Liquid crystals: Lecture 2 Topological defects, Droplets and Lamellar phases

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Support: NSF

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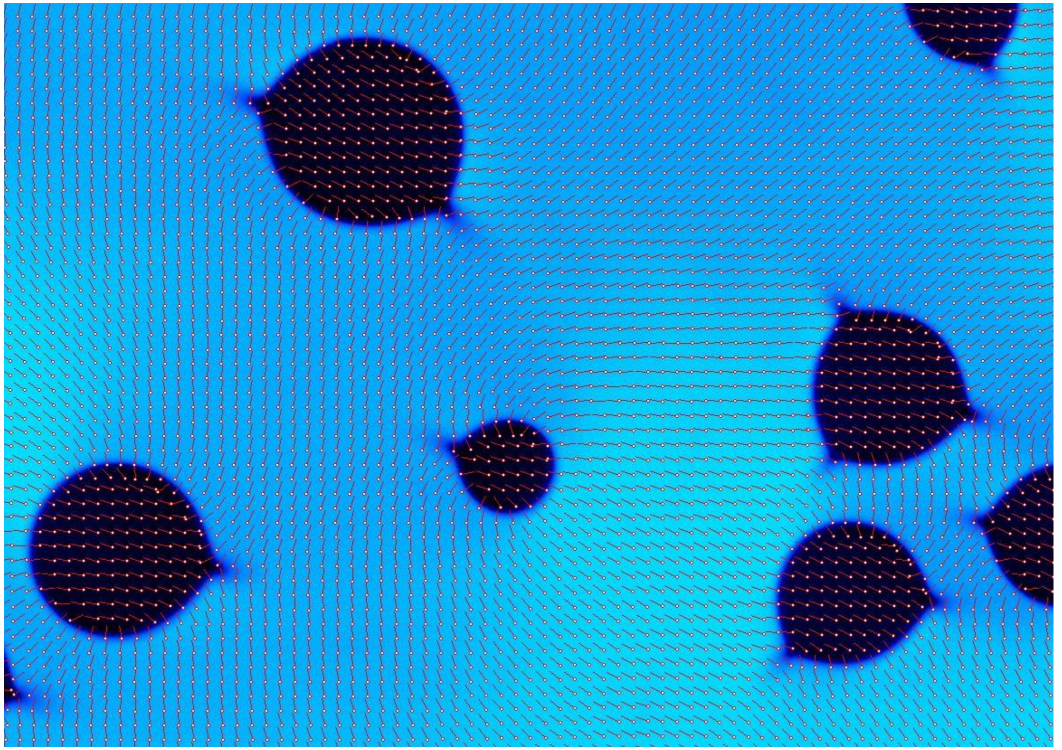
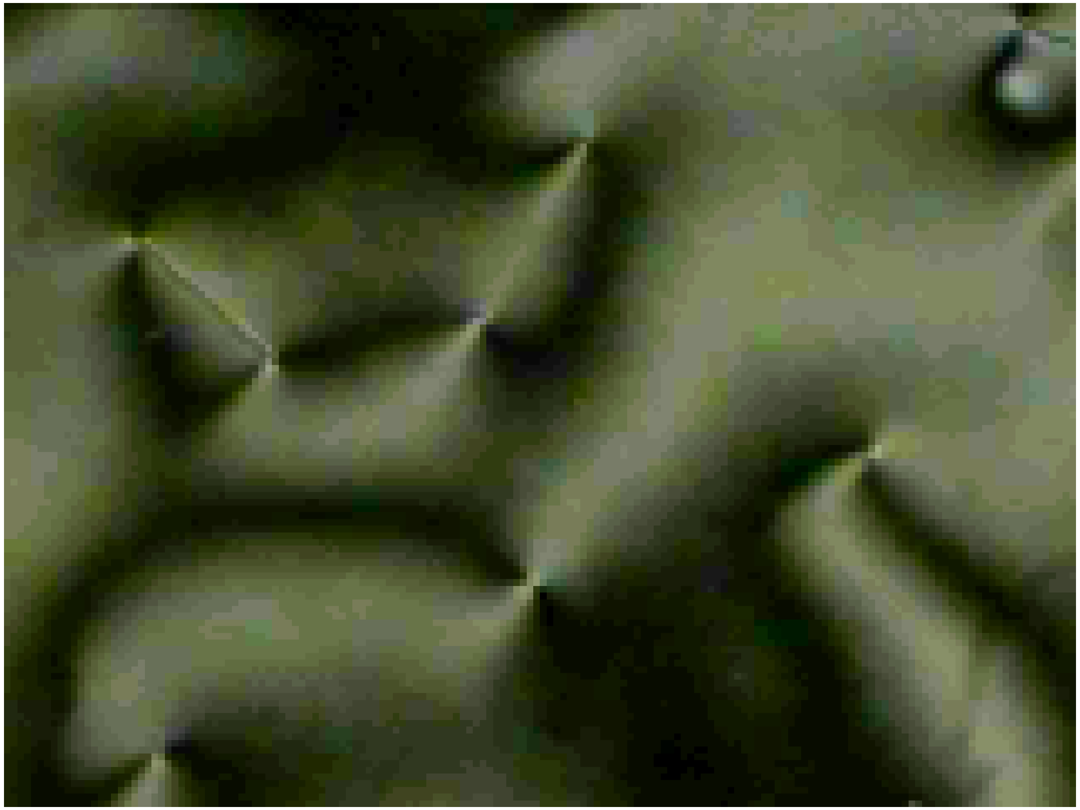
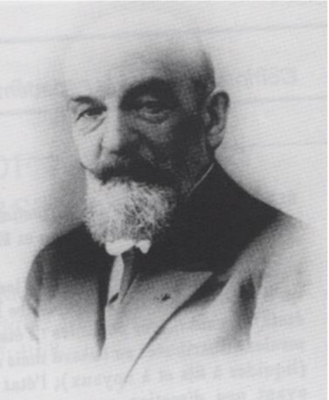


Boulder School for Condensed Matter and Materials Physics,
Soft Matter In and Out of Equilibrium,
6-31 July, 2015

Nematic LC: νεμα=thread; aka "disclination"



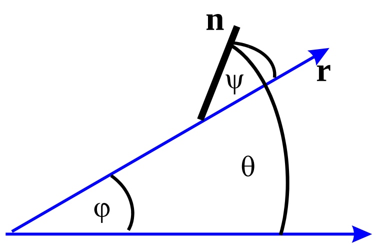


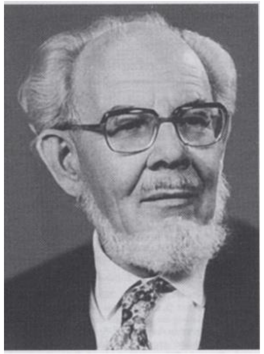
1922, G. Friedel:
Named "nematics", the simplest LC, after observing linear defects, νεμα=thread, under a polarized light microscope

Frank's model of disclinations in N

The simplest form (one constant) approximation:

$$f = \frac{1}{2} K\left[(\mathrm{div}\hat{\mathbf{n}})^2 + (\mathrm{curl}\hat{\mathbf{n}})^2\right]$$

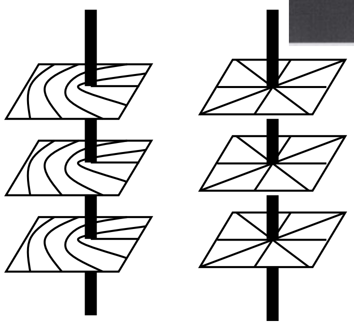




$$\{n_r, n_\varphi, n_z\} = \{\cos\psi(\varphi), \sin\psi(\varphi), 0\}$$

$$\mathrm{div}\,\hat{\mathbf{n}} = \frac{1}{r}\frac{dn_\varphi}{d\varphi} + \frac{n_r}{dr} = \frac{\cos\psi}{r}\left(1 + \frac{d\psi}{d\varphi}\right)$$

$$\mathrm{curl}_z\hat{\mathbf{n}} = -\frac{1}{r}\frac{dn_r}{d\varphi} + \frac{n_\varphi}{r} = \frac{\sin\psi}{r}\left(1 + \frac{d\psi}{d\varphi}\right)$$



k=1/2 k=1

$$F_{1length} = \frac{1}{2} K \int_S \left(1 + \frac{\partial\psi}{\partial\varphi}\right)^2 \frac{1}{r^2} r\,d\varphi\,dr = \frac{1}{2} K \int_{\varphi=0}^{\varphi=2\pi} \left(1 + \frac{\partial\psi}{\partial\varphi}\right)^2 d\varphi \int_{r=0}^{r=R} \frac{dr}{r}$$

Euler-Lagrange equation $\Rightarrow \dfrac{\partial^2\psi}{\partial\varphi^2} = 0 \quad \Rightarrow \psi = A\varphi + c$

$$\oint d\psi = 2\pi k \Rightarrow A = 0, \pm 1/2, \pm 1, \ldots \quad (n_r, n_\varphi) = \left(\cos[\varphi(k-1)+c],\ \sin[\varphi(k-1)+c]\right) \quad (n_x, n_y) = \left(\cos[\varphi k + c],\ \sin[\varphi k + c]\right)$$

$$F_{1length} = \pi k^2 K \int_{r=0}^{r=R} \frac{dr}{r} = \pi k^2 K \ln\frac{R}{r_{core}} + F_{core}$$

$$F_{core} = k_B (T_{NI} - T) \times \pi r_{core}^2 \times \rho N_A / M$$

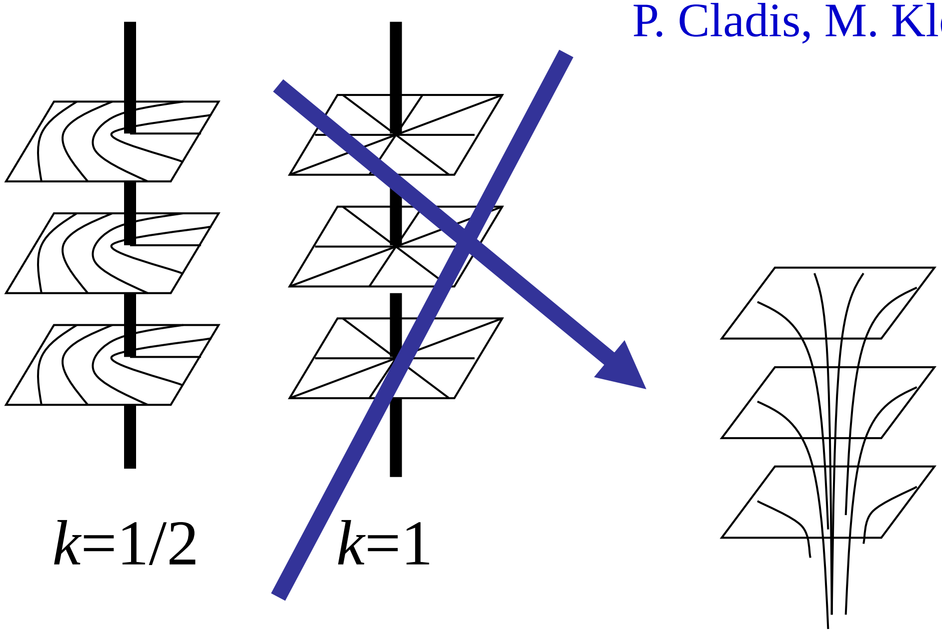
Energy per degree of freedom # degrees of freedom

$$r_{core} = k\sqrt{\frac{MK}{\rho N_A k_B (T_{NI} - T)}} \sim \textit{few molecular lengthes};\ F_{core} \sim \pi k^2 K$$

Kleman, ODL Soft Matter Physics, p. 393

Escape into the 3rd dimension

P. Cladis, M. Kleman (1972), R.B. Meyer (1972)



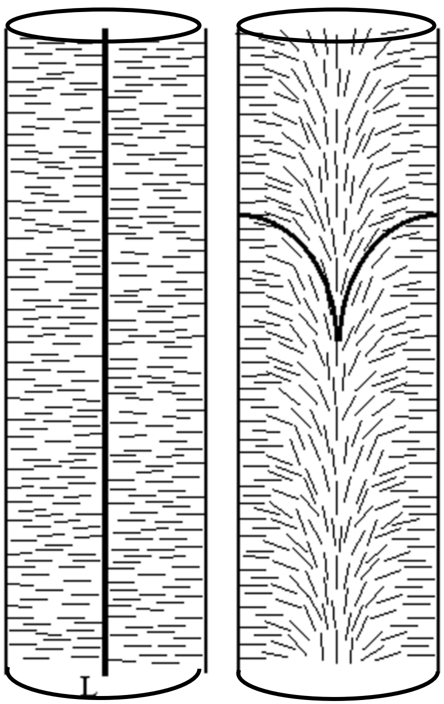
k=1/2 k=1

k=1

Escape into the 3rd dimension

$$n_r = \cos\chi(r), \quad n_\varphi = 0, \quad n_z = \sin\chi(r)$$

$$f = \frac{1}{2}K\left[(\mathrm{div}\hat{\mathbf{n}})^2 + (\mathrm{curl}\hat{\mathbf{n}})^2\right]$$


(a)

$$\chi(r=R)=0$$

$$\chi(r=0)=\pi/2$$

$$\mathrm{div}\,\hat{\mathbf{n}} = \frac{1}{r}\frac{d(rn_r)}{dr} = -\sin\chi\frac{d\chi}{dr} + \frac{\cos\chi}{r} \qquad \mathrm{curl}_\varphi\hat{\mathbf{n}} = -\frac{dn_z}{dr} = -\cos\chi\frac{d\chi}{dr}$$

$$F_{1length} = \frac{1}{2}K\int_{\varphi=0}^{\varphi=2\pi} d\varphi \int_{r=0}^{r=R}\left[\left(\frac{\partial\chi}{\partial r}\right)^2 + \frac{\cos^2\chi}{r^2} - \frac{1}{r}\sin 2\chi\frac{d\chi}{dr}\right] r dr \qquad r \to \exp\xi$$

$$F_{1length} = \pi K \int_{r=0}^{r=R}\left[\left(\frac{\partial\chi}{\partial\xi}\right)^2 + \cos^2\chi - \sin 2\chi\frac{d\chi}{d\xi}\right] d\xi$$

Euler-Lagrange equation $\quad \dfrac{\partial^2\chi}{\partial\xi^2} = -\cos\chi\sin\chi$

$$\Rightarrow \left(\frac{\partial\chi}{\partial\xi}\right)^2 = \cos^2\chi + const; \quad \left.\frac{\partial\chi}{\partial\xi}\right|_{r\to 0} \to 0 \Rightarrow const = 0$$

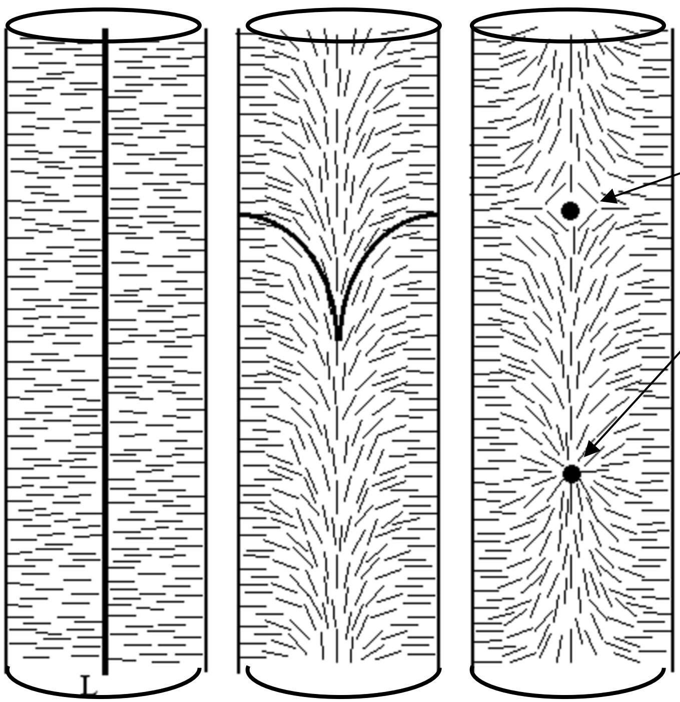
$$\frac{\partial\chi}{\partial\xi} = -\cos\chi \quad \Rightarrow \int_r^R \frac{dy}{y} = -\int_\chi^0 \frac{dp}{\cos p} \qquad \chi = 2\arctan\left(\frac{R-r}{R+r}\right)$$

$$F_{1length}^{escaped} = 3\pi K \qquad F_{1length}^{singular} = \pi K \ln\frac{R}{r_{core}} + F_{core}$$

Escape is preferred when $R > 10 r_{core}$

P. E. Cladis, M. Kleman J. Physique 33, 591 (1972), R.B. Meyer, Phil. Mag. 27, 405 (1972)

Escape into the 3rd dimension



(a) $\chi(r=R)=0$ (c)

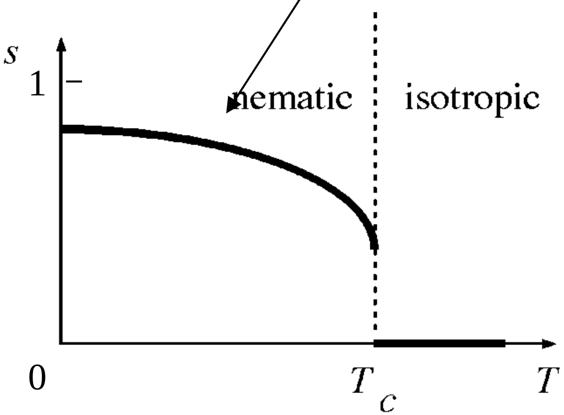
$\chi(r=0)=\pi/2$

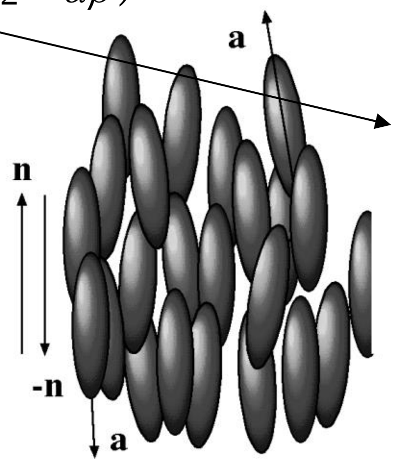
Point defects in the nematic bulk
-hedgehogs

LCI KENT STATE UNIVERSITY

Homotopy classification: Uniaxial nematic N_u

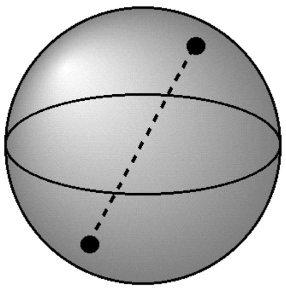
$$Q_{\alpha\beta} = s\left(n_\alpha n_\beta - \tfrac{1}{2}\delta_{\alpha\beta}\right)$$





S^2 / Z_2

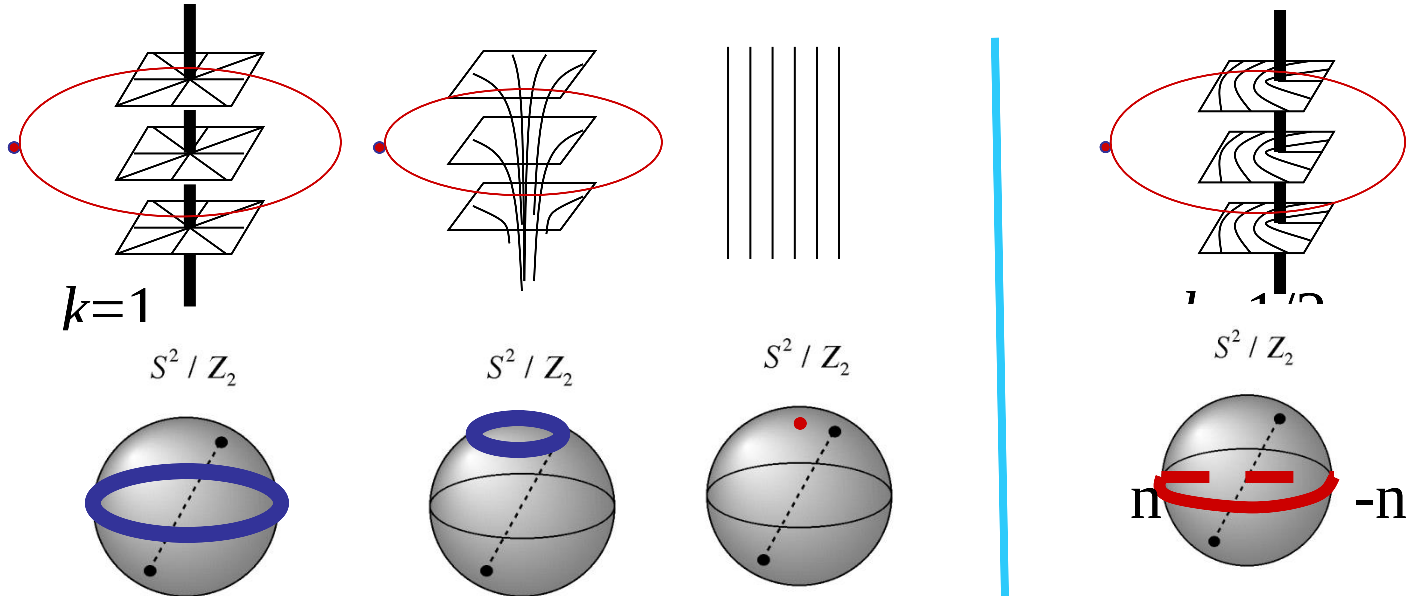
n=-n



Degeneracy space

Topological stability is established by mappings from real space onto the degeneracy (or order parameter) space

Homotopy classification: Lines in N_u



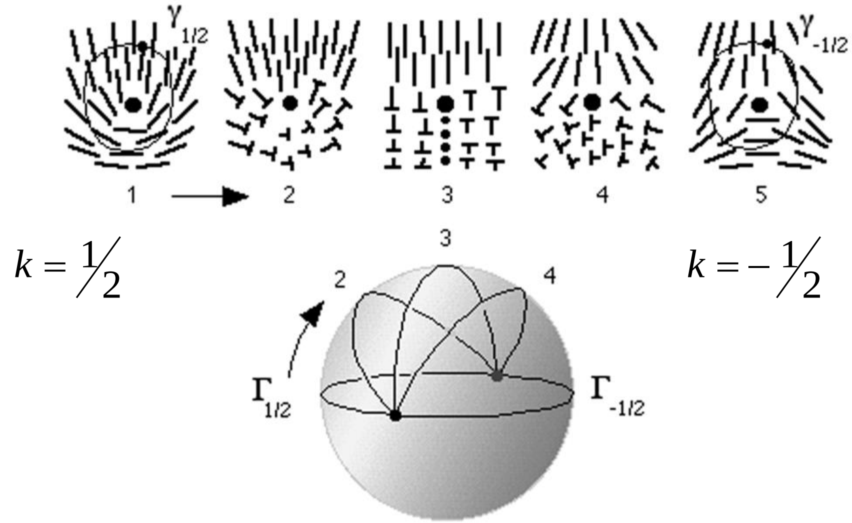
Topologically unstable

Topologically stable

Topologically stable defect: A non-uniform configuration of the order parameter that cannot be reduced to a uniform state by a continuous transformation. In practical terms, to destroy a topological effect, one needs an energy exceeding the self energy of the defects by many orders of magnitude; e.g. melt the entire sample.

