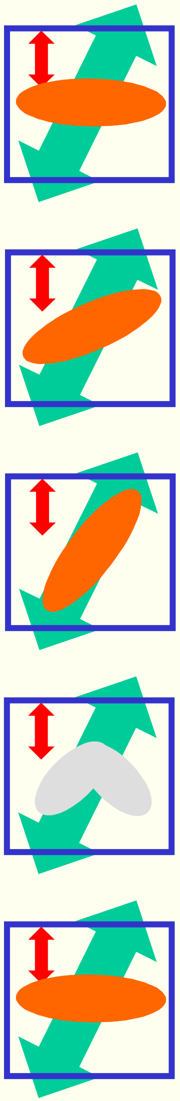
dye molecules parallel to pump polarization are excited & diffuse over barrier

∴ steady rotation: dye is light driven molecular motor

torque results from rotation of dye;
no momentum transfer from light.

P. Palffy-Muhoray, T. Kosa and Weinan E, *Appl. Phys. A* **75**, 294 (2002)

Schematic of Brownian motor:



dye in *trans*-state starts to rotate towards director

it exerts torque on director & vice versa

as it becomes parallel to pump polarization

it is excited into *cis*-state, undergoes diffusion

relaxes into *trans*-state, rotates towards director...

Dynamics

- dye: Fokker-Planck

$$\frac{\partial \rho_{\mathrm{t}}}{\partial \mathrm{t}} = D_t \nabla^2 \rho_t + \nabla \cdot (M_t \rho_t \nabla U_t) - \rho_t f_t + \rho_c f_c$$

$$\frac{\partial \rho_{\mathrm{c}}}{\partial \mathrm{t}} = D_c \nabla^2 \rho_c + \nabla \cdot (M_c \rho_c \nabla U_c) - \rho_c f_c + \rho_t f_t$$

- transition rates

$$f_t = f_{to} \mathrm{e}^{\mathrm{U_t}/kT} + \nu e_t^{\,2} (\hat{\mathbf{I}}_d \cdot \hat{\mathbf{E}})^2$$

$$f_c = f_{co} \mathrm{e}^{\mathrm{U_c}/kT} + \nu e_c^{\,2} (\hat{\mathbf{I}}_d \cdot \hat{\mathbf{E}})^2$$

Dynamics

- liquid crystal
  - bulk:

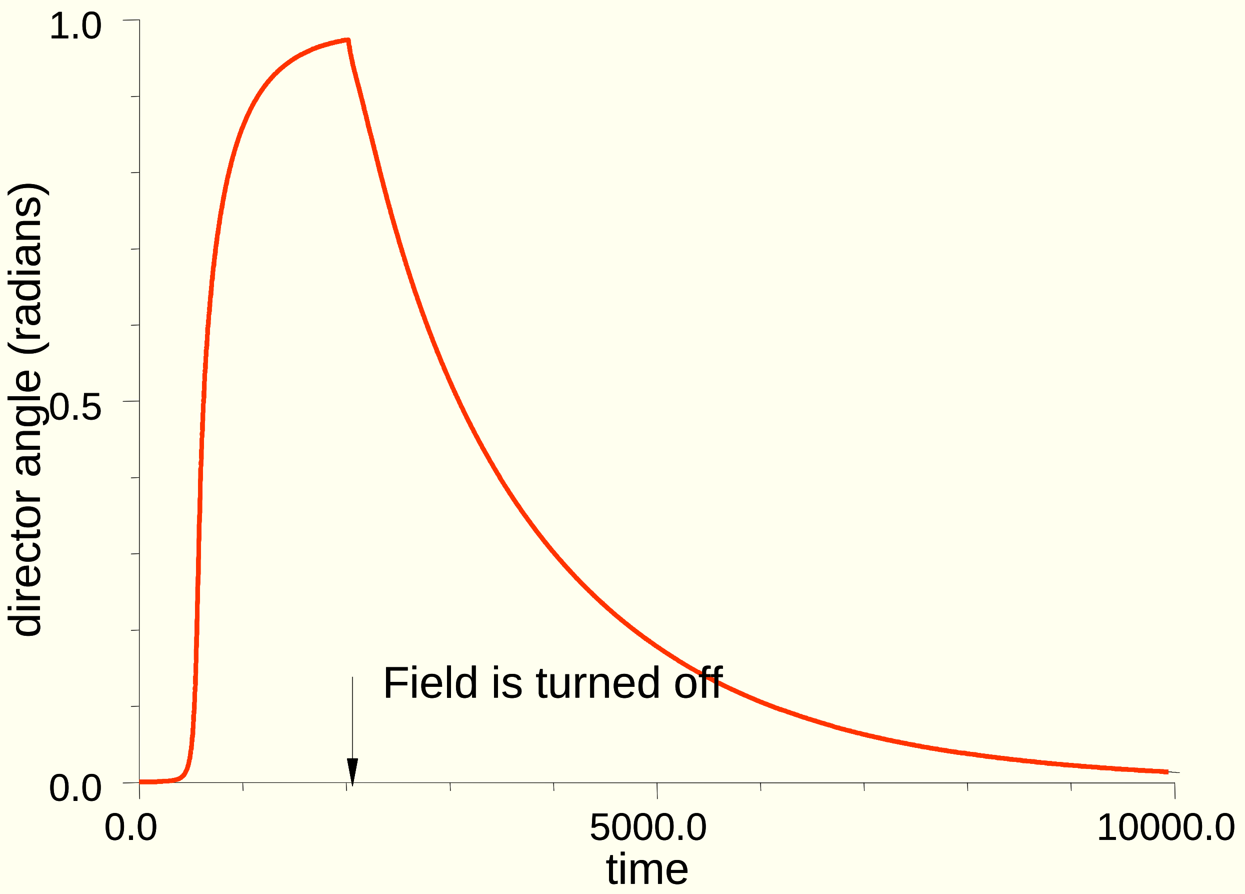
$$\gamma \frac{\partial \hat{\mathbf{n}}}{\partial t} = \mathrm{K}\nabla^2 \hat{\mathbf{n}}(I - \hat{\mathbf{n}}\hat{\mathbf{n}})$$

  - surface:

$$\gamma_s \frac{\partial \hat{\mathbf{n}}}{\partial t} = \{\mathrm{K}(\hat{\mathbf{N}}\nabla \cdot \hat{\mathbf{n}} + \hat{\mathbf{N}} \times \nabla \times \hat{\mathbf{n}})$$

$$- d_d < \rho_{\mathrm{t}} \frac{\partial U_t}{\partial \hat{\mathbf{n}}} > - d_d < \rho_{\mathrm{c}} \frac{\partial U_c}{\partial \hat{\mathbf{n}}} > \}(I - \hat{\mathbf{n}}\hat{\mathbf{n}})$$

Simulations



- optical field drives orientational current
- dye exerts steady torque on nematic

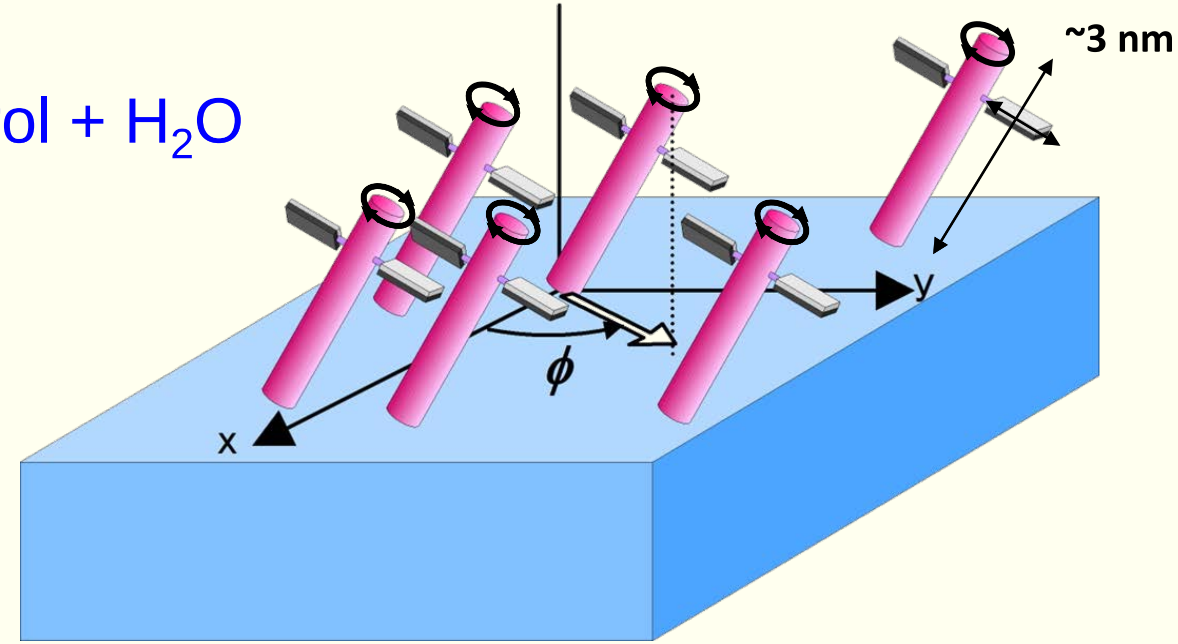
Summary of Anomalous Photoalignment

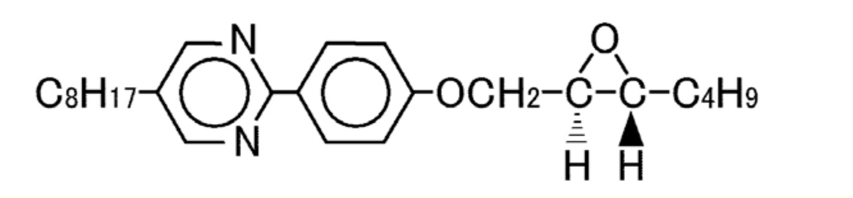
- light-driven molecular motors
- dye* molecules are rotors in nematic potential
- energy (but not momentum) from light
- steady unidirectional rotation
- orientational ratchet / Landauer's blowtorch mechanism
- work: steady torque on director by viscous stress + dissipation
- achiral

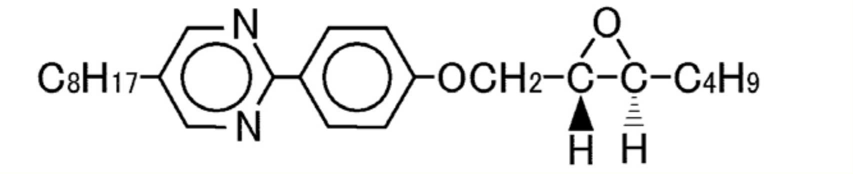
Molecular Motors 2.
Yokoyama - Tabe Experiment

Yokoyama – Tabe Experiment

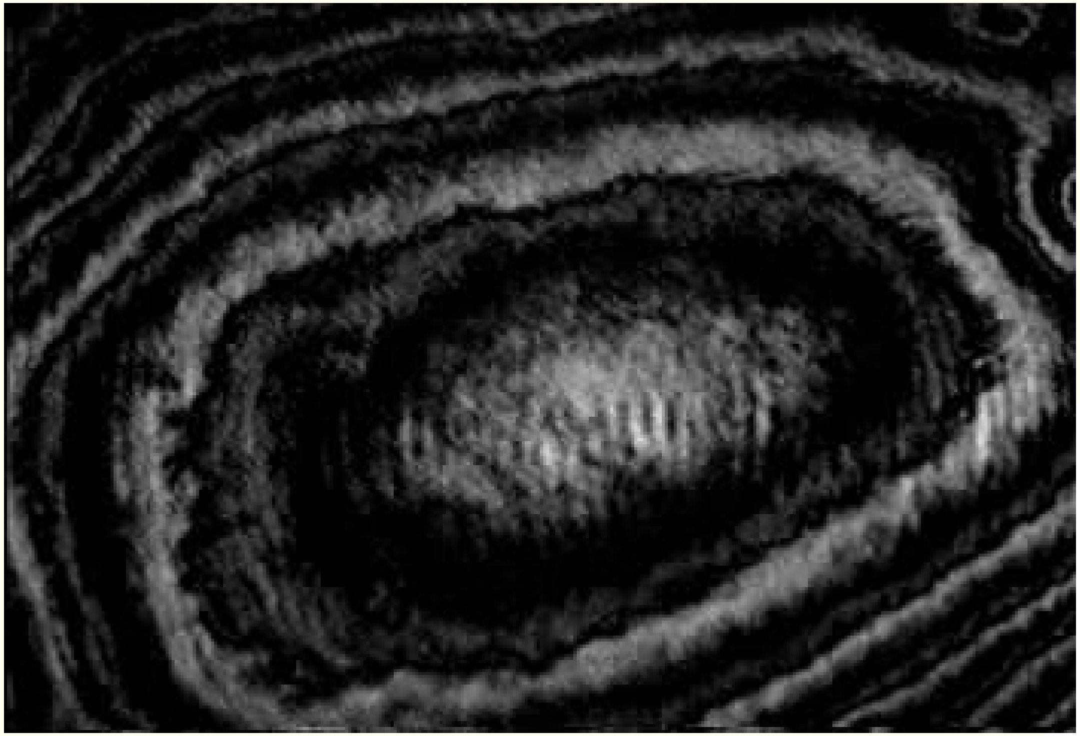
- chiral Langmuir monolayer
- substrate: glycerol + H_2O

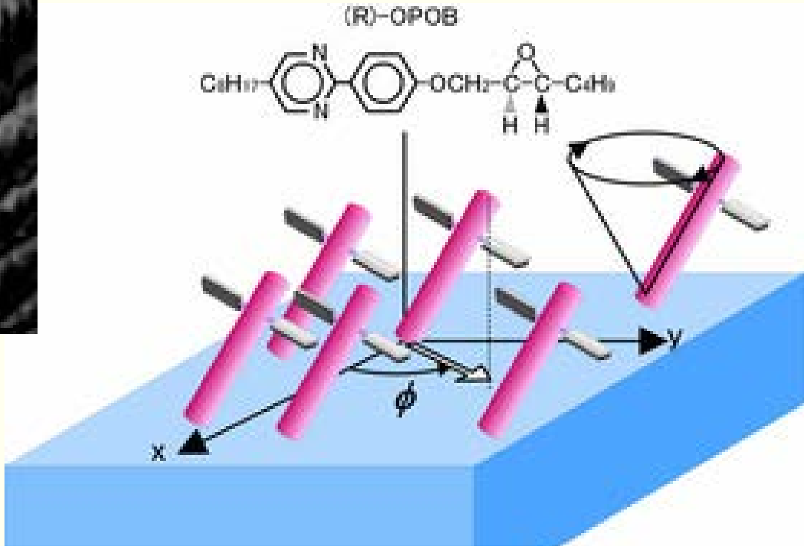






Collective Molecular Rotor/Pump

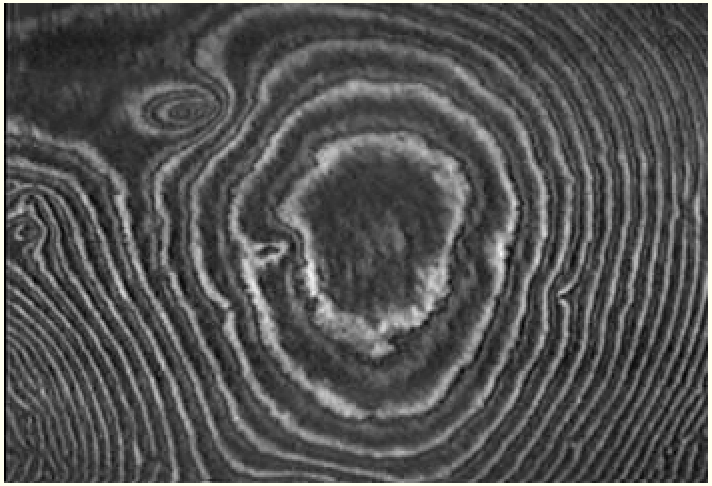


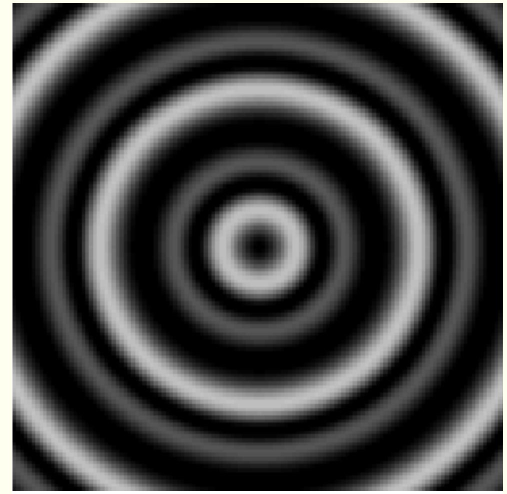


Yuka Tabe and H. Yokoyama, *Nature Materials*, 2, 806(2003).

Chiral LC molecules on glycerol

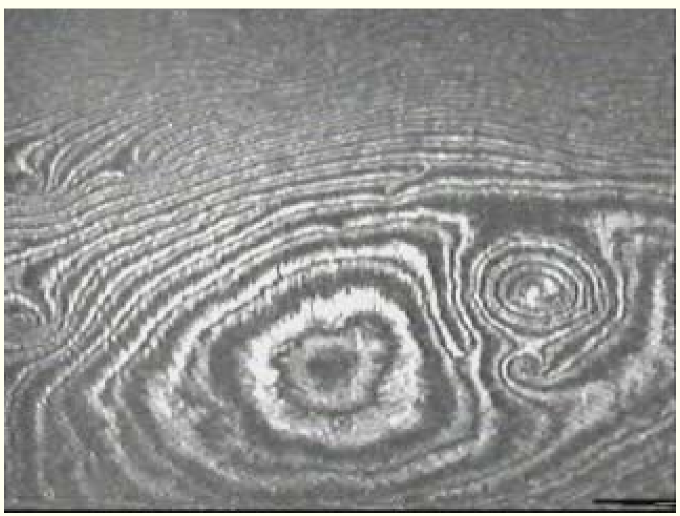
FELIX013 on pure glycerol (SmC* phase)

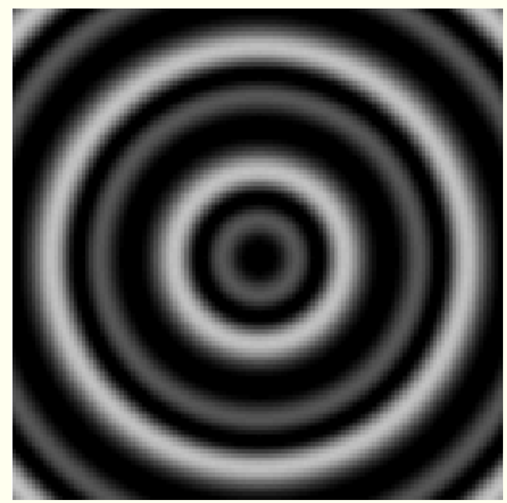




counter-clockwise rotation

CS4001 on pure glycerol (SmCA* phase)



