Soft nematic solids:
textures, defects, and deformations

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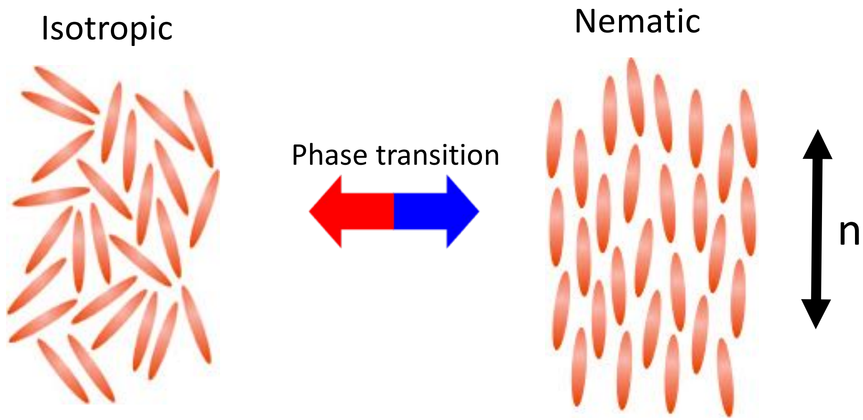
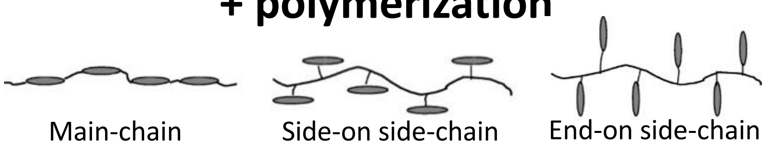
Liquid crystalline elastomers

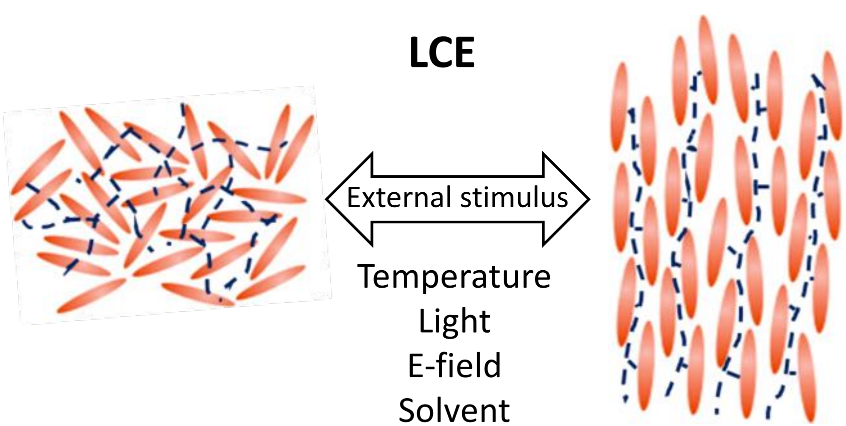
Nematic ordering in liquid crystals



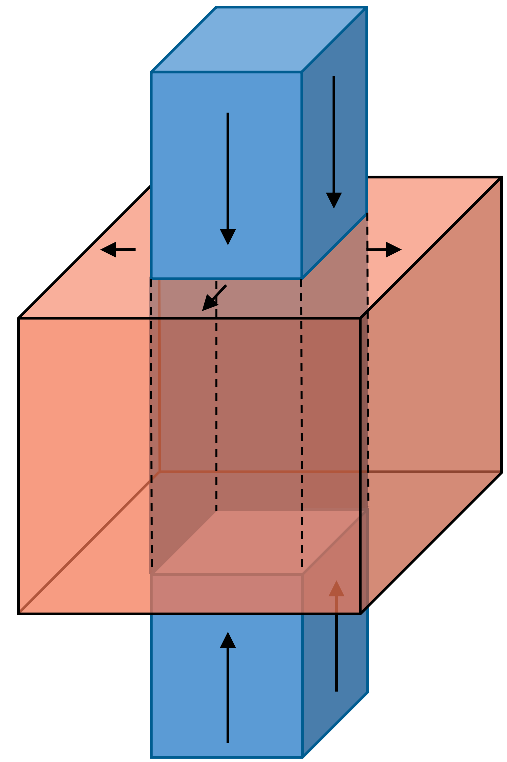
+ polymerization



LCE



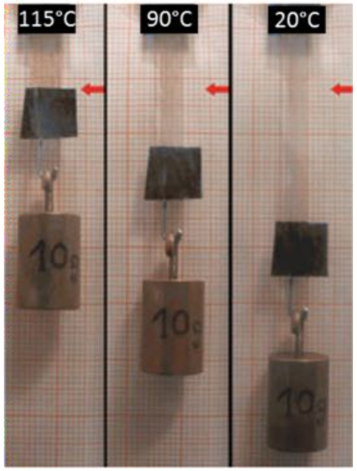
Elastic response



LCE actuators

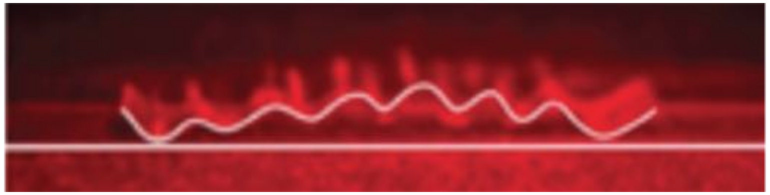
Caused by:

Heat



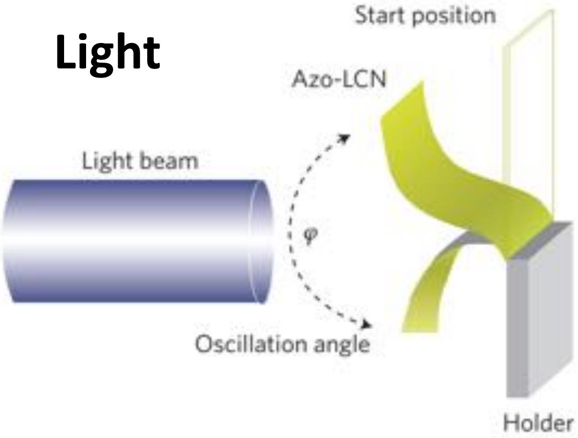
Finkelmann, *e-Polymers* **1**, 111-123 (2001)

reversible extension up to 60%



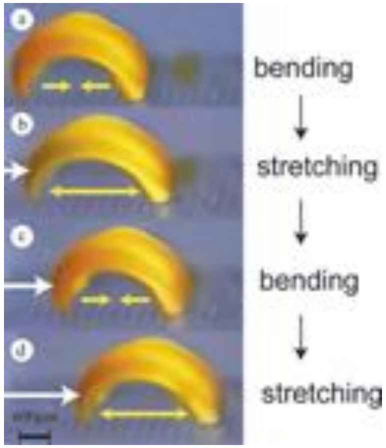
M Rogoz, et al, Adv. Optical Mater. **4,** 1689 (NOV 2016)

Light



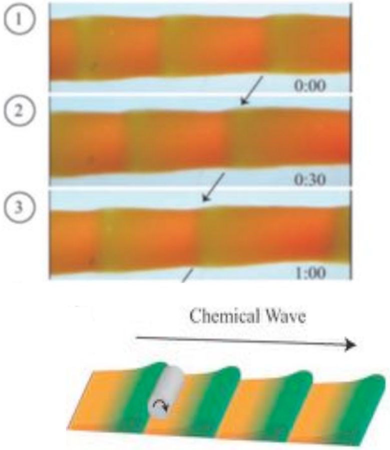
Serak et al., *Soft Matter* **6**, 779-783 (2010)

Self-walking



Hashimoto et al.,
Adv.Materials **19.21** (2007)