G. Toulouse, M. Kleman J. Phys. Lett. 37, L149 (1976), G.Volovik, V. Mineev, JETP 46, 1186 (1977)

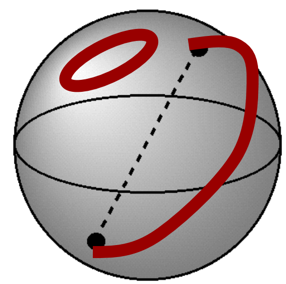
Homotopy classification: Lines in N_u



All semi-integer disclinations are topologically equivalent to each other and can be smoothly transformed one into another

Disclinations in N are described by the 1st homotopy group, comprised of two elements

$$\pi_1\left(S^2/Z_2\right) = Z_2 = \left(0, \tfrac{1}{2}\right)$$



G. Toulouse, M. Kleman J. Phys. Lett. 37, L149 (1976),
G.Volovik, V. Mineev, JETP 46, 1186 (1977)

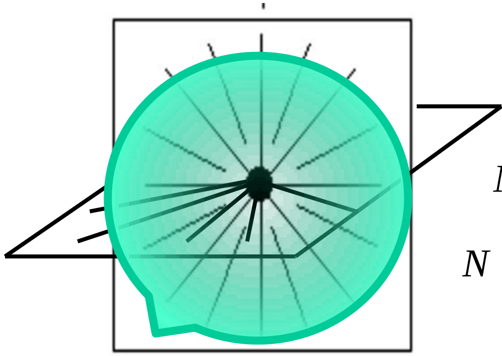
Homotopy classification: Points in 3D N_u

Hedgehogs (point defects) in uniaxial N

$$\pi_2\left(S^2/Z_2\right) = N = 0, \pm 1, \pm 2, \ldots$$

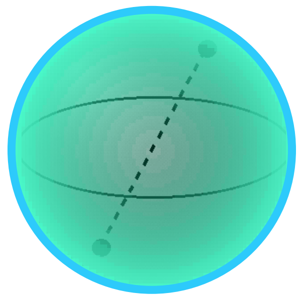
Radial hedgehog

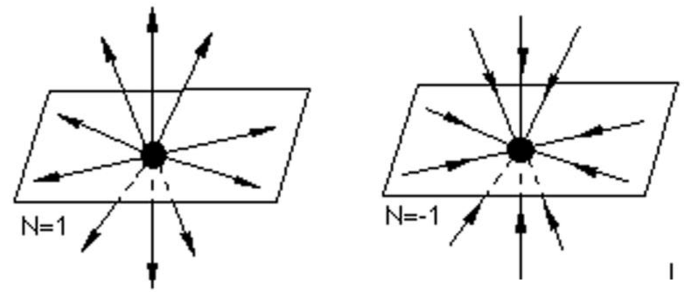
S^2/Z_2



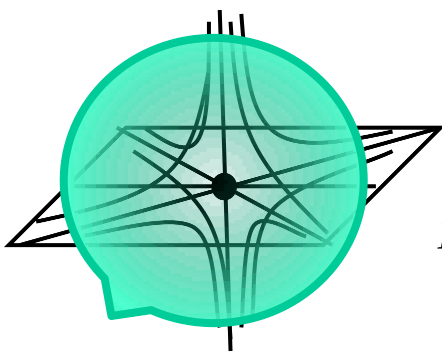
$N=1?$

$N=-1?$



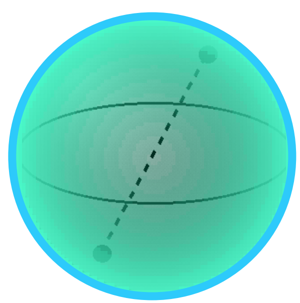


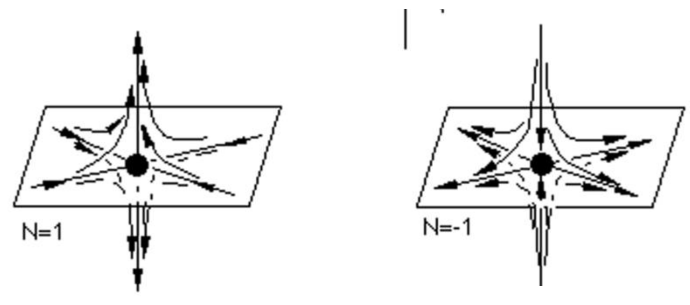
Hyperbolic hedgehog



$N=1?$

$N=-1?$





Topological charges of points, vector fields, t-space

t-dimensional vector field:

$$\mathbf{n} = \left(n^1, n^2, \ldots n^t\right)$$

(t-1)-coordinates specified on the sphere around the defect

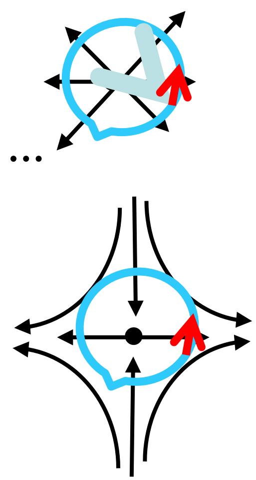
$$\left(u^1, u^2, \ldots u^{t-1}\right)$$

$$N^{(t)} = \frac{1}{\Omega} \int_{S^{t-1}} \begin{vmatrix} n^1 & \ldots & \ldots & n^t \\ \dfrac{\partial n^1}{\partial u^1} & \ldots & \ldots & \dfrac{\partial n^t}{\partial u^1} \\ \ldots & \ldots & \ldots & \ldots \\ \dfrac{\partial n^1}{\partial u^{t-1}} & \ldots & \ldots & \dfrac{\partial n^t}{\partial u^{t-1}} \end{vmatrix} du^1 \ldots du^{t-1}$$

Definition of t-dimensional topological charge:
E. Dubrovin et al, Modern Geometry, Springer, 1984

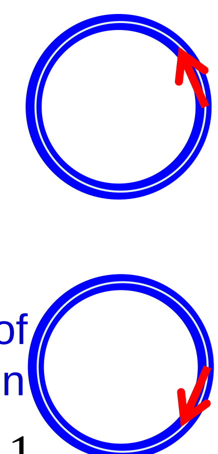
Point defects in 2D:

$$N^{(2)} \equiv k = \frac{1}{2\pi} \oint_{loop} \left(n^1 \frac{dn^2}{dl} - n^2 \frac{dn^1}{dl} \right) dl = \pm 1, \pm 2, \ldots$$



$k = 1$

Circle of all possible orientations of magnetization

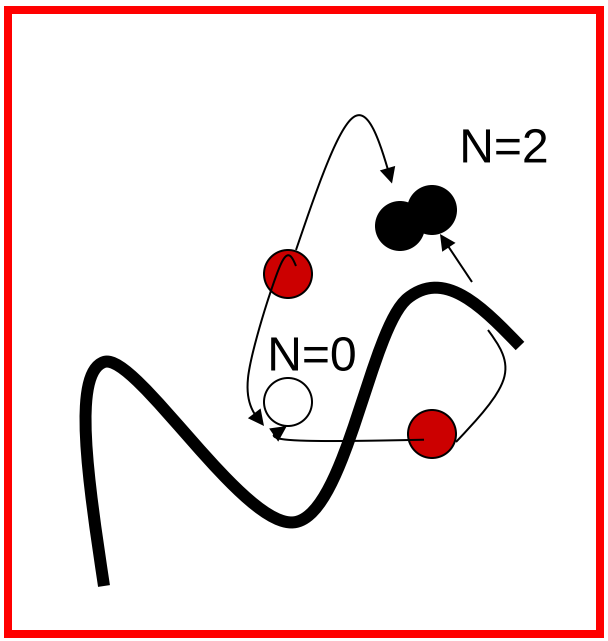


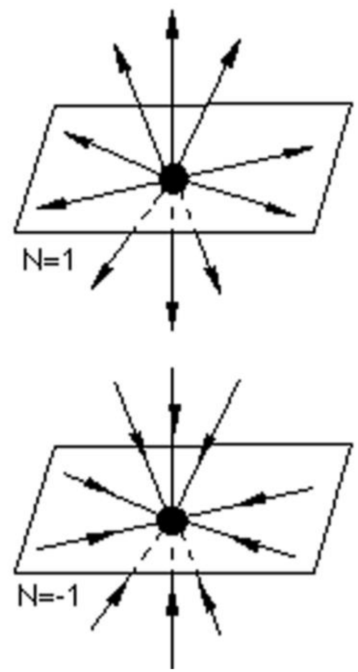
$k = -1$

Homotopy: Points in 3D N_u

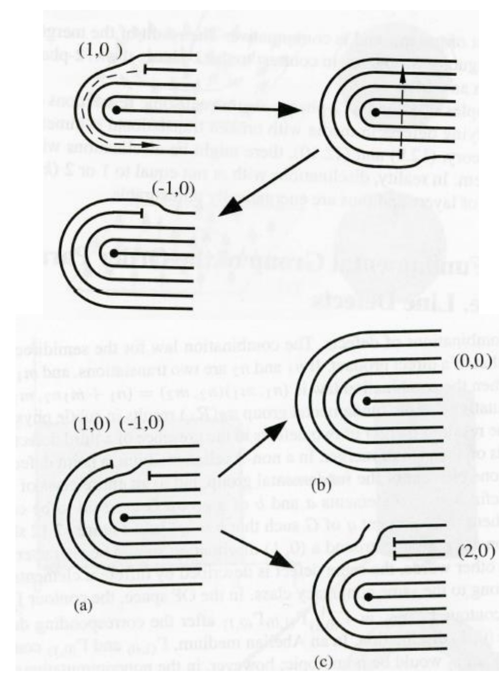
Result of merger of 2 hedgehogs in a uniaxial N in presence of a disclination depends on the pathway of merger

$$N + N = \begin{cases} 2N \\ 0 \end{cases}$$



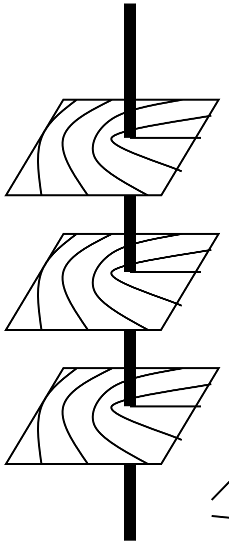


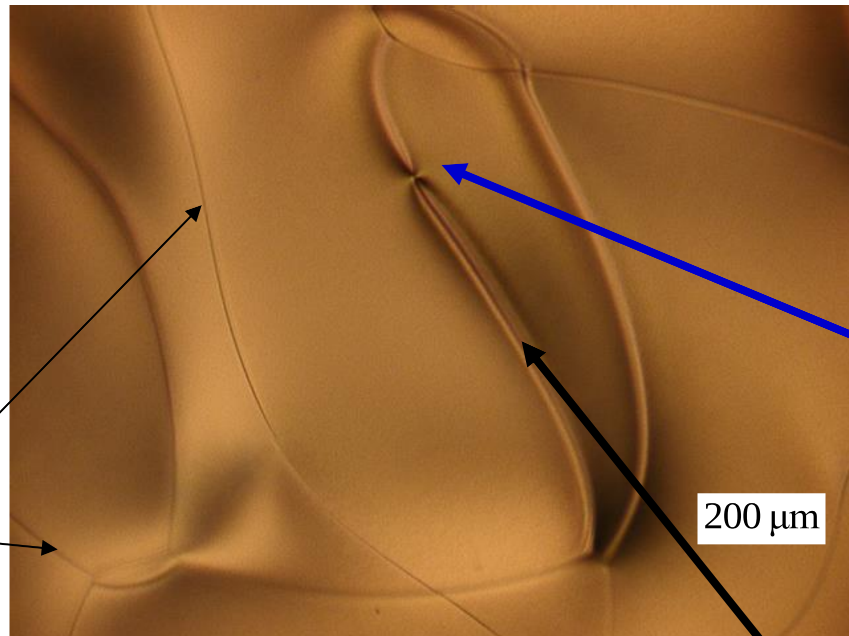
Similar example for dislocations in presence of disclinations:

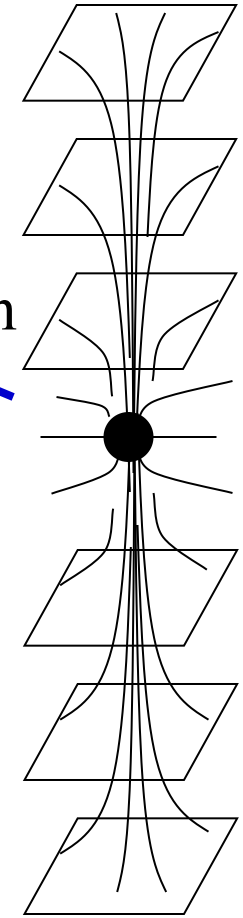


G. Toulouse, M. Kleman J. Phys. Lett. 37, L149 (1976),
G.Volovik, V. Mineev, JETP 46, 1186 (1977)

Typical texture of a (thick) N_u



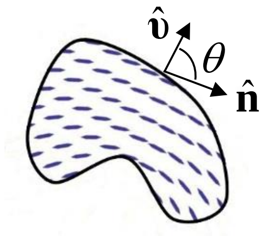




Eventually, all the defects will disappear, except
maybe one line and one point defect,
mostly through annihilation, as ½+½=0 and 1+1=0!

Defects in equilibrium: LC droplets

The structure is determined by the balance of anisotropic surface tension and internal elasticity



- Anisotropic surface energy $F_{surface} = \sigma_o + f\left(\hat{\mathbf{n}}\cdot\hat{\boldsymbol{\upsilon}}\right)$

$f\left(\hat{\mathbf{n}}\cdot\hat{\boldsymbol{\upsilon}}\right) = W_2\left(\hat{\mathbf{n}}\cdot\hat{\boldsymbol{\upsilon}}\right)^2 = W_2\cos^2\theta$ Rapini-Papoular surface anchoring potential

S. Faetti et al, PRA **30**, 3241 (1984): N-I thermotropic interface is weakly anisotropic:

$$\sigma_o \sim 10^{-5}\ \mathrm{J/m^2};\ W_2 \sim 10^{-6}\ \mathrm{J/m^2};\ W_2/\sigma_o \sim 0.1-0.01$$

- Elasticity:

$$F_{elastic} \sim KR \qquad K_i \sim 5\ \mathrm{pN} \qquad R \geq 10\ \mu\mathrm{m} \Rightarrow$$

$$\frac{\sigma_0 R^2}{KR} \geq 10;\quad \frac{W_2 R^2}{KR} \geq 1$$

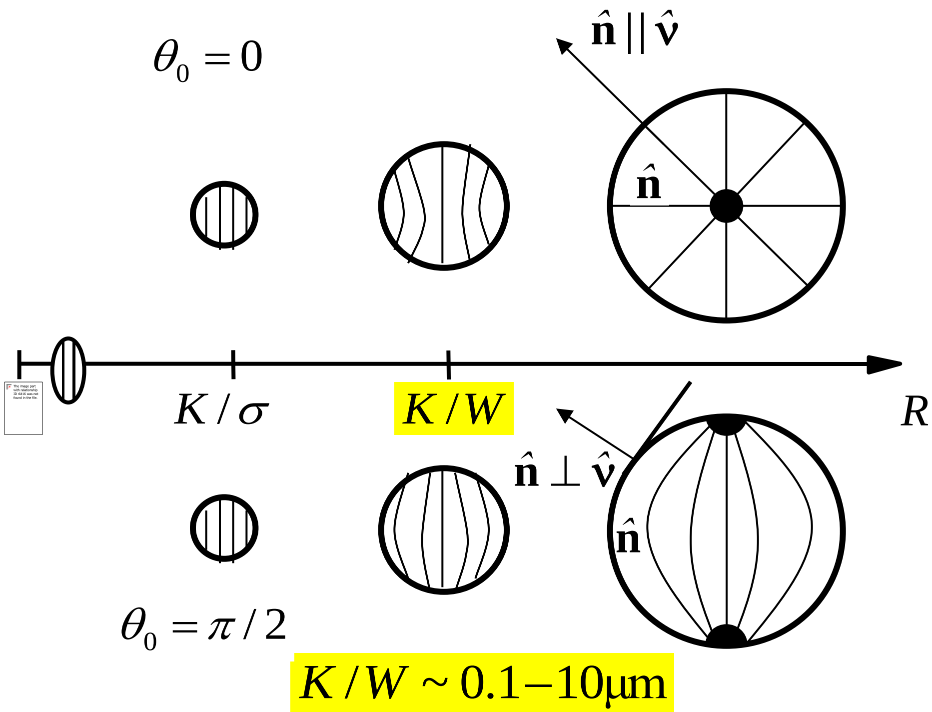
The droplets of thermotropic N in isotropic melt are spherical and contain defects to satisfy surface anchoring conditions

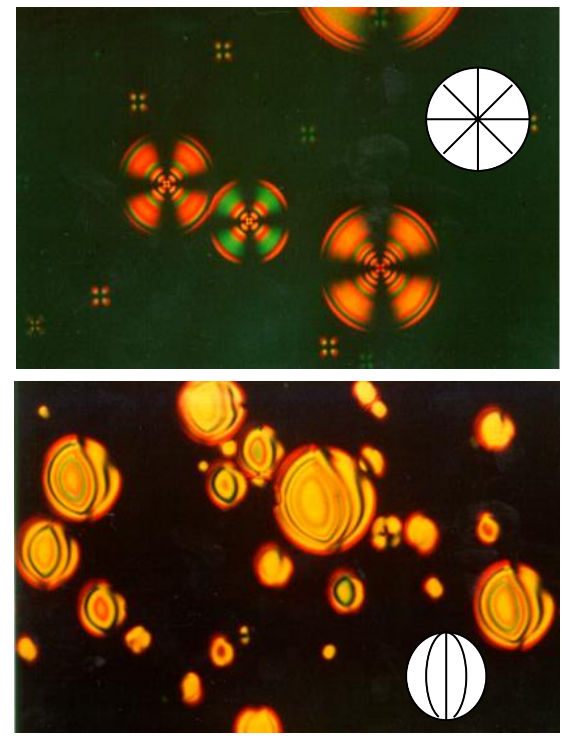
Defects in equilibrium: LC droplets

Balance of elasticity and surface anchoring

$$F_{elastic} \sim KR \qquad F_{anchoring} \sim WR^2$$

leads to the following expectation for scaling behavior:



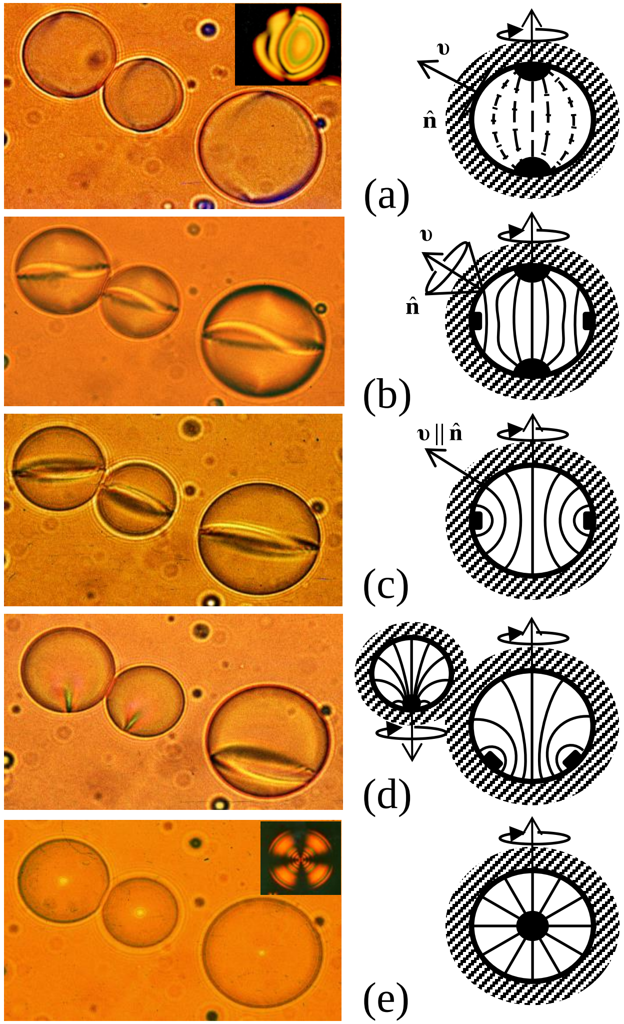


Defects correspond to the equilibrium state of the (large) system

Liquid Crystals **24**, 117 (1998)

Defects in equilibrium: LC droplets

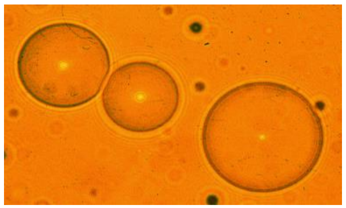
N droplets in glycerine with temperature varied anchoring axis; topological dynamics of boojums, disclination loops and hedgehogs
NB: Defects correspond to the equilibrium state of the system; they help to minimize the sum of the anisotropic surface tension and bulk energy.

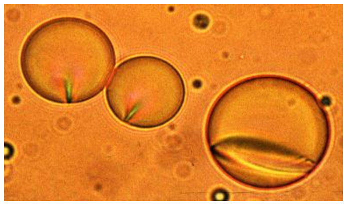


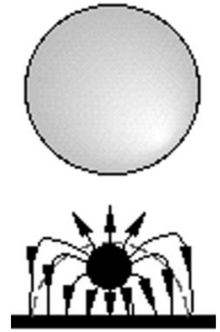
Do we really want to minimize the energy for each and every surface angle?!