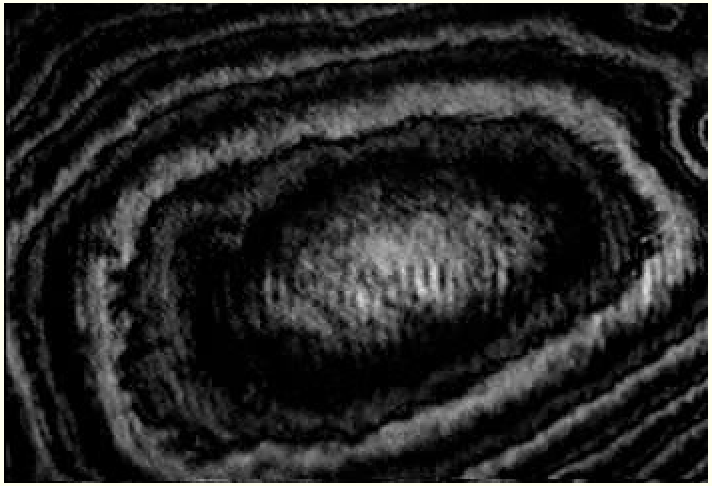


clockwise rotation

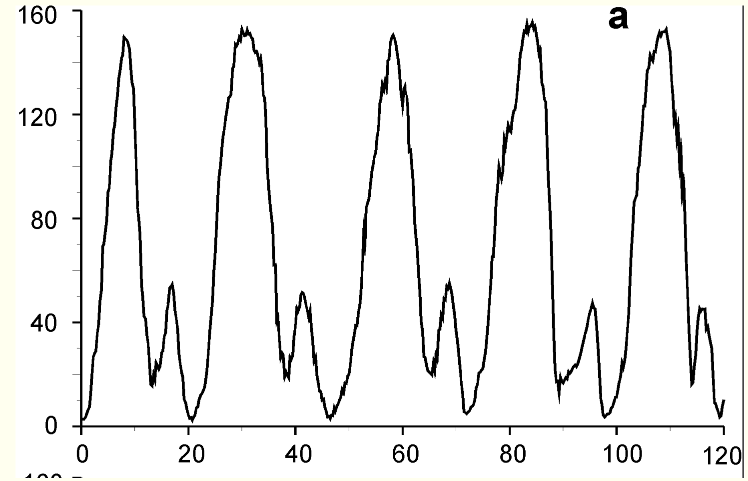
Chirality inversion

(R)-OPOB

on pure glycerol

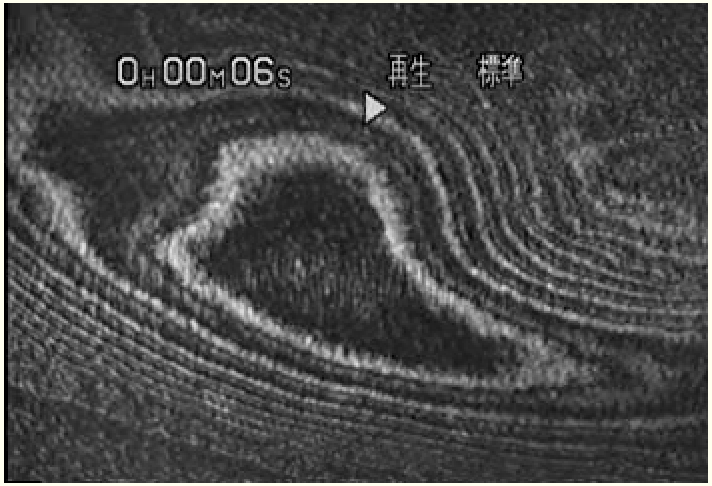


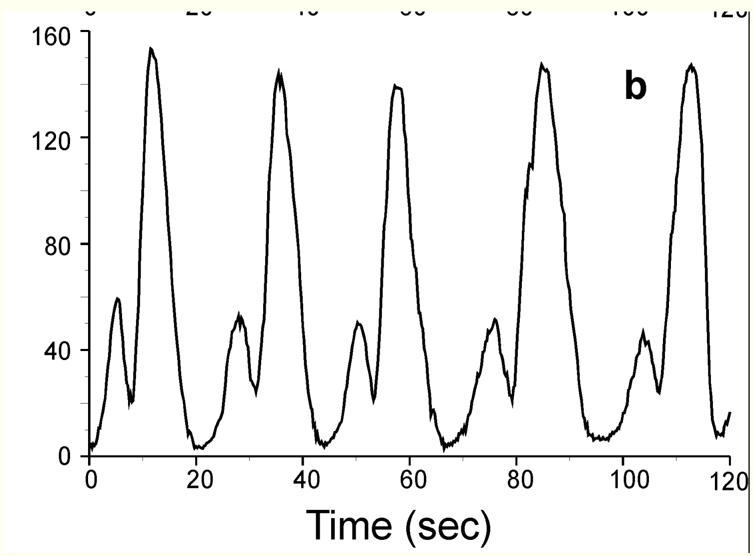
100µm



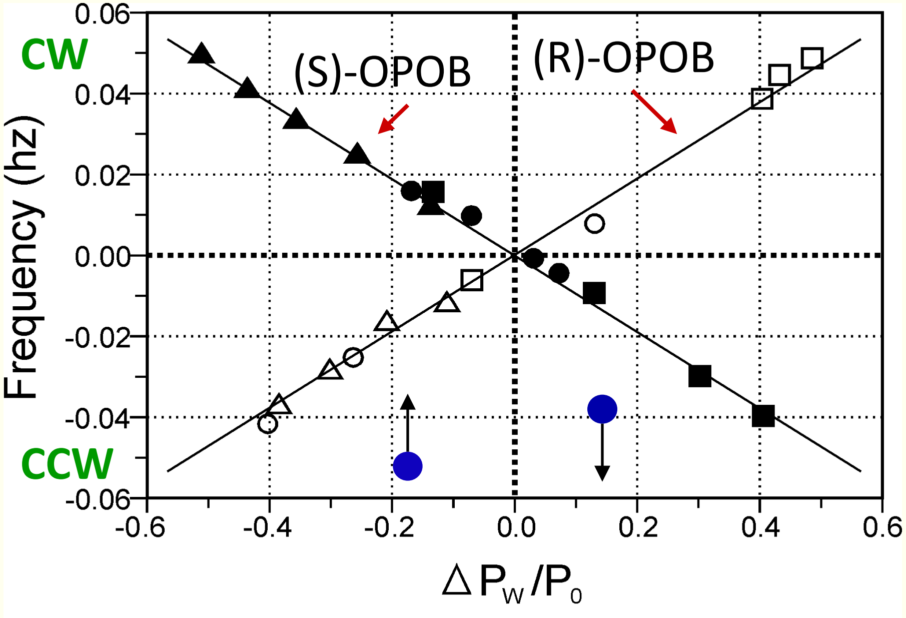
(S)-OPOB

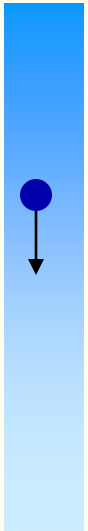
on pure glycerol

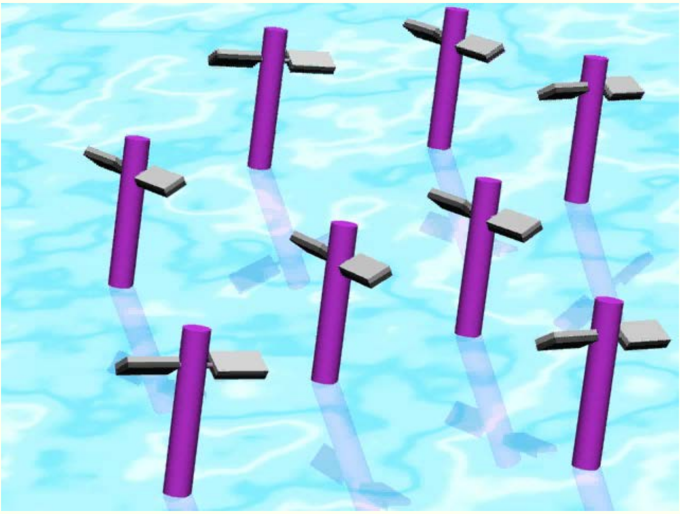


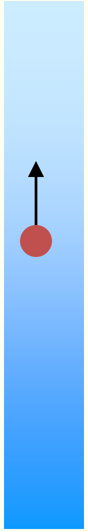


Precession speed linearly depends on $\Delta P_W/P_0$









$\Delta P_w/P_0 = P_v - P_s$

P_v: actual water vapor pressure

P_s: saturated water vapor pressure

Onsager Reciprocal Relations

Entropy Production:

$$T\dot{S} = \tau \frac{\partial \phi}{\partial t} + J \cdot \upsilon_m \Delta P$$

Onsager Relations:

$$\frac{d\phi}{dt} = \frac{1}{\gamma}\tau + b\ \upsilon_m\ \Delta P$$

$$J = b\tau + \frac{1}{\eta}\upsilon_m \Delta P$$

υ_m: molecular volume of water in vapor

γ: rotational viscosity of LC director

η: water mobility through the film

b: Lehmann coefficient ($\propto$ chirality strength)

Phenomenological Theory of Lehmann effect

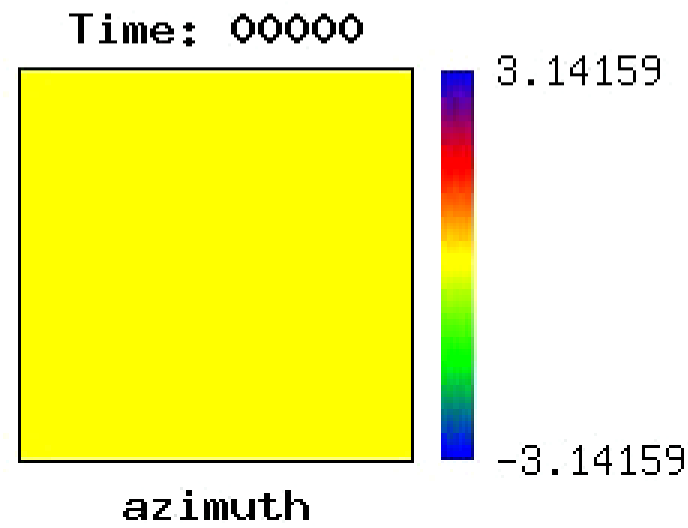
- Shibata & Mikhailov, Europhys. Lett., 73 (2006)
- H. Brand et al., Phys. Rev. Lett. 96 (2006)
- Tsori & de Gennes, Euro.Phys. J. E 14 (2004)
- T. Okuzono, Kyoto Workshop (2005)

Equation of motion :

$$\gamma \frac{\partial \mathbf{c}}{\partial t} = -\frac{\delta F}{\delta \mathbf{c}} + \underline{\nu\, \mathbf{c} \times \frac{\partial P}{\partial \mathbf{z}}}$$

↑ Lehman term

$$F = \int dr \left[\frac{K}{2} \sum_{i=x,y} |\nabla c_i|^2 - \frac{\tau}{2} |\mathbf{c}|^2 + \frac{u}{4} |\mathbf{c}|^4 \right.$$



Simulated by T. Okuzono

Summary of Yokoyama – Tabe experiment

- substrate & monolayer system is motor
- energy stored in chemical potential of H_2O
- vapor current drives rotation of chiral molecules
- work: produces circulating flow, dissipation

Molecular Motors 3. ATP Synthase

F_1F_O ATP Synthase

- enzyme that synthesizes

  adenosine-5'-triphosphate (ATP)

  from

  adenosine diphosphate (ADP) + phosphate

- reaction:

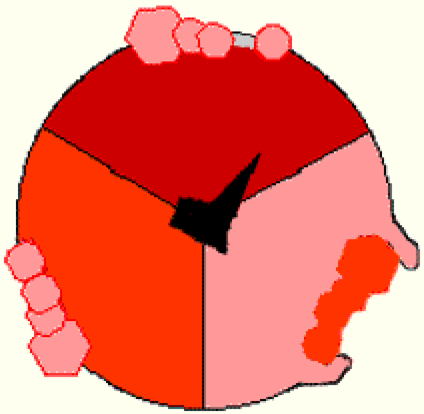
$$ADP + P_i \rightarrow ATP$$

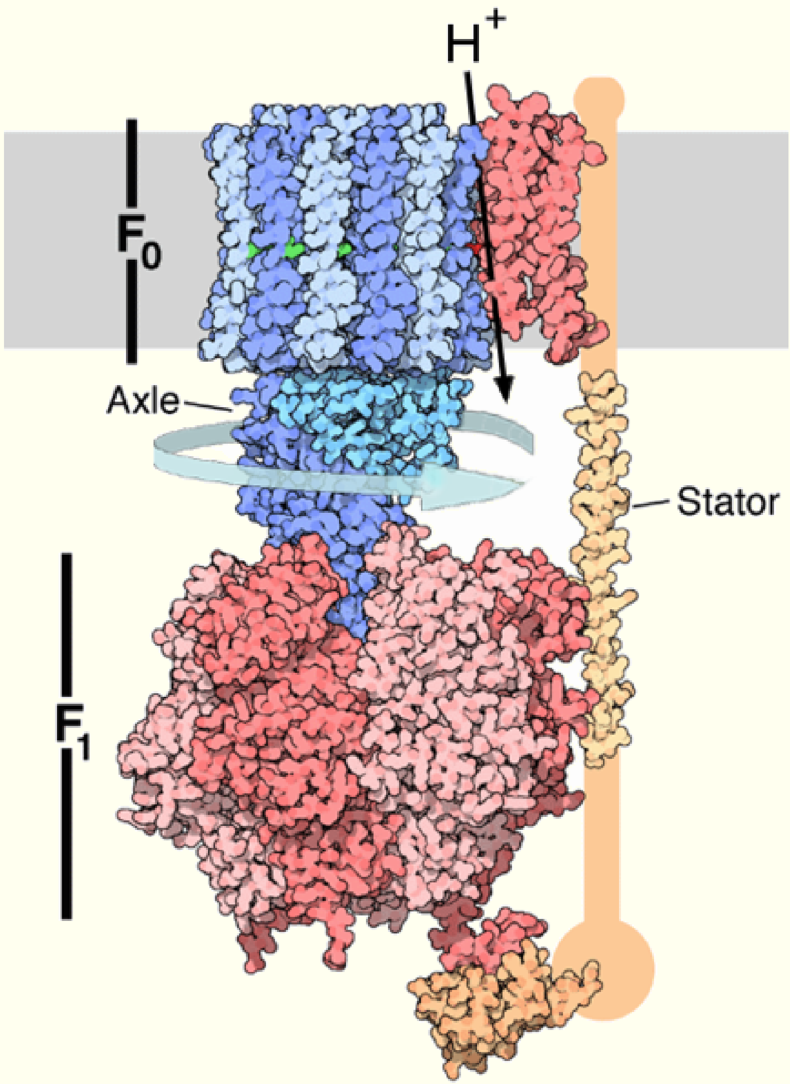
- ATP:

  "molecular unit of currency" of intracellular energy transfer

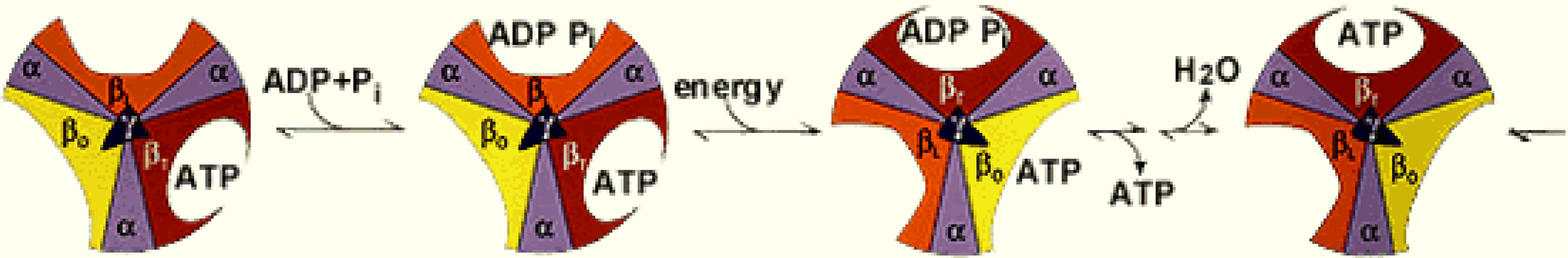
F_1F_O ATP Synthase

- energy from glucose sets up H^+ gradient
- H^+ current drives motor
- stator opens & closes, producing ATP





F_1F_O ATP Synthase



A complete ATP molecule is bound to β_T.

β_L binds ADP and inorganic phosphate (P_i).

The γ subunit has rotated. β_T becomes open and ATP is released. β_L becomes tight and β_O becomes loose.

The phosphate ion reacts with the ADP molecule so that a new ATP molecule is formed. We are back to the first stage.

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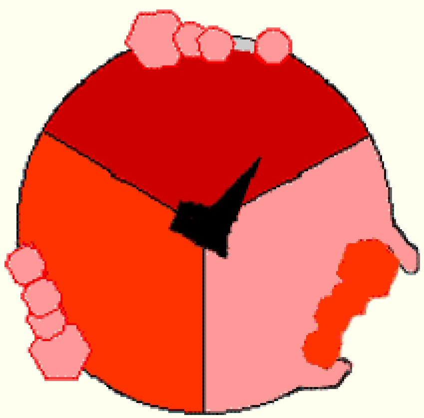
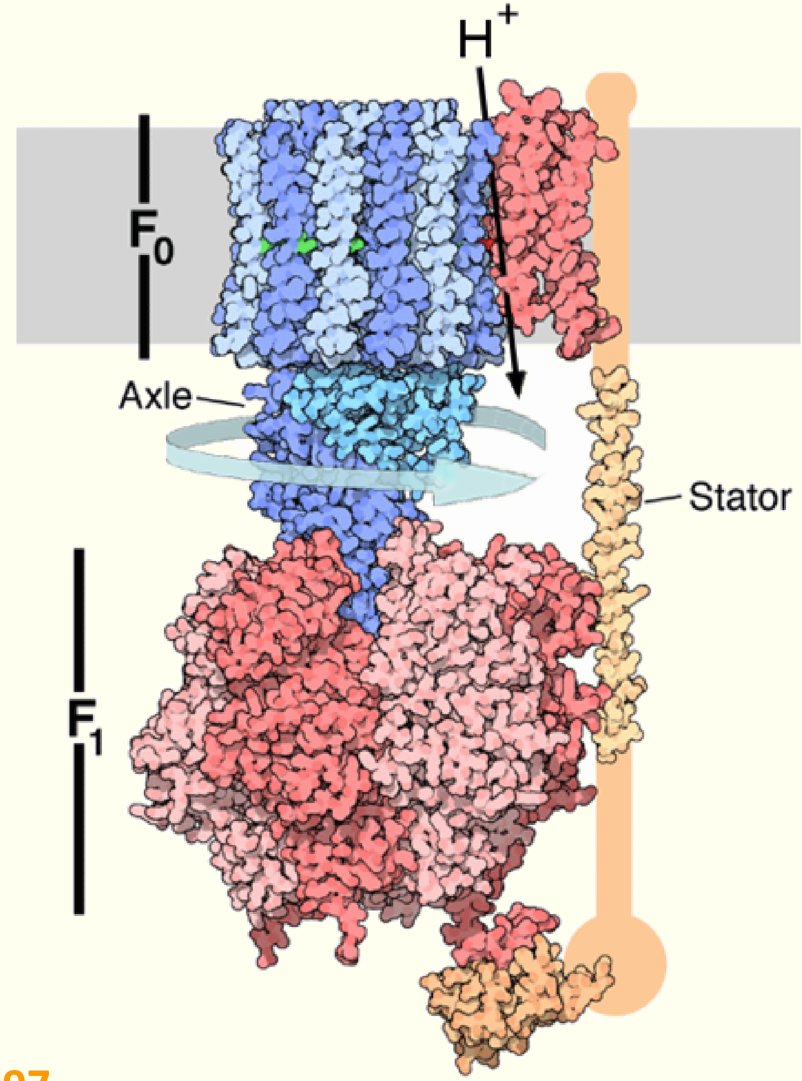
F_1F_O ATP Synthase

- normal human produces ~100lbs of APT/day

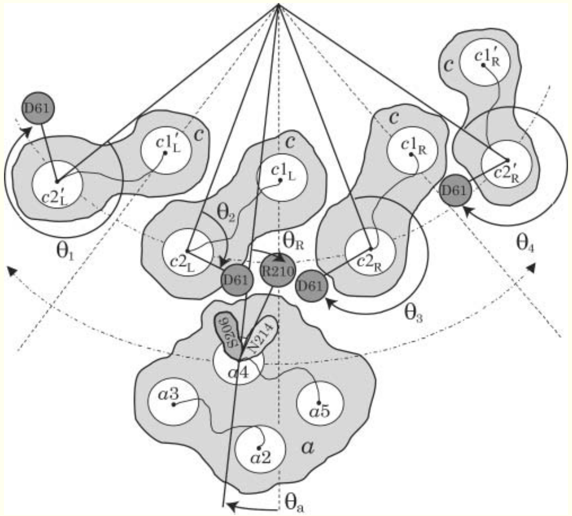
- motor can run backwards



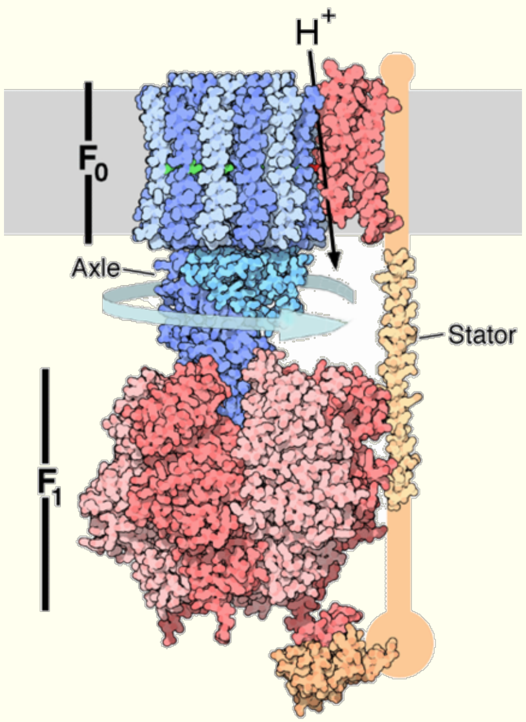


Boyer & Walker, Nobel Prize in Chemistry, 1997

Why does rotor turn?