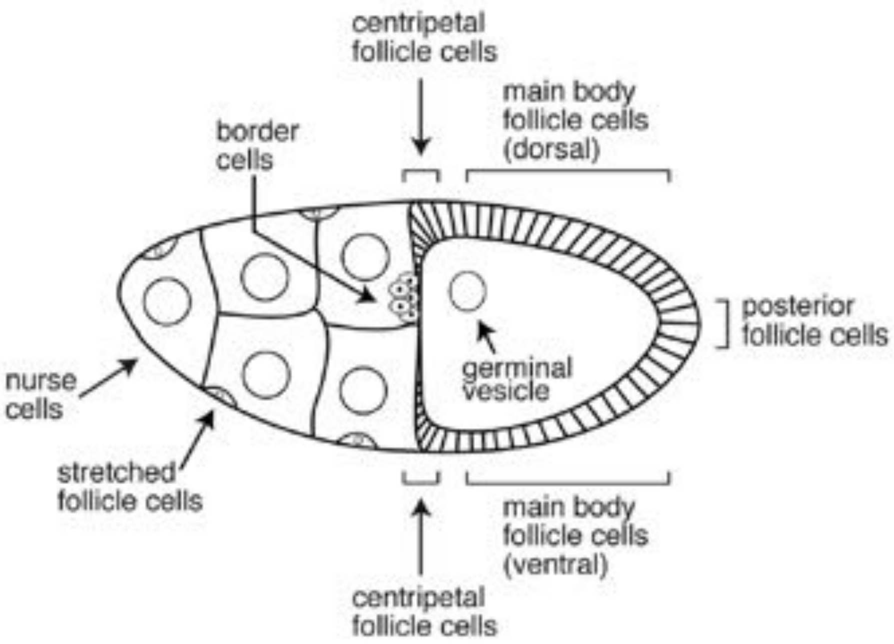
Peristaltic Motion



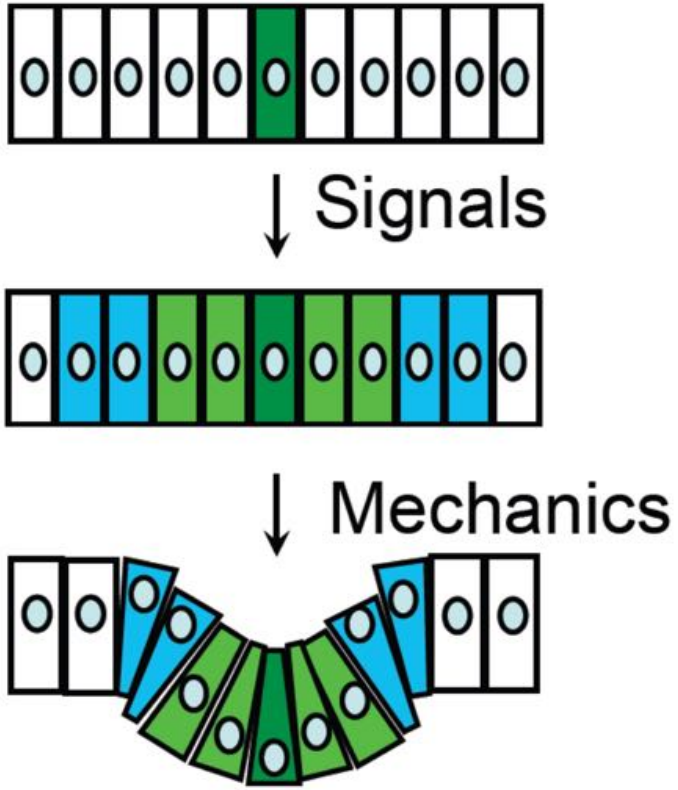
Hashimoto et al., *Ang. Chem.* **47**, 6690-6693 (2008)

Compare to biology?

Drosophila egg shell at early stage

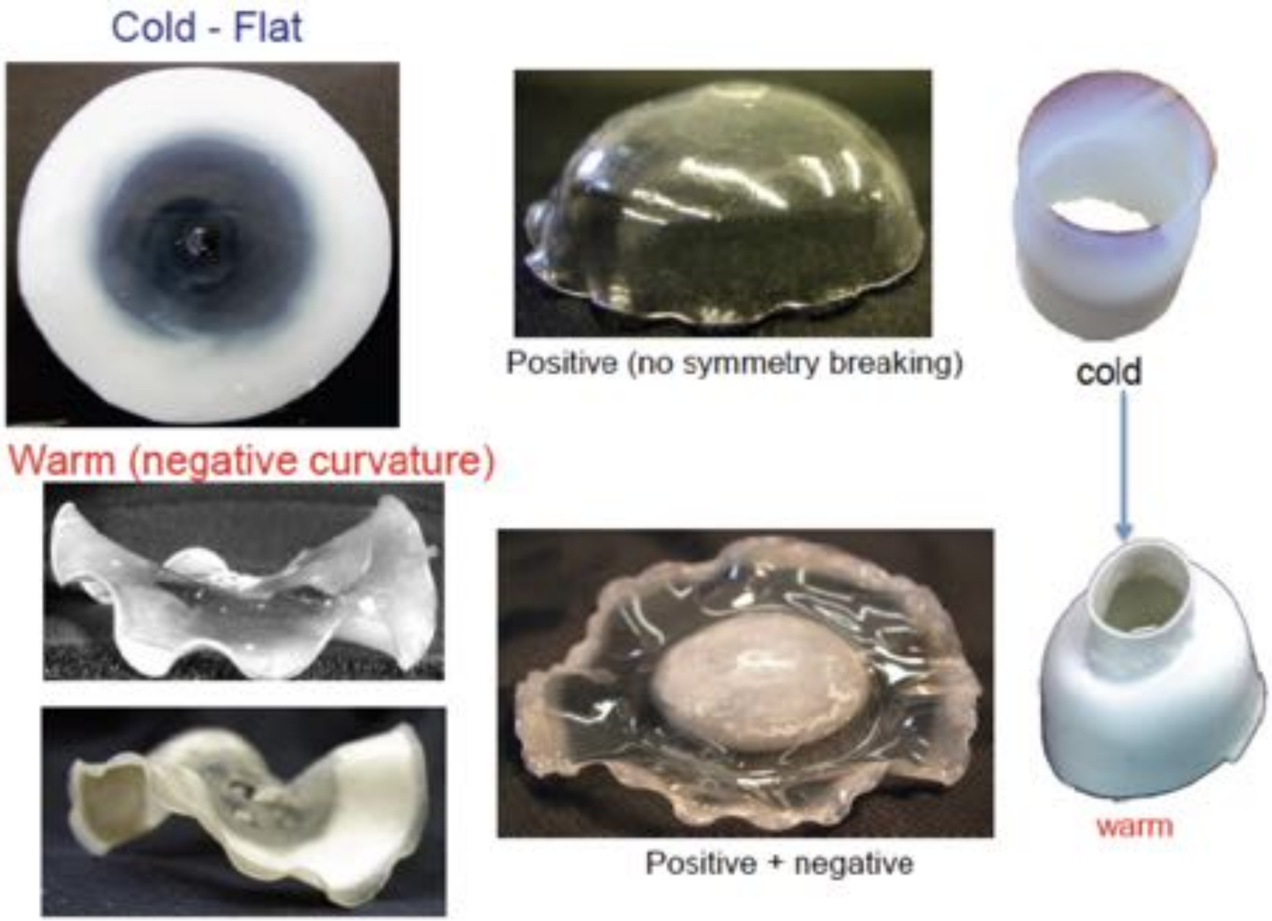


Cavaliere et al., Dev. Dyn. 2008, 237:2061-2072



Zartman & Shvartsman, Annu. Rev. Biomol. Eng. 2010, 1:231-246

Examples of 3D shapes



Y. Klein, E. Efrati and E. Sharon, Science. **315**, 1116 (2007)

Governing equations

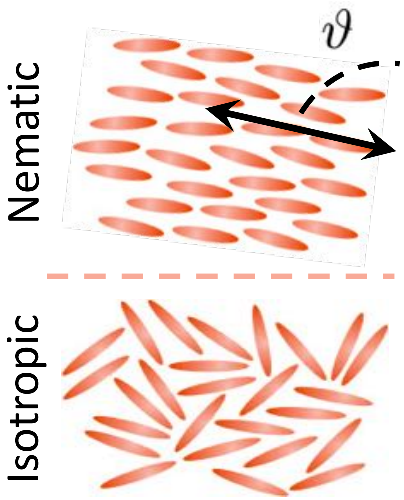
Free energy: elastic + nematic + compositional

$$\mathcal{F}\{U(\mathbf{x})\} = \mathcal{F}_{\mathrm{el}} + \mathcal{F}_{\mathrm{n}} + \mathcal{F}_{\mathrm{c}} = \int (\mathcal{L}_{\mathbf{el}} + \mathcal{L}_{\mathrm{n}} + \mathcal{L}_{\mathrm{c}})\, \mathrm{d}^2\mathbf{x}$$

Variables: $U=\{$polarization, deformation, composition$\}$

Dynamics $$\frac{\partial \mathbf{x}_i}{\partial t} = -\frac{\delta \mathcal{F}}{\delta \mathbf{x}_i}$$ + non-equilibrium terms

Nematic and Elastic Energy



2D tensor nematic order parameter

$$\mathbf{Q} = \begin{pmatrix} p & q \\ q & -p \end{pmatrix} = \frac{S}{\sqrt{2}} \begin{pmatrix} \cos 2\vartheta & \sin 2\vartheta \\ \sin 2\vartheta & -\cos 2\vartheta \end{pmatrix}$$

Nematic energy

$$\mathcal{F}_\mathrm{n} = \int \mathcal{L}_\mathrm{n} \mathrm{d}^2\mathbf{x}$$

$$\mathcal{L}_\mathrm{n} = -\frac{\alpha_1}{4} Q_{ij} Q_{ij} + \frac{\alpha_2}{16} \left(Q_{ij} Q_{ij}\right)^2 Q_{ij} + \frac{\kappa_1}{2} |\nabla_i Q_{ij}|^2 + \frac{\kappa_2}{4} \sum_{ijk} \left(\nabla_i Q_{jk}\right)^2$$

- $\overline{u}_{ij}$ is elastic deformation
- H is the mean curvature

Elastic energy

$$\mathcal{F}_\mathrm{e} = \frac{\nu}{2} \int h\, \overline{u}_{ij}^2 \mathrm{d}^2\mathbf{x} + \frac{\nu}{2c} \int h^3 H(\mathbf{x})^2 \mathrm{d}^2\mathbf{x}$$

in-shell deformation

bending

Avoid stress by bending in 3D!