Topological dynamics of defects in LC drops

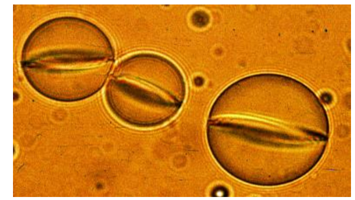
Bulk point defect hedgehog: $N=1$







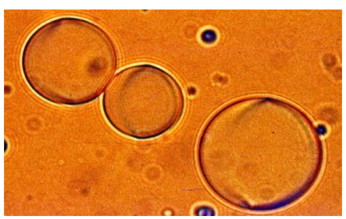
Hedgehog spreadable into a disclination loop:

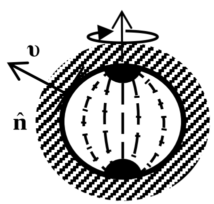


$N=1$

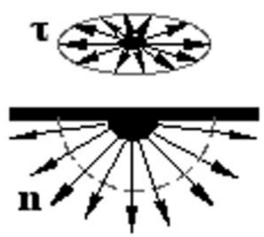
Replace director with a vector

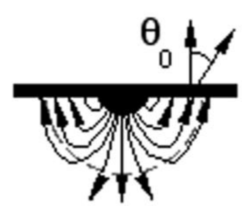
Surface point defect boojum: two topological charges, 2D and 3D;

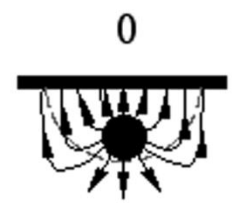




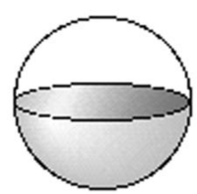
$k=1$



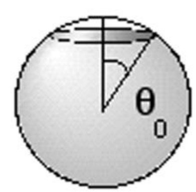




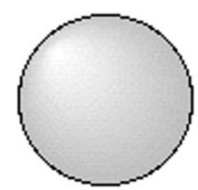
$$C_{k,N}=\frac{1}{4\pi}\int_{\sigma}d\theta d\phi\,\mathbf{n}\left[\frac{\partial\mathbf{n}}{\partial\theta}\times\frac{\partial\mathbf{n}}{\partial\phi}\right]=\frac{k}{2}(\mathbf{n}\cdot\boldsymbol{\nu}-1)+N$$



$C=1/2$



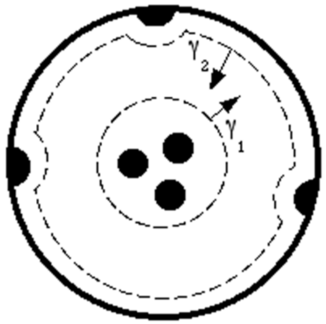
$C=\cos^2\frac{\theta_0}{2}$



$C=1$

G.E. Volovik et al, Sov. Phys. JETP **58** 1159 (1983)

Topological dynamics of defects in LC drops



$$\sum_{i=1}^{b} C_{k_i,N_i} + C_s + \sum_{j=b+1}^{h+b} N_j = \left(-1+\frac{1}{2}\sum_{i=1}^{b} k_i\right)(\mathbf{n}\cdot\boldsymbol{\nu}-1) + \sum_{j=b+1}^{h+b} N_j - 1 = 0$$

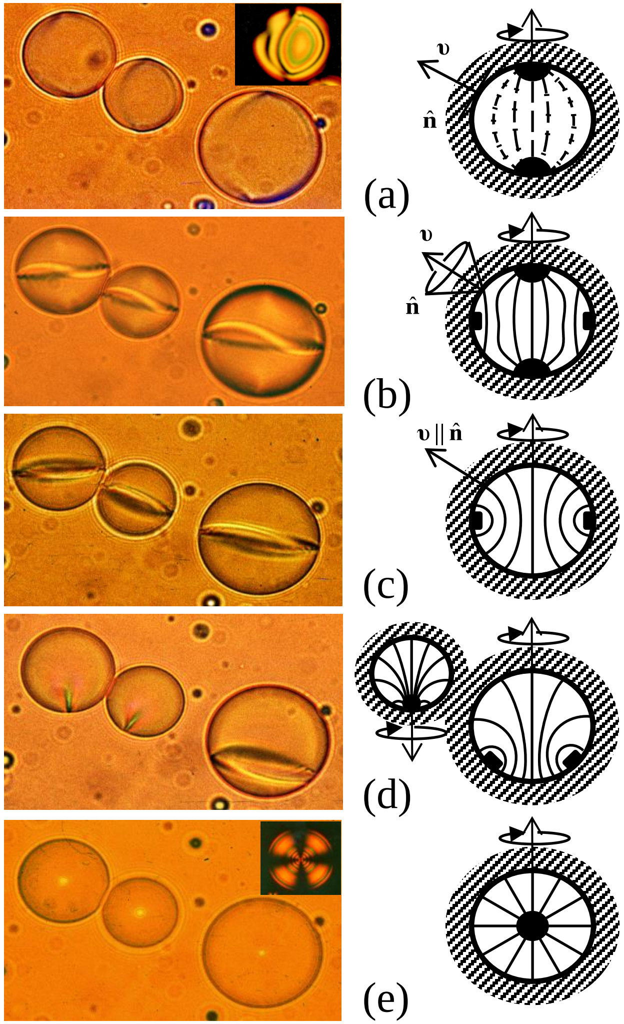
Poincare theorem: conservation law for vector fields tangential to the surface

$$\sum_{i}^{b} k_i = E$$

Gauss theorem: conservation law for vector fields perpendicular to the surface

$$\sum_{j=1}^{h+b} N_j = E/2$$

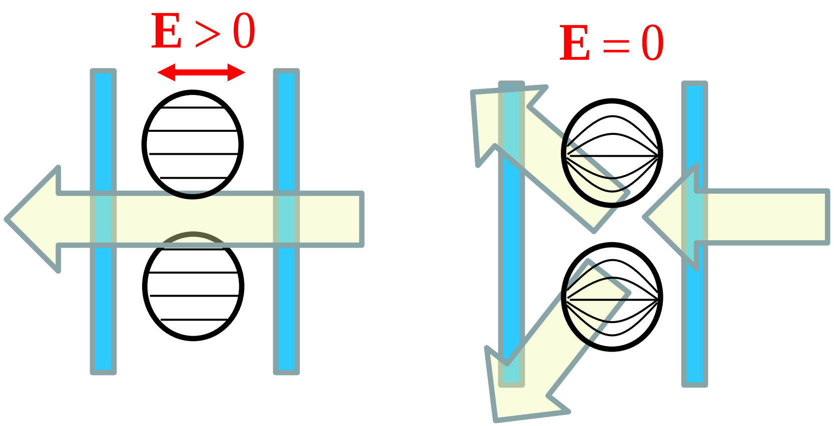
Euler characteristic for sphere $E = 2$



G.E. Volovik et al, Sov. Phys. JETP **58** 1159 (1983)

Applications of LC drops

Privacy windows:
Polymer Dispersed Liquid Crystals
(JW Doane et al, LCI, Kent)



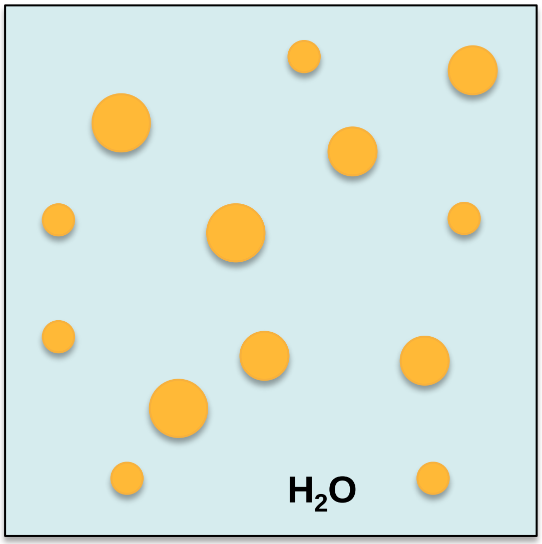
$n_o = n_{polymer}$ $n_{effective} \neq n_{polymer}$

Droplets as Biosensors:

Abbott and Lynn (UW-Madison)

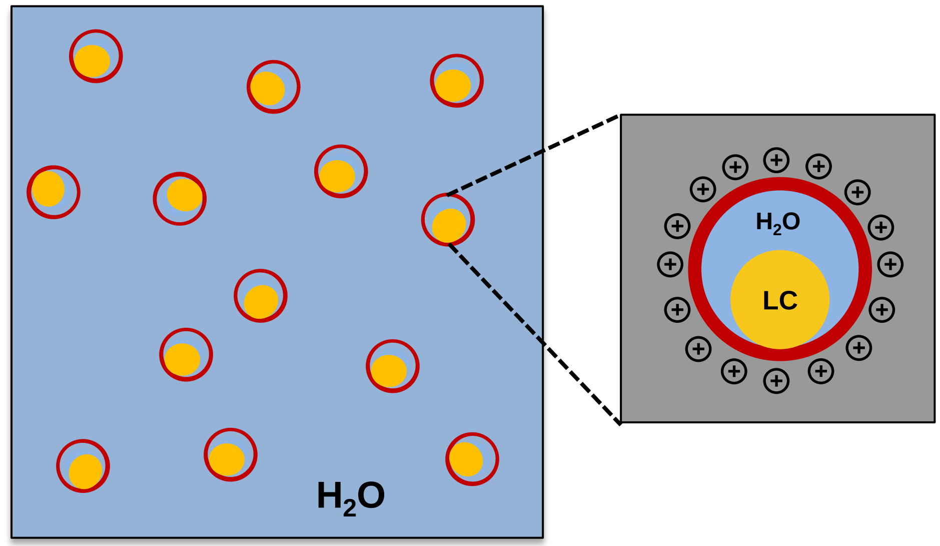
Microscale LC Droplets

(Oil-in-Water Emulsion)



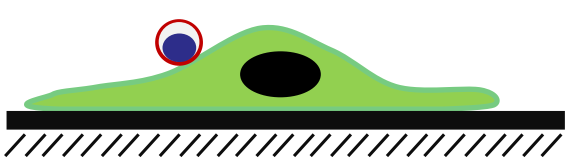
'Caged' LC Droplets

(Droplets in Polymer Capsules)

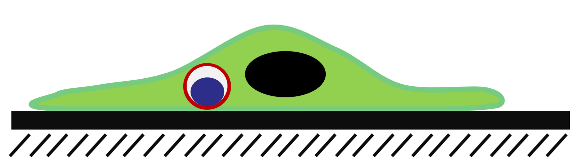


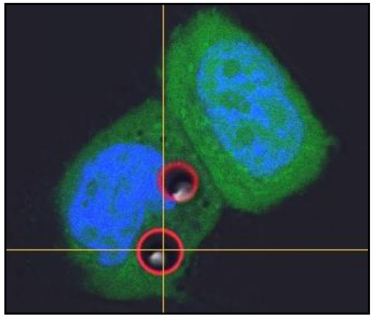
Sensing in Biological Environments:

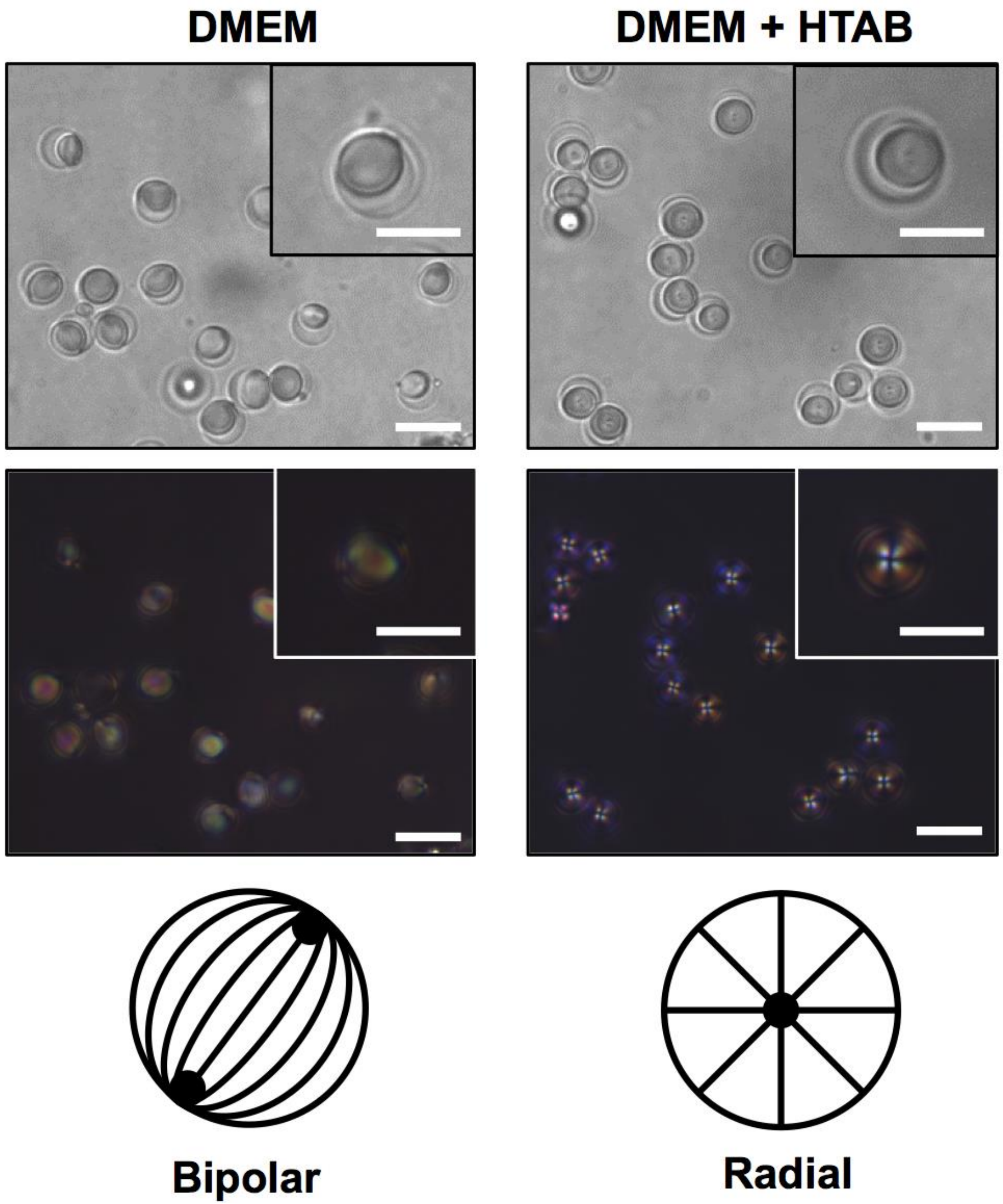
Immobilized LC Droplets

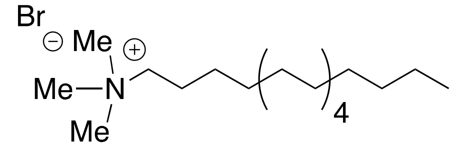


Internalized LC Droplets









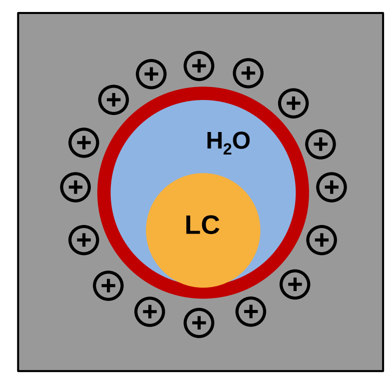
HTAB
(10 μm)

Transitions triggered by:

- **Cationic surfactants**
- **Anionic surfactants**
- **Bacterial endotoxin**

Not by:

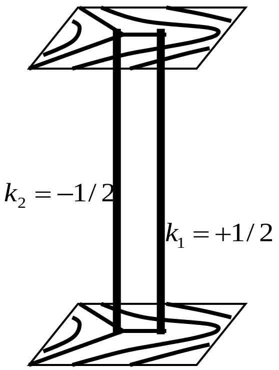
- **Proteins, serum, etc.**



Abbott and Lynn (UW-Madison)

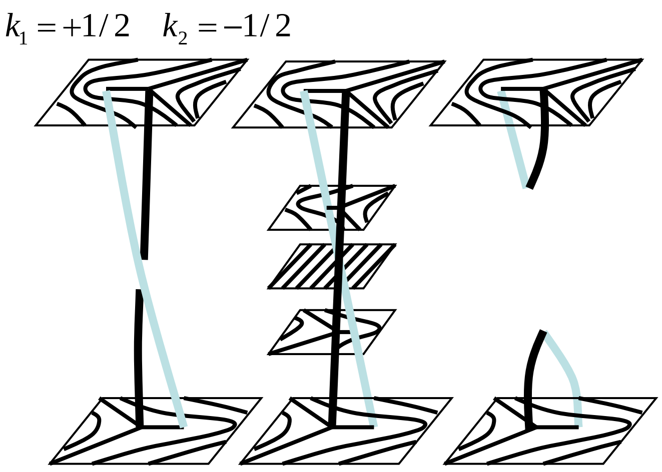
Angew. Chem. **2013**; *Langmuir* **2014**

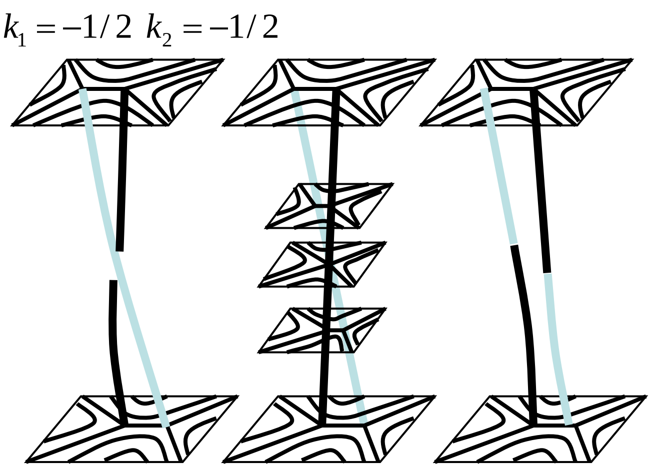
Reconnection of disclinations in N_u



Disclinations are not “material” lines and can cross each other.

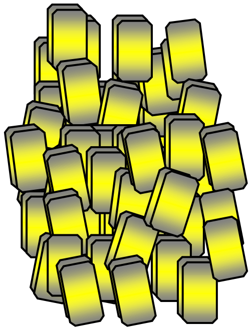
Two disclinations connecting opposite plates of a nematic cell; plates are twisted; disclination ends reconnect



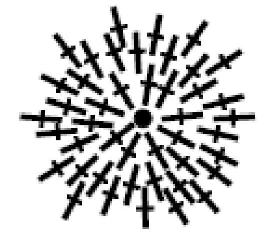


T.Ishikawa et al, Europhys. Lett. (1998)

Reconnection of disclinations in biaxial N_{bx}

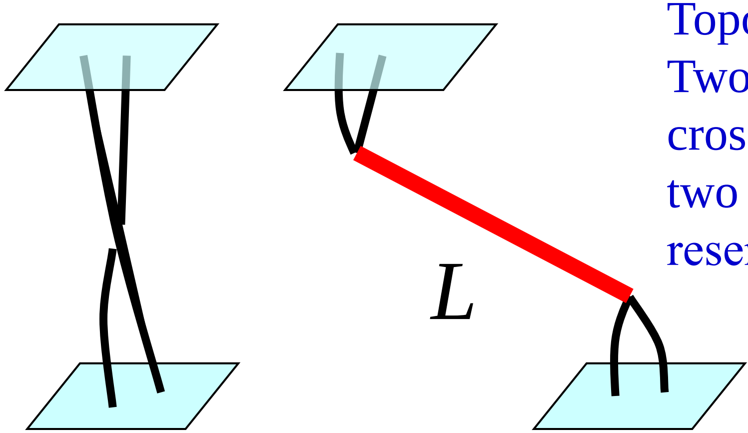


Degeneracy space: Solid sphere; each point describes a state of three directors, n,m,l. In biaxial nematics, the strength 1 disclinations cannot escape (strength 2 can). There are three different classes of ½ disclinations with *k* semi-integer and one with k=1



$k = 1$ does not escape!

$$\pi_1\left(S^3 / D_2\right) = Quaternion\ units = \left(0; 1; 1/2_x; 1/2_y; 1/2_z\right)$$



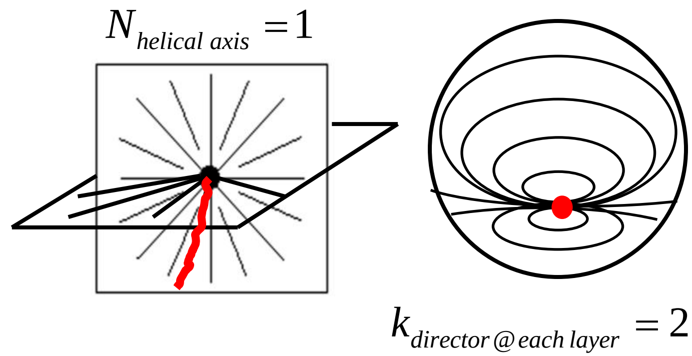
Topological test for biaxiality of a nematic:
Two disclinations ½ belonging to different classes cannot cross each other, the trace is a third line of strength 1; the two separated disclinations interact through a potential that resembles interaction of …. Quarks!

$$U \propto KL$$

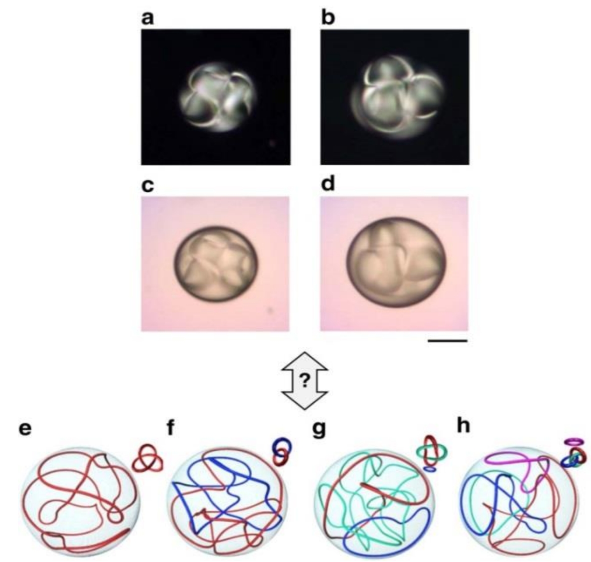
G. Toulouse, J. Phys. Lett. **38**, L67 (1977)

Cholesteric drops and Dirac monopole

Two orthogonal vector fields: helical axis and director (magnetic field and vector-potential)



Point hedgehog in helical axis (magnetic) field and an attached disclination (Dirac string) in the director field

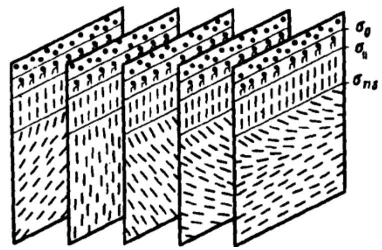


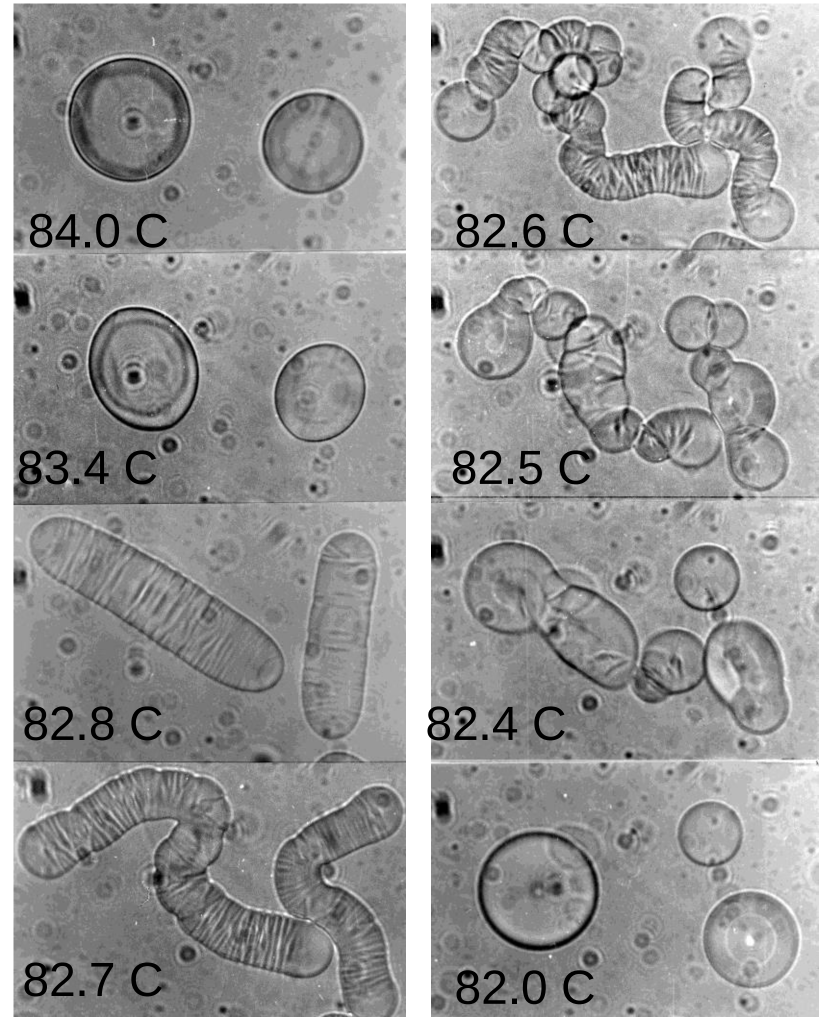
P. Dirac, Proc. Roy. Soc. (London) A133, 60 (1931)
Ch droplet, called Robinson spherulite or Frank-Price structure,
C. Robinson et al, Disc. Faraday Soc. 25, 29 (1958);
Kurik et al, JETP Lett **35**, 444 (1982)