- sequential protonation & deprotonation of side groups coupled with rotation



- chemical potential difference of H^+ drives current, which drags surface of C-rotor.

- pot. diff. $\rightarrow$ current $\rightarrow$ rotation.

A. Aksimentiev *et al.* Biophysical Journal **86** ,1332 (2004)

Modeling

- system of Langevin equations

$$\xi_i \frac{d\theta_i}{dt} = -\frac{\partial \Psi(\theta_a, \theta_R, \theta_1, \theta_2, \theta_2, \theta_4)}{\partial \theta_i} + \eta_i(t),$$
$$i = a, R, 1, \ldots, 4.$$

- Lennard-Jones + hydrophobic +screened Coulomb

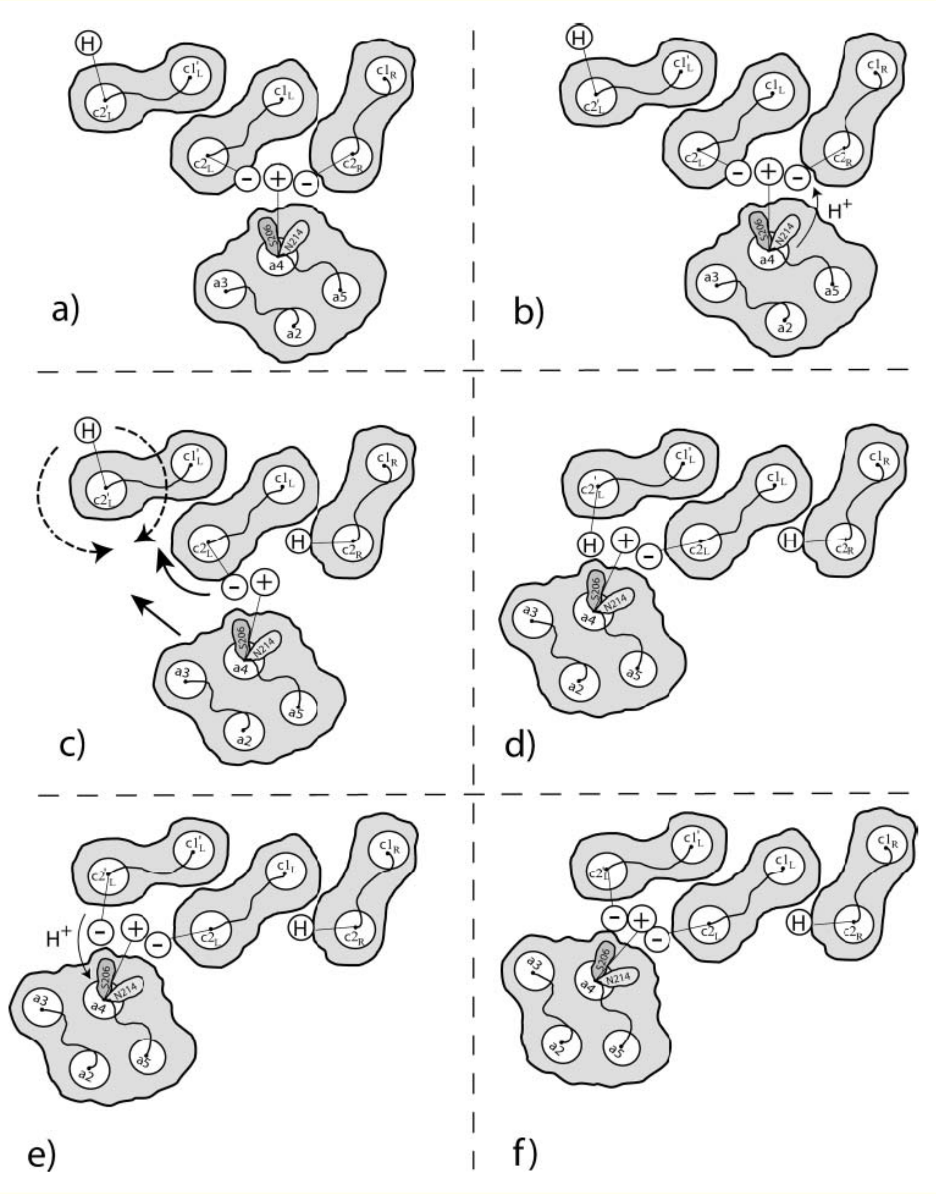
$$U_{EL}(\vec{r}) = \frac{e^2}{4\pi\varepsilon_0\varepsilon}\frac{q_1 q_2}{|\vec{r}|}\exp(-\lambda|\vec{r}|);$$

A. Aksimentiev *et al.* Biophysical Journal **86** ,1332 (2004)

Modeling

- proposed sequence

  based on simulations



A. Aksimentiev *et al.*
Biophysical Journal **86** ,1332 (2004)

Summary of ATP Synthase

- rotary molecular motor
- rotation driven by proton current
- energy from stored electrochemical potential
- work: creation of ATP + dissipation

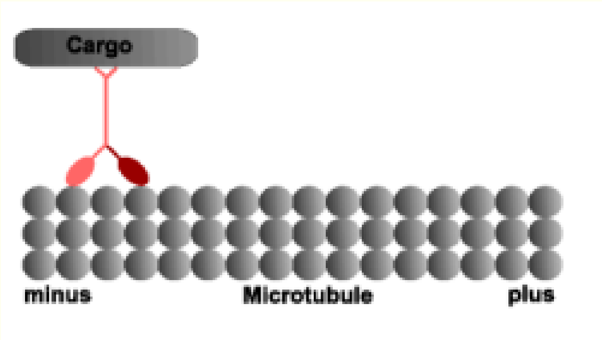
Molecular Motors 4.
Actin & Myosin

Biological transport

- all organisms (eukaryotic cells of yeasts, plants, animals) contain ‘motor proteins’

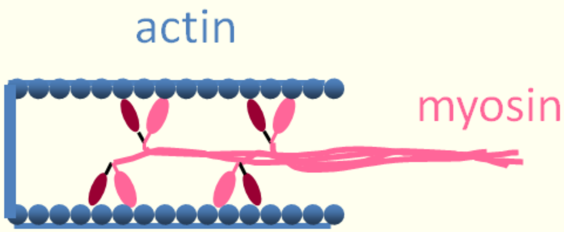
- two well known examples:

  - kinesins
    - two active heads
    - hydrolyses ATP
    - moves along microtubules



  - myosins
    - two active heads
    - hydrolyses ATP
    - moves along actin fibers

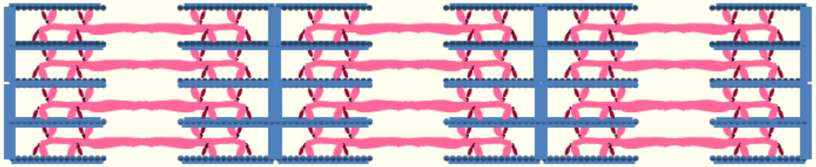
Muscle force and movement



F=5.3pN /cross-bridge
step-size=5.5nm
1 step/ATPase reaction

sarcomere

myosin filament length=1.55µm



muscle fiber

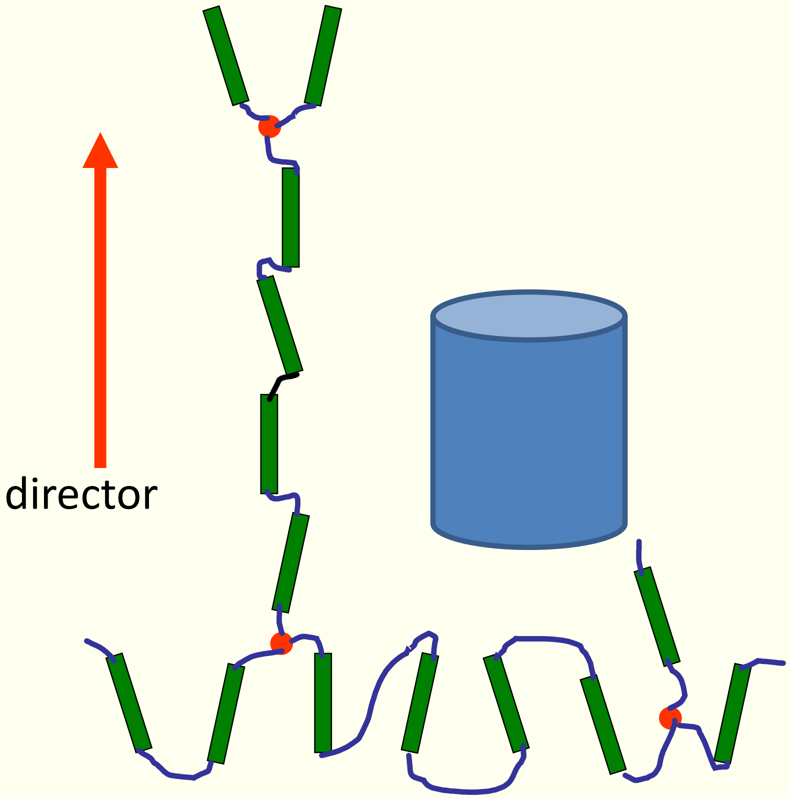
C.J. Pennycuick, *Newton Rules Biology* (Oxford, 1995)

Summary of Actin &Myosin

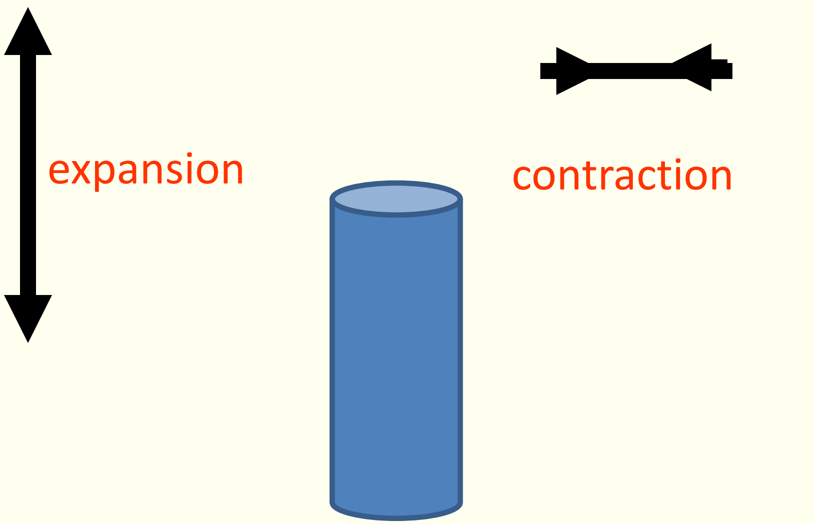
- processive motor (unidirectional translation)
- hand-over-hand motion
- driven by chemical energy of ATP
- work: translation of cargo against force, dissipation

Molecular Motors 5.
LC elastomers

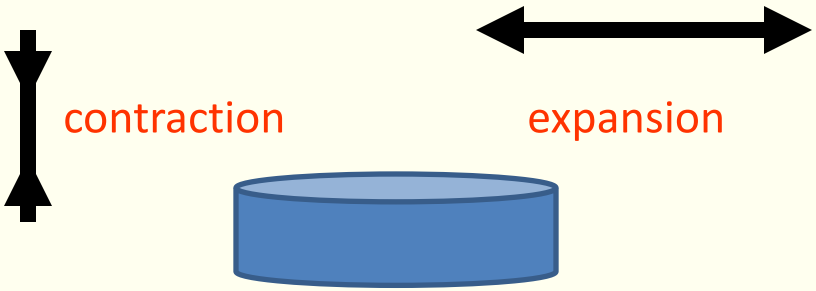
LC elastomer network changes shape



If orientational order increases,



If orientational order decreases,



Summary of LC elastomers

- elongational motor:
  - change in orientational order produces stress
  - stress produces change in shape
- driven by heat, light, or impurities
- work: motion against force, dissipation

Broken Symmetry

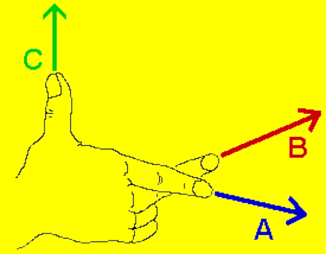
Proper- and pseudo-tensors

tensor rank	0	1	2	3	4
proper	π , x	$\mathbf{E}$, $\mathbf{P}$, $\mathbf{D}$	$\delta_{\alpha\beta}$, $Q_{\alpha\beta}$ $\varepsilon_{\alpha\beta}$, $\mu_{\alpha\beta}$	$d_{\alpha\beta\gamma}$	etc.
pseudo	$\mathbf{A}\bullet(\mathbf{B}\times\mathbf{C})$	$\mathbf{H}$, $\mathbf{M}$, $\mathbf{B}$	$\Gamma_{\alpha\beta}$	ε_{ijk}	

scalar vector

changes sign on inversion

does not change sign on inversion



handedness = pseudoscalar c*!

Symmetry and motors

- symmetry of the system determines motion of motor!

Translational motion

YAHOO! ANSWERS

My rugs are alive and moving!?

I have wall to wall carpets in my apartment. I have placed large rugs on top of the carpet. Without damaging the carpet or the rug, how can I stop them from wrinkling and moving? Is it caused by static electricity?

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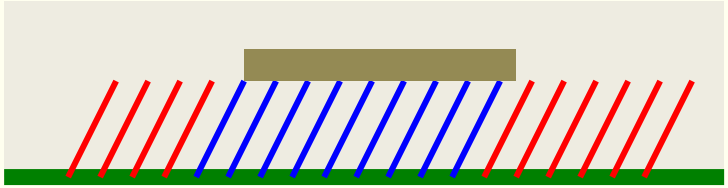
tilted strands



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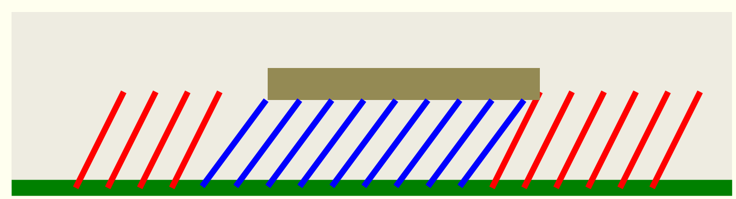

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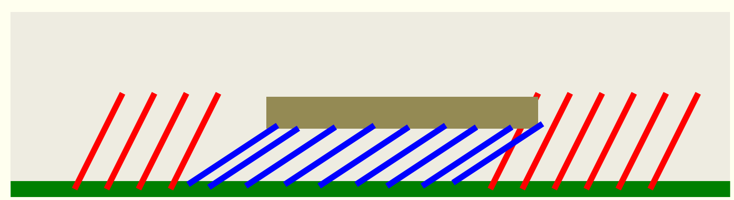

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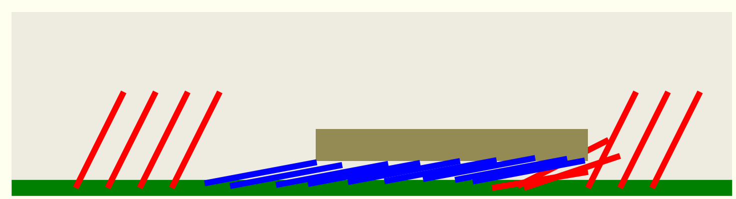

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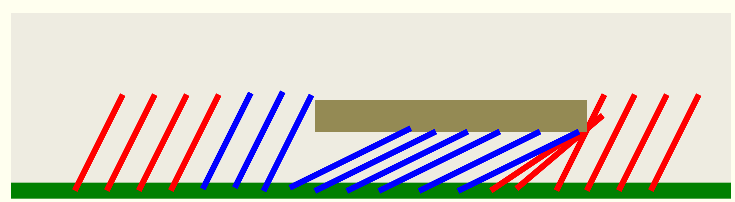

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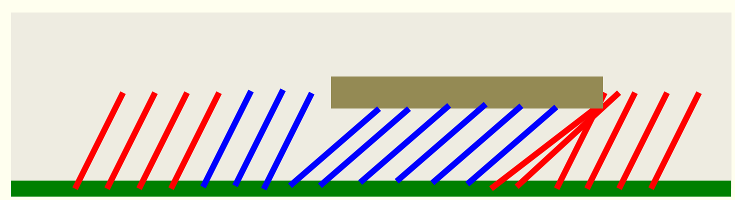

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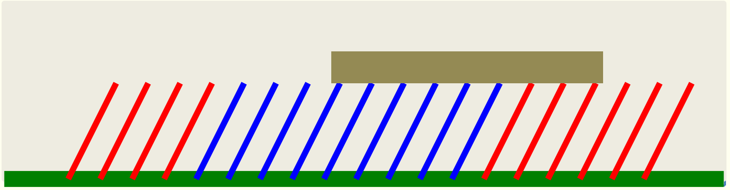


Symmetry and motors

- symmetry of the system determines motion of motor!
- broken left-right symmetry:
  - proper vector exists in system
  - translation in direction of vector (carpet, kinesin, myosin)

Symmetry and motors

- symmetry of the system determines motion of motor!

- broken translational symmetry:
  - proper vector exists in system
  - translation in direction of vector (carpet, kinesin, myosin)

  [Q: is there a vector in Landauer's blow torch?]

- broken chiral symmetry
  - pseudoscalar c* exists in system

- broken chiral + broken translational symmetry
  - pseudoscalar + proper vector = pseudovector
  - rotation (Yokoyama – Tabe, ATP Synthase, etc.)