How to find 3D shape

construct the metric of the deformed sheet

$$\mathrm{d}\xi^\alpha = T^\alpha{}_\beta \mathrm{d}x^\beta, \quad T^\alpha{}_\beta = N^{-1/2}\left(\delta^\alpha_\beta + a\widetilde{Q}^\alpha{}_\beta\right)$$

a = extension coefficient

The original metric tensor $\mathbf{g}^0$ is transformed to $\mathbf{g} = \mathbf{T}\mathbf{g}^0\mathbf{T}$; det($\mathbf{T}$) $= 1$ (area-preserving) when $N = 1 - a^2\widetilde{S}^2$

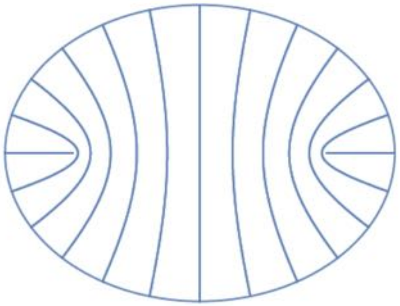
$$g_{\alpha\beta} = (1 - a^2\widetilde{S}^2)^{-1}\left[(1 + a^2\widetilde{S}^2)g^0_{\alpha\beta} - 2aQ_{\alpha\beta}\right)$$

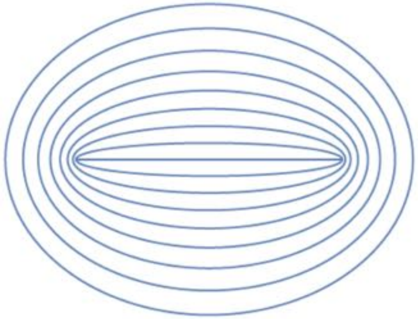
given a metric, one can compute Gaussian curvature

find the shape analytically? only in simplest cases

Elliptic domain: metric and texture

Elliptic coordinates
x = cosh v cos u
y = sinh v sin   u





Metric

$$\mathbf{g} = g\,\mathrm{diag}\left(\ell^{-2}, \ell^{2}\right), \quad g = \frac{1}{2}(\cosh 2v - \cos 2u) \quad \ell = \sqrt{\frac{1+a}{1-a}}$$

Gaussian curvature

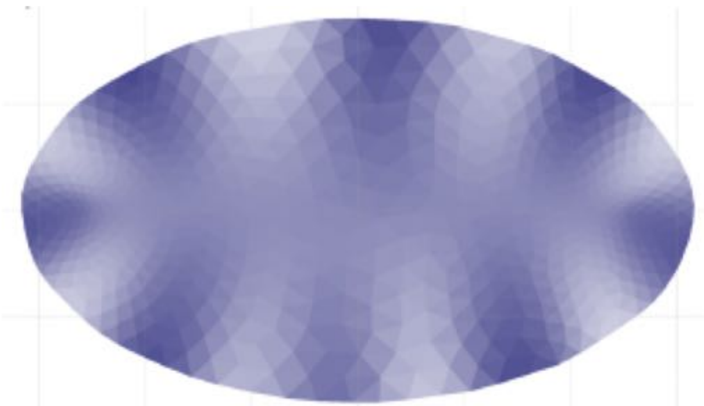
$$K = \pm\frac{1}{g}\left[\frac{\partial}{\partial u}\left(\frac{1}{g}\frac{\partial g}{\partial u}\right) + \frac{\partial}{\partial v}\left(\frac{1}{g}\frac{\partial g}{\partial v}\right)\right] = \pm\frac{16a(\cosh 2v \cos 2u - 1)}{(1-a^2)(\cosh 2v - \cos 2u)^2}$$

Regularisation near a defect

$$S''(r) + r^{-1}S'(r) + S\left(1 - r^{-2} - S^2\right) = 0$$

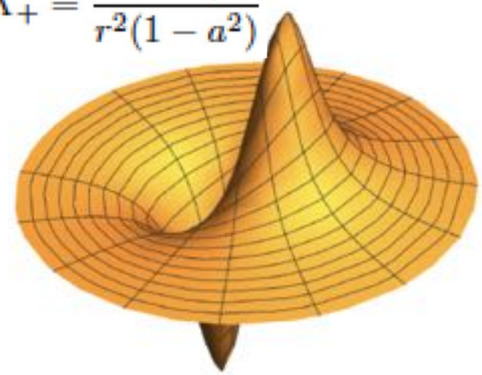
Deformation

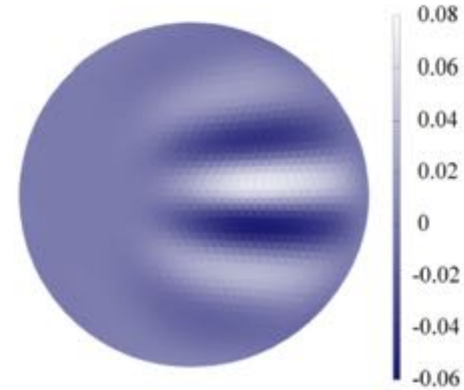
Vicinity of defects



Normal anchoring

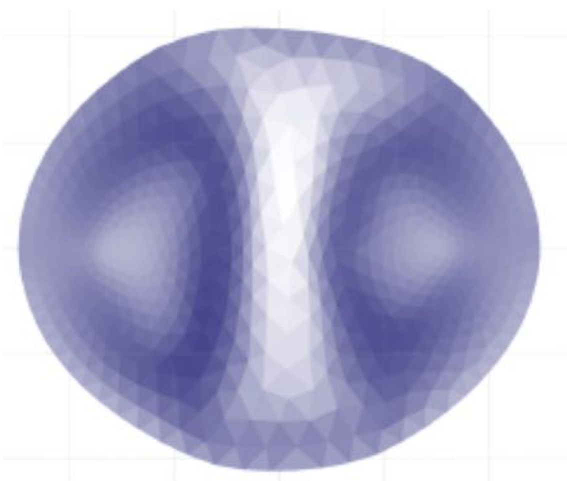
$$K_+ = \frac{a\cos\phi}{r^2(1-a^2)}$$



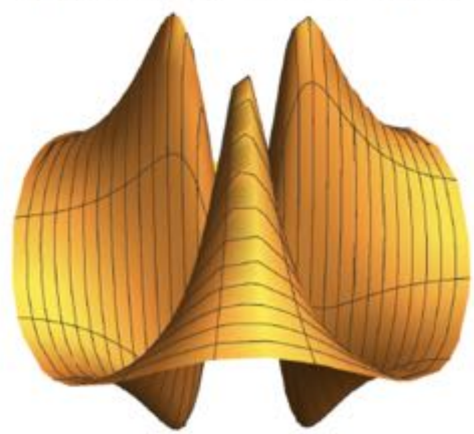


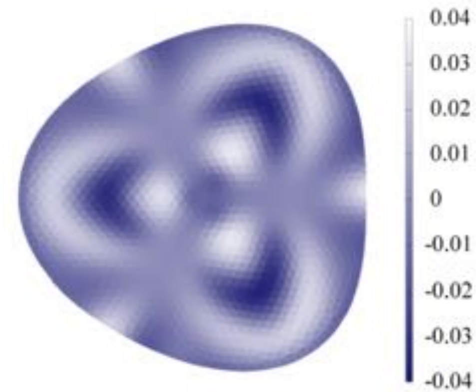
Gaussian curvature

deformed shapes



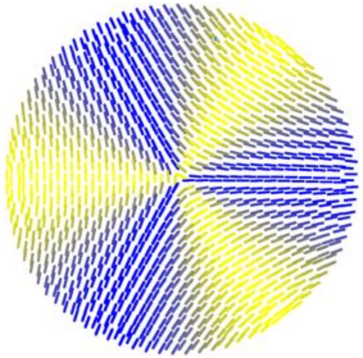
Tangential anchoring



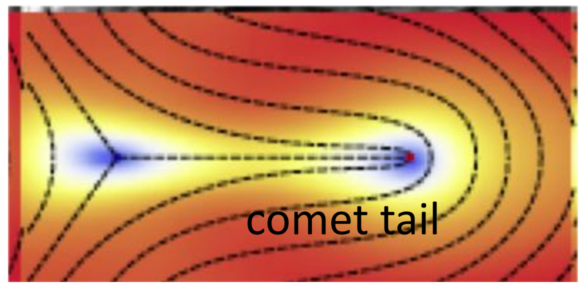


$$K_- = -\frac{3a\cos 3\phi}{r^2(1-a^2)}$$

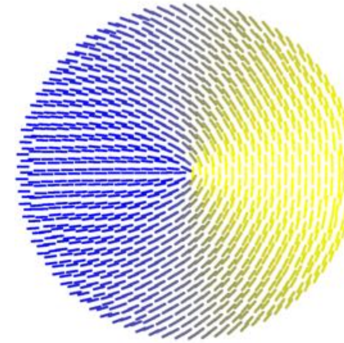
Topology: Defects



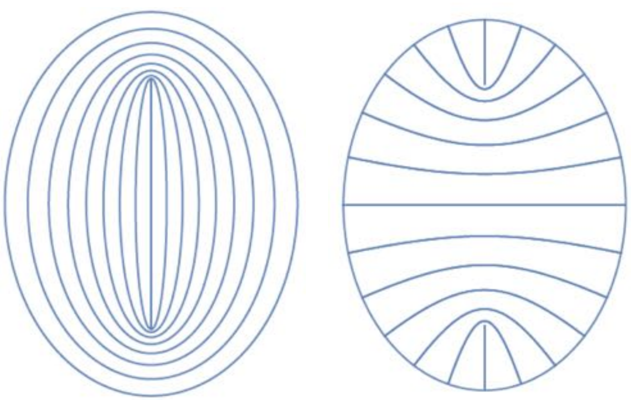
Charge –1/2



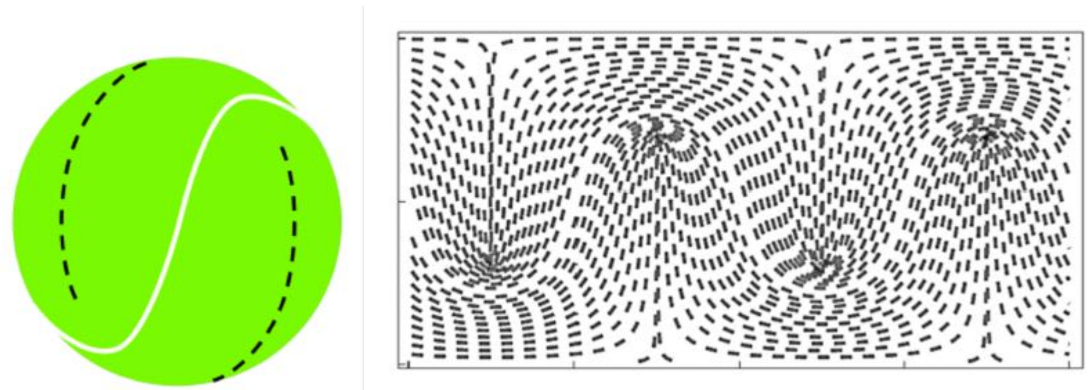
plane or cylinder: charge 0



charge +1/2:

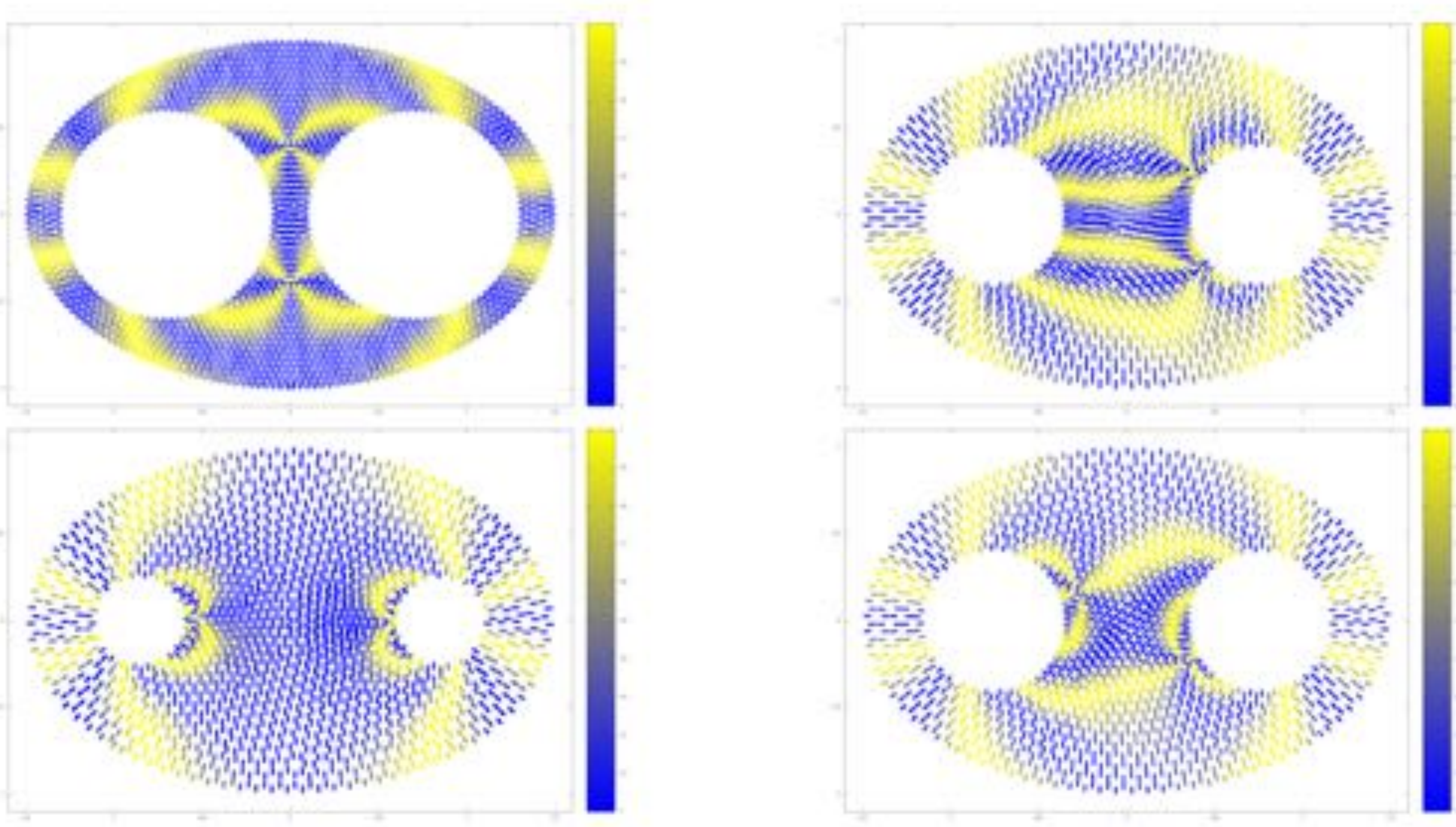


Ellipse: 2 defects, charge 1



sphere: 4 defects, charge 2

Domains with holes



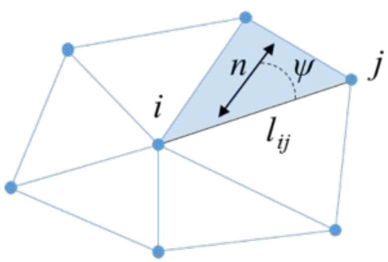
Elastic energy: numerical implementation

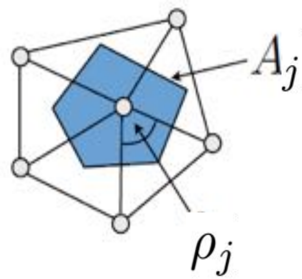
$$\mathcal{F}_e = \frac{1}{2}\sum_{\text{nodes}}\left[\frac{h_i}{2}\sum_{\text{adj.n}}\left(\frac{l_{ij}}{\bar{l}_{ij}}-1\right)^2 + \frac{h_i^3}{9}\sum_{\text{adj.t}}\left\langle\frac{1-\mathbf{m}_i\cdot\mathbf{m}_{ij}}{l_{ij}^2}\right\rangle_j\right]$$

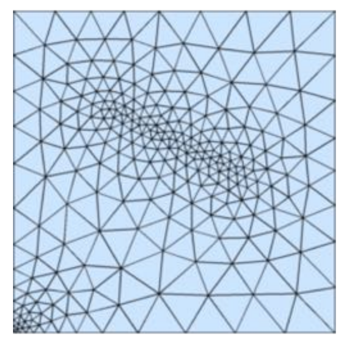
$$\bar{l}^2 = \frac{1}{4}\left(\sqrt{\lambda}-\frac{1}{\lambda}\right)^2\sin^2 2\psi + \left(\sqrt{\lambda}\sin^2\psi + \frac{\cos^2\psi}{\lambda}\right)^2$$