T. Orlova et al, Nat. Comm. **6**, 7603 (2015)

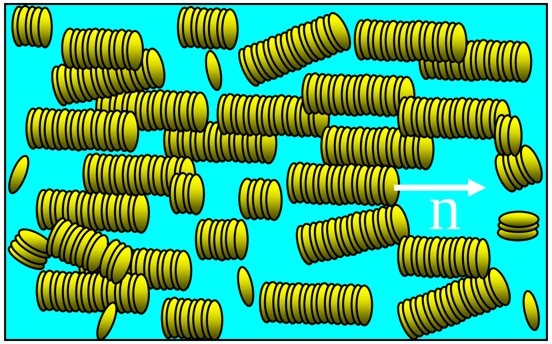
Rare exception of round cohesive droplets: Ch-SmA phase transition

Ch droplets in glycerine+lecithin; cooling down leads to extended shapes, then nucleation of spherical SmA sites; the process often results in division of droplets (Nastishin et al Sov Phys JETP Lett 1984; EurophysLett 1990)





$(LC)^2$: Lyotropic Chromonic Liquid Crystals



$$\sigma_o \sim \alpha \frac{k_B T}{LD} \sim \left(10^{-7} - 10^{-6}\right) \text{J/m}^2$$

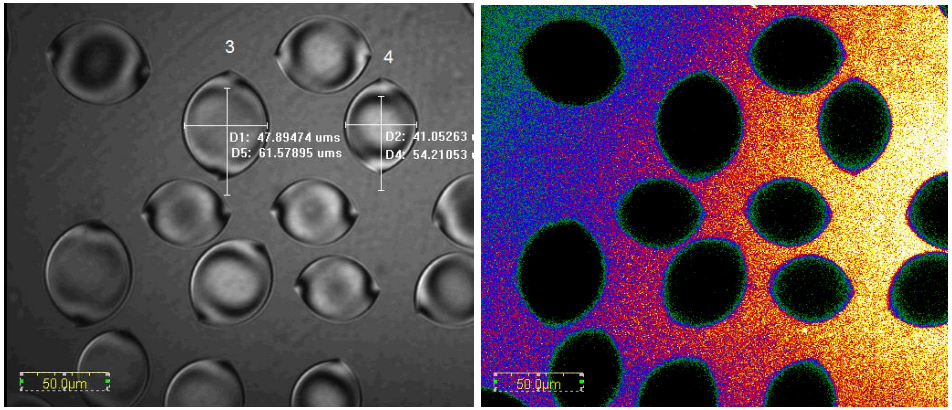
$$W \sim 10^{-5} \ \text{J/m}^2$$

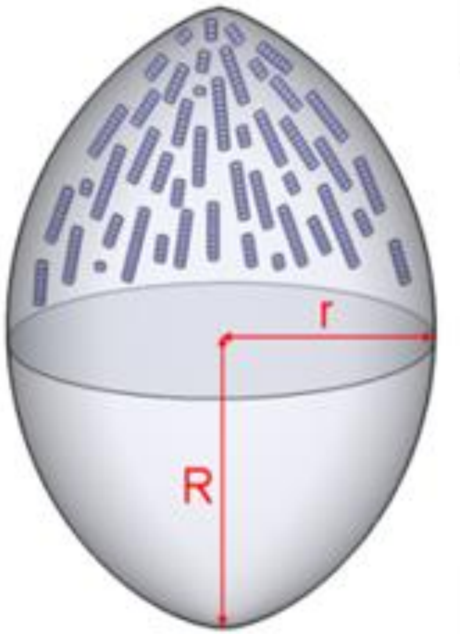
Model of surface tension: P. van der Schoot J. Phys. Chem B **103**, 8804 (1999)

Lyotropic I-N interface might be strongly anisotropic and be influenced by elasticity

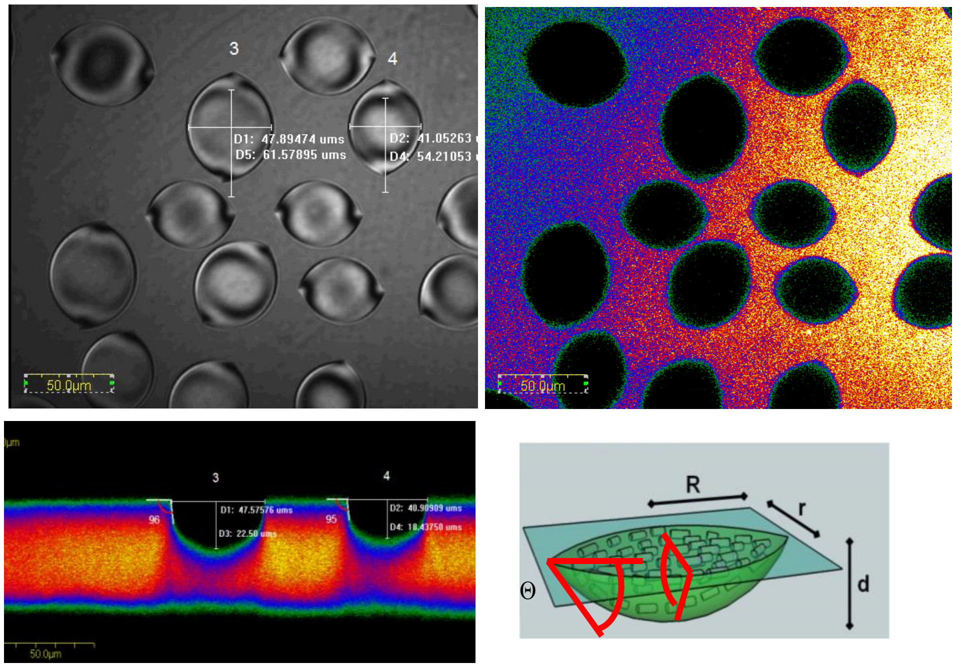
J. Bernal and I. Fankuchen, J. Gen. Physiol. (1941): tactoids as N nuclei in tobacco mosaic virus dispersions

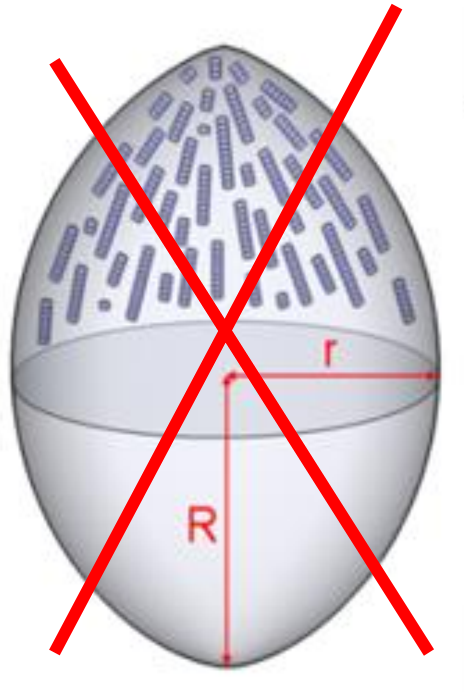
Droplets of chromonic N in isotropic melt (tactoids)





Surprise #1: Surface-located, not bulk

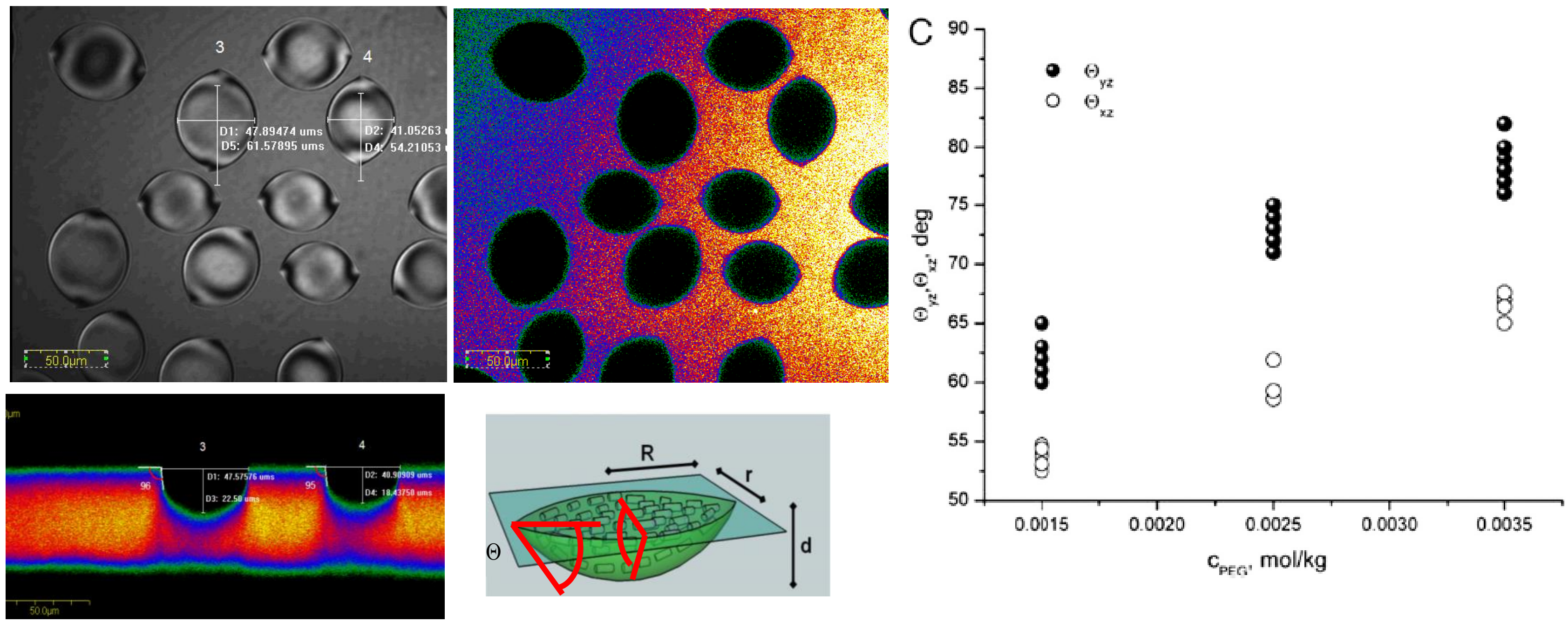




Vertical cross-section image; fluorescent confocal microscopy

Tortora et al., PNAS **108**, 5163 (2011)

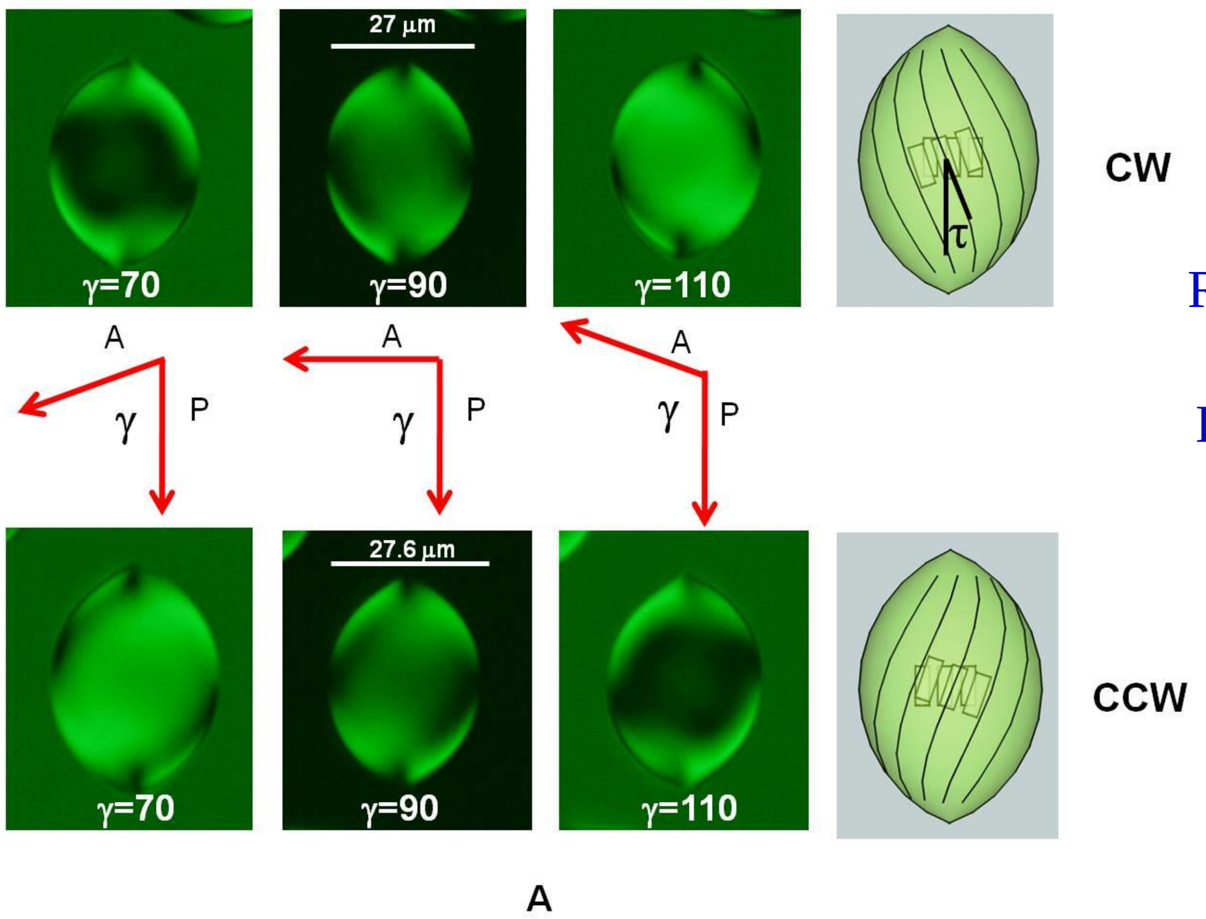
Surprise #2 (mild): Contact angle changes along the perimeter



Vertical cross-section image; fluorescent confocal microscopy

Tortora et al., PNAS **108**, 5163 (2011)

Surprise #3: Twist

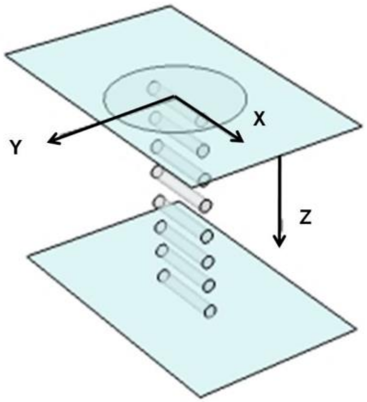


Right-twisted tactoid

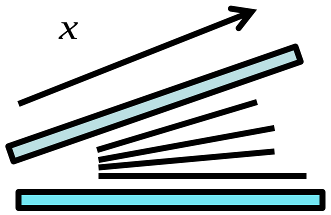
Left-twisted tactoid

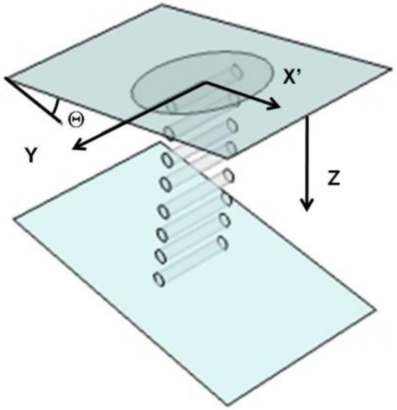
Tortora et al., PNAS **108**, 5163 (2011)

Mechanism: “Geometrical” anchoring+large K_1/K_2

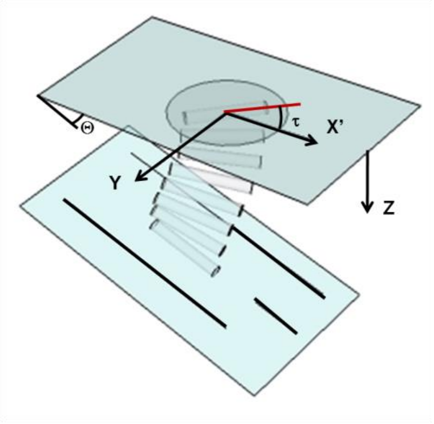


Nematic between two isotropic parallel boundaries: Degenerate in-plane orientation





One plate tilts: alignment perpendicular to the thickness gradient is the only one without distortions; other directions cause splay



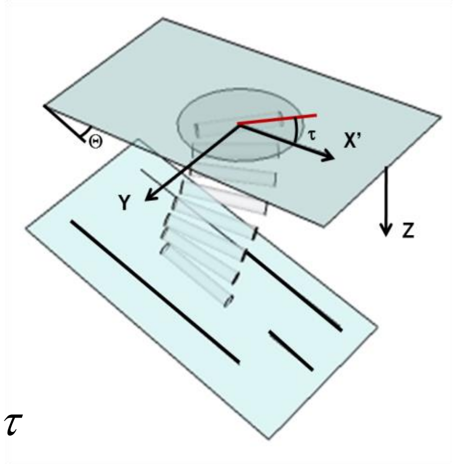
One plate tilts, the other sets “physical anchoring” say, along the long axis of the tactoid’s footprint: balance of twist and splay establishes a twist angle τ

Tortora et al., PNAS **108**, 5163 (2011)

Mechanism: "Geometrical" anchoring+large K_1/K_2

Elastic energy of a tilted element:

$$f \approx K_1\left(\frac{\partial\theta}{\partial z}\right)^2 + K_2\left(\frac{\partial\varphi}{\partial z}\right)^2$$



Bulk equilibrium:

$$\frac{\partial^2\theta}{\partial z^2} = 0; \frac{\partial^2\varphi}{\partial z^2} = 0$$

$$\theta(z=d) = -\arcsin(\sin\Theta\cos\tau) \approx \Theta\left(1-\tau^2/2\right); \;\; \varphi(z=d) \approx \tau$$

Twist deformations reduce the cost of splay deformations

$$F \approx \frac{K_1}{2d}\Theta^2\left(1-\tau^2\right) + \frac{K_2}{2d}\tau^2$$

Condition for the twist: $K_2 / K_1 < \Theta^2$

Easy to fulfill as in chromonics, $K_2 / K_1 \sim 0.1 - 0.03$

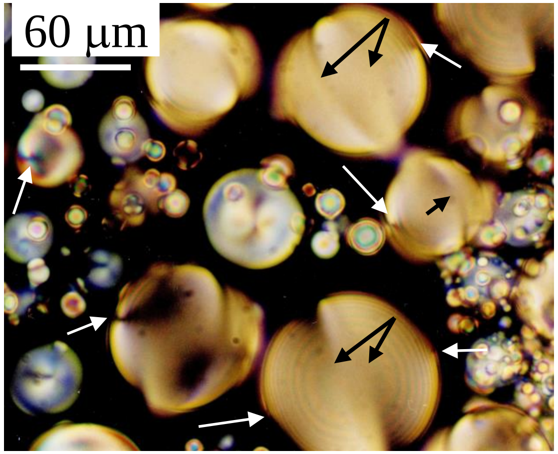
S. Zhou et al., Soft Matter **10**, 6571 (2014)

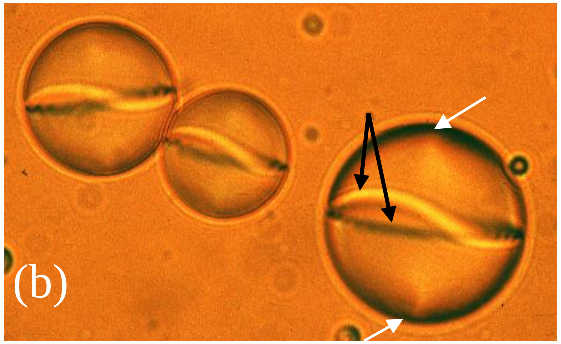
Twisted tactoids: An example of chiral symmetry braking in a molecularly non-chiral system; only spatial confinement and elastic anisotropy are needed to produce macroscopic chiral purity.