Symmetry and motors

- if system has proper dyad (director)
  - strain (elongation)
- if system has proper dyad and gradient (vector),
  - proper vector (curvature, bend)
- if system has proper dyad, gradient & pseudoscalar
  - pseudovector (twist)

Symmetry & deformation/motion

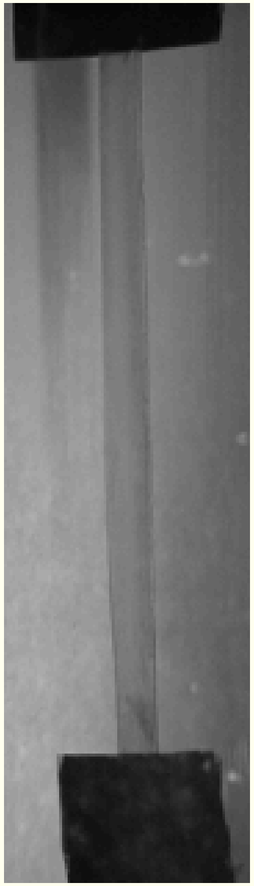
Symmetry	can construct	deformation/motion	material
→	vector	translation	in kinesin, actin
↔	dyad	uniaxial strain	nematic networks
c*	-	-	
c* →	pseudovector	rotation	Lehman, ATP, Tabe
→ ↔ c*	pseudovector	twist	LCE twist
→ ↔	proper vector	bend	LCE photoactuation

Connecting molecular & macrosopic scales

- cumulative effect of many molecular motors $\rightarrow$ macroscopic response
  - rotating dye system, Yokoyama-Tabe expt:
    - distributed local vorticity $\rightarrow$ bulk torque & bulk flow
  - ATP synthase:
    - produces bulk ATP
  - myosin & actin
    - muscle fibers form long muscles, these contract
  - effective shape change
    - contraction, elongation and bend and twist

Smooth shape change: elongation

- liquid crystal elastomers:
  - coupling of orientational order and strain
  - large mechanical response to excitations



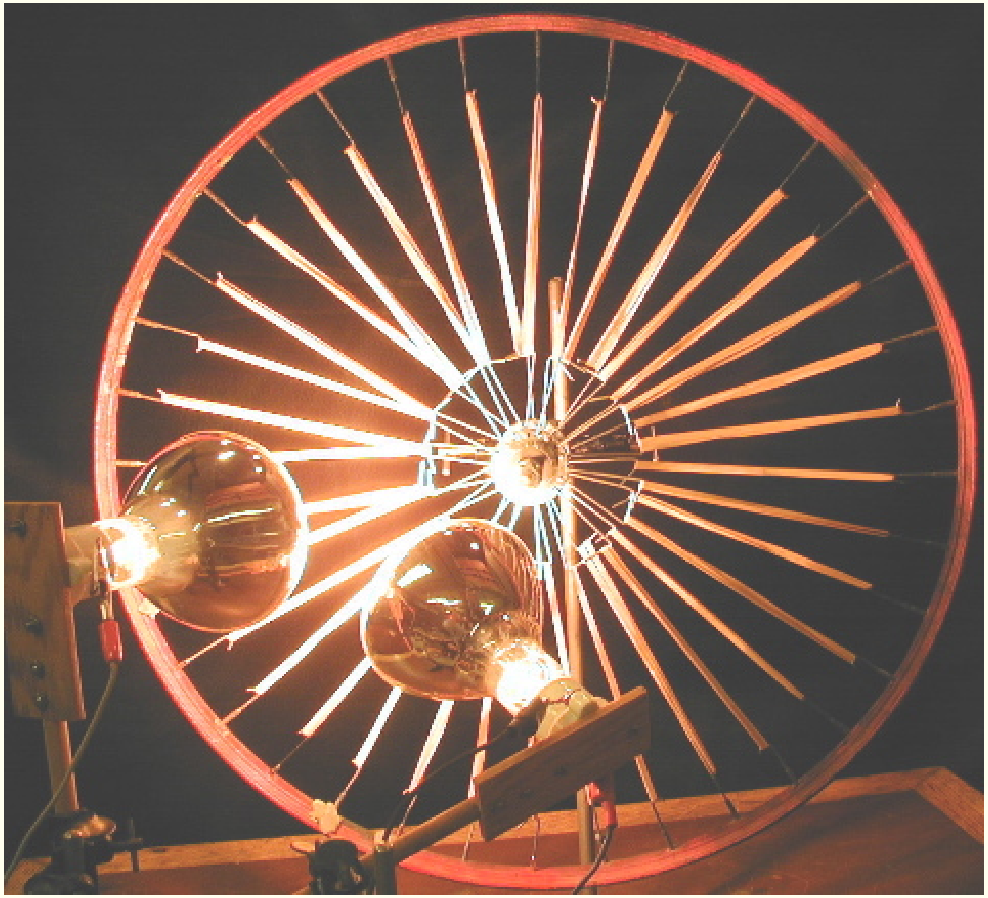
- elongation due to temperature change

- motor based on elongation

H. Finkelmann, nematic LCE

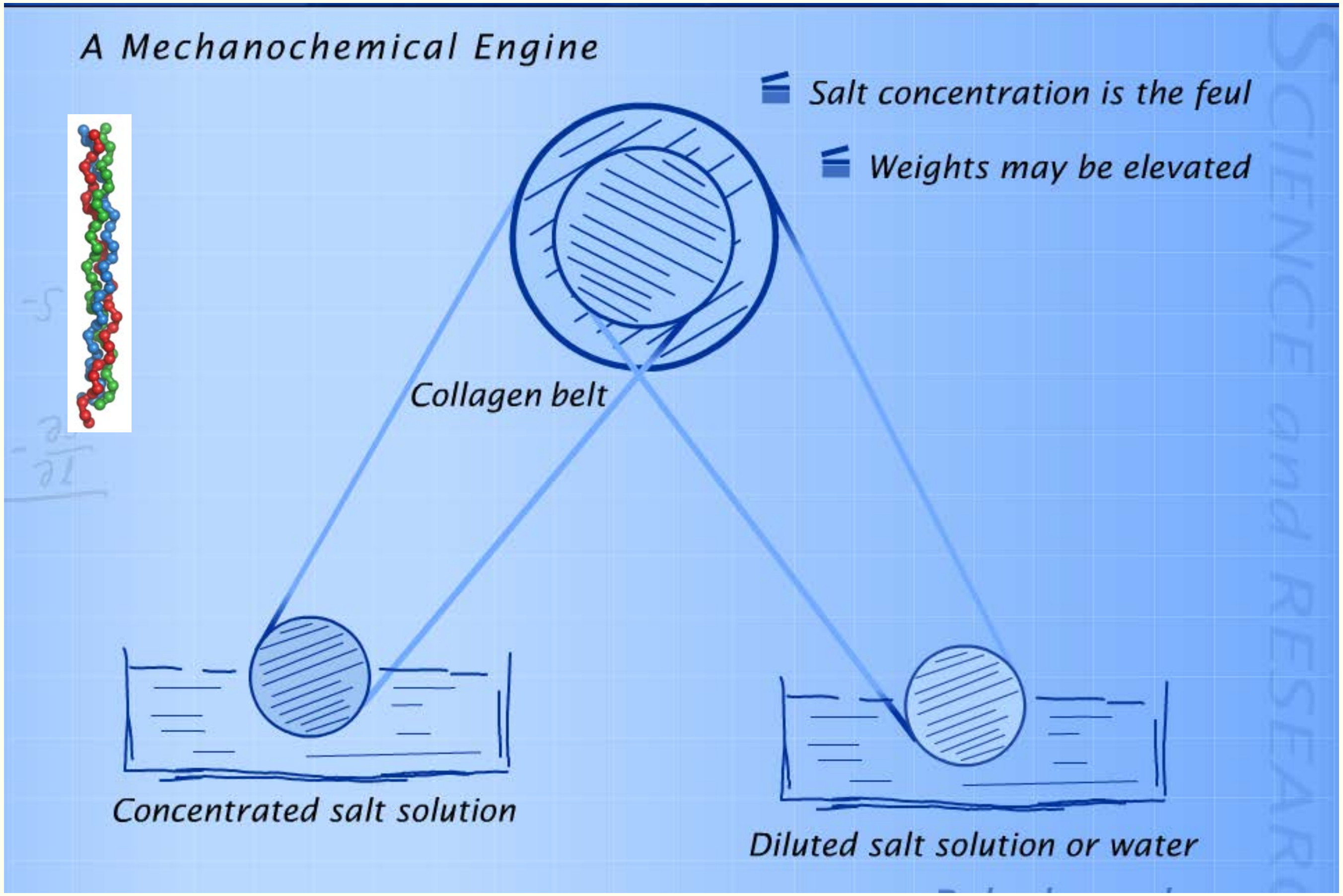
Another motor based on elongation

- rubber band heat engine



Another motor based on elongation

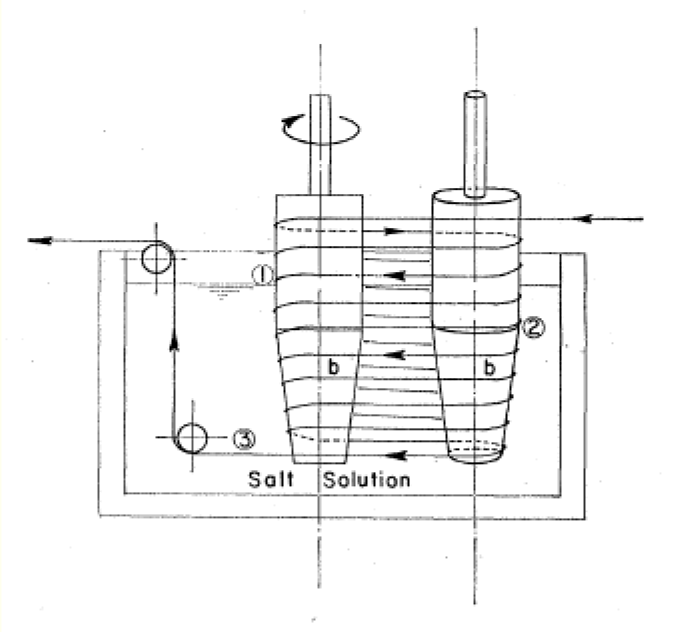
- collagen contracts in salt water

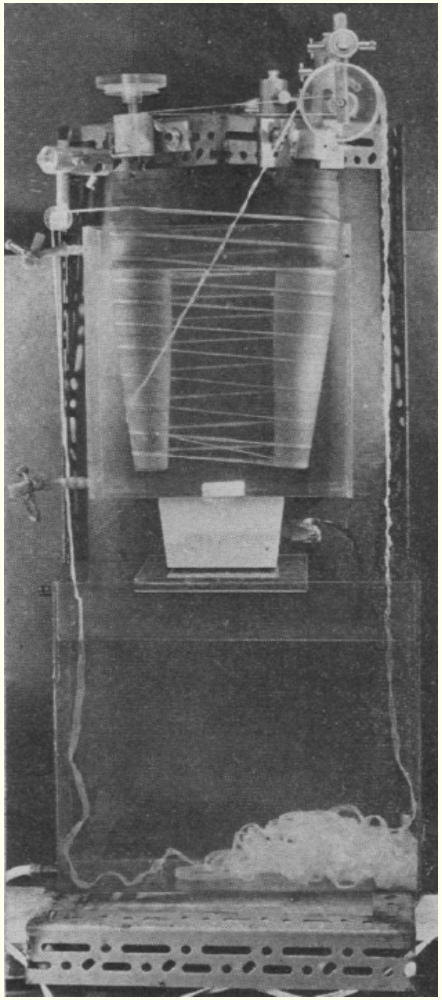


Aharon Katzir-Katchalsky 1913-1972

Another motor based on elongation

- a modified version





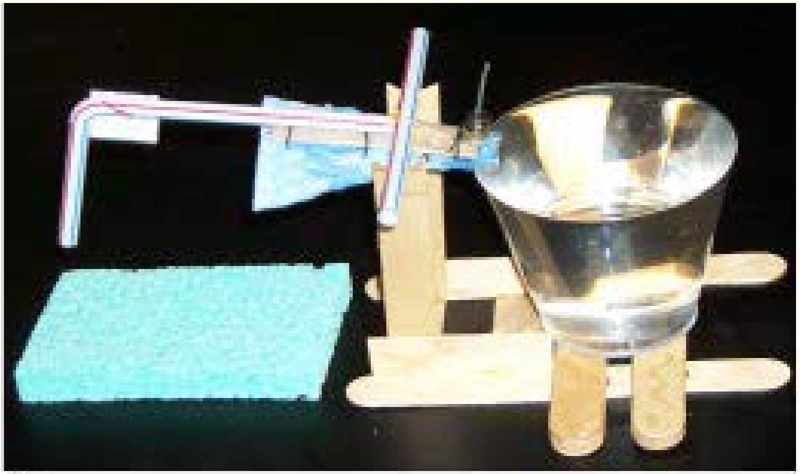
M. V. Sussman and A. Katchalsky, Science, **167**, 45 (1970)

Dunking bird of the first kind

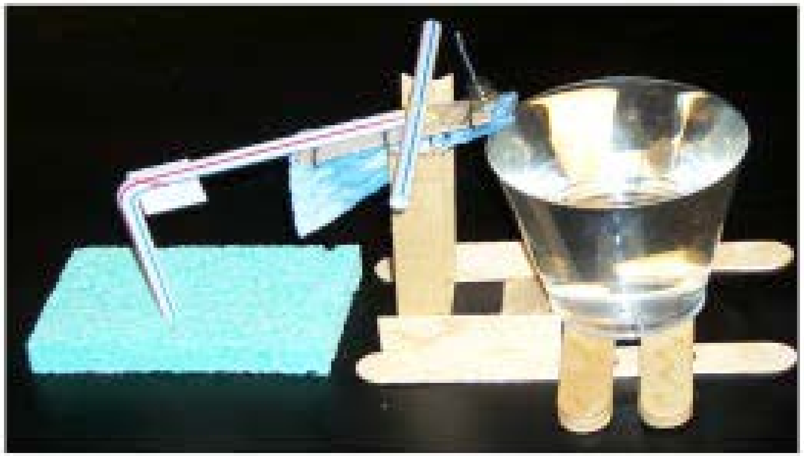
- heat engine
  - Carnot efficiency limit

Dunking bird of the second kind

- not a heat engine
- isothermal
- involves shape change



(a)

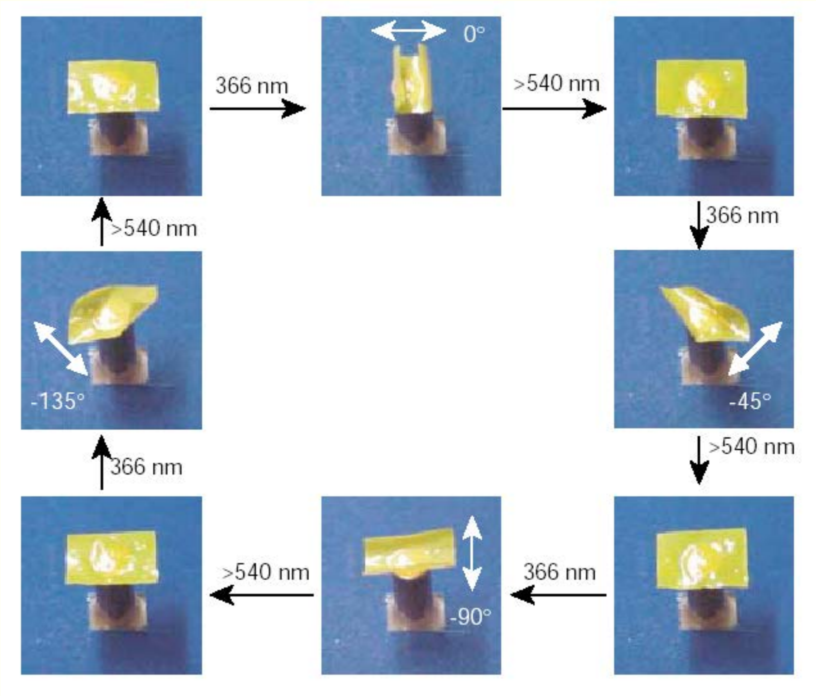


(b)

N. Abraham, P. Palffy-Muhoray., *Am.J. Phys.* **72**, 782 (2004)

Bend Motors

- samples of liquid crystal elastomers with azo dye bend on exposure to light

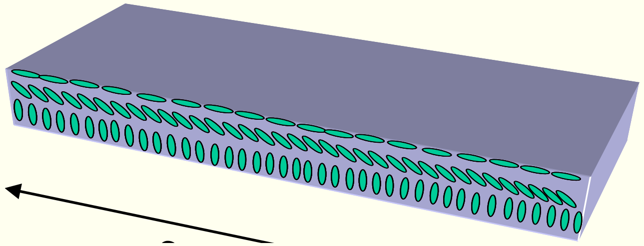


LC + diacrylate network
+ functionalized
azo-chromophore

timescale: 10 s

Yanlei Yu, Makoto Nakano, Tomiki Ikeda, *Nature* **425**, 125 (2003)