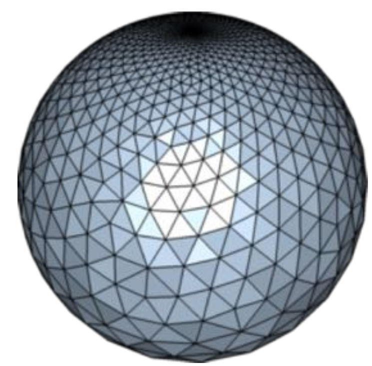
m is the normal to a tile

ψ is the angle between an edge and the director





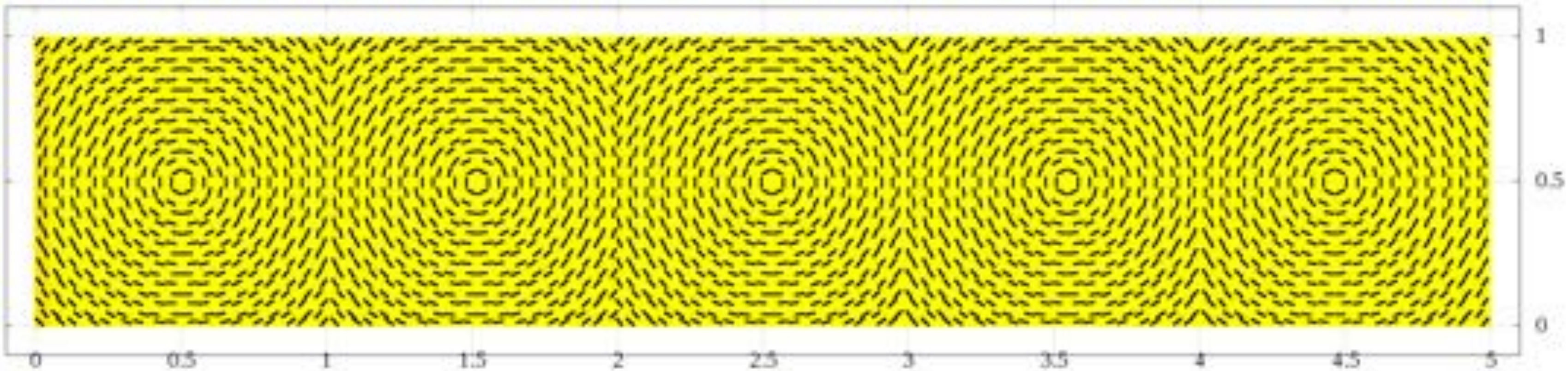




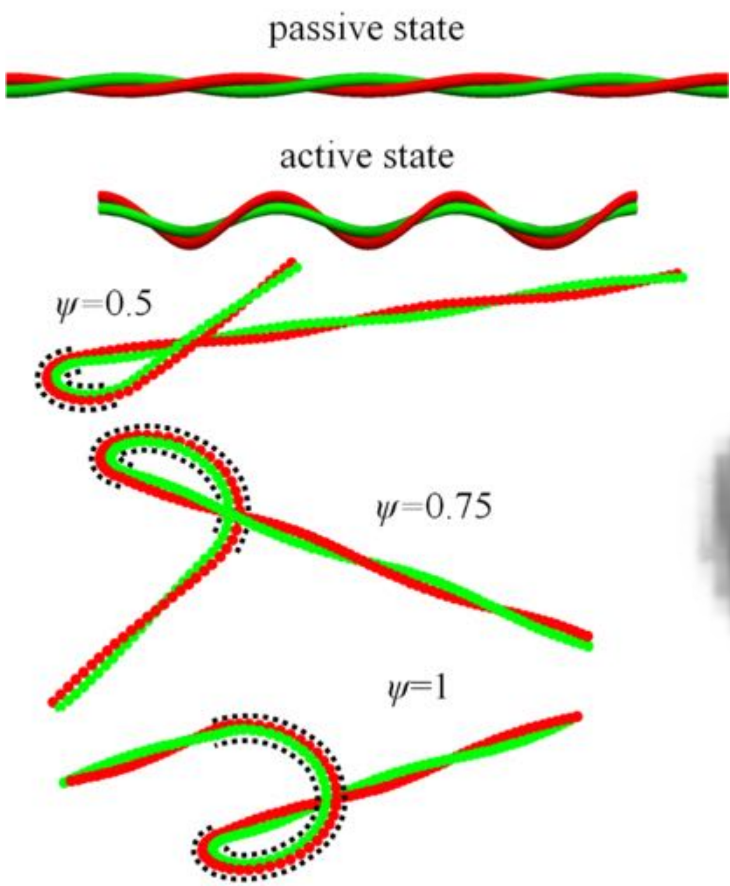
$$C_i^2 = 4H_i^2 - 2K_i$$

$$K_i = (2\pi - \textstyle\sum \rho_j)/A_i \quad H_i = \textstyle\sum(l_{ij}\eta_j)/(4A_i)$$

A crawler



A swimmer made of Janus fiber



ψ= ratio of the excited region to the pitch

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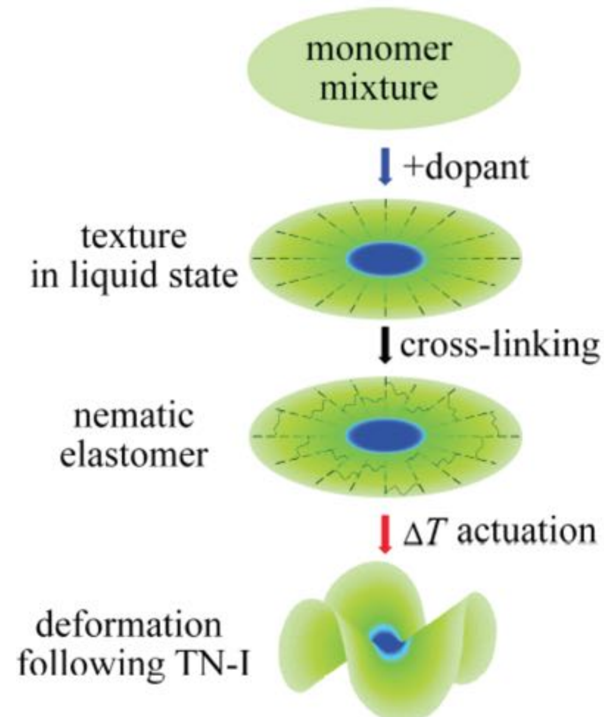
Nematic energy: doped nematics

Concentration dependent ordering

$$\mathcal{L}_{\mathrm{n}} = -\frac{\alpha_1 - \alpha_c c}{4} Q_{ij}Q_{ij} + \frac{\alpha_2}{16}\left(Q_{ij}Q_{ij}\right)^2 - \beta\nabla_i c \nabla_j Q_{ij} + \frac{\kappa_1}{2}\left|\nabla_i Q_{ij}\right|^2 + \frac{\kappa_2}{4}\sum_{ijk}\left(\nabla_i Q_{jk}\right)^2$$



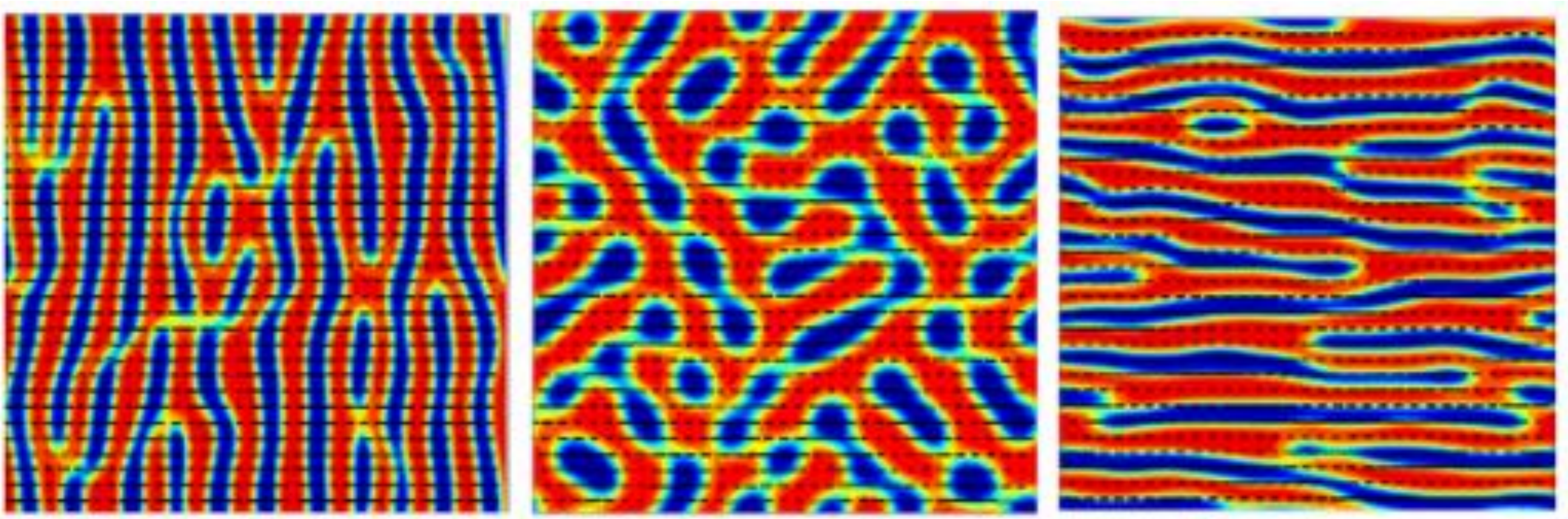
Chemical signal:

$$\mathrm{D}_t c = \nabla_i(D\nabla_i c) + f(c)$$

Near a phase front:

$$\mathscr{L}_{\mathrm{n}} = -\frac{1-\alpha c}{2}S^2 + \frac{1}{4}S^4 - \frac{\beta}{\sqrt{2}}c'(r)S'(r)\underline{\cos 2\phi_0} + \frac{\kappa}{4}S'(r)^2$$

Phase separation and spontaneous anchoring



$\beta > 0 \Rightarrow \vartheta = \pi/2$ $\beta=0$ $\beta < 0 \Rightarrow \vartheta = 0$

Köpf and Pismen Eur. Phys. J. E (2013)

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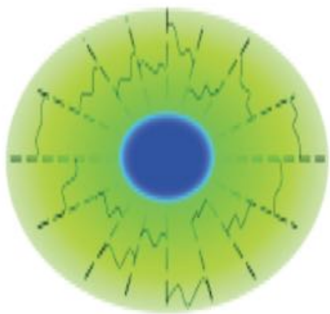
Reshaping a disk

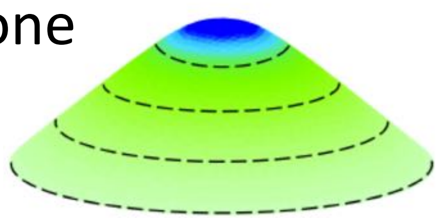
point source of an isotropic dopant at the center



concentration distribution

$$\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}c}{\mathrm{d}r}\right)-k^2c(r)=0$$

cone



Shorten the circumference of each circle with the radius r by the factor $\lambda = 1 + aS$ and extend the radius and the thickness by the factor $\lambda^{1/2}$

diagonal metric tensor:

$$\gamma_{11} = z'(r)^2 + \rho'(r)^2 = \lambda,\ \ \gamma_{22} = \rho^2 = (r/\lambda)^2$$

compute the elevation $z(r)$

$$z(r) = \int\sqrt{1 + aS(r) - \left[\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{r}{1 + aS(r)}\right)\right]^2}\,\mathrm{d}r$$

$S = \sqrt{1 - \alpha c}$ outside the isotropic circle

at $r = r_0 + \varepsilon x,\ S \sim \sqrt{\varepsilon x},\quad S'(r) \sim 1/\sqrt{\varepsilon x}$

approximate the concentration $c(x) = c_0 - qx$

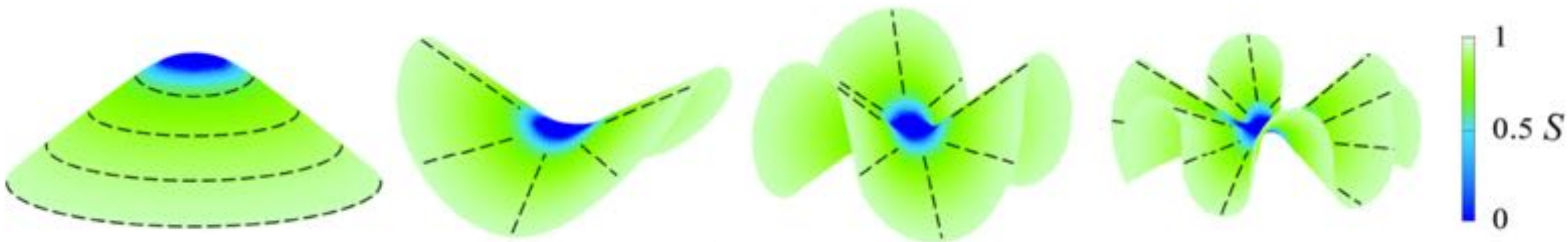
add elastic energy terms: $\kappa S''(x) + qxS = 0$

$$S(x) = s_0\left[\sqrt{3}\mathrm{Ai}\left(-(q/\kappa)^{1/3}x\right) - \mathrm{Bi}\left(-(q/\kappa)^{1/3}x\right)\right]$$