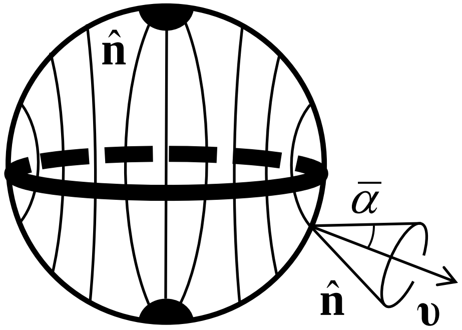
L. Tortora et al., PNAS 108, 5163 (2011)

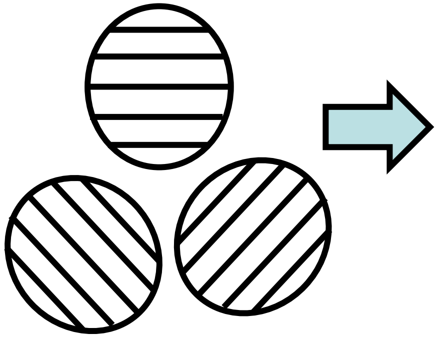
2D tactoids and Kibble mechanism

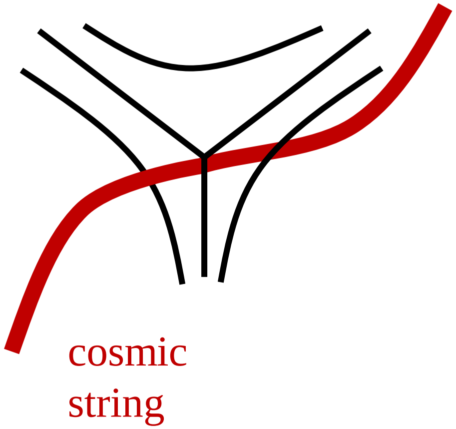
Isotropic-Nematic transition: Anchoring-induced topological defects in each and every nuclei of the N phase, as long as it is large enough, $R > K/W$





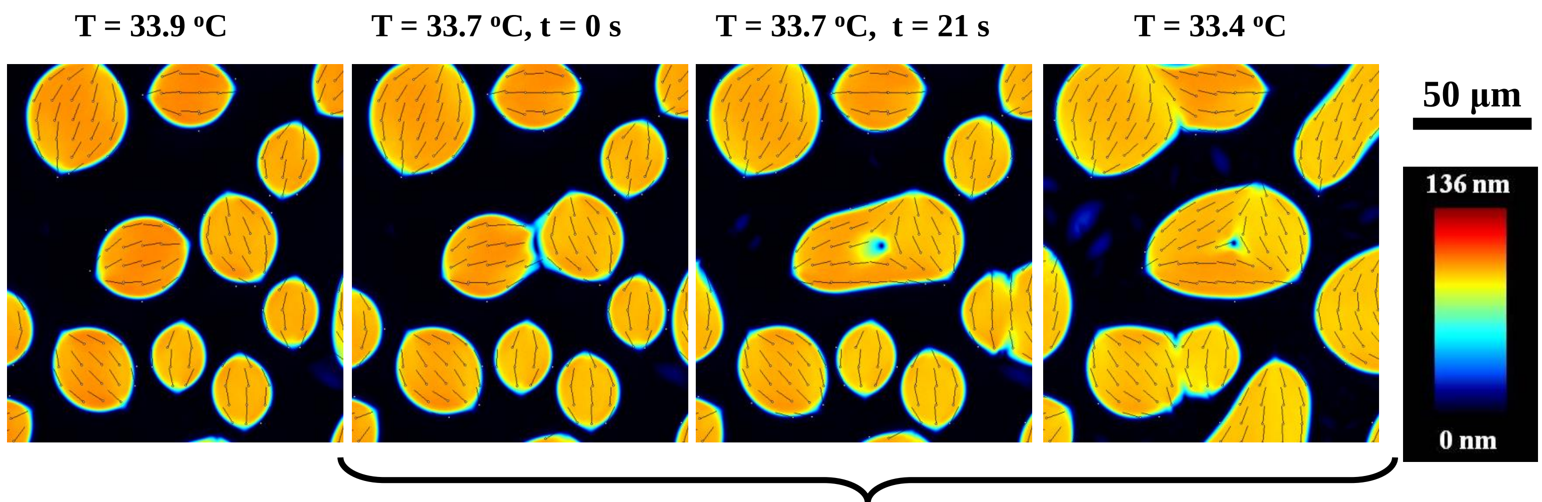






Kibble (1976) Model of formation of cosmic domains and strings

2D tactoids and Kibble mechanism in (LC)^2

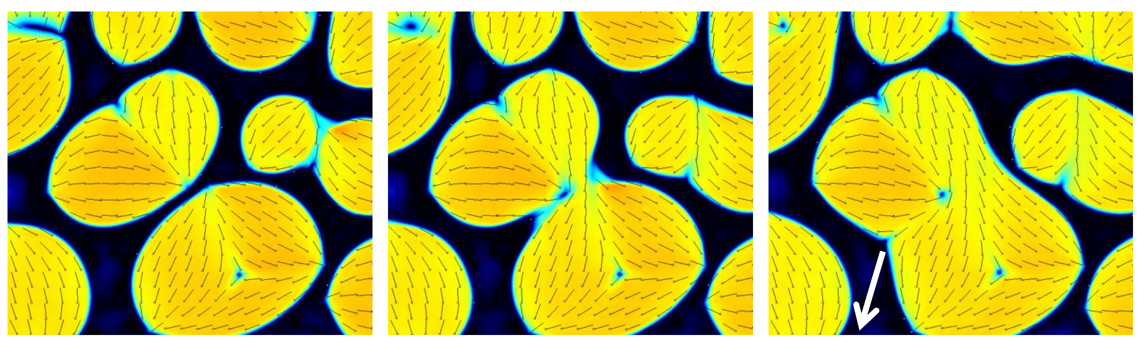


Anchoring-produced surface defects-boojums

Kibble-like production of disclinations as a result of tactoids merger

Conservation law for positive and negative cusps:

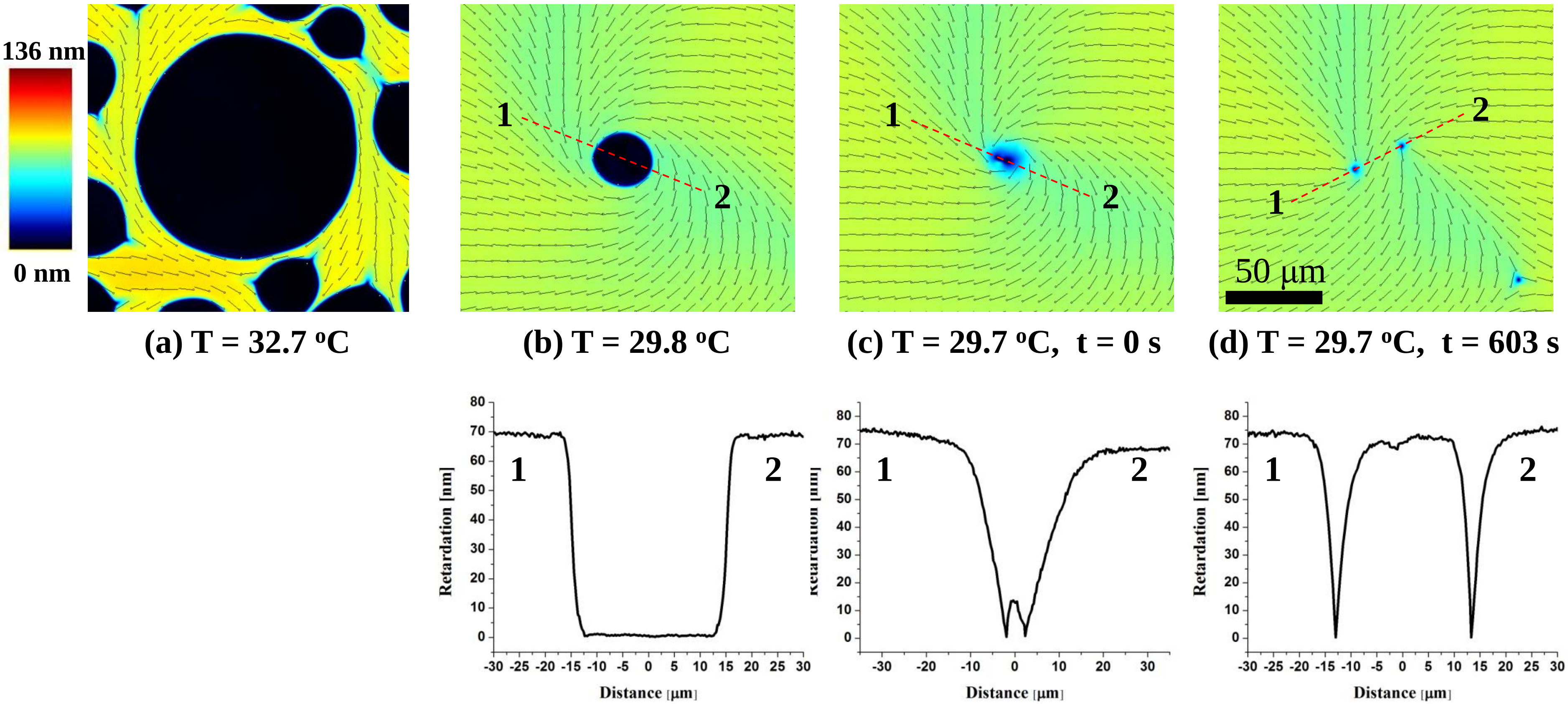
$$c^{+} - c^{-} = 2\left(1 - \sum_{k}^{n} m_k\right)$$



negative cusp

YK Kim et al., J Phys C ond Matt **25** 404202 (2013)

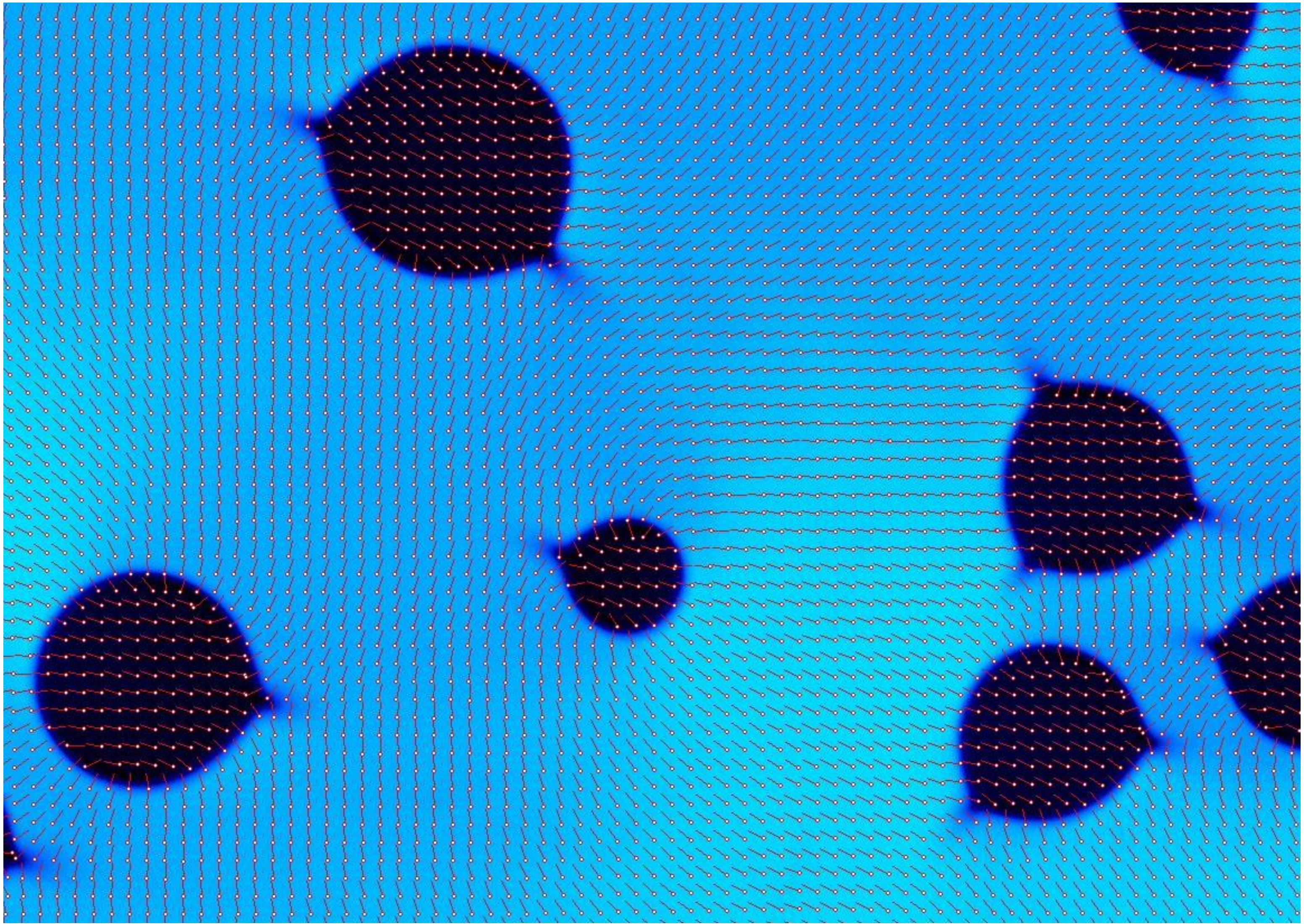
2D tactoids and k=1 disclinations



$$f_1 - f_{pair} = \frac{\pi K}{2} \ln \frac{L}{\sqrt{2} r_1} + \sqrt{2} \pi r_1 \sigma_0 \left(\sqrt{2} - 2 - w \right)$$

YK Kim et al., J Phys C ond Matt **25** 404202 (2013)

Drops of isotropic phase in N environment with distroted director: A balance of surface tension, anchoring, and elasticity



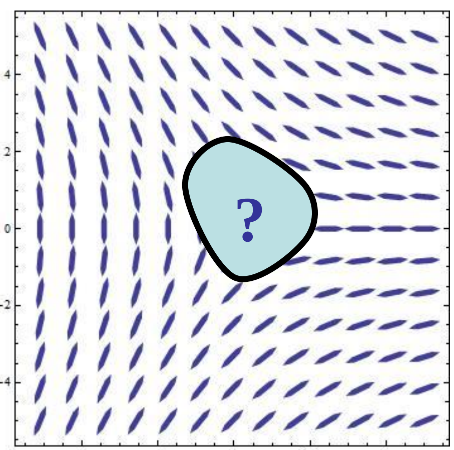
Equilibrium shape+director?

Difficult problem, requires to minimize both the anisotropic surface energy and elastic interior/exterior

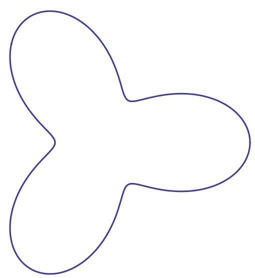
$$\iiint_V f_{FO}\left(\hat{\mathbf{n}}(\mathbf{r})\right)dV + \iint_S \left[\sigma + W\left(\hat{\mathbf{n}}\cdot\boldsymbol{\upsilon}\right)^2\right]dS \to \min$$

First step: Assume "infinite" elasticity (frozen director); then calculate the equilibrium shape of the I tactoid at the core, using the angular dependence of the surface tension for each disclination

$$\sigma(\theta) = \sigma_0\left\{1 + w\cos^2\left[(k-1)\theta\right]\right\}$$

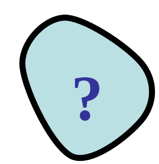


k = -1/2



$w = 2$

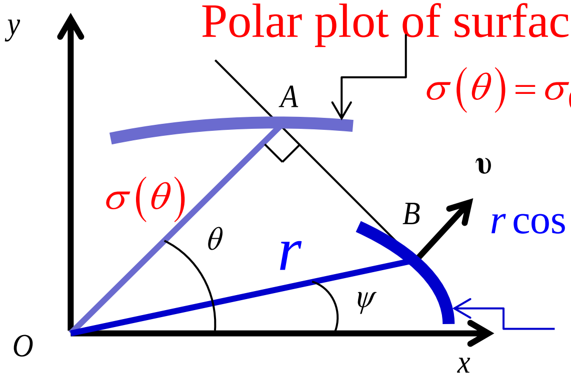
Polar plot of surface tension of an isotropic island inside a nematic region representing a disclination of -1/2 strength;
Problem: Find the shape that minimizes the anisotropic surface tension



YK Kim et al., J Phys C ond Matt **25** 404202 (2013)

Equilibrium shape by Wulff construction for distorted director

Wulff construction for crystals:
L. Landau, E. Lifshits, Statistical Physics (1964)



$$\sigma(\theta)=\sigma_0\left\{1+w\cos^2\left[(k-1)\theta\right]\right\}$$

$$r\cos(\psi-\theta)=\sigma(\theta) \qquad \frac{\partial\left[r\cos(\psi-\theta)=\sigma(\theta)\right]}{\partial\theta}\Rightarrow r\sin(\psi-\theta)=\sigma'(\theta)$$

$$r=\sqrt{\sigma^2+\sigma'^2};\ \psi=\theta+\arctan\frac{\sigma}{\sigma'}$$

Radius of curvature: $R=\sqrt{r'^2+r^2\psi'^2}=\sigma+\sigma''$

Round shape, all orientations of I-N interface: $\sigma+\sigma''>0$

Missing orientations and cusps: $\sigma+\sigma''<0$

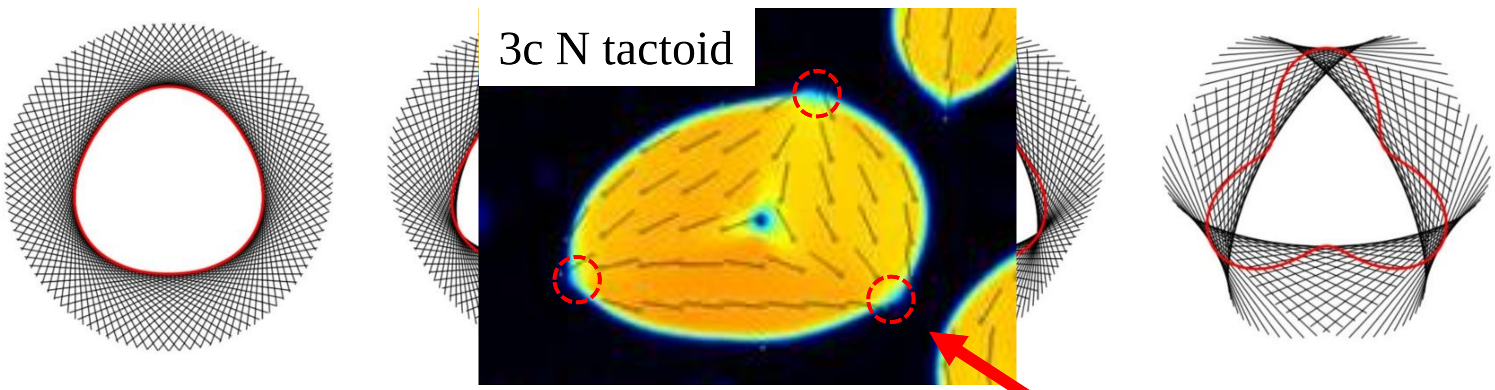
$$1+w\left[1-4(k-1)^2\right]\cos^2(k-1)\psi+2(k-1)^2w<0$$

YK Kim et al., J Phys C ond Matt **25** 404202 (2013)

Wulff construction by Mathematica

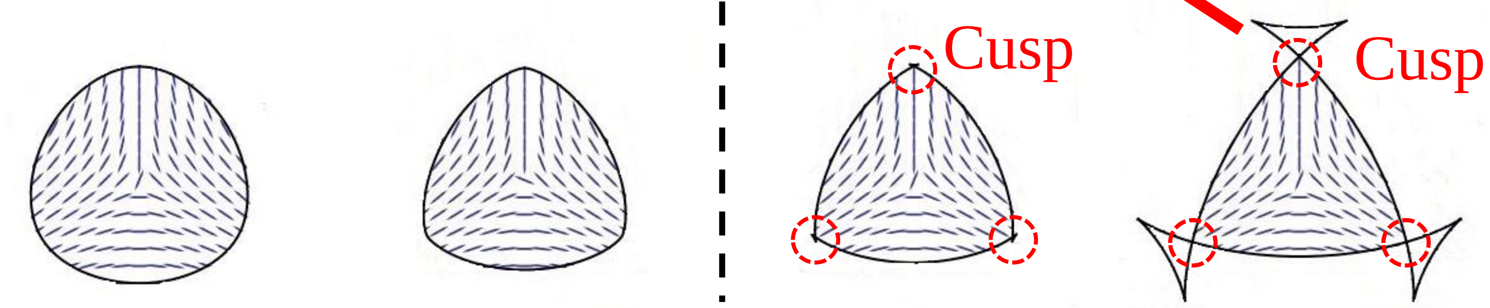
Draw the tangent lines at each point in a polar plot of σ (θ)

Wulff Construction



The interior envelope describes the shape in equilibrium

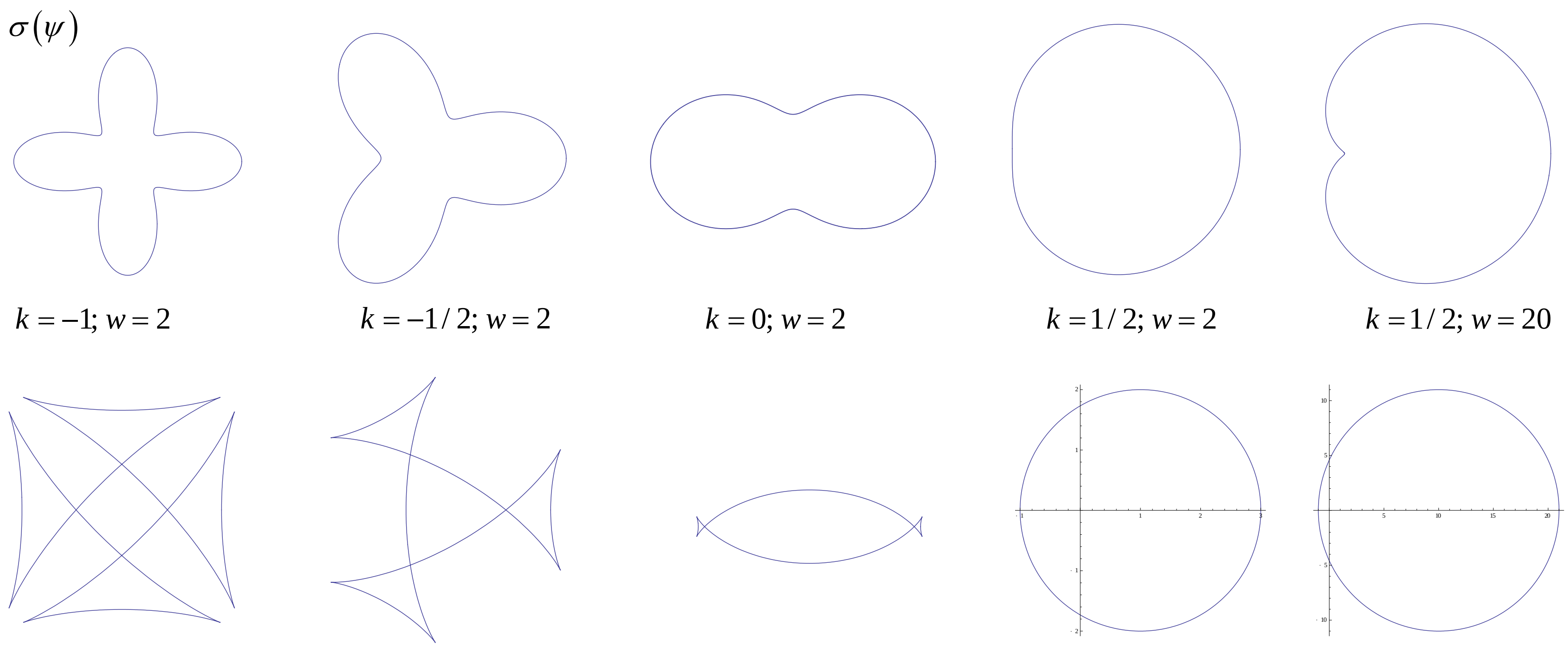
Shape of Domain



w_c=2/7

YK Kim et al., J Phys C ond Matt **25** 404202 (2013)

Equilibrium shape by Wulff construction for distorted director



Missing orientations and cusps: $$1+w\left[1-4(k-1)^2\right]\cos^2(k-1)\psi+2(k-1)^2 w<0$$

Never the case for k=1/2 and k=1; for k=0, w_c=1; for k=-1/2, w_c=2/7; for k=-1, w_c=1/7

YK Kim et al., J Phys C ond Matt **25** 404202 (2013)

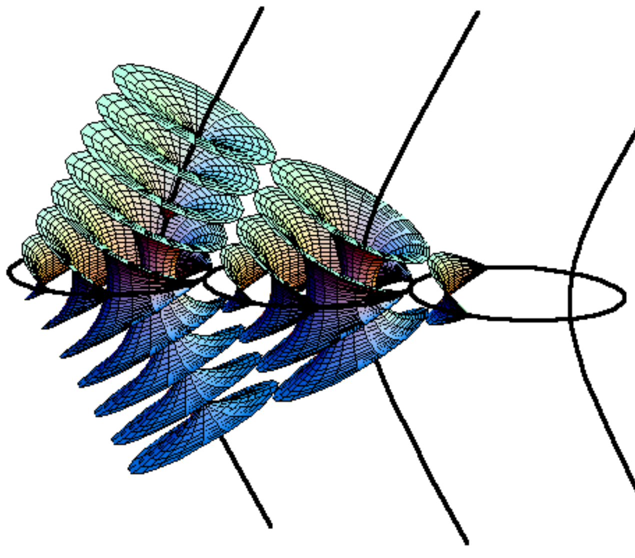
Summary/What have you learned

- Disclinations: Frank model, line energy ~ln of size, $\sim k^2$
- Integer disclinations: Escape into the third dimension
- Semi-integer: Stable
- Homotopy classification: A natural language to describe defects in any medium, LCs and superfluid He-3 including
- Surface anchoring: Controls topology and energy of defects;
- Defects occur as equilibrium features in LC droplets, …Including the nuclei during the phase transition from the isotropic phase
- Cholesteric: Dirac monopoles
- Chromonic droplets: Spontaneous chiral symmetry broken; shape is strongly dependent on director deformations, the problem of full energy (elastic+surface tension+anchoring) minimization not solved yet