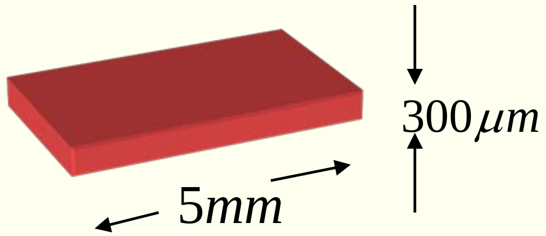
Water vapor sensitive network

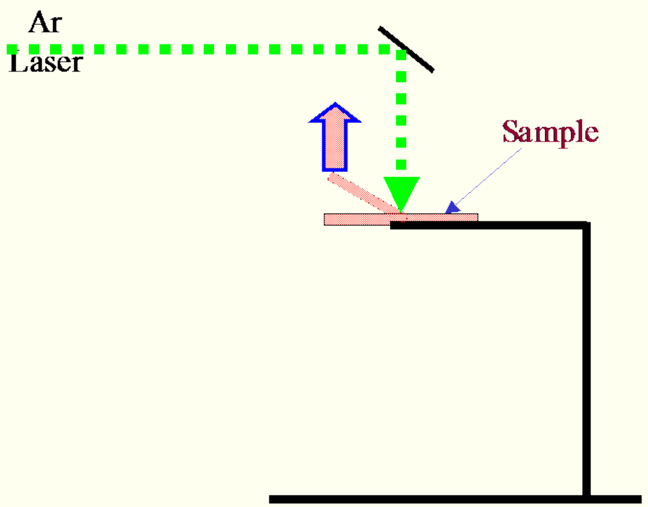


K. Harris, C. Bastiaansen, D. Broer, *J. MEM Syst.*, **16**, 480 (2007)

Bend Motors

sample: nematic elastomer EC4OCH3
+ 0.1% dissolved
Disperse Orange 1 azo dye

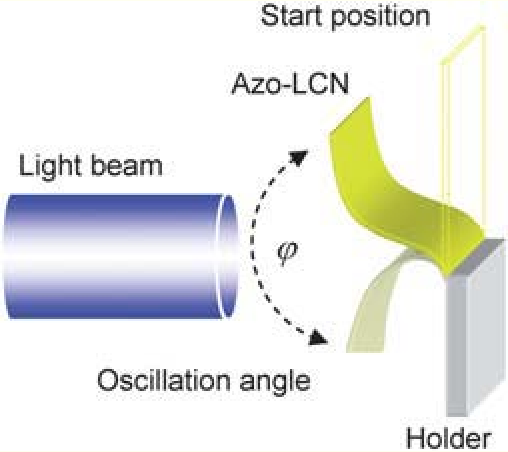


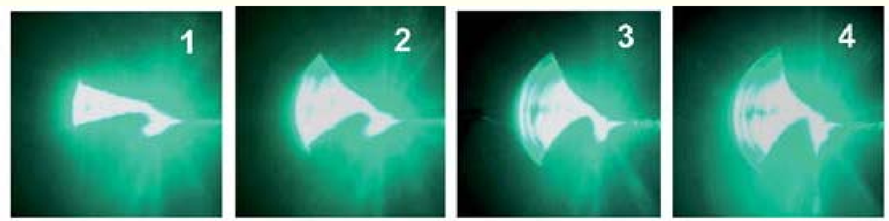


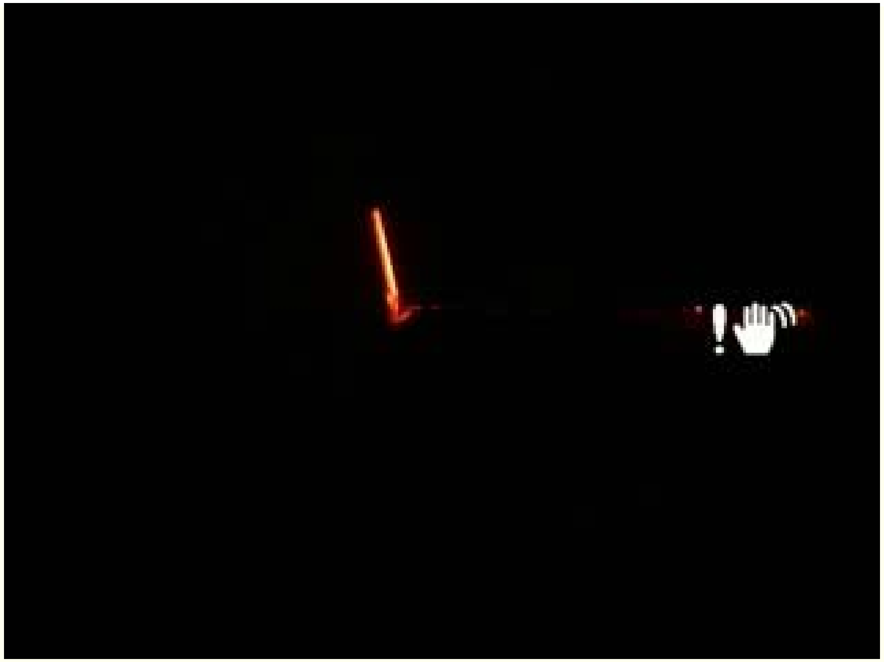
Response time: 70ms

Photoinduced oscillations

- if sample bends $> 90^o$ both sides are illuminated, producing oscillations







nematic azo-elastomer

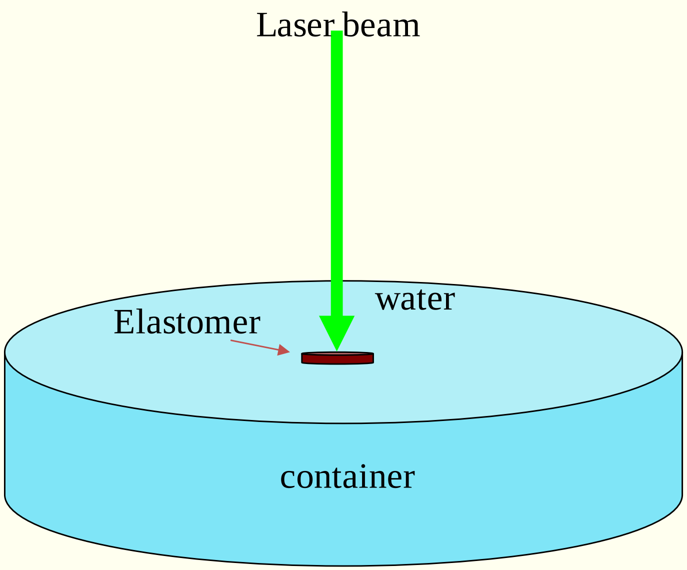
sample size: 5 mm 0.8 mm 0.05 mm

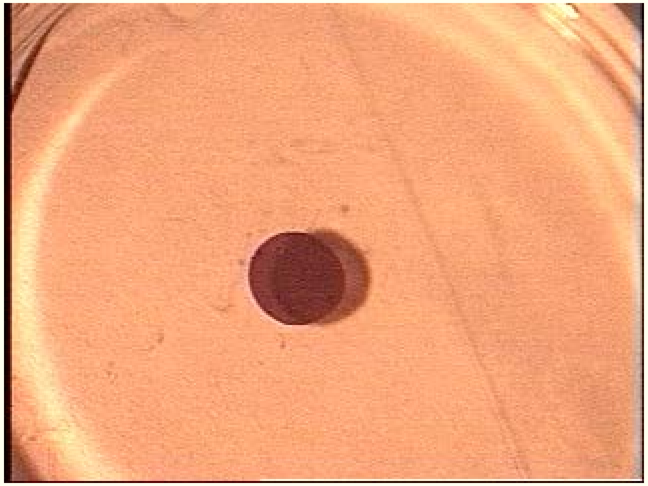
max. frequency = 270Hz

S. Serak, N. Tabiryan, R. Vergara, T. White, R. Vaia, T. Bunning, *Soft Matter* **6**, 779–783 (2010)

Bend Motors

- floating nematic LCE sample illuminated from above

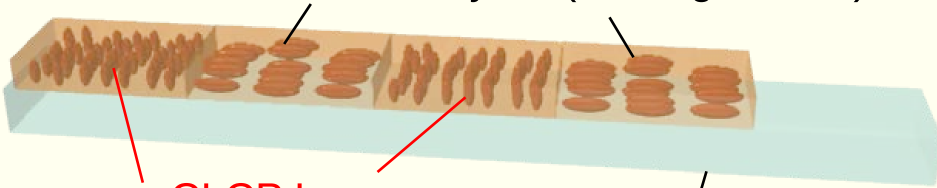


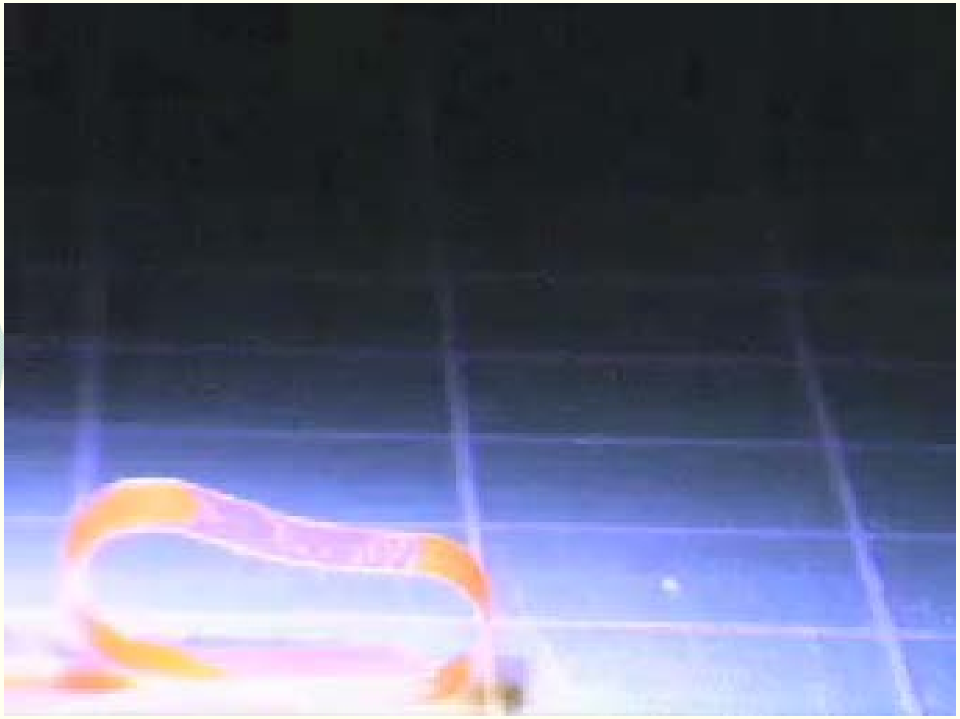


M. Chamacho-Lopez, H. Finkelmann, P. Palffy-Muhoray, M. Shelley, *Nature Mat.* **3**, 307, (2004)

Bend Motors

- robotic arm





T. Ikeda, Chuo University (priv. comm.)

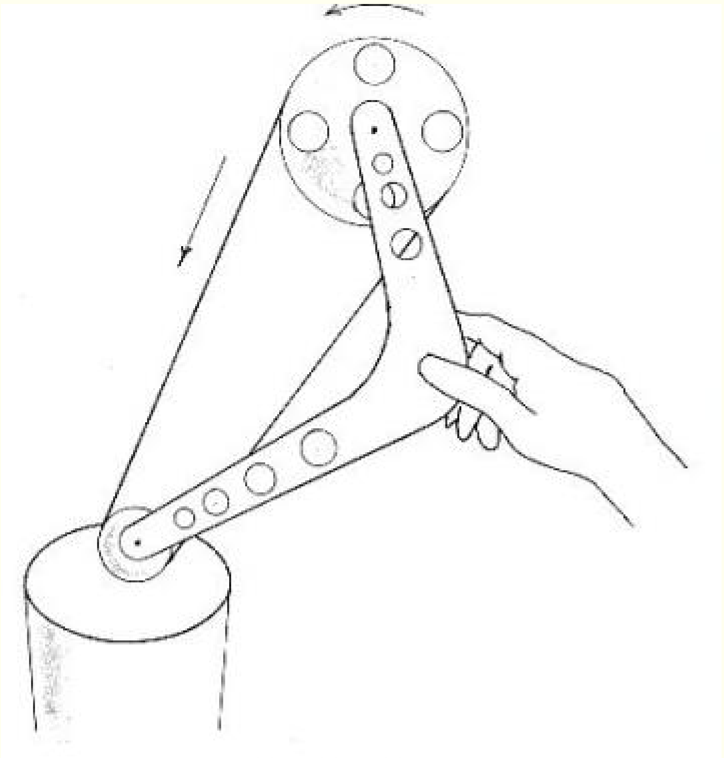
Bend Motor: focus of current interest

- azo-dye doped liquid crystal elastomer

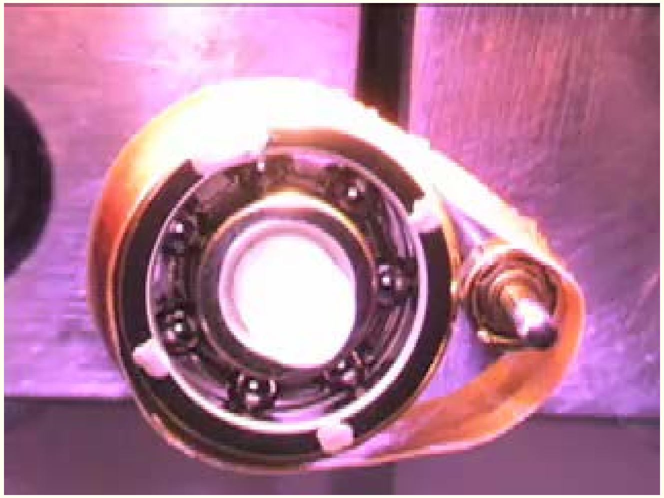
M. Yamada, M. Kondo, J. Mamiya, Y. Yu, M. Kinoshita, C. Barrett, T. Ikeda, *Angew. Chem.* **47**, 4986 (2008)

Bend Motor: focus of current interest

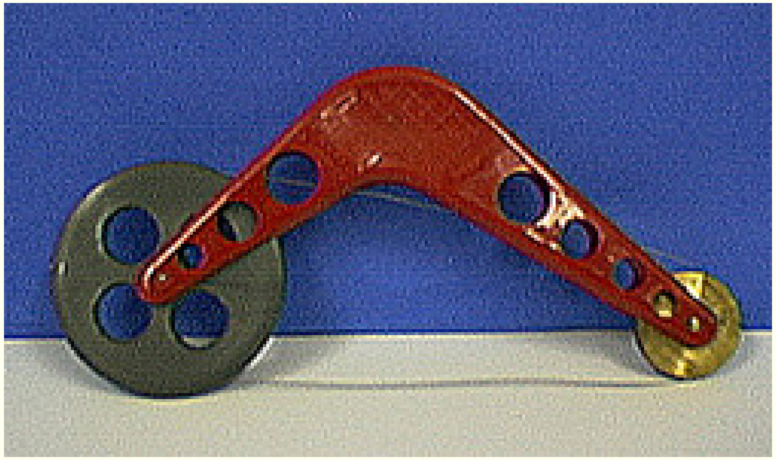
- shape-memory Ni-Ti alloy,
  - two phases:
    - orthorhombic martensite (cold)
    - cubic austenite (hot)



Existing rotary bend motors



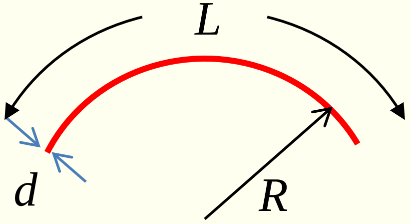
LCE bends on exposure to light

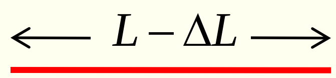


wire becomes stiff when heated

Model

- bend vs. compression:
  - if ends are brought closer, will filament compress or bend?





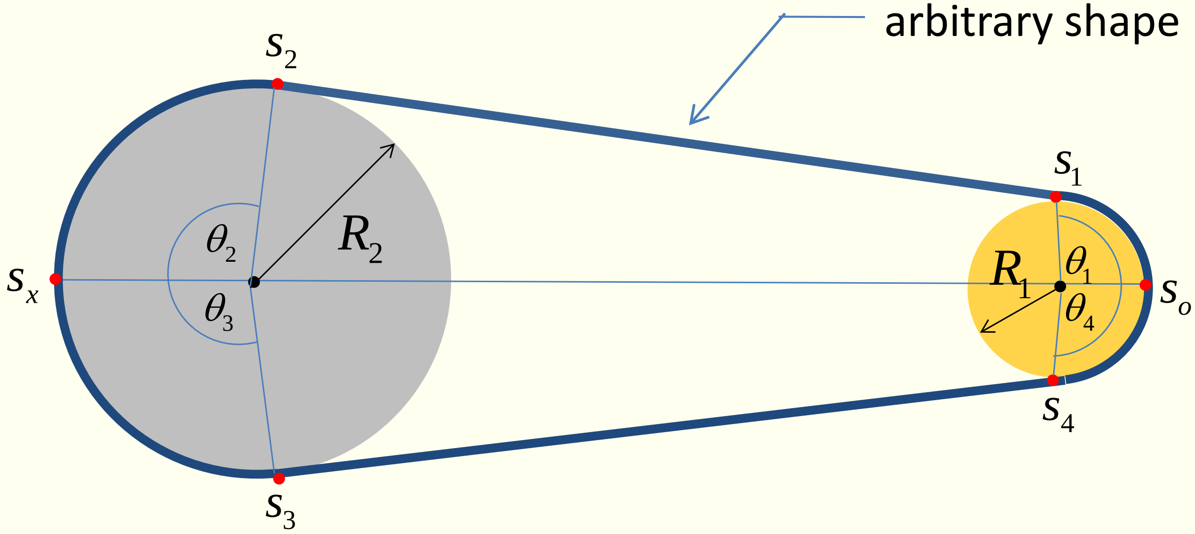
$$\frac{\Delta L}{L} \simeq \frac{1}{24}\left(\frac{L}{R}\right)^2$$

$$\mathcal{E}_b / l = \frac{1}{2} E\left(\frac{d}{R}\right)^2 \frac{wd}{12} \qquad \mathcal{E}_c / l = \frac{1}{2} E\left(\frac{\Delta L}{L}\right)^2 wd \qquad \boxed{\frac{\mathcal{E}_c}{\mathcal{E}_b} \sim \left(\frac{L}{d}\right)^2\left(\frac{L}{R}\right)^2}$$

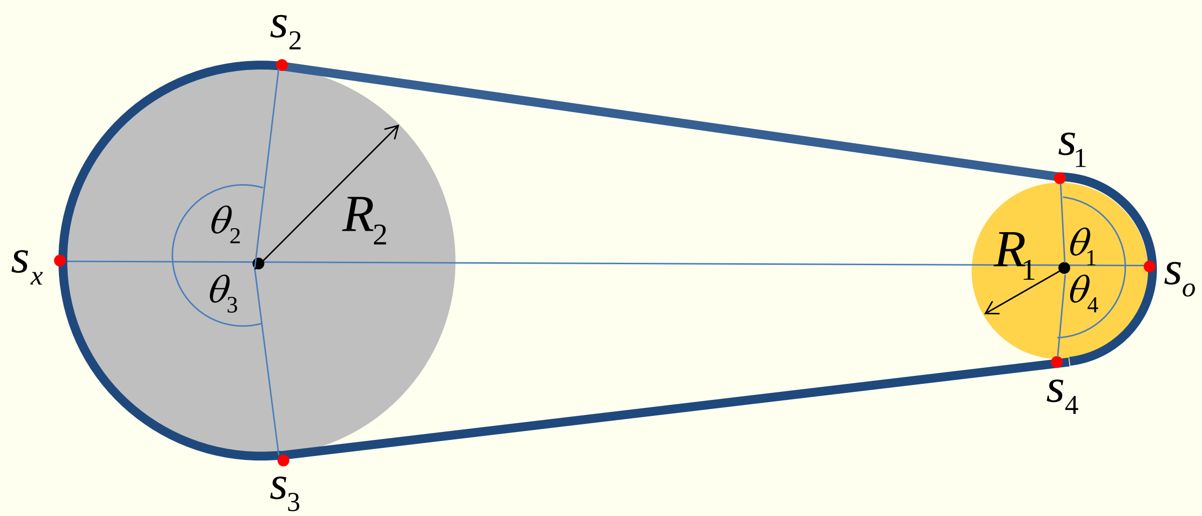
Bend is *much* cheaper energetically than stretch;

→ <u>length is constant</u>.

Model

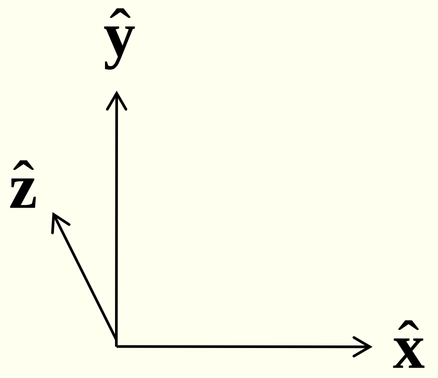

arbitrary shape
s_2
s_1
θ_2
R_2
s_x
θ_3
R_1
θ_1
θ_4
s_o
s_4
s_3

Model



s – arc length along filament

$\mathbf{R}(s)$ – position vector of point on filament



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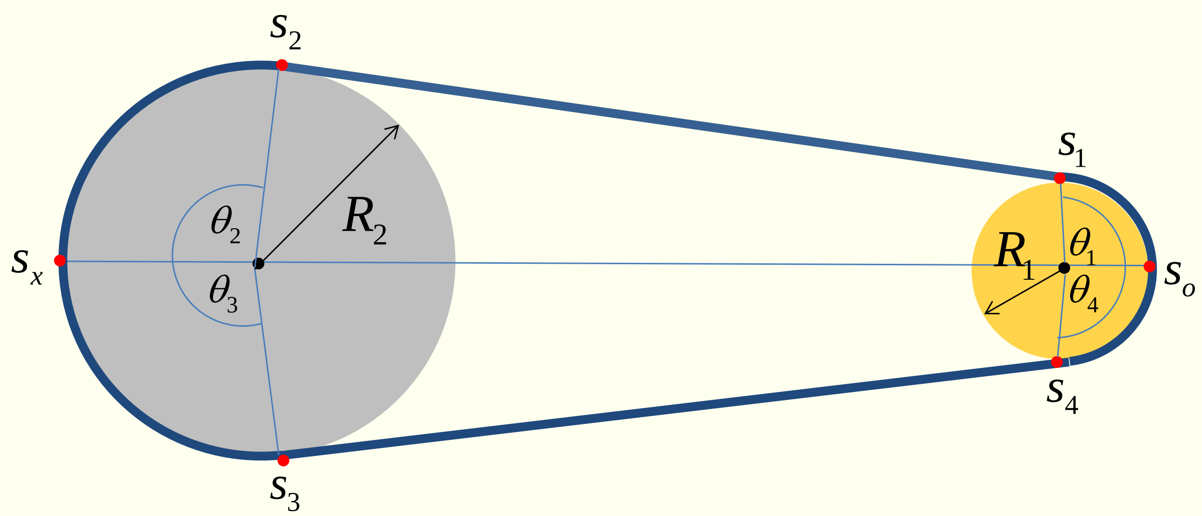


– bend energy density:

$$\mathcal{E}_b / l = \frac{1}{2} EI \frac{1}{R^2} = \frac{c}{R^2}$$

stiffness fn. of position

natural curvature fn. of position

$$\mathcal{E} = \int_{s_o}^{s_1} c\left(\frac{1}{R_1} - \kappa\right)^2 ds + \int_{s_1}^{s_2} c\left(\frac{\partial^2 \mathbf{R}}{\partial s^2} - \kappa\left(\frac{\partial \mathbf{R}}{\partial s} \times \hat{\mathbf{z}}\right)\right)^2 ds +$$

$$\int_{s_2}^{s_3} c\left(\frac{1}{R_2} - \kappa\right)^2 ds + \int_{s_3}^{s_4} c\left(\frac{\partial^2 \mathbf{R}}{\partial s^2} - \kappa\left(\frac{\partial \mathbf{R}}{\partial s} \times \hat{\mathbf{z}}\right)^2 ds + \int_{s_4}^{s_o} c\left(\frac{1}{R_1} - \kappa\right)^2 ds,$$