$S'(0) = 2(q/3\kappa)^{1/3}/\Gamma(1/3)$ finite, no singularity

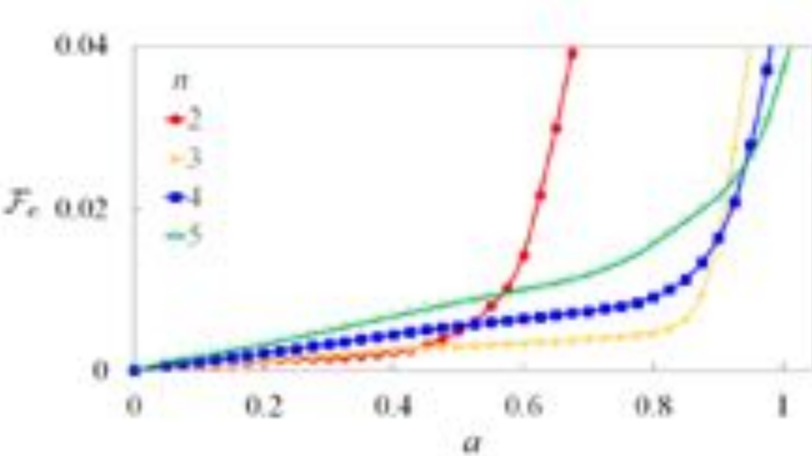
Reshaping a disk

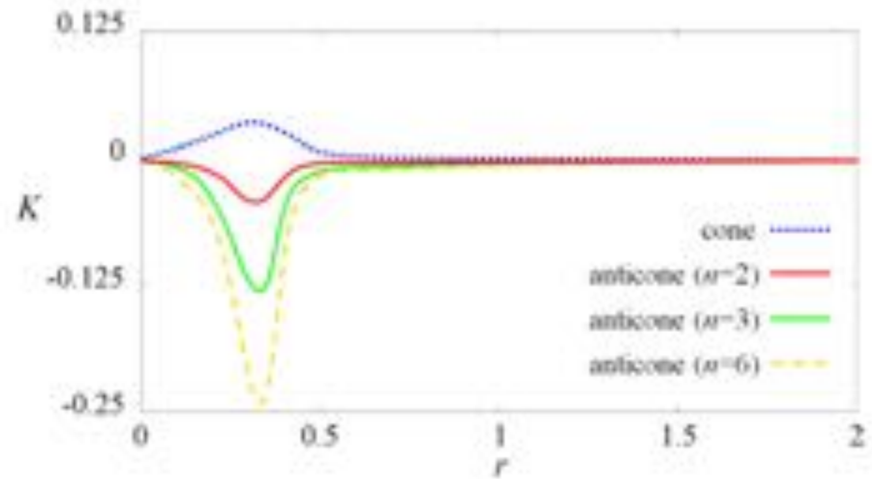
point source of an isotropic dopant at the center



cone

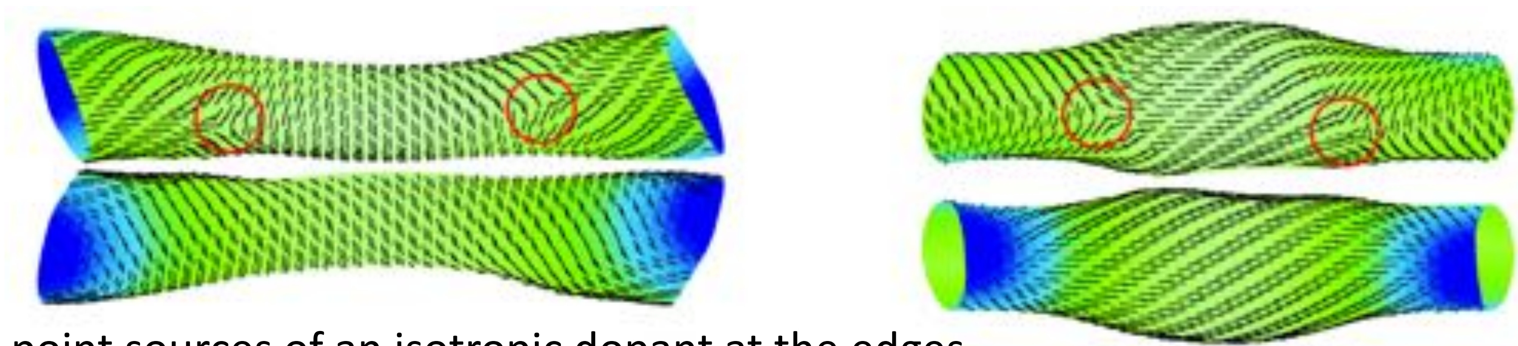
anticone



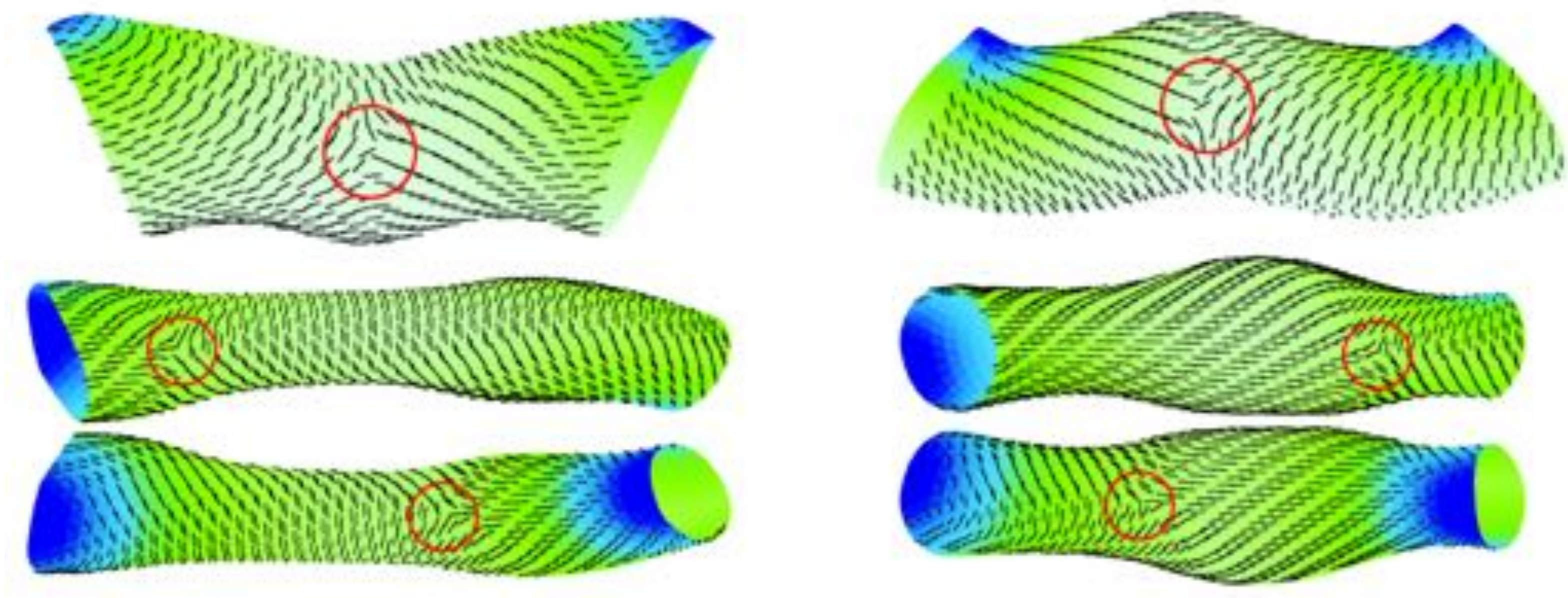


Zakharov and Pismen Soft Matter (2017)