Liquid crystals: Lecture 2.2
Lamellar phases

Oleg D. Lavrentovich

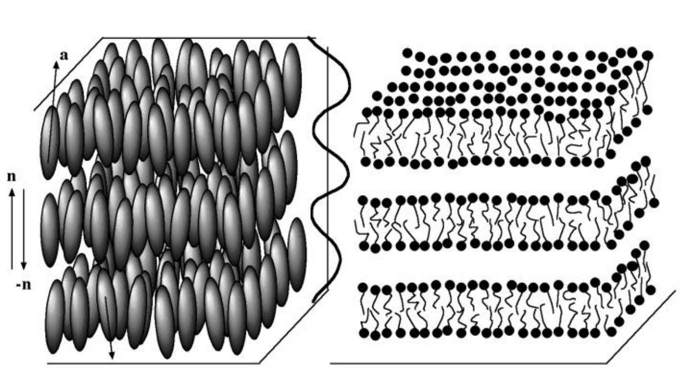
Support: NSF



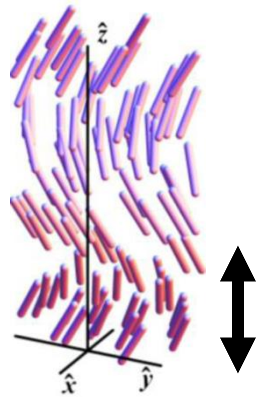
Boulder School for Condensed Matter and Materials Physics,
Soft Matter In and Out of Equilibrium,
6-31 July, 2015

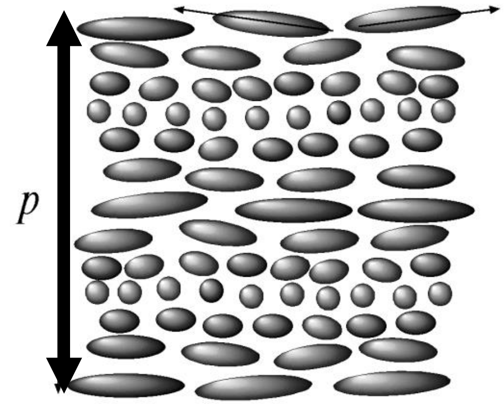
LCI KENT STATE UNIVERSITY

Lamellar phases



(a) (b)





1-10 nm

>0.1 μm

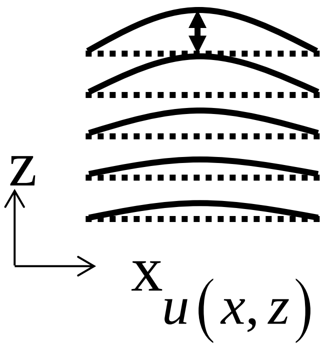
Smectics A (thermotropic)

Smectic A (lyotropic)

Twist-bend nematic

Cholesteric (chiral N)

Elasticity of lamellar phase; 1D translational order, weak distortions



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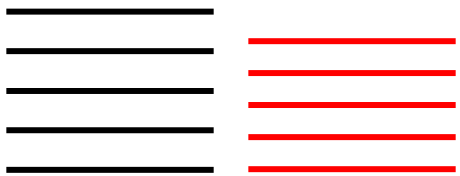
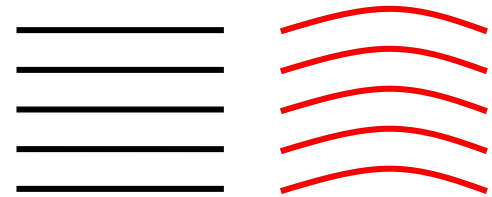


$$\frac{\partial u}{\partial z}$$

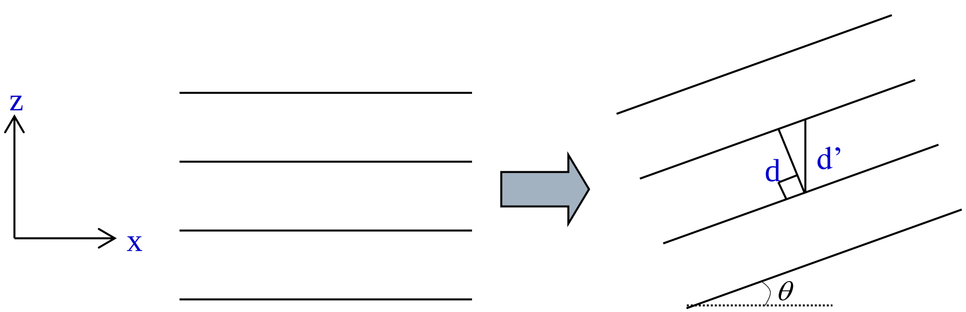
Curvature:



$$\left(\frac{\partial^2 u}{\partial x^2}\right)$$

$$f = \frac{1}{2}B\left\{\frac{\partial u}{\partial z} - \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2\right\}^2 + \frac{1}{2}K\left(\frac{\partial^2 u}{\partial x^2}\right)^2$$

Correction to make the model invariant w.r.t. uniform rotations:



$$\frac{\partial u}{\partial z} - \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2$$

$$d' = d / \cos\theta$$

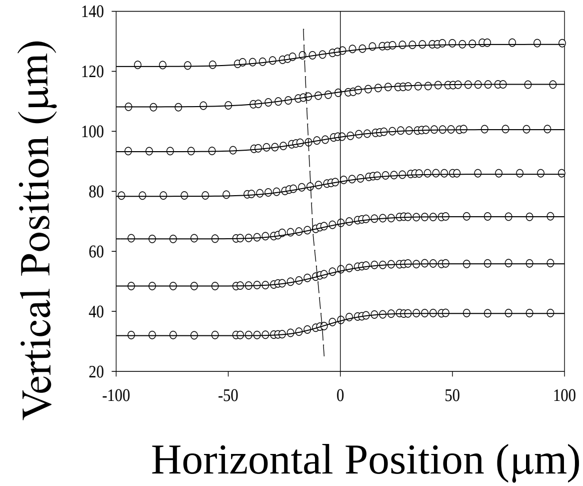
Material length $\lambda = \sqrt{\frac{K}{B}} \sim period\,?$

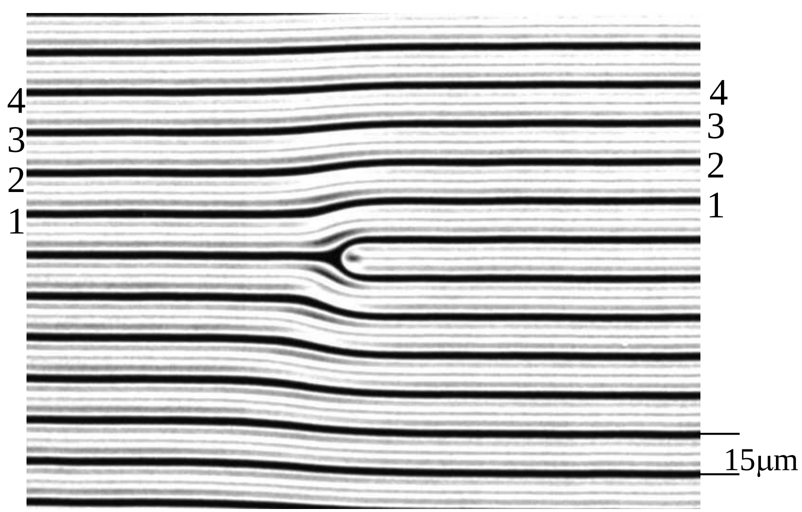
Elasticity of Smectics: Dislocation

$$u(x,y) = 2\lambda \ln\left\{1 + \frac{exp(b/4\lambda) - 1}{2}\left[1 + erf\left(\frac{x}{2\sqrt{\lambda z}}\right)\right]\right\}$$

Brener and Marchenko PRE'99

By fitting $u(x,z)$, one can measure $\lambda = \sqrt{\frac{K}{B}}$





$$period = 14.9\ \mu m$$

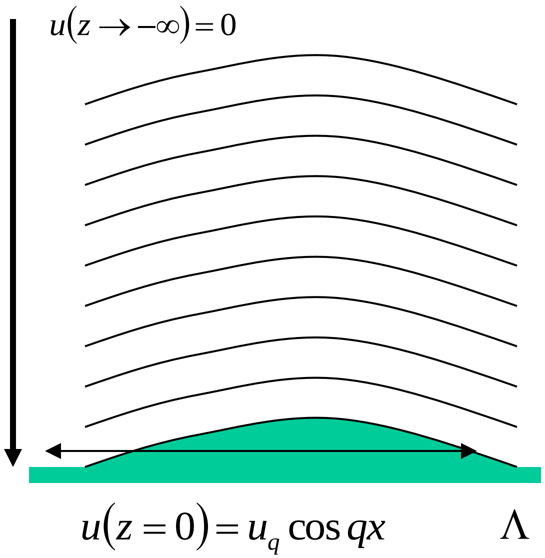
$$\lambda = 2.7\ \mu m$$

$$\lambda \approx 0.2 \times period$$

T.Ishikawa, ODL *Phys Rev E* (1999)

Long range effect of layers deformations

$u(x,z)$ E-L equation $K\dfrac{\partial^4 u}{\partial x^4} - B\dfrac{\partial^2 u}{\partial z^2} = 0$



Look for solution of the type: $u = u_q \cos qx \exp\left(\dfrac{z}{L}\right)$

$$u(z=0) = u_q \cos qx \qquad u(z\to -\infty) = 0$$

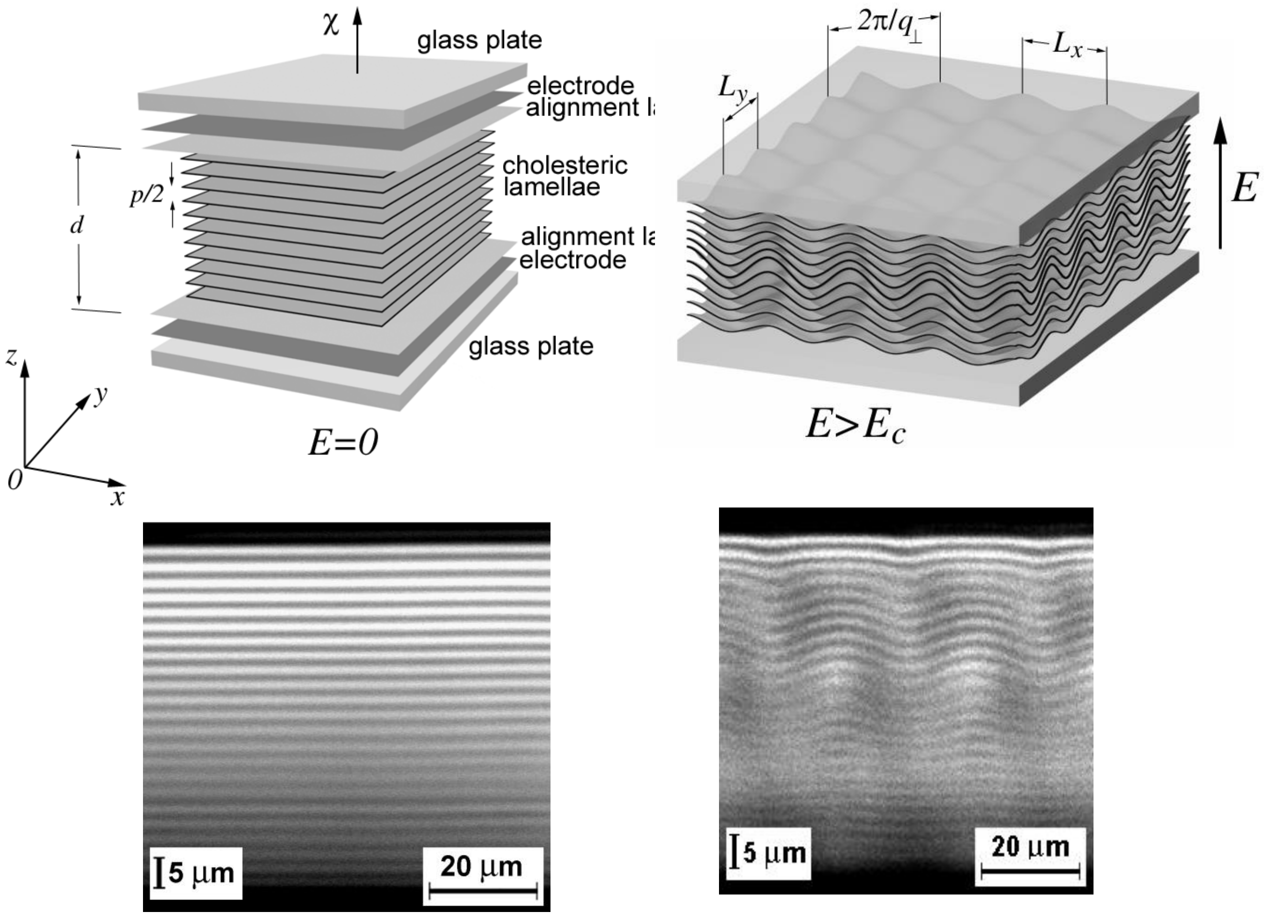
$$K_1 q^4 - B\frac{1}{L^2} = 0 \quad \Rightarrow \quad L = \frac{1}{q^2}\sqrt{\frac{B}{K}} \propto \frac{\Lambda^2}{\lambda}$$

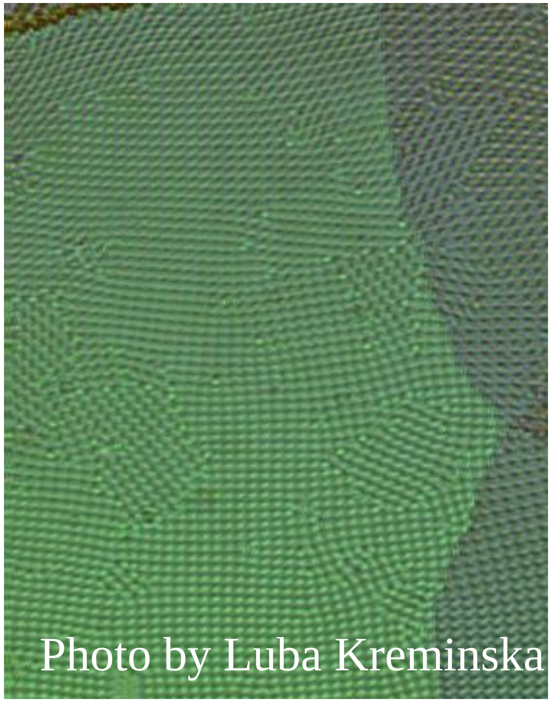
$$L == \frac{\text{macroscopic scale}^2}{\text{microscale}} = \Lambda\left(\frac{\Lambda}{\lambda}\right) >> \Lambda$$

Saint-Venaint principle $L \sim \Lambda$ is not applicable to SmA materials;
Smectics: A good model of "la Princesse sur la graine de pois"
If a pea is 1 mm, layer thickness 10 nm, then the pea is felt over 100 m!

G. Durand (1968)

Undulations in Cholesteric caused by E field





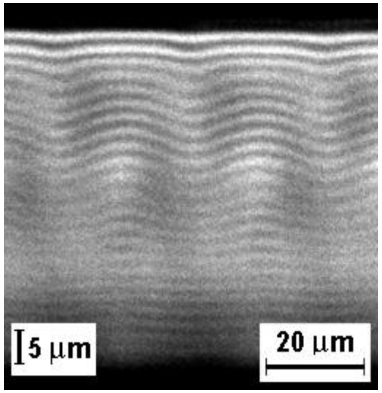
Senyuk et al PRE 74, 011712 (2006)

Undulations in Cholesteric (2D)

$$f = \frac{1}{2}K\left(\frac{\partial^2 u}{\partial x^2}\right)^2 + \frac{1}{2}B\left\{\frac{\partial u}{\partial z} - \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2\right\}^2 - \frac{1}{2}\varepsilon_0\varepsilon_a E^2\left(\frac{\partial u}{\partial x}\right)^2 \qquad f_{anchoring} = \frac{1}{2}W\left[\left(\frac{\partial u}{\partial x}\right)^2\right]_{z=0,d}$$

$$u(x,z) = u_0\varphi(z)\sin q_x x \quad \Rightarrow \quad \begin{cases} B\phi'' - q_x^2\left(Kq_x^2 - \varepsilon_0\varepsilon_a E^2\right)\phi = 0 \\ B\varphi' \pm Wq_x^2\varphi = 0\Big|_{z=\pm a/2} \end{cases}$$

$$\varphi = const \times \cos q_z z$$

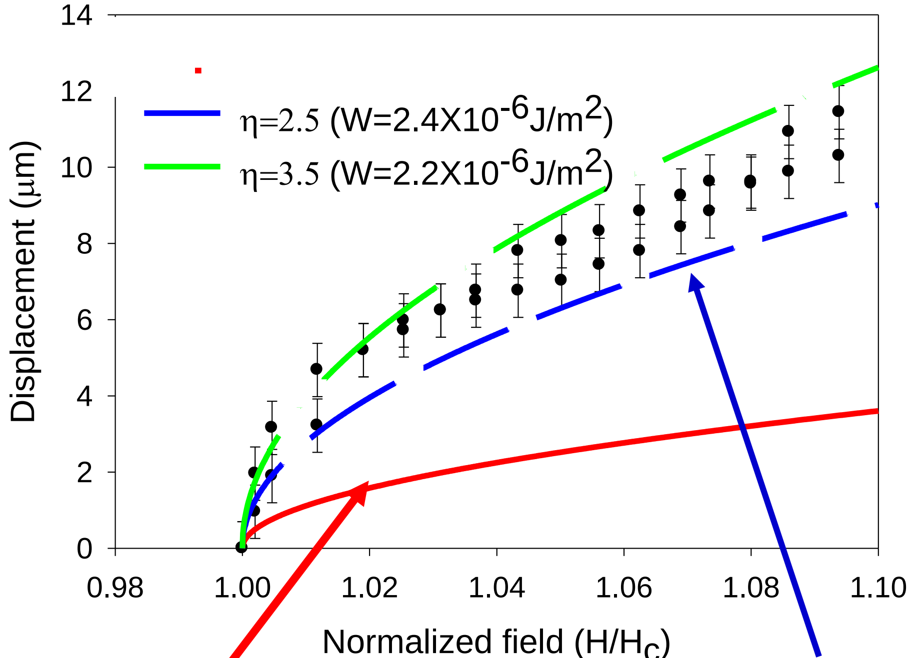


$$\begin{cases} q_z = q_x\sqrt{\kappa - \lambda^2 q_x^2} \\ W = \dfrac{B\sqrt{\kappa - \lambda^2 q_x^2}}{q_x \cot\left(\dfrac{dq_x}{2}\sqrt{\kappa - \lambda^2 q_x^2}\right)} \end{cases} \qquad \kappa = \varepsilon_0\varepsilon_a E^2 / B \quad \Rightarrow \quad E_c \approx \sqrt{\frac{2\pi K}{\varepsilon_0\varepsilon_a \lambda a}}$$

$$u_0(W \to \infty) = \frac{8\lambda}{3}\sqrt{\frac{E^2}{E_c^2} - 1} \qquad u_0 = \frac{8\lambda\eta}{3}\sqrt{\frac{E^2}{E_c^2} - 1}$$

3D version: Senyuk et al PRE 74, 011712 (2006)

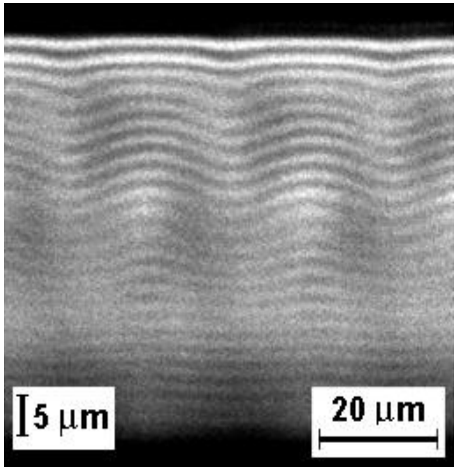
Undulations in Cholesteric (2D)



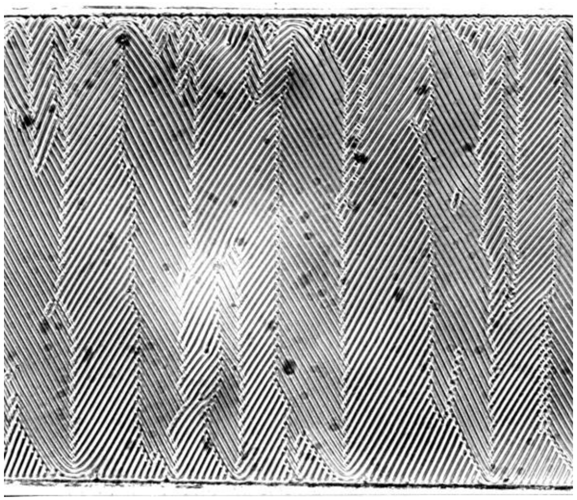
$$u_0\left(W \to \infty\right) = \frac{8\lambda}{3}\sqrt{\frac{E^2}{E_c^2}-1} \qquad u_0 = \frac{8\lambda\eta}{3}\sqrt{\frac{E^2}{E_c^2}-1}$$

Ishikawa et al PRE 63, 030501(R) (2001)

Undulations in Cholesteric above threshold

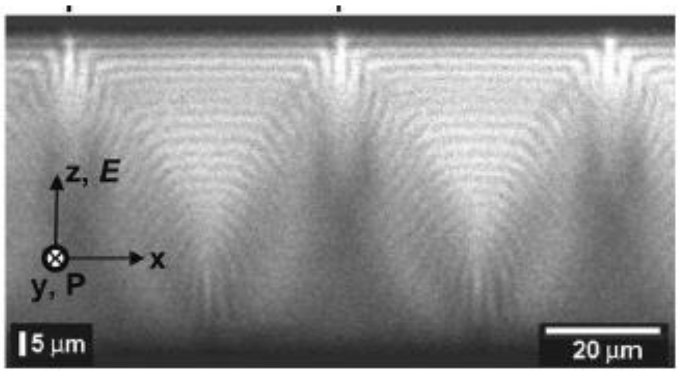


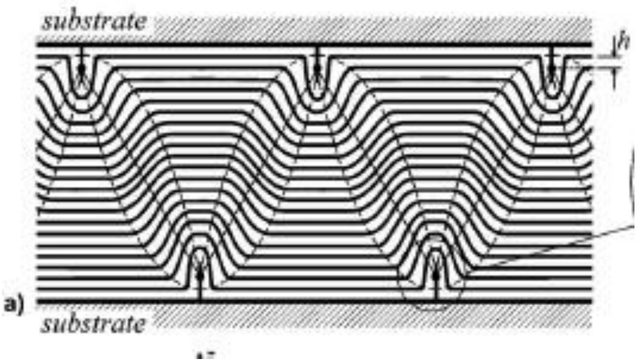
Immediately above the threshold



Well above the threshold, 2D cell; broken surface anchoring

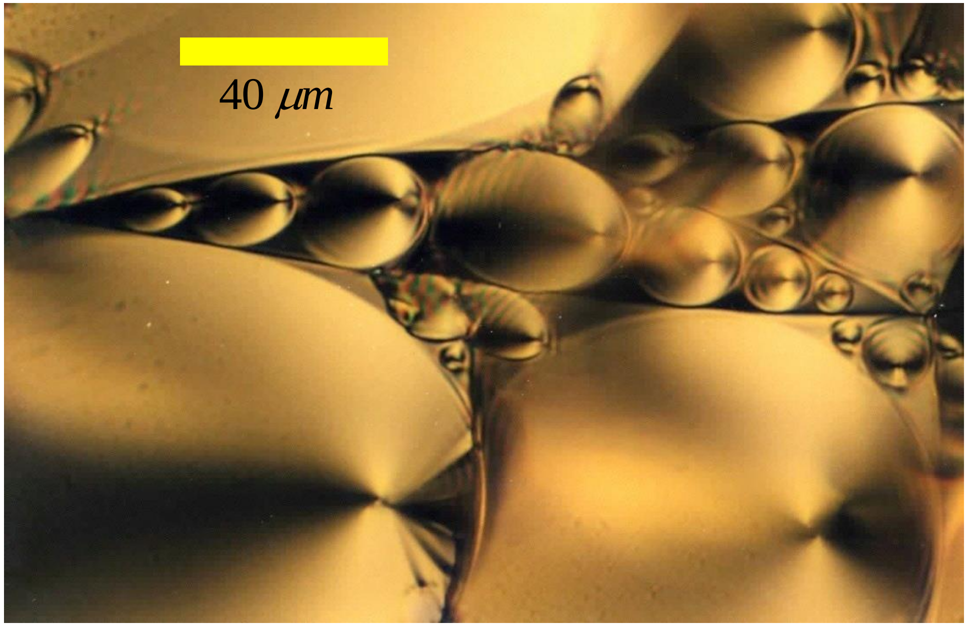
Well above the threshold, 3D,
Anchoring takes over, forcing parabolic domain walls