Model

s_2

s_1

s_x θ_2 R_2 R_1 θ_1 s_o

θ_3 θ_4

s_4

s_3

– constraints:

- filament length is constant
- displacement in x-dir. is fixed

$$R_1(1-\cos\theta_1) - \int_{s_1}^{s_2} \hat{\mathbf{t}}\cdot\hat{\mathbf{x}}ds + R_2(1-\cos\theta_2) = L + R_1 + R_2,$$

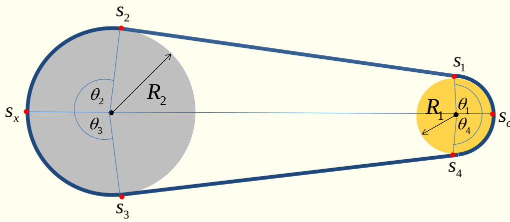
$$R_1(1-\cos\theta_4) + \int_{s_3}^{s_4} \hat{\mathbf{t}}\cdot\hat{\mathbf{x}}ds + R_2(1-\cos\theta_3) = L + R_1 + R_2.$$

- displacement in y-dir. is fixed

$$R_1\sin\theta_1 + \int_{s_1}^{s_2} \hat{\mathbf{t}}\cdot\hat{\mathbf{y}}ds - R_2\sin\theta_2 = 0,$$

$$R_1\sin\theta_4 + \int_{s_3}^{s_4} \hat{\mathbf{t}}\cdot\hat{\mathbf{y}}ds - R_2\sin\theta_3 = 0$$

Model: Energy with constraints



$$\mathcal{E} = \int_0^{s_1} c(\frac{1}{R_1} - \kappa)^2 ds + \int_{s_1}^{s_2} c(\hat{\mathbf{t}}' - \kappa(\hat{\mathbf{t}} \times \hat{\mathbf{z}}))^2 ds + \int_{s_2}^{s_3} c(\frac{1}{R_2} - \kappa)^2 ds$$

$$+ \int_{s_3}^{s_4} c(\hat{\mathbf{t}}' - \kappa(\hat{\mathbf{t}} \times \hat{\mathbf{z}}))^2 ds + \int_{s_4}^{1} c(\frac{1}{R_1} - \kappa)^2 ds$$

$$+ f_{1x}\{R_1(1 - \cos\frac{s_1}{R_1}) - \int_{s_1}^{s_2} \hat{\mathbf{t}} \cdot \hat{\mathbf{x}} ds + R_2(1 - \cos(\frac{s_x - s_2}{R_2})) - (L + R_1 + R_2)\}$$

$$+ f_{1y}\{R_1 \sin\frac{s_1}{R_1} + \int_{s_1}^{s_2} \hat{\mathbf{t}} \cdot \hat{\mathbf{y}} ds - R_2 \sin(\frac{s_x - s_2}{R_2})\}$$

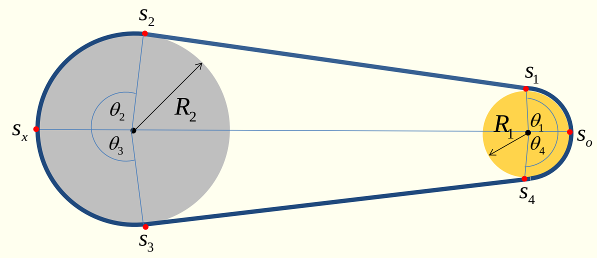
$$+ f_{2x}\{R_1(1 - \cos(\frac{1 - s_4}{R_1})) + \int_{s_3}^{s_4} \hat{\mathbf{t}} \cdot \hat{\mathbf{x}} ds + R_2(1 - \cos(\frac{s_3 - s_x}{R_2})) - (L + R_1 + R_2)\}$$

$$+ f_{2y}\{R_1 \sin(\frac{1 - s_4}{R_1}) + \int_{s_3}^{s_4} \hat{\mathbf{t}} \cdot \hat{\mathbf{y}} ds - R_2 \sin(\frac{s_3 - s_x}{R_2})\}$$

Lagrange multipliers are components of forces in top and bottom filaments.

BOULDER SCHOOL

Model: Energy minimization



- ODEs are obtained by minimizing $\mathcal{E}$ w.r.t. $\hat{\mathbf{t}} = (\cos\theta, \sin\theta)$

$$-2(c\theta'' + c'\theta' + (c\kappa)') + f_{1x}\sin\theta + f_{1y}\cos\theta = 0, \quad \text{if} \quad s \in (s_1, s_2)$$

$$-2(c\theta'' + c'\theta' + (c\kappa)') - f_{2x}\sin\theta + f_{2y}\cos\theta = 0, \quad \text{if} \quad s \in (s_3, s_4).$$

- these govern the shape of the filaments on top and bottom
  - BC for θ is obtained by minimizing $\mathcal{E}$ w.r.t. s_1, s_2, s_3, s_4
  - this gives <u>continuous tangent</u> and <u>curvature</u> at contact pts.

Numerical Solution

1. Assign initial values for s_1, s_2, s_x and f_{1x}, f_{1y} and solve ODE

$$-2(c\theta'' + c'\theta' + (c\kappa)') + f_{1x}\sin\theta + f_{1y}\cos\theta = 0$$

with BCs.

2. Assign initial values for s_3, s_4 and f_{2x}, f_{2y} and solve ODE

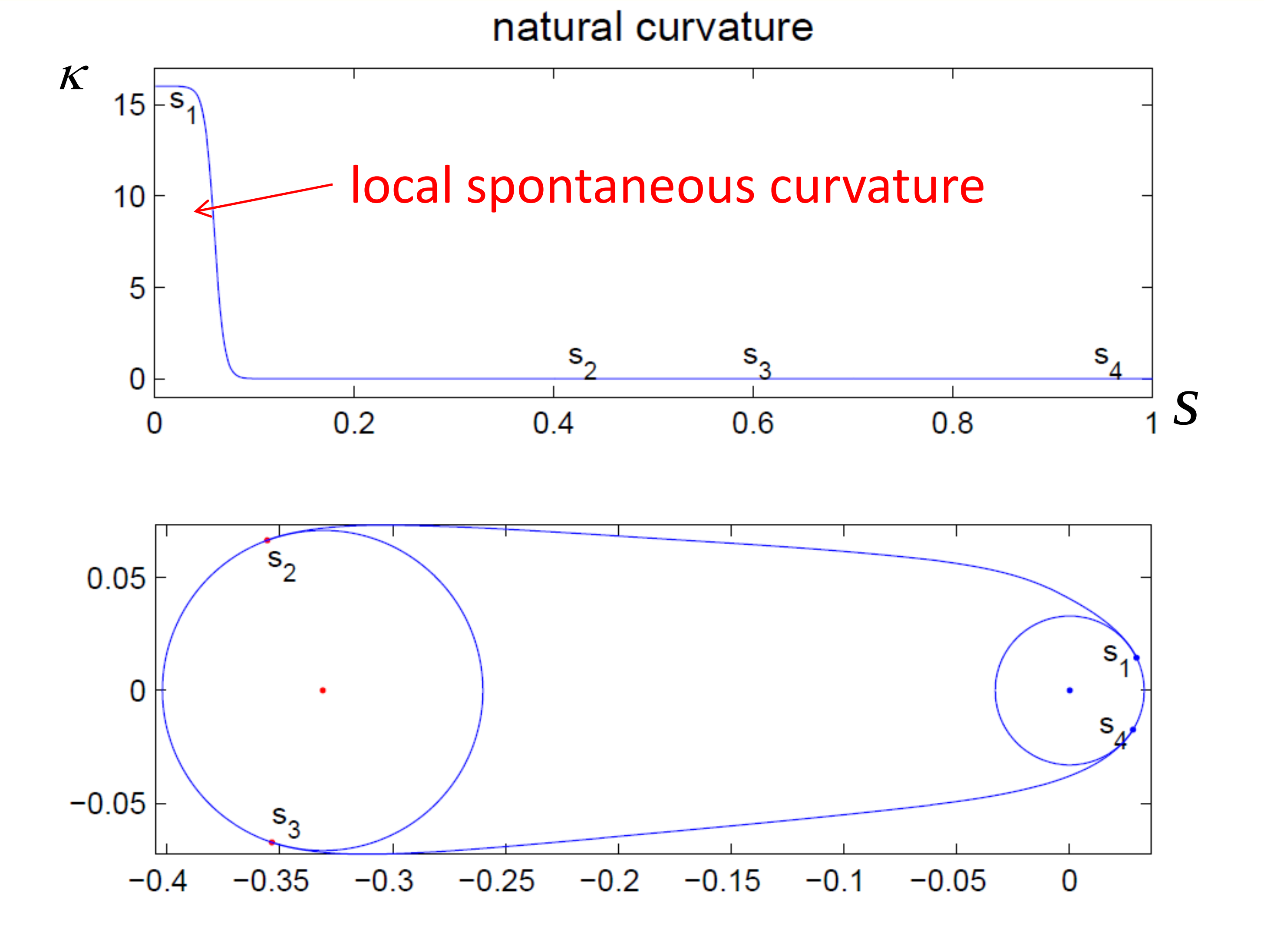
$$-2(c\theta'' + c'\theta' + (c\kappa)') - f_{2x}\sin\theta + f_{2y}\cos\theta = 0$$

with BCs.

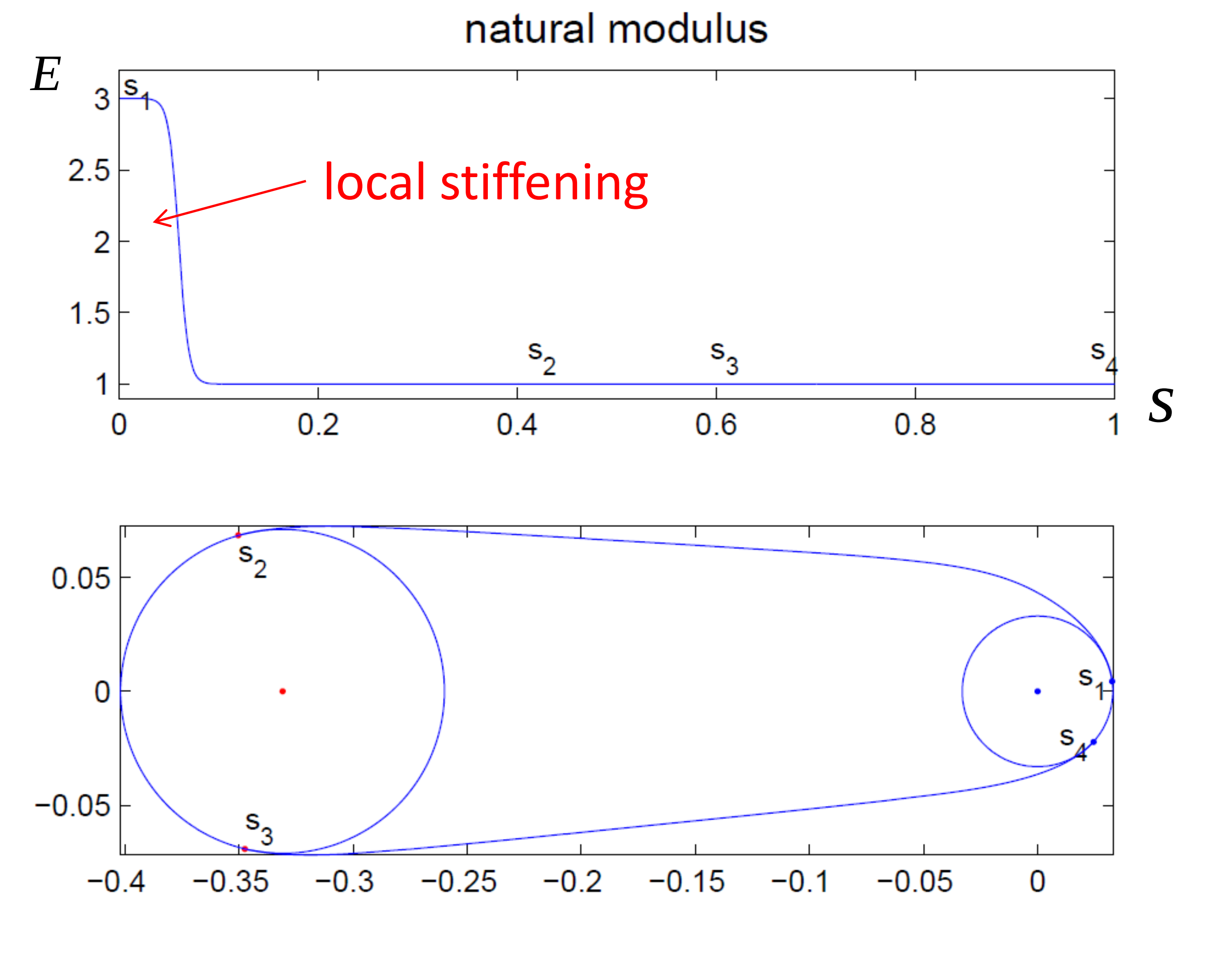
3. Vary the forces $f_{1x}, f_{1y}, f_{2x}, f_{2y}$ to satisfy constraints (root finding)

4. Vary s_1, s_2, s_3, s_4, s_x and go to 1. until $\dfrac{\partial \mathcal{E}}{\partial s_i} = 0, \quad i = 1, \ldots 4, x.$

Numerical Solution: varying the curvature



Numerical Solution: varying the stiffness



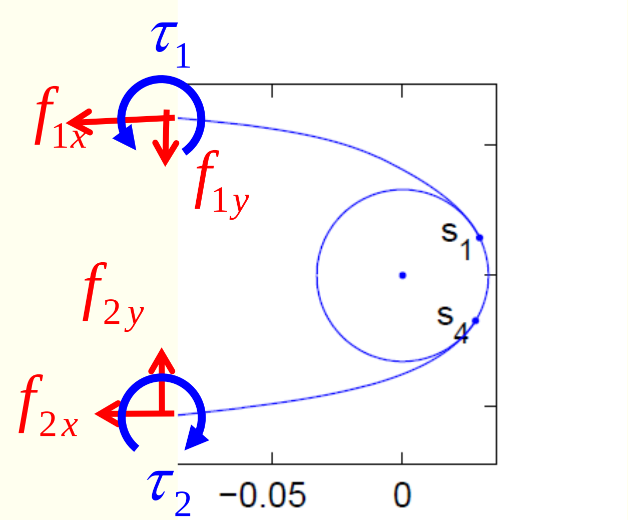
Calculating torques

– to calculate the net torque, we consider <u>part</u> of system

– look at forces

– look at point torques

$$\tau = 2c(\hat{\mathbf{t}}' - \kappa(\hat{\mathbf{t}} \times \hat{\mathbf{z}}))$$



Note: integrating the ODE w.r.t. to *s* gives

$$2c(\theta' + \kappa) - f_{1x}\int_0^s \sin\theta(\tilde{s})d\tilde{s} - f_{1y}\int_0^s \cos\theta(\tilde{s})d\tilde{s} = K_1, \text{(upper part)}$$

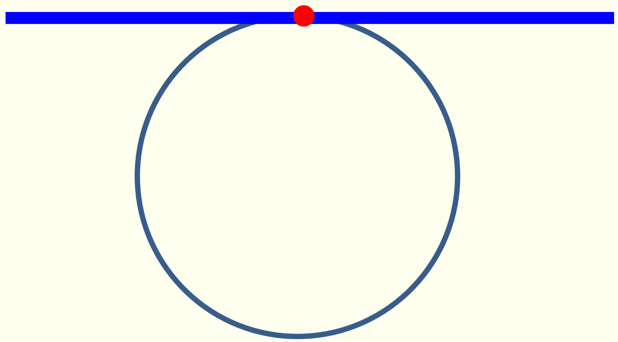
ODE is *precisely* the condition that the torque on wheel remain constant, regardless of where the filament is cut!

What happens on the pulleys?

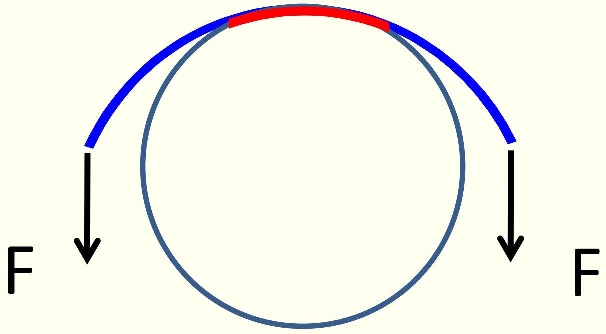
- Problem: elastic beam on rigid cylinder