Reshaping a a cylinder: Topology change



point sources of an isotropic dopant at the edges

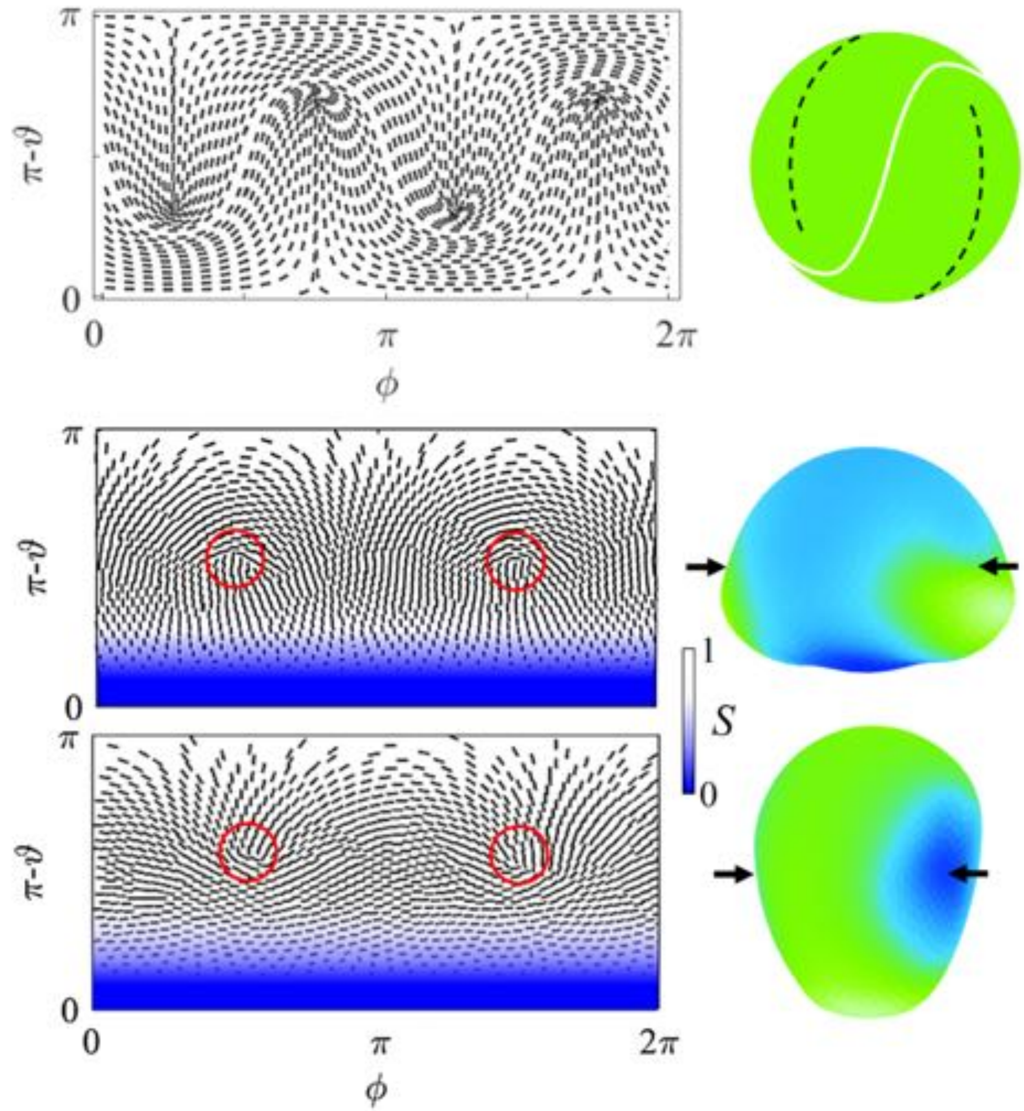


Zakharov and Pismen Soft Matter (2017)

Reshaping a sphere: Topology change

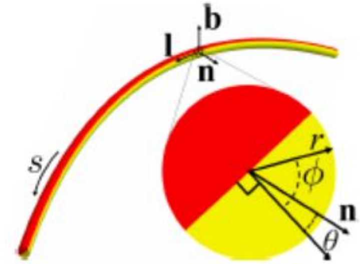
nematic texture on a sphere: 4 defects

point source of an isotropic dopant at the south pole: 2 defects



Zakharov and Pismen Soft Matter (2017)

Janus filaments

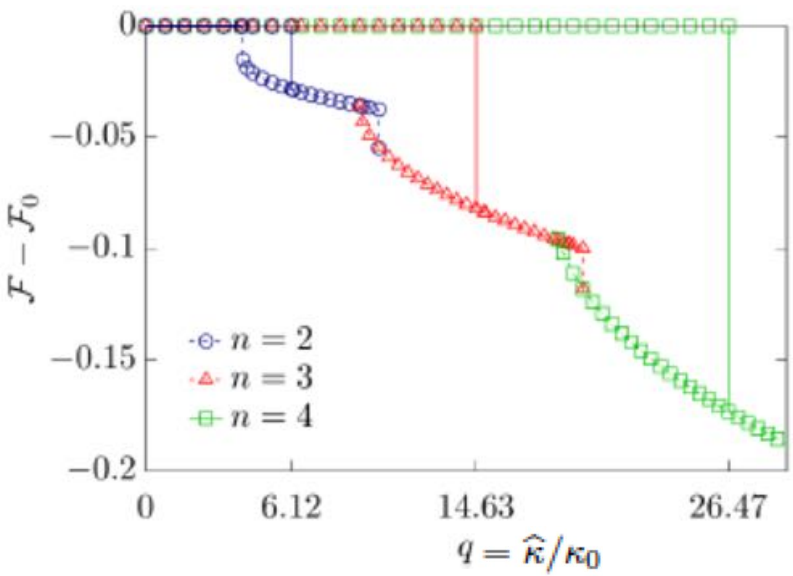


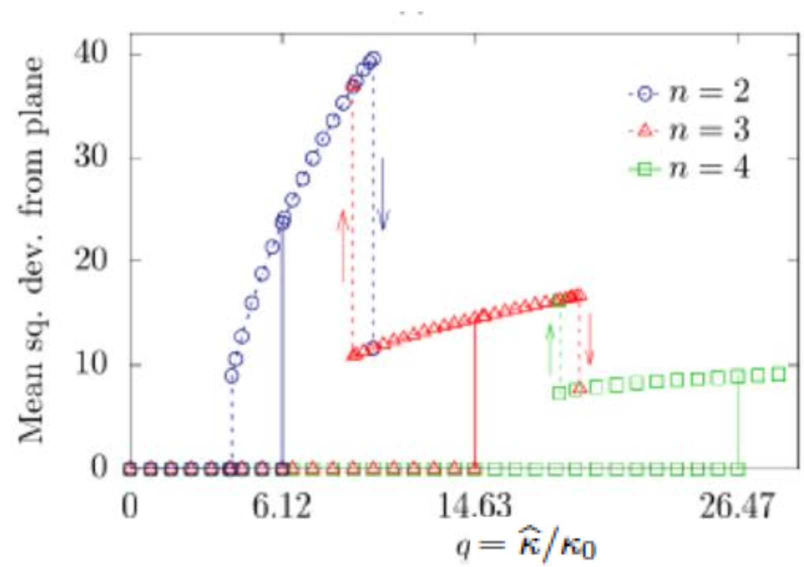
Energy

$$\mathcal{F} = \frac{1}{2}AEr^2 \int \left[\frac{1}{4}\kappa(\kappa - 2\widehat{\kappa}\cos\theta) + \frac{1}{2}\widehat{\tau}^2 \right] ds.$$

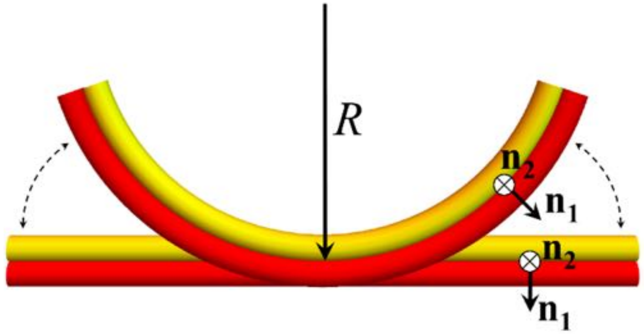
Energy increment

$$\delta\overline{\mathcal{F}} = (\kappa_0 - \widehat{\kappa})\overline{\kappa} + 2|\widetilde{\kappa}|^2 + 2(\kappa_0\widehat{\kappa} + 2k^2)|\widetilde{\theta}|^2 + 4|\widetilde{\tau}|^2 + 2\mathrm{i}k(\widetilde{\tau}^*\widetilde{\theta} - \widetilde{\tau}\widetilde{\theta}^*).$$

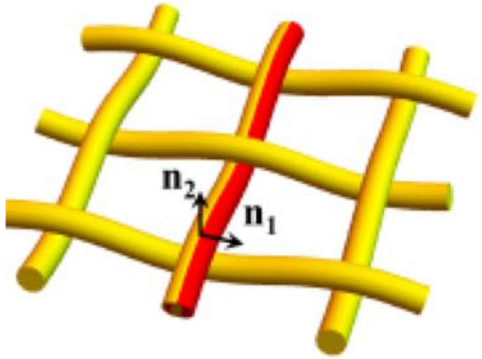




Active textiles



A **Janus fibre** made of two linked filaments before and after actuation.



A piece of textile made as a woven regular structure with passive fibres

Energy $$\mathcal{F}^e = \frac{1}{2} E A \left(\mathcal{F}^s + \mathcal{F}^c\right), \quad \mathcal{F}^s = u_z^2, \quad \mathcal{F}^c = I(R)$$

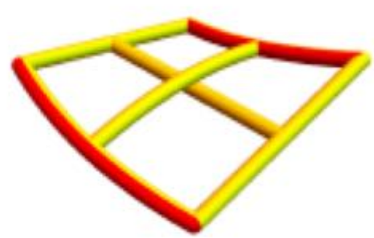
Bending moment of a Janus-fibre $$I(R) = \frac{1}{4}\left(\frac{r_a}{R}\right)^2 - \frac{4\,\epsilon}{3\pi}\frac{r_a}{R} + \frac{\epsilon^2}{2}$$