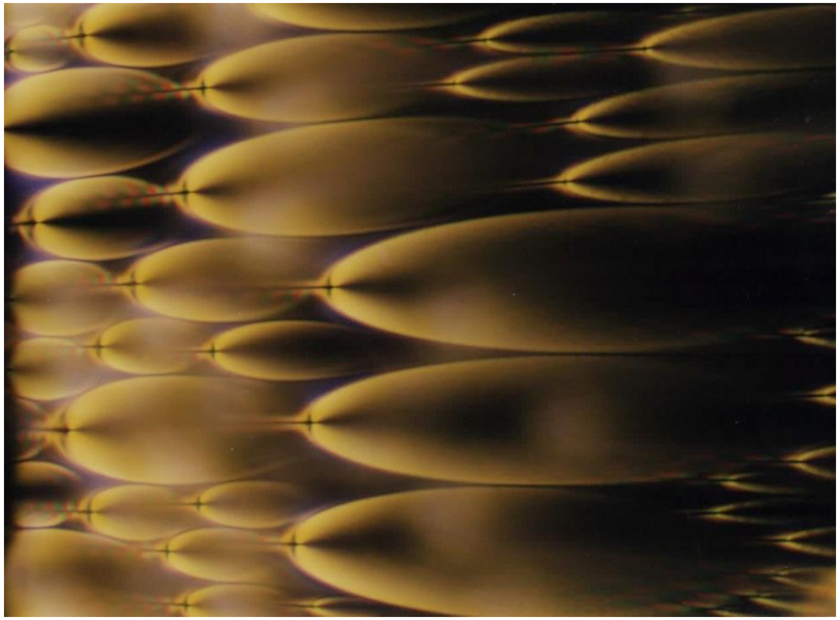


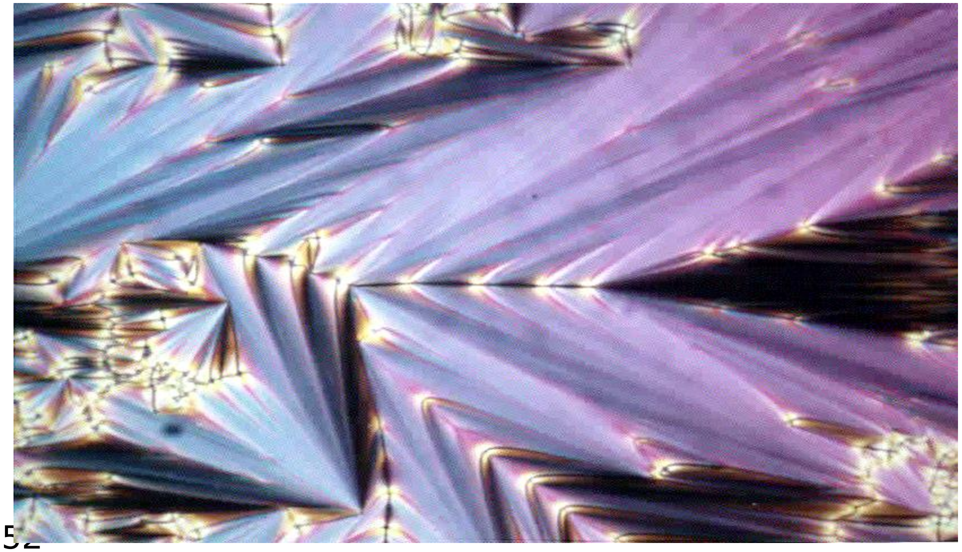


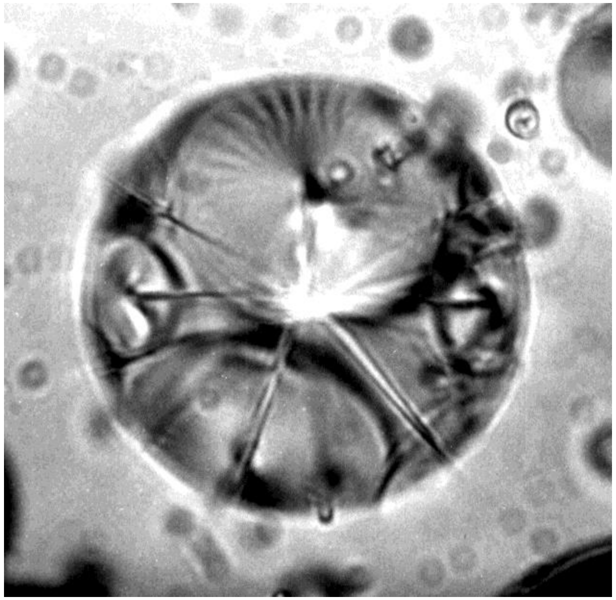
Senyuk et al PRE 74, 011712 (2006)

Strong perturbations: Focal conic domains



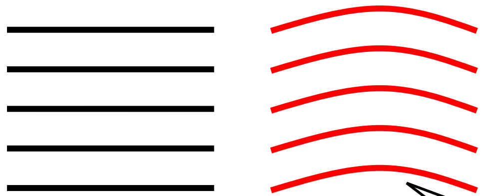




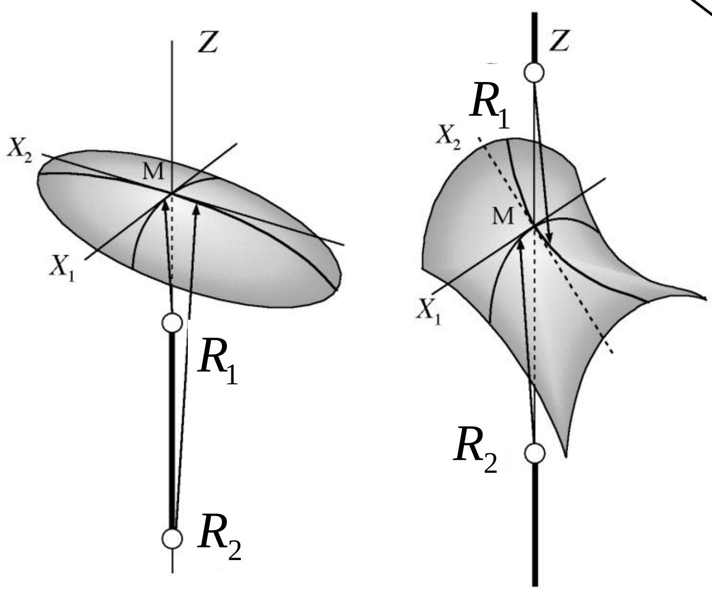


Elasticity of Smectics: Strong distortions

Curvature:



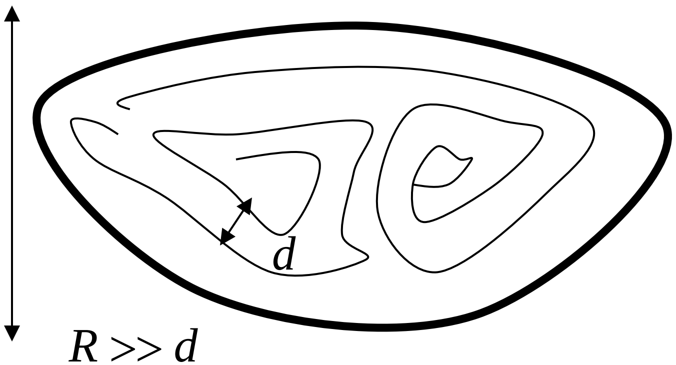
Compression/Dilation:



principal radii

$$f = \tfrac{1}{2}K\left(\frac{1}{R_1}+\frac{1}{R_2}\right)^2 + \overline{K}\,\frac{1}{R_1R_2} + \tfrac{1}{2}B\left(\frac{d}{d_0}-1\right)^2$$

Elasticity of Smectics



$R >> d$

$$f = f_{curv} + \cancel{f_{dilat}} = \tfrac{1}{2} K \left(\frac{1}{R_1} + \frac{1}{R_2} \right)^2 + \bar{K} \left(\frac{1}{R_1 R_2} \right) + \tfrac{1}{2} B \cancel{\left(\frac{d - d_0}{d_0} \right)}^2$$

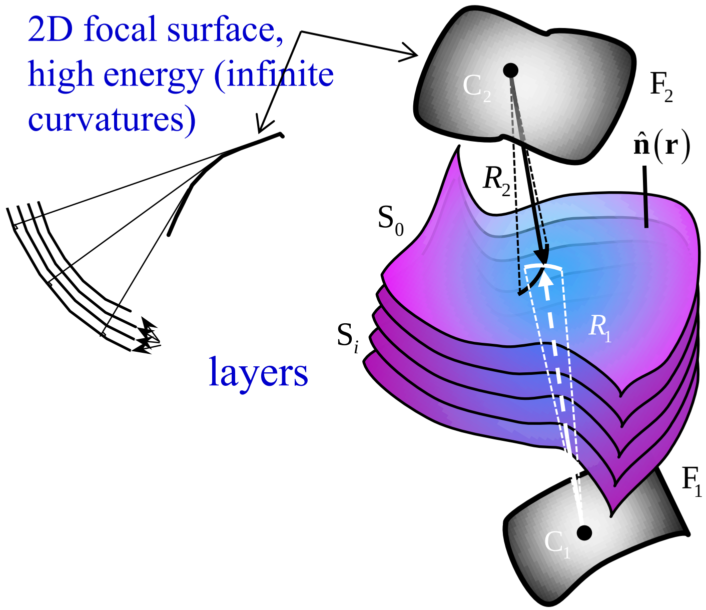
$$\lambda = \sqrt{\frac{K}{B}} \sim d_0$$

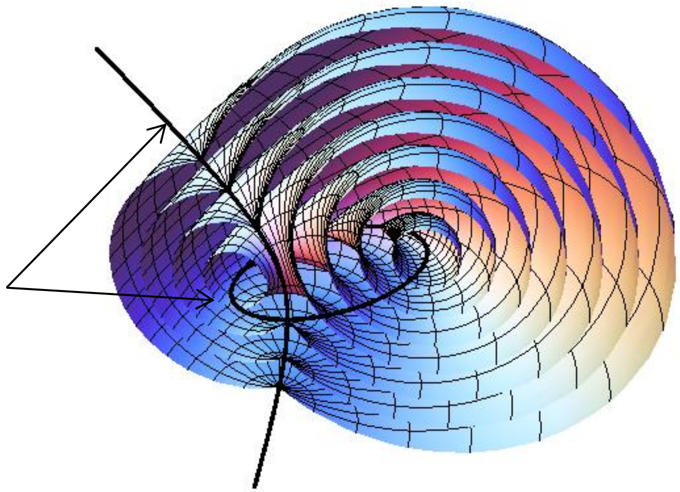
$$\frac{F_{curv}}{F_{dilat}} \sim \frac{KR}{BR^3} \sim \left(\frac{\lambda}{R} \right)^2 << 1 \quad \text{if } R >> \lambda$$

$$\Downarrow$$

At large scales of deformations, the curved layers are equidistant

Curved smectic layers: Dupin Cyclides



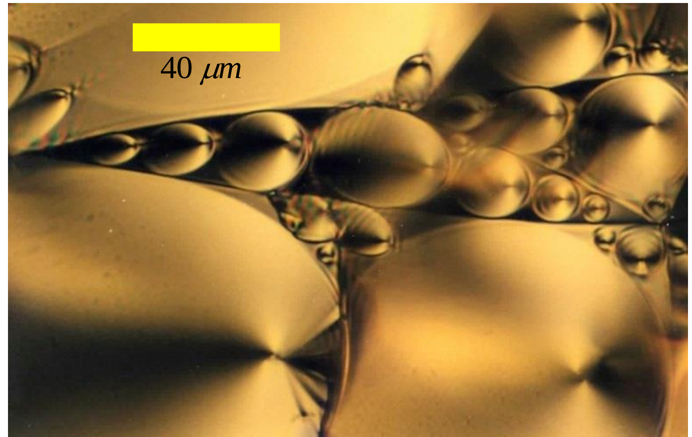


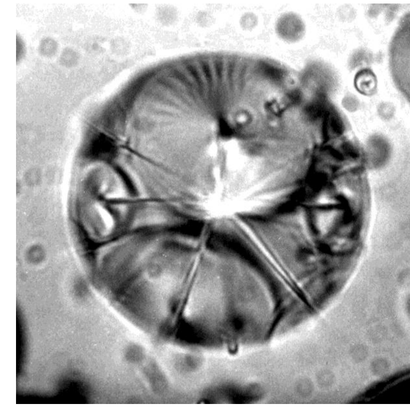
To reduce the energy, focal surfaces in SmA
degenerate into 1D focal lines, that can be only of three types:
(a) circle and straight line, or
(b) confocal ellipse and hyperbola,
(c) two confocal parabolae
producing a Focal Conic Domain (FCD); the smectic layers are Dupin cyclides

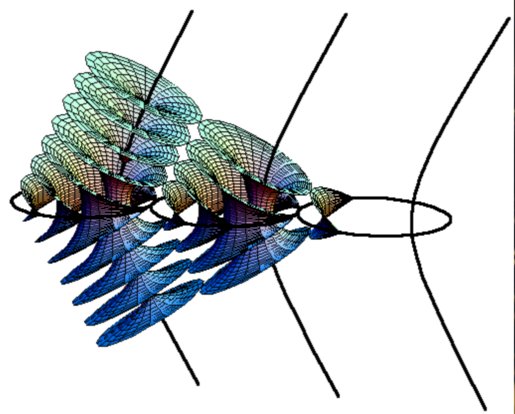
C.P. Dupin, Applications de Géométrie (Paris, 1822)
J. Maxwell, On the cyclide, Q. J. Pure Appl. Math **9**, 111 (1868)

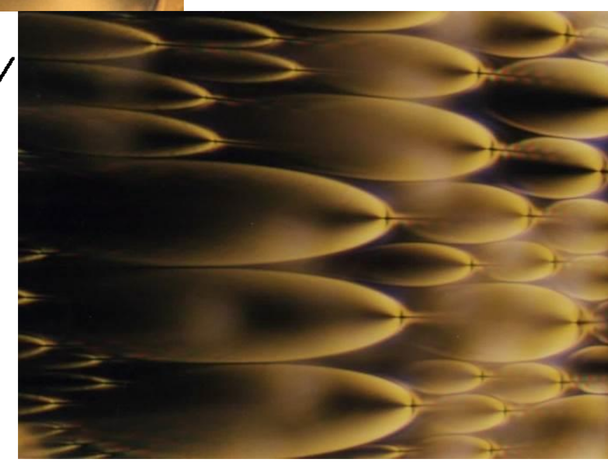
Smectics and focal conic domains

1910, G. Friedel, F. Grandjean:
Deciphered SmA structure
from observation of
focal conic domains;
X-ray was not available

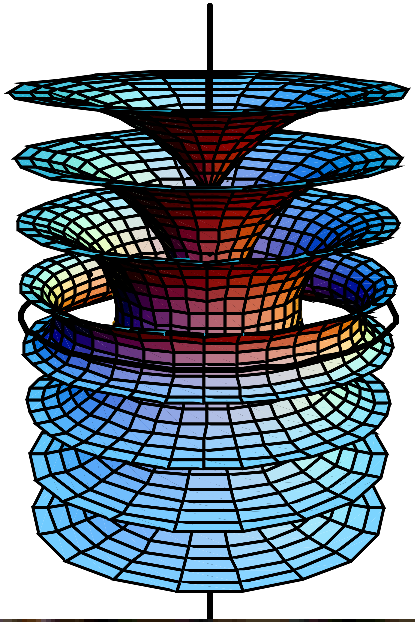


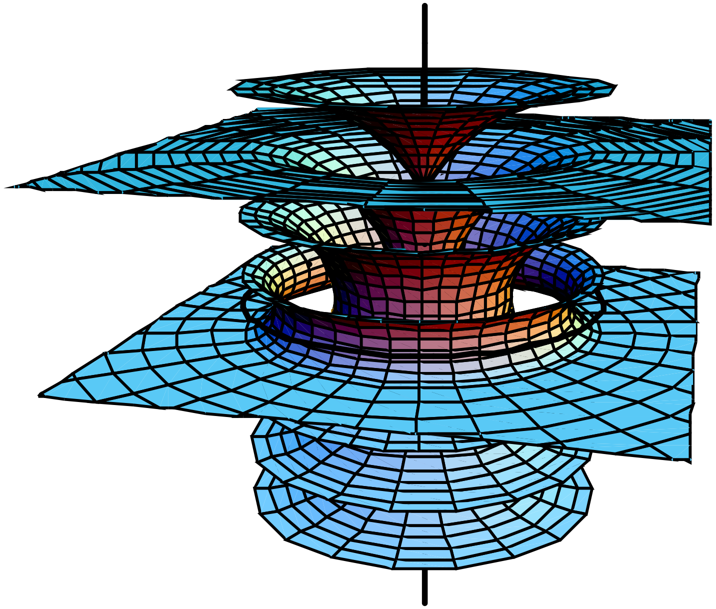


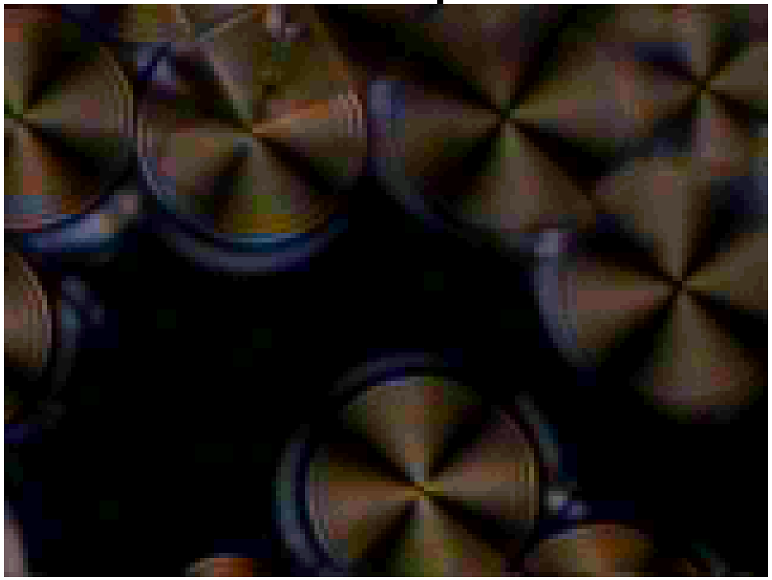




Toroidal Focal Conic Domains



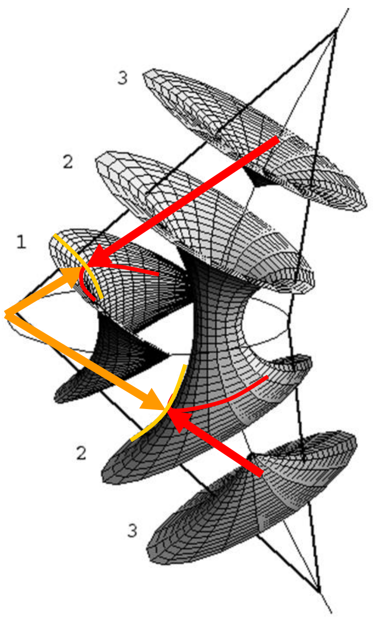




Smoothly fits into the system of parallel layers

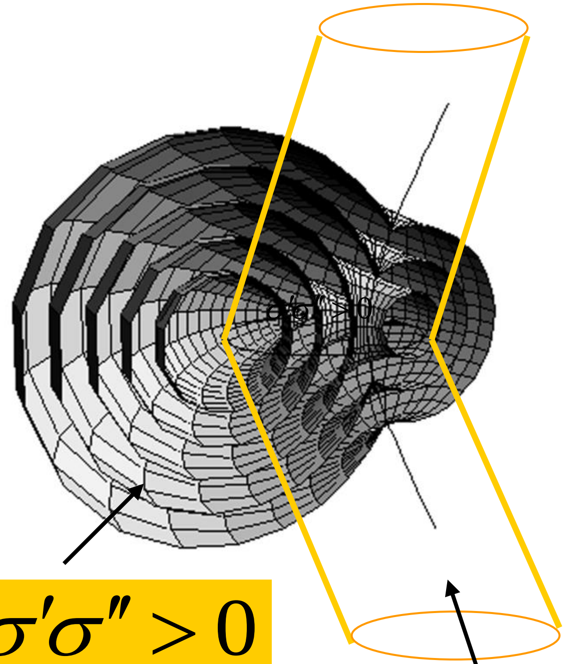
Classification of FCDs by Gaussian curvature

FCD-I



$\sigma'\sigma'' < 0$

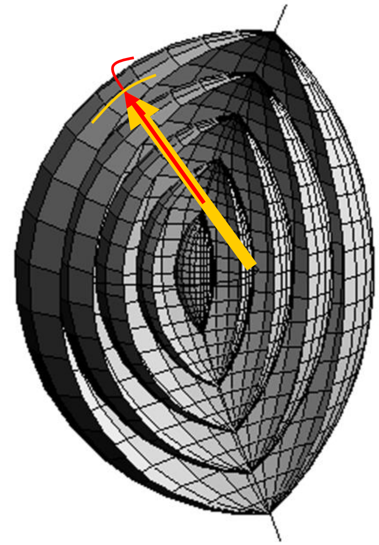
FCD-III



$\sigma'\sigma'' > 0$

$\sigma'\sigma'' < 0$

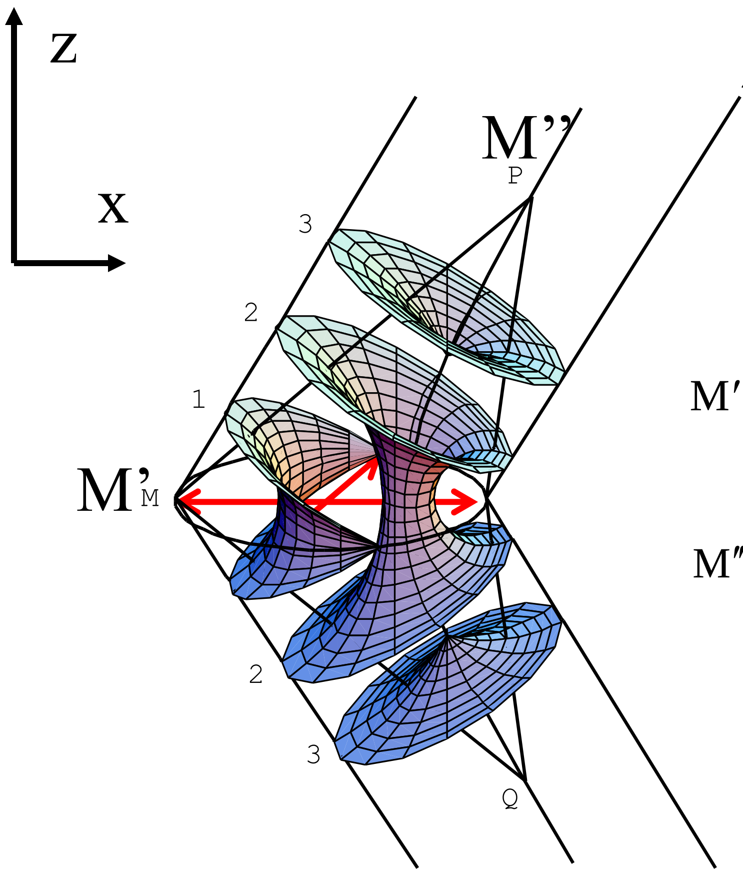
FCD-II



$\sigma'\sigma'' > 0$

How to describe the FCD analytically?