Interesting observation

– straight beam touches cylinder along one line

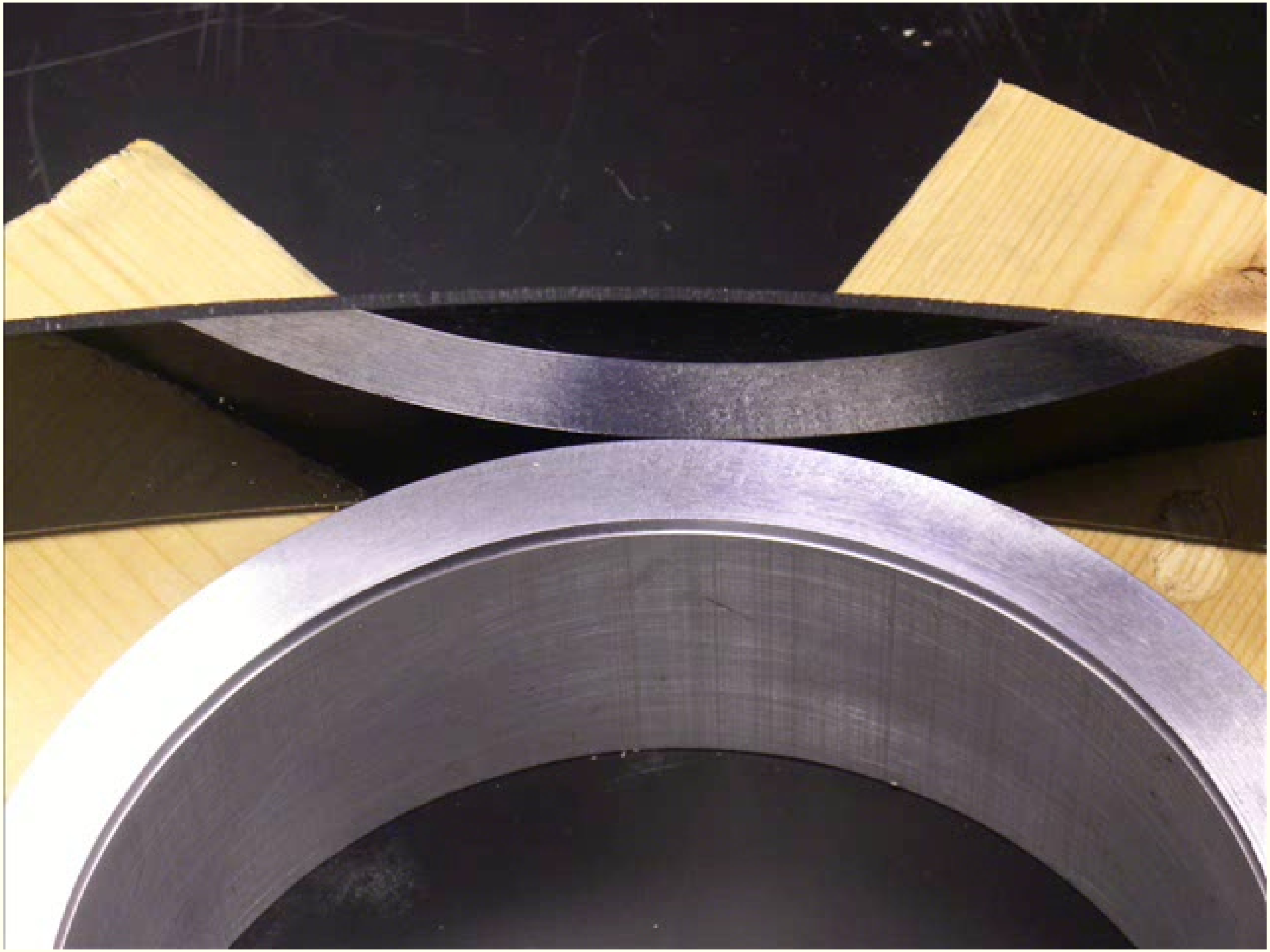


– curved beam touches cylinder over extended area

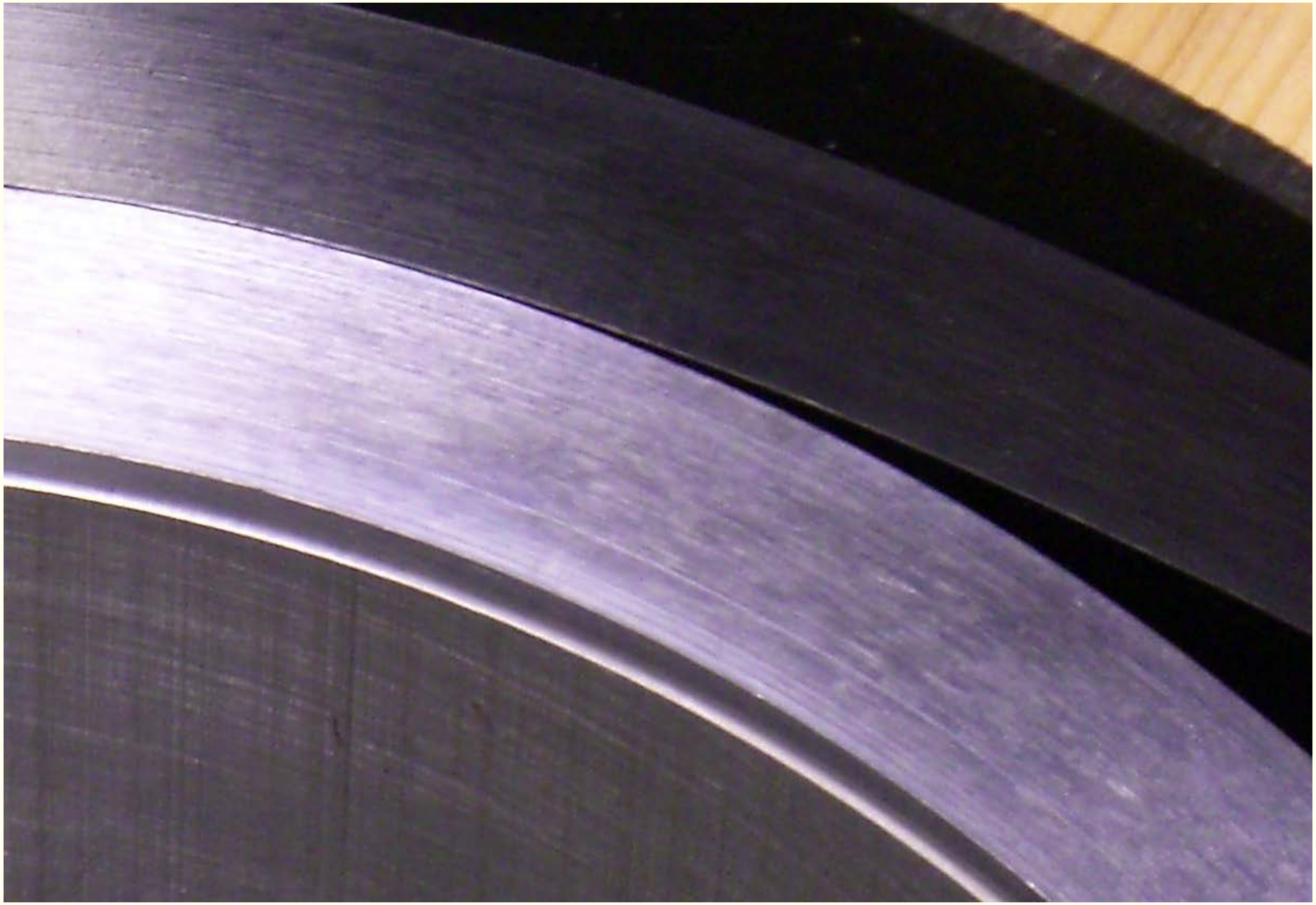


Transition?

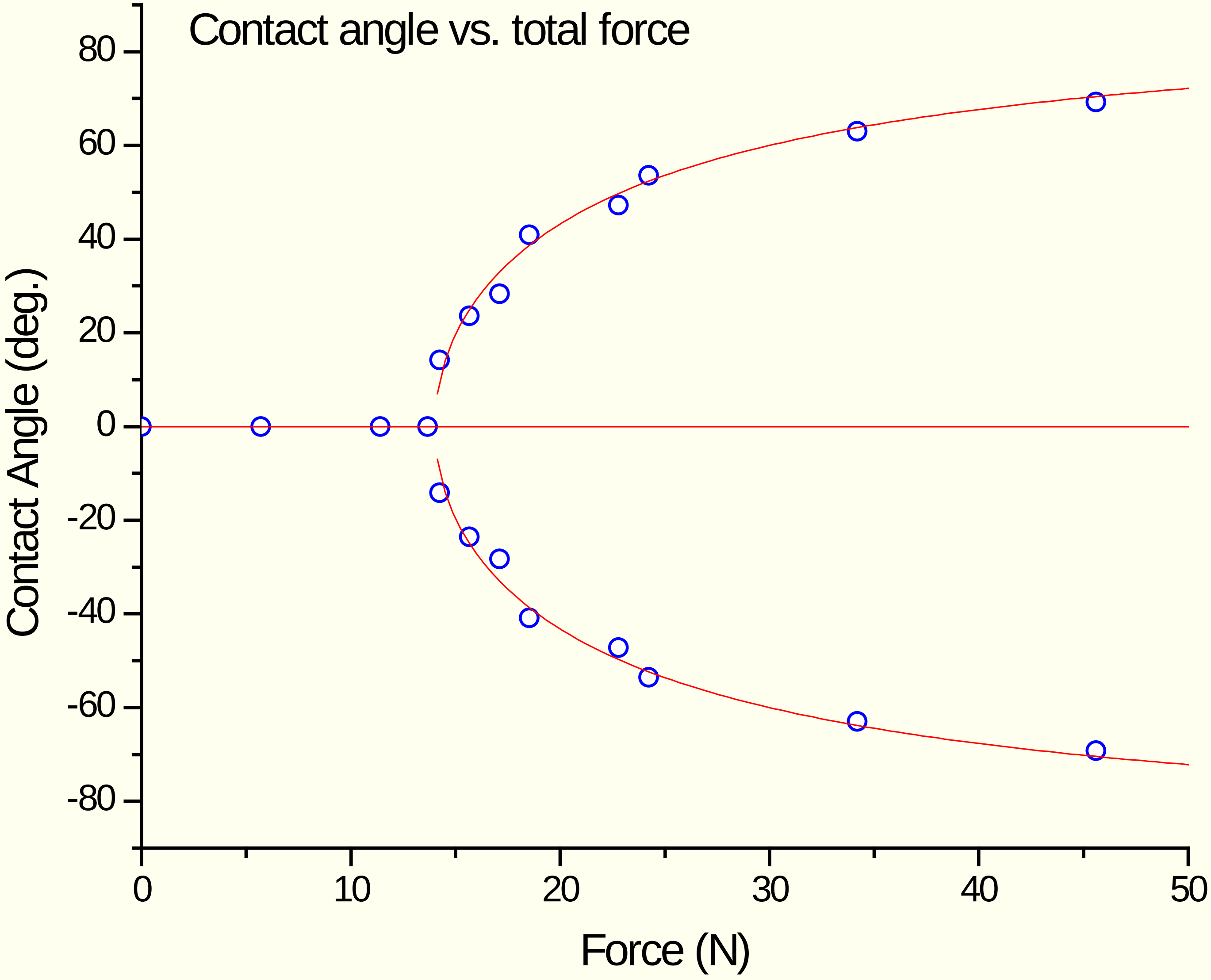
Experiment



Determination of point of contact

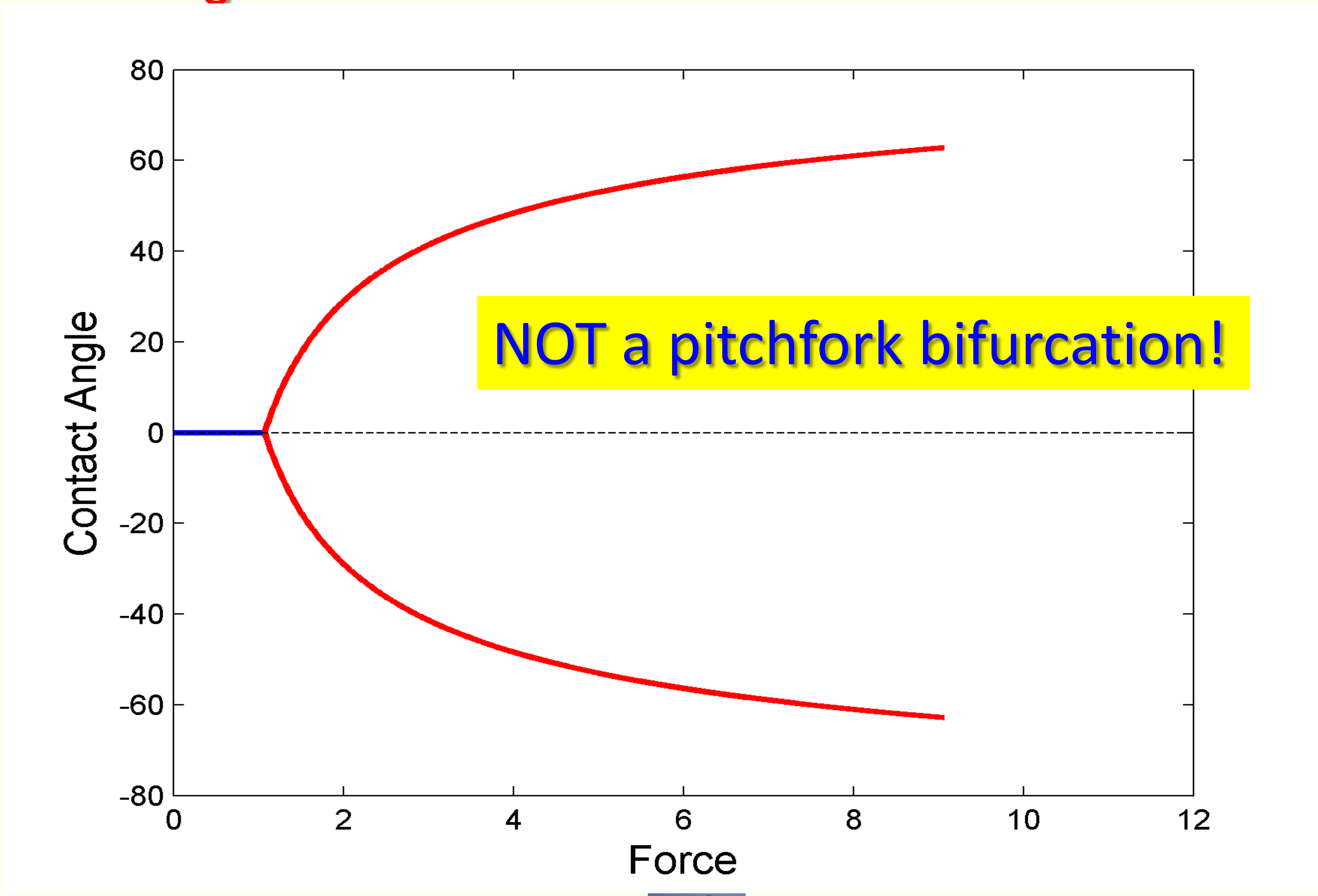


Data

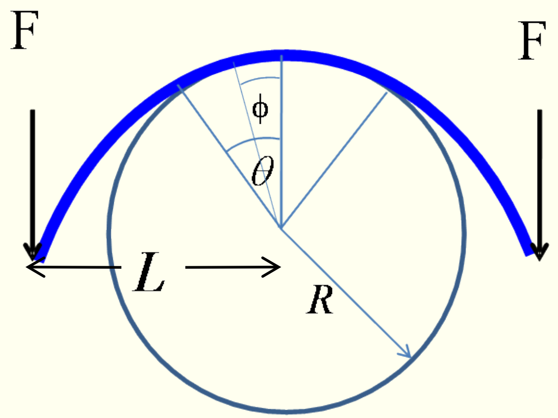


Contact angle vs. total force
Contact Angle (deg.)
80
60
40
20
0
-20
-40
-60
-80
0
10
20
30
40
50
Force (N)

Modelling: as before



Force distribution on pulleys



- when force **F** is applied to filament,
  - point contact if $F \le F_c$
  - extended contact if $F > F_c$

$$F_c = \frac{EI}{LR}$$

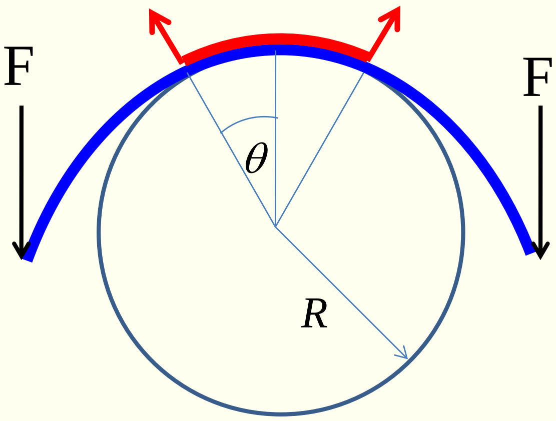
- torque balance:

force density on pulley

$$F(L - R\sin\theta) - \int_{\theta}^{\theta_c} R\sin(\phi-\theta) f(\phi) R\, d\phi = \frac{EI}{R}$$

- Volterra integral equation of first kind.

Force distribution on pulleys



- When force $\mathbf{F}$ is applied to filament,

L

  - point contact if $F \le F_c$
  - extended contact if $F > F_c$

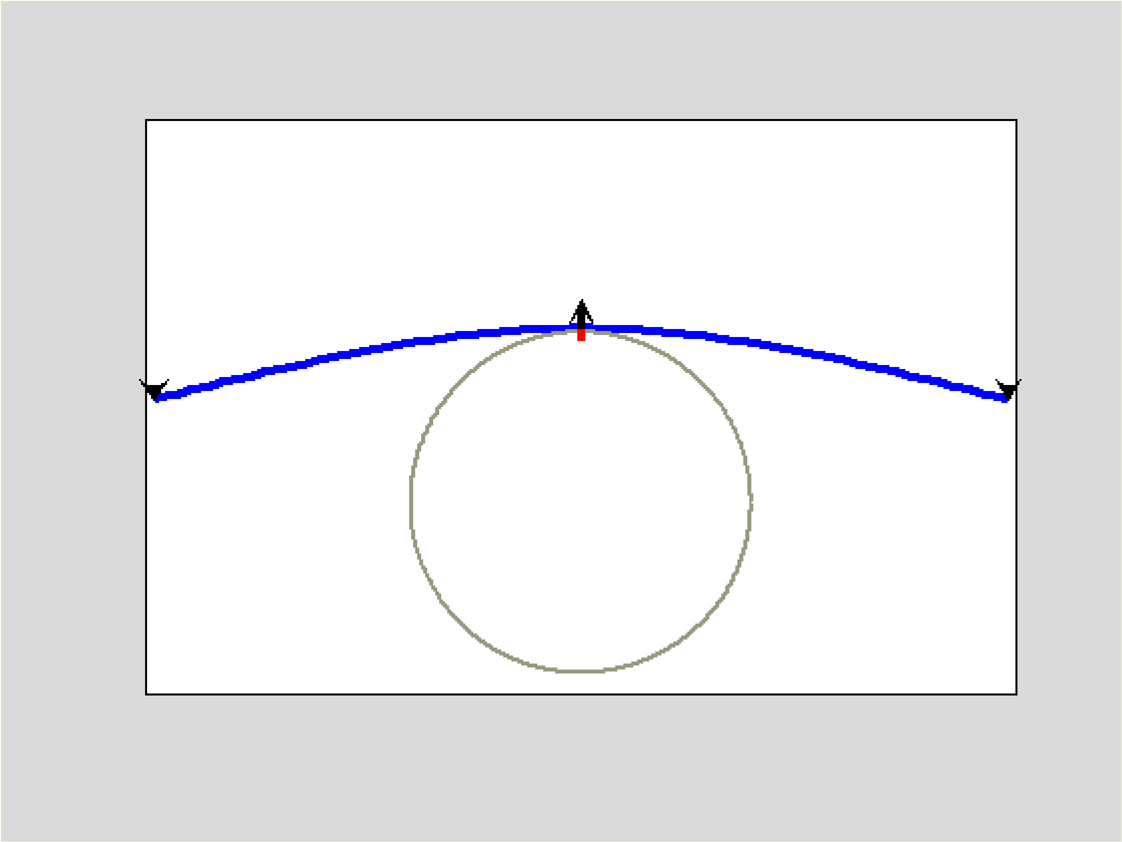
$$F_c = \frac{EI}{LR}$$

- Solution for force density:

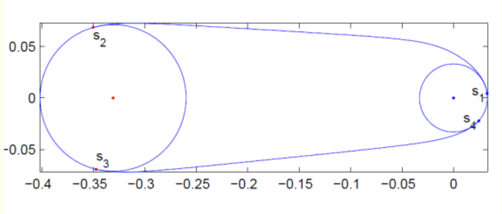
$$f(\theta) = \frac{F}{R}(\delta(\theta - \theta_c)\cos\theta_c + \sin\theta_c)$$

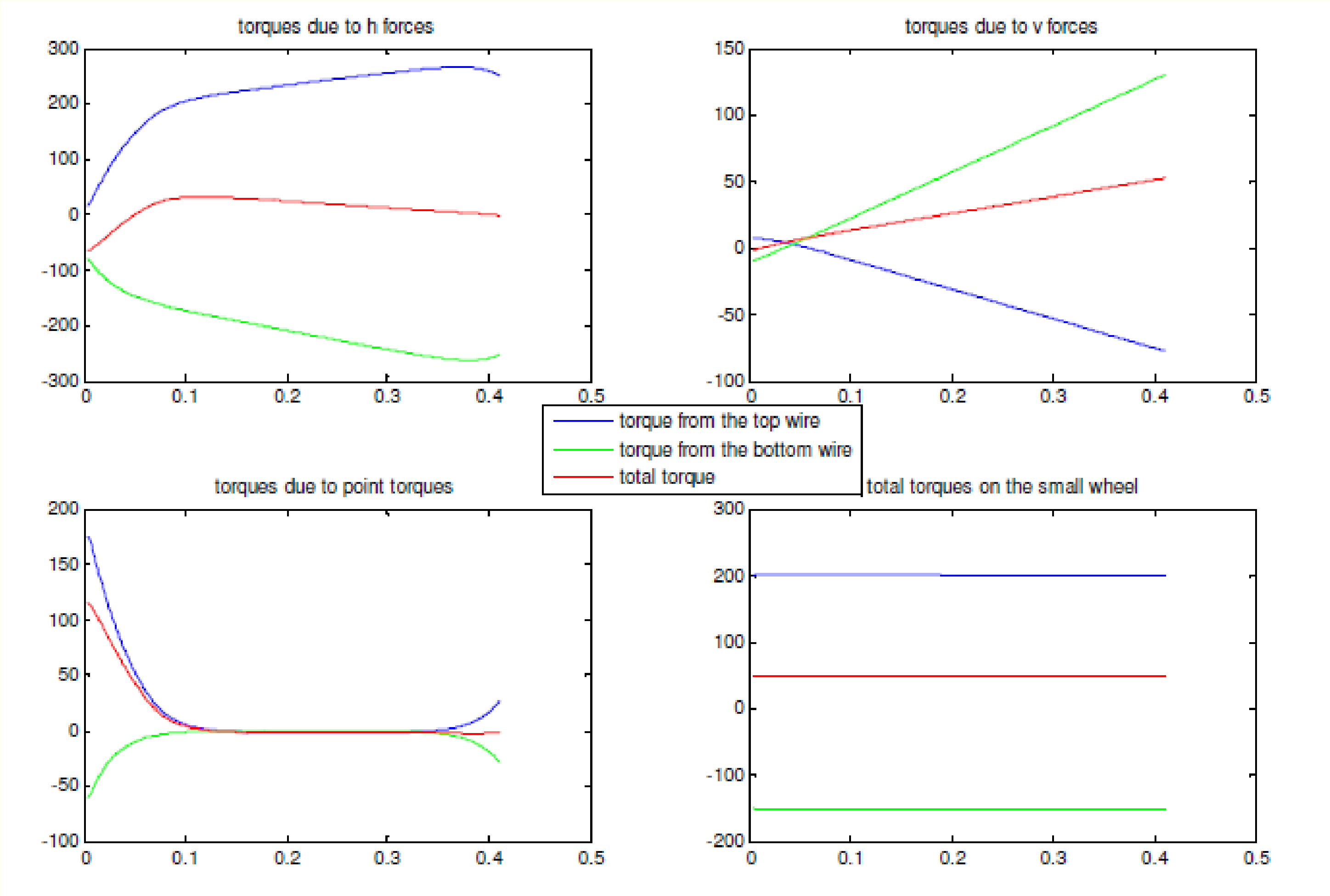
where $\sin\theta_c = (\frac{F - F_c}{F})\frac{L}{R}$

Force distribution



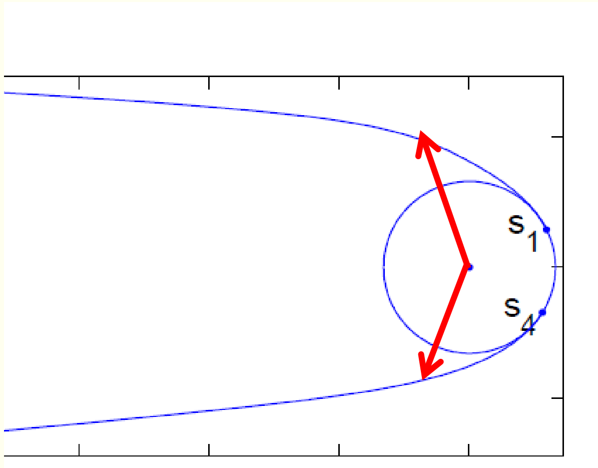
How does rotation come about?