1. Zakharov and Pismen *Soft Matter* **14** 676 (2018)

Active textile: the simplest structure

Energy

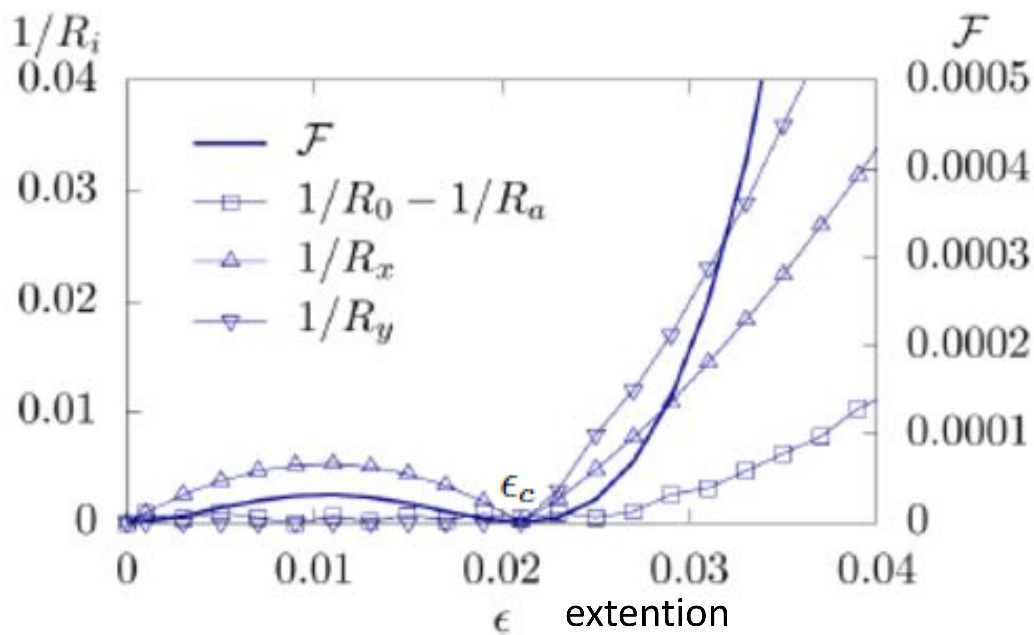
$$\mathcal{F} = \frac{\rho^4}{8}\left(\frac{1}{R_y^2} + \frac{2}{R_x^2} + \frac{1}{R_c^2}\right) + \chi^4 I_a(R_a)$$



Non-planar shape
Optimal at $\epsilon < \epsilon_c$,

Planar shape
Optimal at $\epsilon > \epsilon_c$,

The inverse optimal curvature radii of the parallel and perpendicular passive fibres, the deviation of the inverse curvature of the active fibres from its optimal value, and the residual energy of planar structures as functions of the relative extension

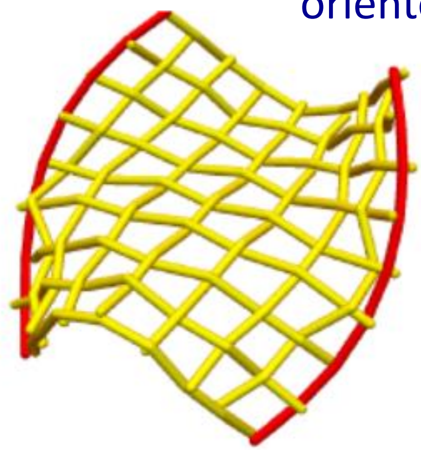


Zakharov and Pismen *Soft Matter* **14** 676 (2018)

Compressive/extensional actuation

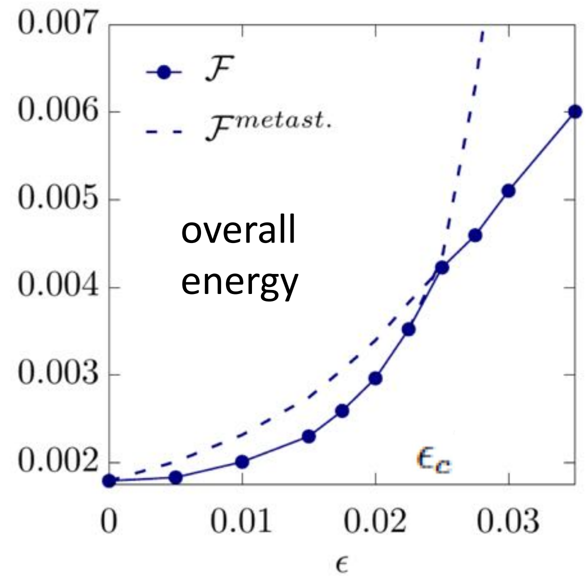
alternative shapes

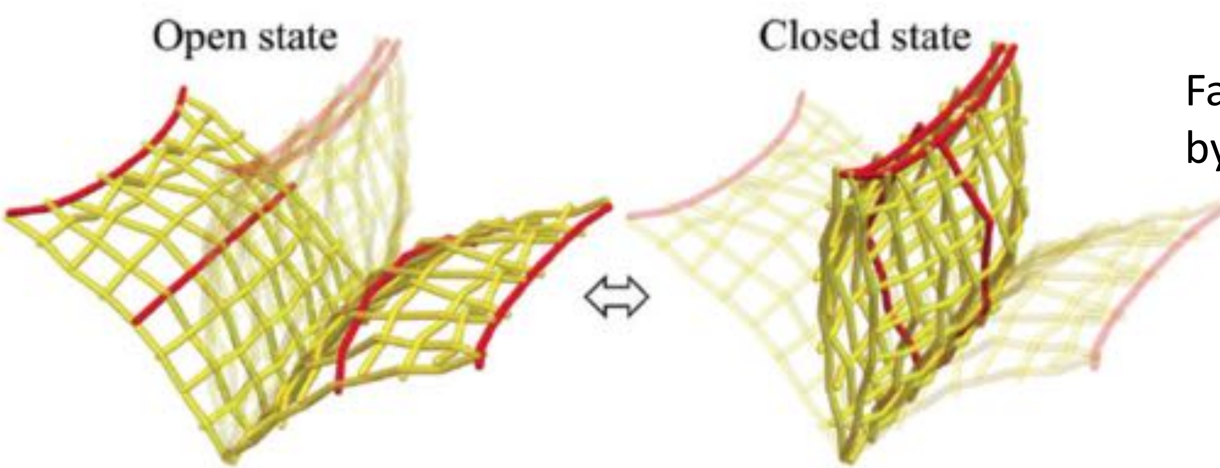
a saddle shape optimal at $\epsilon < \epsilon_c$,



a monkey saddle optimal at $\epsilon > \epsilon_c$,

Both curvature radii are originally oriented in-plane inward





Fast closure of a flytrap by snap-through

Summary

- Liquid crystal elastomers, made of cross-linked polymeric chains with embedded mesogenic structures, combine orientational properties of liquid crystals with the shear strength of solids. Their flexibility and sensitivity to chemical and physical signals comes close to that of biological tissues.

- A variety of three-dimensional forms can arise following a phase transition in elastomeric textures.

- Transitions to a deformed polarized state may be frustrated in constrained geometry leading to the formation of defects.

- Phase separation and a change of topology of nematic textures may take place due to the coupling between gradients of the nematic order and chemical composition.

- Reversible local phase transitions causing repeated reshaping can be used to construct soft crawling and swimming robots with the gait and speed dependent on flexural rigidity and substrate friction.

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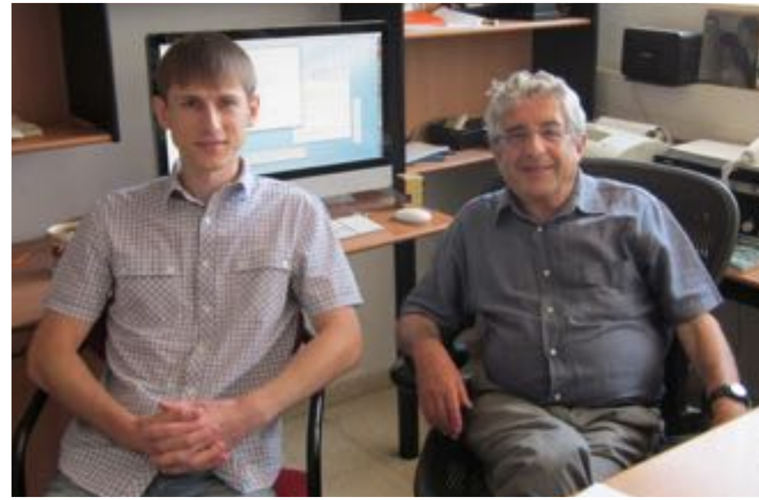
Thank you for your attention!



Further reading:

1. Zakharov A. P. and Pismen L. M. "Reshaping nemato-elastic sheets." Eur. Phys. J. *E* **38** 75 (2015)

1. Zakharov A. P. and Pismen L. M. "Nematoelastic crawlers." *Physical Review E* **93** 022703 (2016)

2. Zakharov A. P., Leshansky A. M. and Pismen L. M. "Flexible helical yarn swimmers” *Eur. Phys. J. E* **39** 87 (2016)

3. Zakharov A. P. and Pismen L. M. "Textures and shapes in nematic elastomers under the action of dopant concentration gradients." *Soft Matter* **13** 2886 (2017)

4. Zakharov A. P. and Pismen L. M. “Phase separation and folding in swelled nematoelastic films” *Physical Review E* **96** 012709 (2017)

5. Zakharov A. P. and Pismen L. M. “Active textiles with Janus fibres” *Soft Matter* **14** 676 (2018)

6. Zakharov A. P. and Pismen L. M. “Reshaping of a Janus ring” ” *Physical Review E* **97** 062705 (2018)

Earlier 2D work

1. Köpf M.H. and Pismen L.M. “Phase separation and disorder in doped nematic elastomers” Eur. Phys. J. E **36** 121 (2013)

2. Köpf M.H. and Pismen L.M. “Spontaneous nematic polarisation and deformation in active media” *Eur. Phys. J. Special Topics* **223**, 1247 (2014)

3. Köpf M.H. and Pismen L.M. “Stressed states and persistent defects in confined nematic elastica” Nonlinearity **28** 3957 (2015)