How does rotation come about?

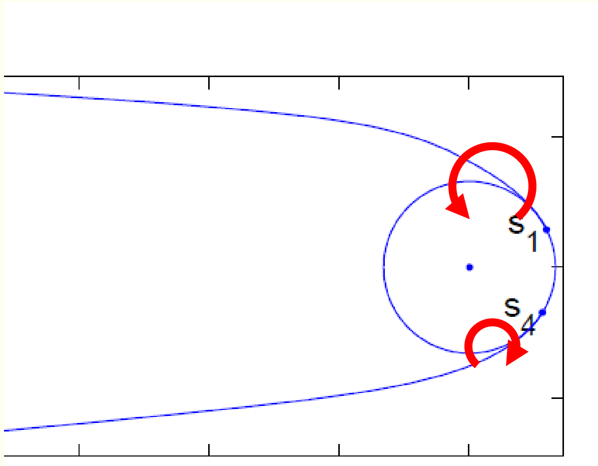
- away from the small wheel,
  - longer lever arm on one side



- near small wheel
  - greater point torque on one side
    - curvature is the same,
      - but stiffer on one side
      - have pontaneous curvature on one side

How does rotation come about?

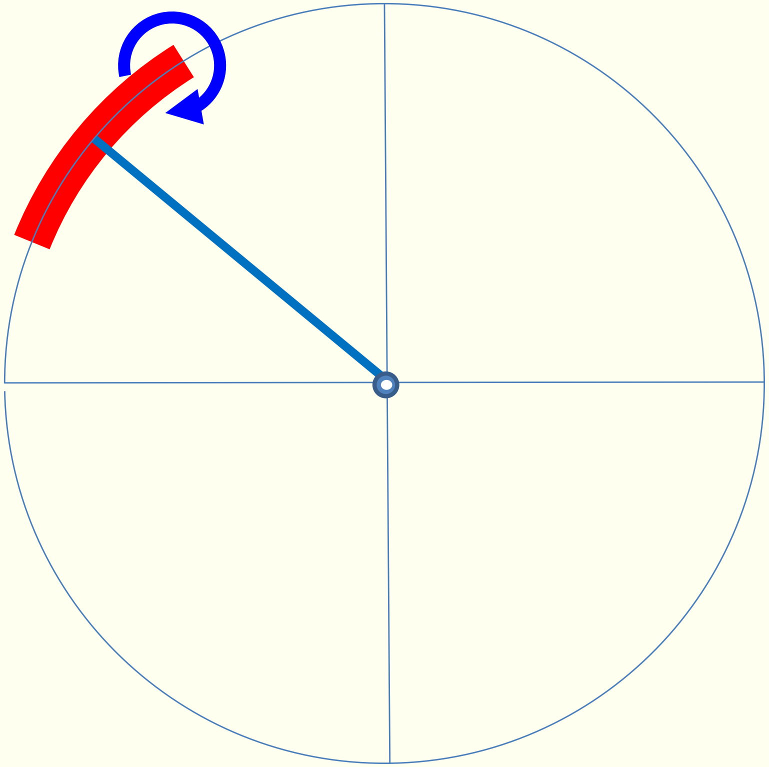
- away from the small wheel,
  - longer lever arm on one side



- near small wheel
  - greater point torque on one side
    - curvature is the same,
      - but stiffer on one side
      - have pontaneous curvature on one side

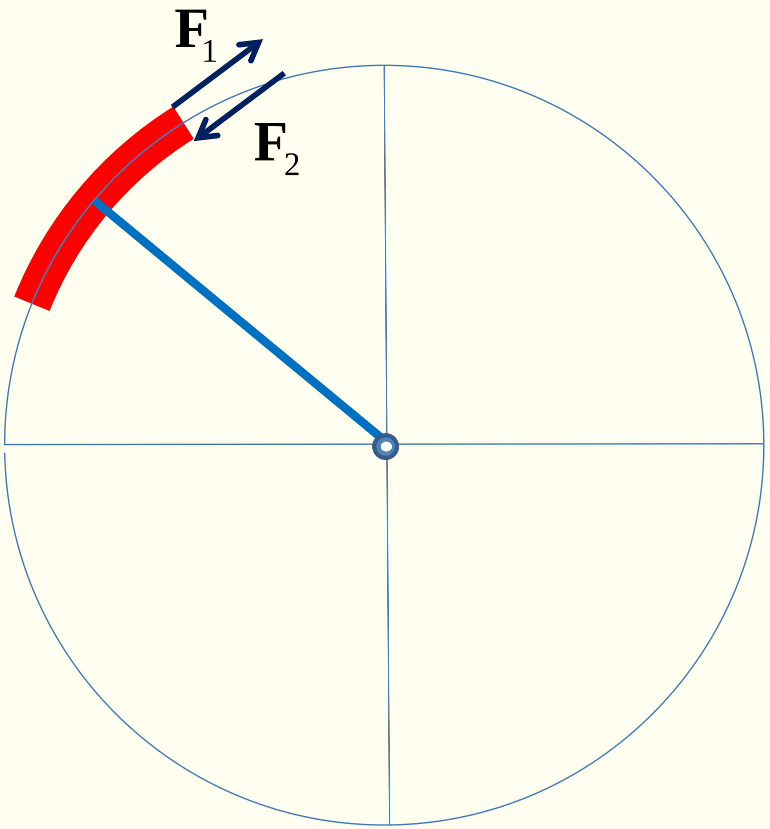
Motion due to point torques

- how can a point torque in filament cause translation?



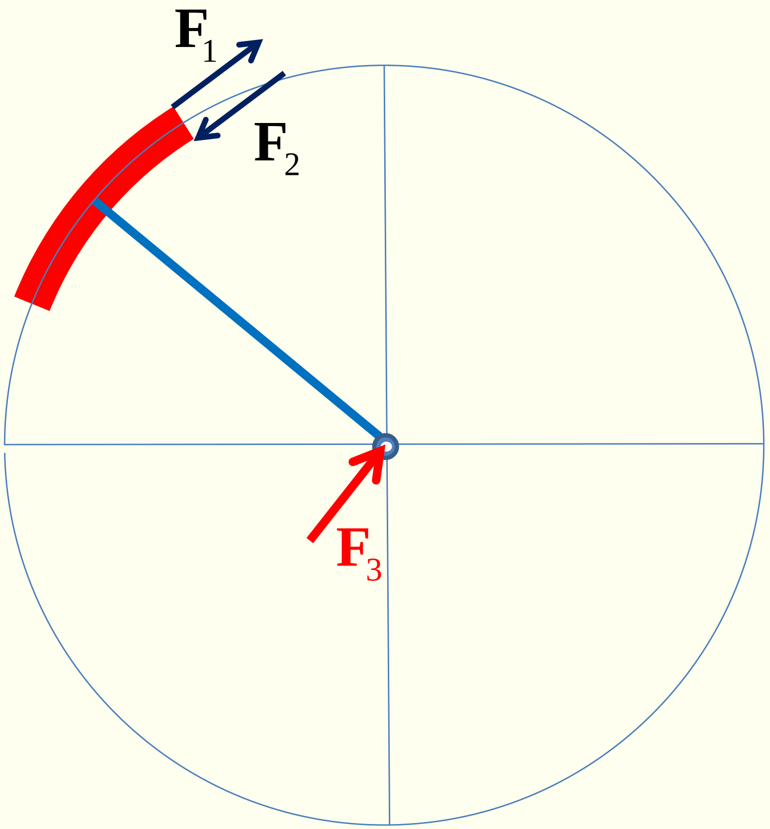
Motion due to point torques

- how can a point torque in filament cause bulk translation?
  - net force is zero,



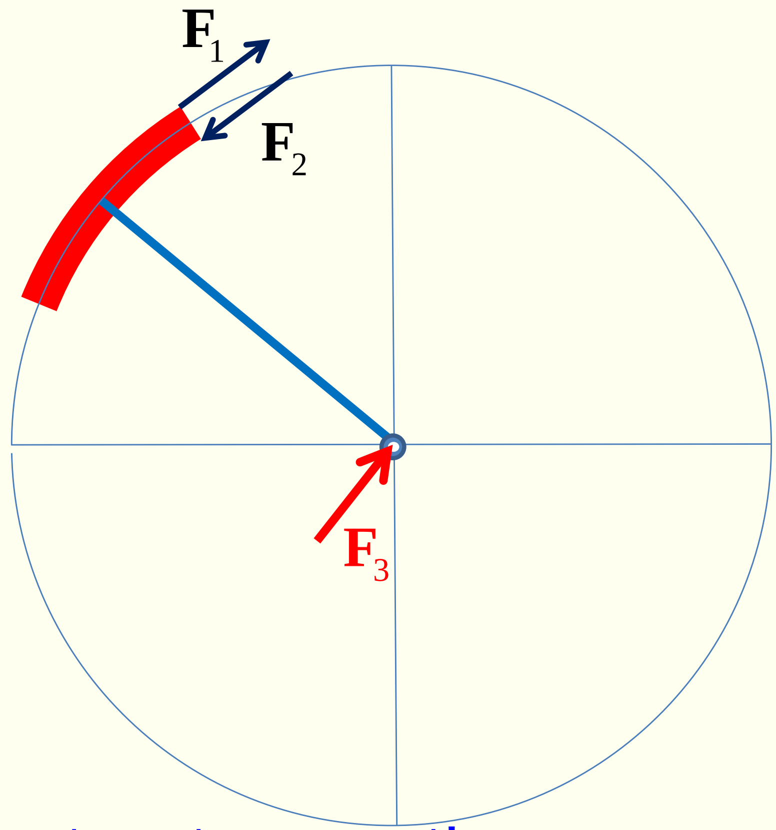
Motion due to point torques

- how can a point torque in filament cause translation?
  - net force is zero, but torque causes constraint force to appear



Motion due to point torques

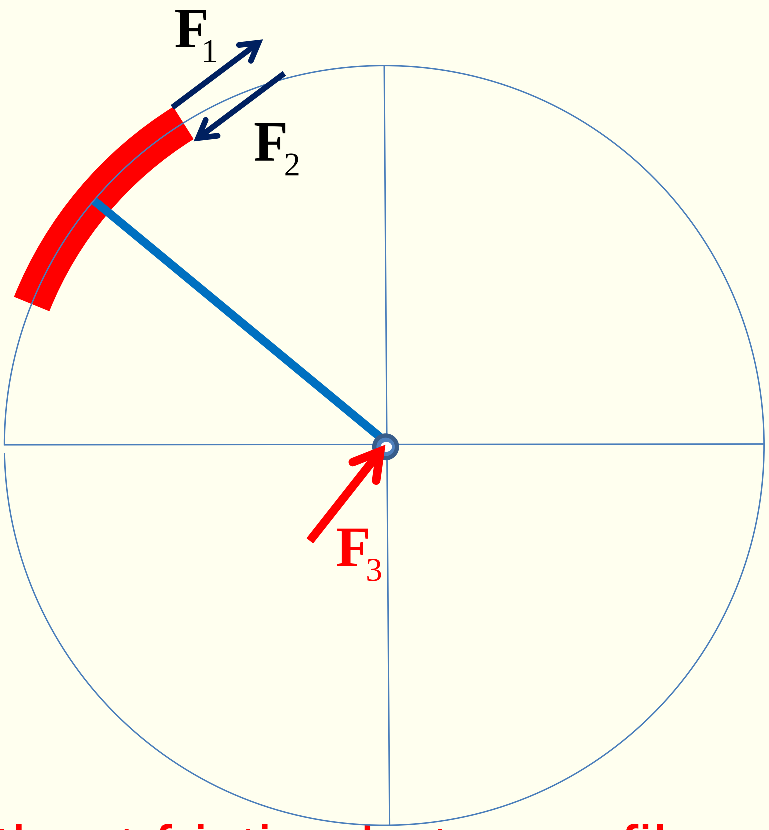
- how can a point torque in filament cause translation?
  - net force is zero, but torque causes constraint force to appear
  - net force along $\mathbf{F}_1$
  - translation



- angular momentum transport!

Motion due to point torques

- how can a point torque in filament cause translation?
  - net force is zero, but torque causes constraint force to appear
  - net force along $\mathbf{F}_1$
  - translation



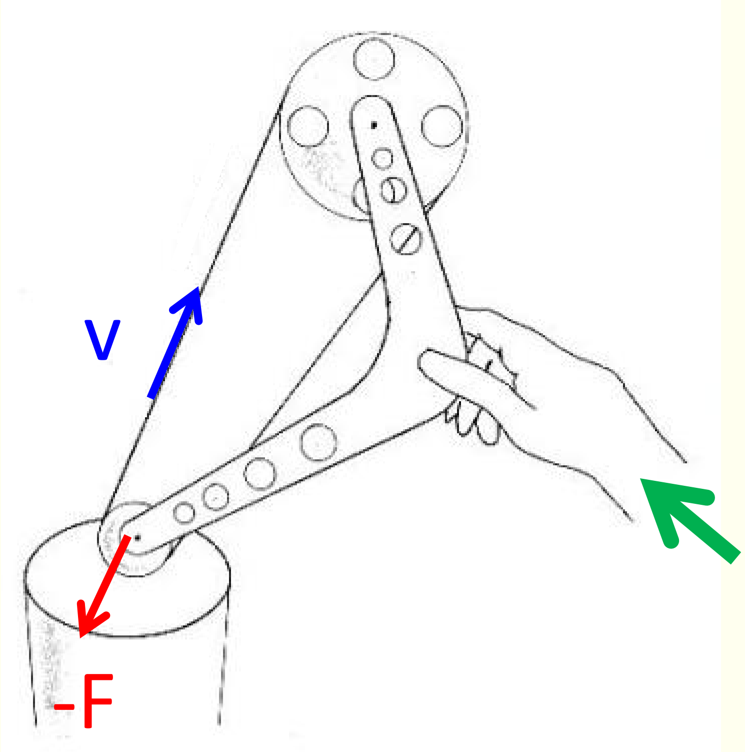
- no rotation without friction between filament & wheel!

Angular momentum current

- point torque in filament causes constraint force F to appear*

- reaction force -F appears;
  exerts torque on hand

- angular momentum current
  flows into bend motor from hand



- * via stress transport: $$\nabla(\nabla \bullet \boldsymbol{\sigma}) = \frac{\rho}{E}\frac{\partial^2 \boldsymbol{\sigma}}{\partial t^2}$$

Summary

- detailed model for bend motors driven by
  - local spontaneous curvature caused by light (LCE-Ikeda)
  - local stiffening caused by heat (Nitinol - Wang)
- corrects/completes existing qualitative explanations
- prediction:
  - LCE motor with perp. alignment runs the other way: confirmed!
- understand angular momentum transport
- efficiency calculation: remains to be done

Angular momentum

stimulus is applied

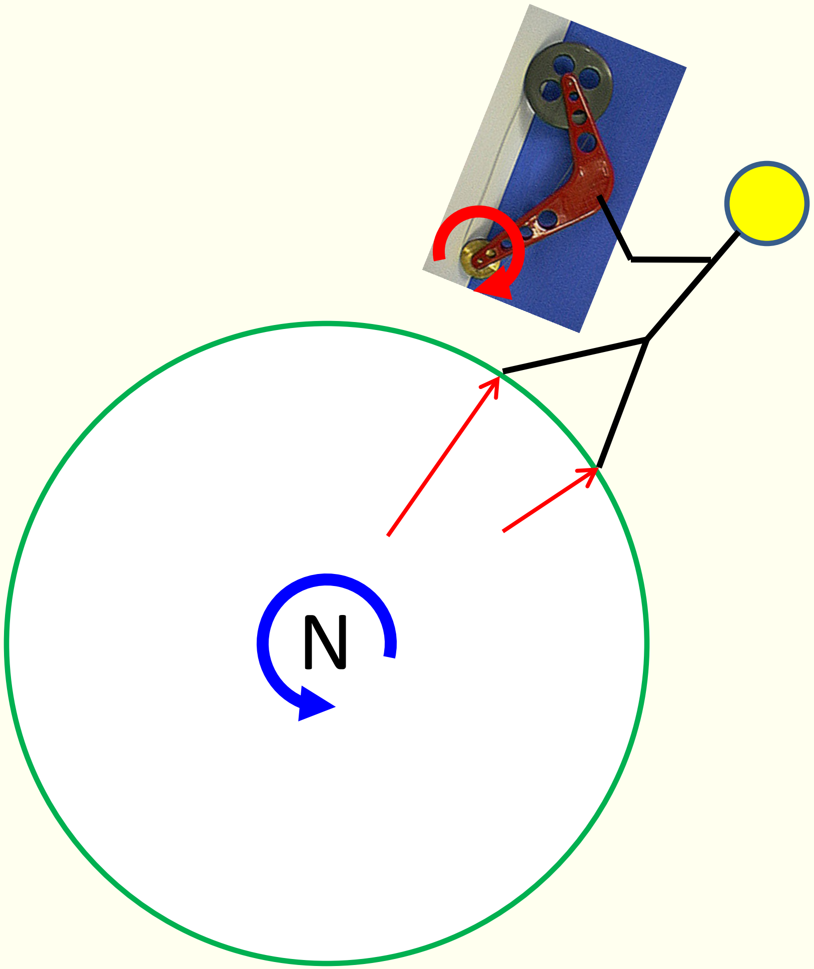
filament bends

torque appears

angular momentum flows into motor

rotation starts

angular momentum is conserved &
earth speeds up



Conclusions

- variety of molecular -scale mechanisms can be exploited
  - rotary (dyes, Yokoyama-Tabe)
  - need better molec. motors with processive translation
  - elongation (LC elastomers/networks)
- symmetry plays important role in determining motion
- macroscopic phenomena are cumulative effects of molecular motors
- understand bend motors well
- many exciting possibilties to explore!