Curvilinear coordinates *r*, *u*, *v*



Ellipse $z = 0, \quad \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$

Hyperbola $y = 0, \quad \frac{x^2}{a^2 - b^2} - \frac{z^2}{b^2} = 1$

Parametrization of conics with coordinates u and v defined within the cyclides

$$M' \begin{cases} x' = a\cos u, \\ y' = b\sin u, \end{cases} \qquad 0 \le u \le 2\pi,$$

$$M'' \begin{cases} x'' = \pm c\cosh v \\ z'' = b\sinh u \end{cases} \qquad -\infty \le v < \infty,$$

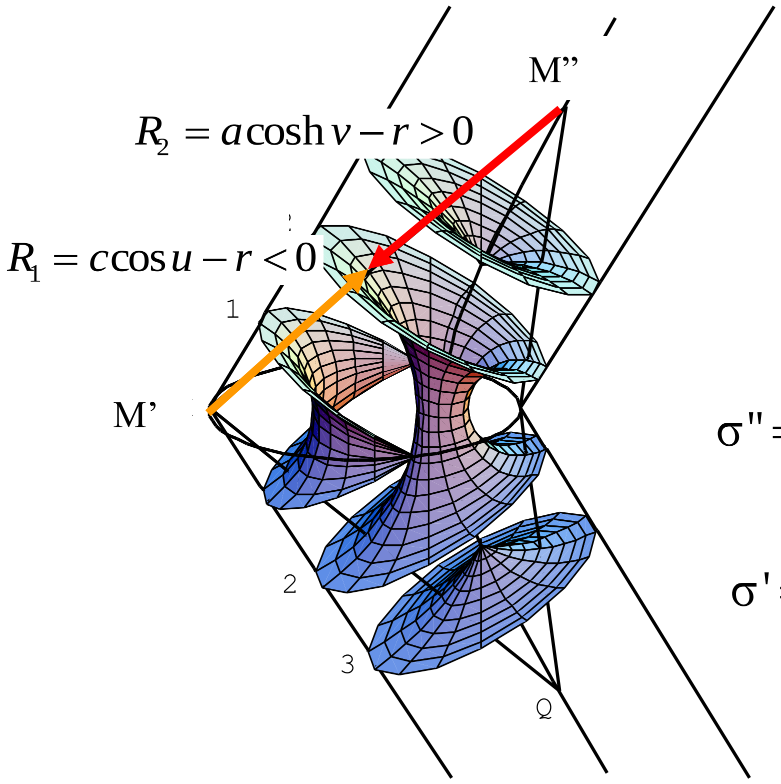
$$c^2 = a^2 - b^2$$

$$\mathrm{M''M'} = a\cosh v - c\cos u$$

Curvature energy functional

Let us introduce the third coordinate r that "counts" the layers

$$\mathrm{M''M'} = a\cosh v - c\cos u = R_2 - R_1 = a\cosh v - r + r - c\cos u$$



$$R_2 = a\cosh v - r > 0 \qquad R_1 = c\cos u - r < 0$$

$$F_{curv} = \int_{FCD} \left[\tfrac{1}{2} K \left(\frac{1}{R_1} + \frac{1}{R_2} \right)^2 + \bar{K} \frac{1}{R_1 R_2} \right] dV$$

$$\sigma'' = \frac{1}{R_2} = \frac{1}{a\cosh v - r} > 0$$

$$\sigma' = \frac{1}{R_1} = \frac{1}{c\cos u - r} < 0$$

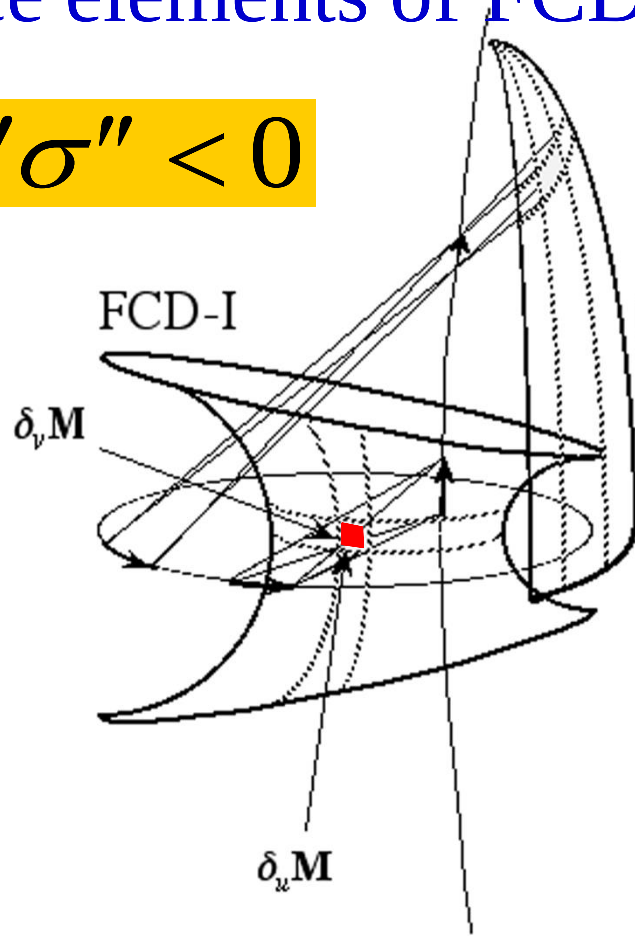
$$dV = dr \times d\Sigma = dr \times \frac{b^2 \left|\sigma'\sigma''\right|}{\left(\sigma' - \sigma''\right)^2} du\, dv$$

Kleman et al PRE 61, 1574 (2000)

Surface elements of FCD I and FCD II

$\sigma'\sigma'' < 0$

$\sigma'\sigma'' > 0$



$$d\Sigma(r) = AB\,du\,dv$$

$$A\,du = |\delta_u \mathrm{M}| = \left|\delta_u \left(\frac{r'}{\Delta}\,\mathrm{M'M}\right)\right| = \pm\frac{b\sigma''}{\sigma - \sigma''}\,du\,,$$

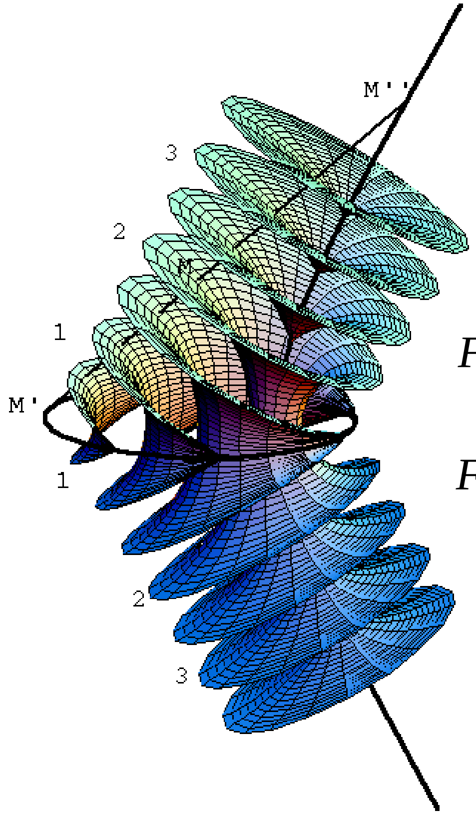
$$\Delta = r'' - r'$$

M'M'' = $|a\cosh v - c\cos u| \; = \; |ex' - e^{-1}x''|$

$$B\,dv = \pm\frac{b\sigma'}{\sigma' - \sigma''}\,dv$$

$$d\Sigma(r) = \frac{b^2|\sigma'\sigma''|}{(\sigma' - \sigma'')^2}\,du\,dv$$

Curvature energy of FCD-I



$$f = \frac{1}{2}K(\sigma' + \sigma'')^2 + \bar{K}\sigma'\sigma''$$

$$F_{curv} = \int_{FCD} f \frac{b^2 |\sigma'\sigma''|}{(\sigma' - \sigma'')^2} dudvdr$$

$$f = \frac{1}{2}K(\sigma' - \sigma'')^2 + (2K + \bar{K})\sigma'\sigma''$$

$$F_{curv} = F_1 + F_2$$

Mathematica© cannot do it….

$$F_1 = -\tfrac{1}{2}K(1-e^2)a\int \frac{du\,dv\,d\rho}{(e\cos u - \rho)(\cosh v - \rho)}$$

$$F_2 = -\left(2K + \bar{K}\right)(1-e^2)\,a\int \frac{du\,dv\,d\rho}{(\cosh v - e\cos u)^2}$$

$$\rho = r / a$$

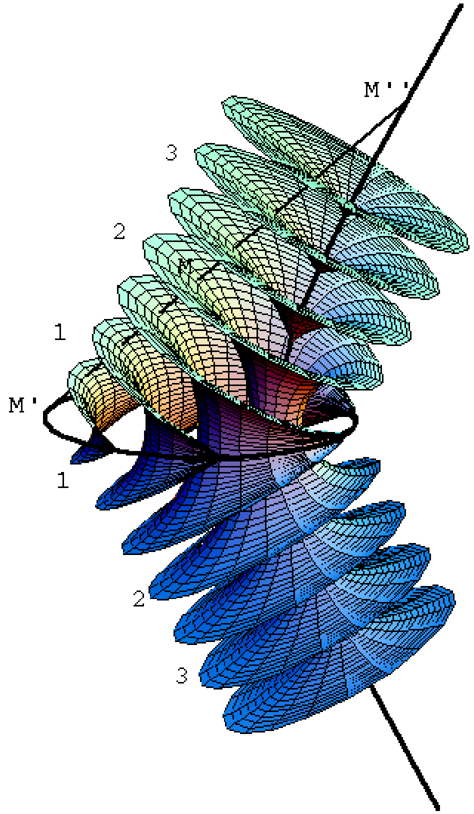
$$r_{cutoff} = a\cosh v - r_c$$

$$r_{cutoff} = c\cos u + r_c$$

substitutions such as $\dfrac{\cosh^2 v - e^2}{1-e^2} = \dfrac{1}{\cos^2 x}$ lead to the desired result...

Kleman et al PRE 61, 1574 (2000)

Curvature energy of FCD-I

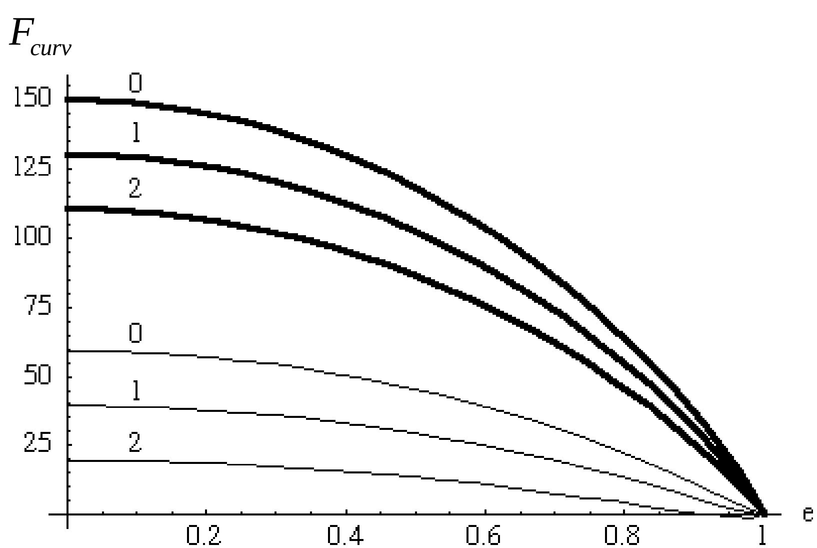


$$F_{curv} = 4\pi a\left(1-e^2\right)\mathbf{K}\left(e^2\right)\left[K\left(\ln\frac{2a\sqrt{1-e^2}}{r_c}-2\right)-\overline{K}\right]+F_{core}$$

$$F_{core} \approx 8\,a\,K\,\mathbf{E}\left(e^2\right)$$

valid for any $0 \le e < 1$

$\mathbf{K}(x), \mathbf{E}(x)$ complete elliptic integrals of the first and second kind

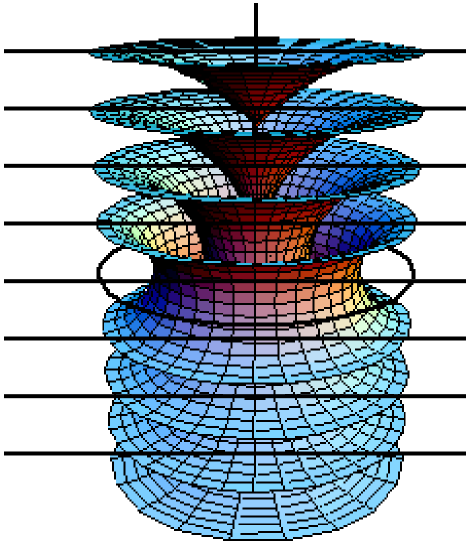


Kleman et al PRE 61, 1574 (2000)

Circular FCDs-I

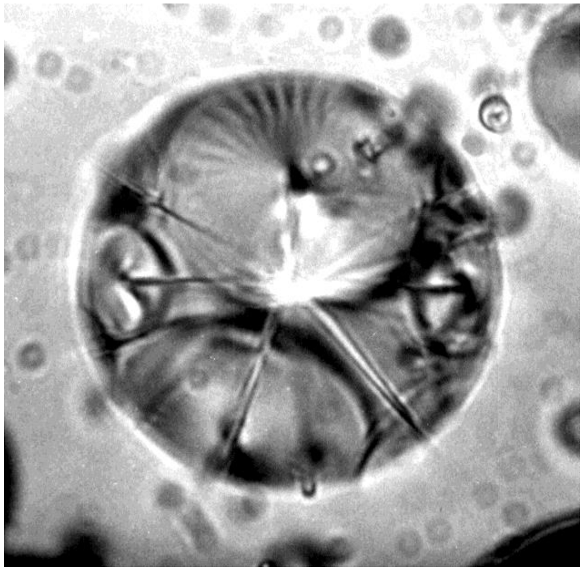
$$F = 2\pi^2 a\left(K \ln\frac{a}{r_c} + K\left(\ln 2 - 2\right) - \bar{K} \right)$$

$$a = b$$
$$e = 0$$
$$\omega = 0$$

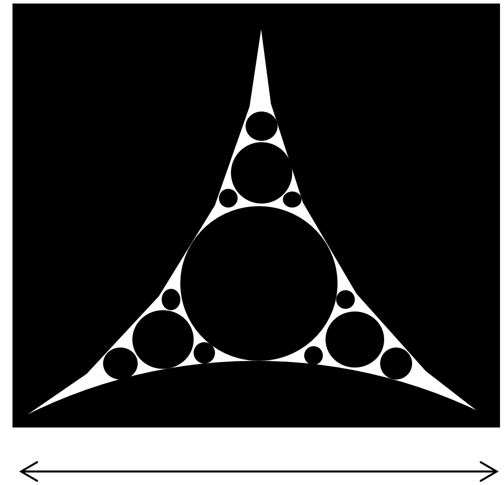


Home assignment: Derive *F* for a circular FCD

Anchoring-Controlled FCD Assembly



Appolonius filling



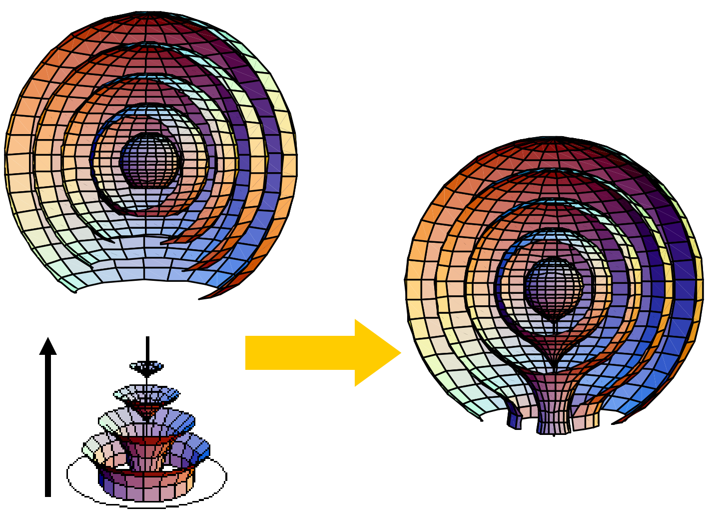
L, sample size

Black: tangential anchoring

White: Normal anchoring

$$F(b) \sim Kb - \Delta\gamma b^2$$

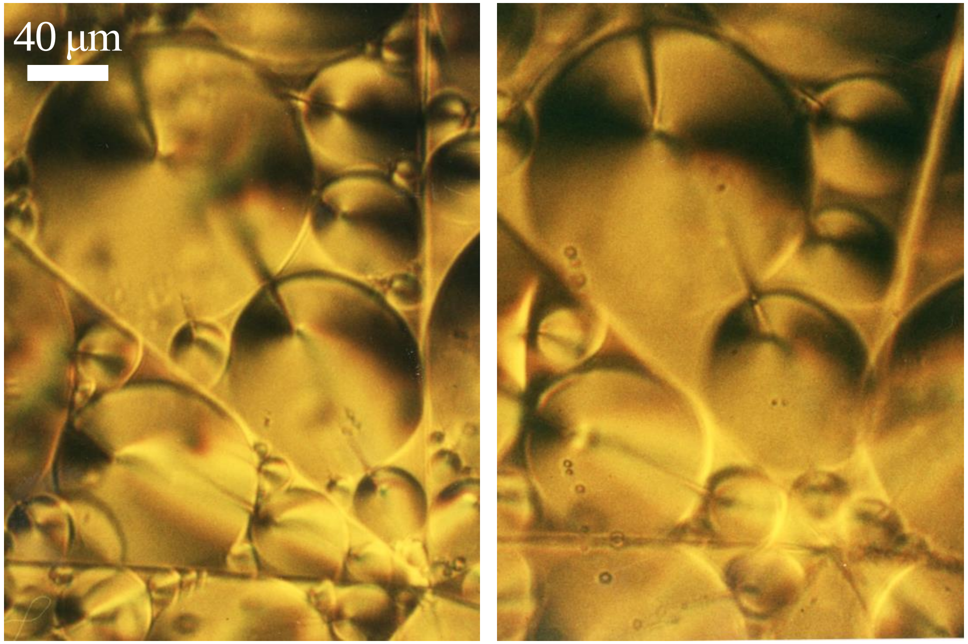
$$\frac{\partial F}{\partial b} = 0 \Rightarrow b^* \sim K / \Delta\gamma >> \lambda$$

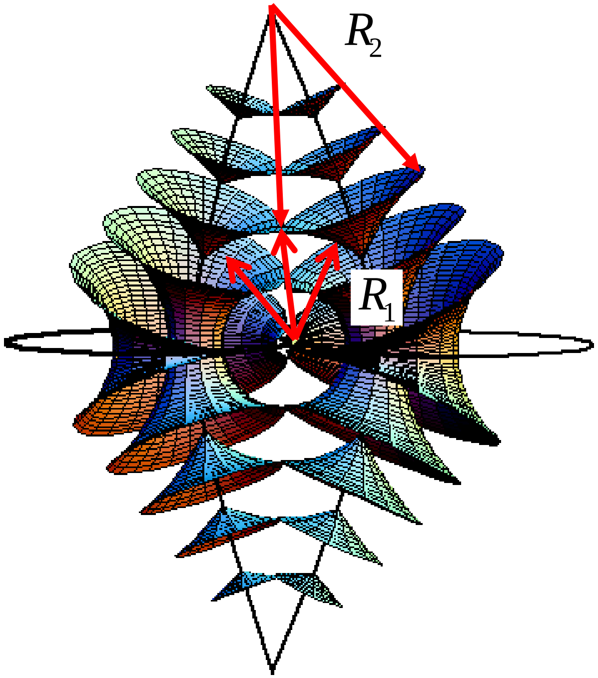


The smallest FCDs are macroscopic

Sov Phys JETP'83

Associations of FCDs

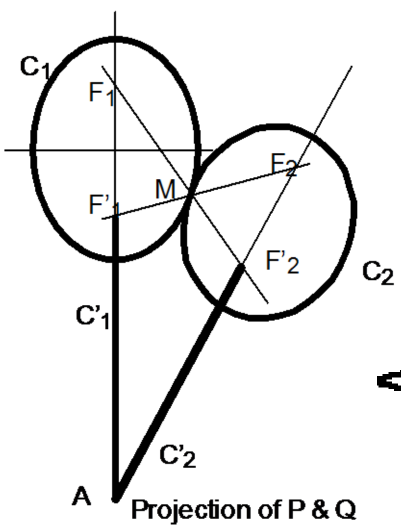


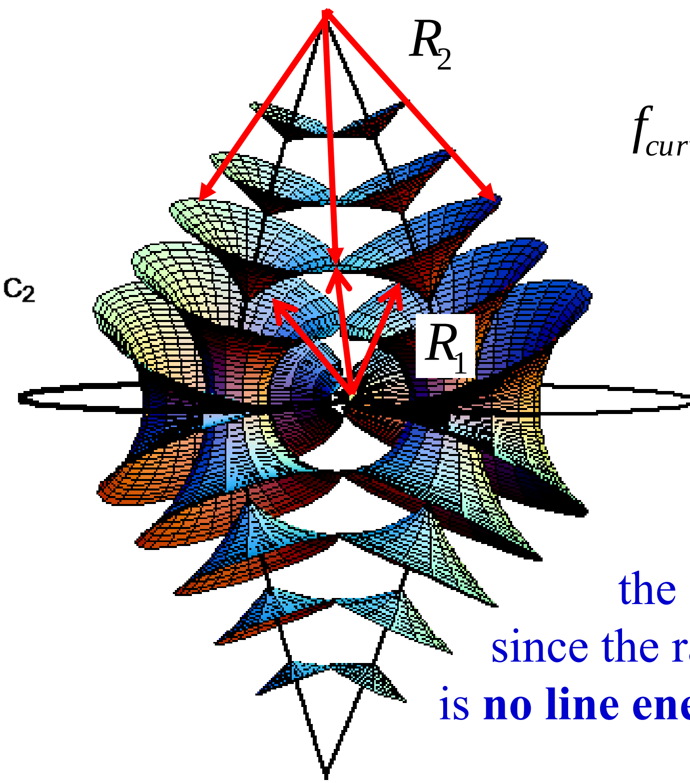


FCDs form families with common apex; Bragg, Nature (1934)

Law of Corresponding Cones

Friedel, 1922: When two coplanar ellipses are in contact at M,
the two corresponding hyperbolae have two points of intersection P and Q
and the domains have two generatrices MP and QM of contact.

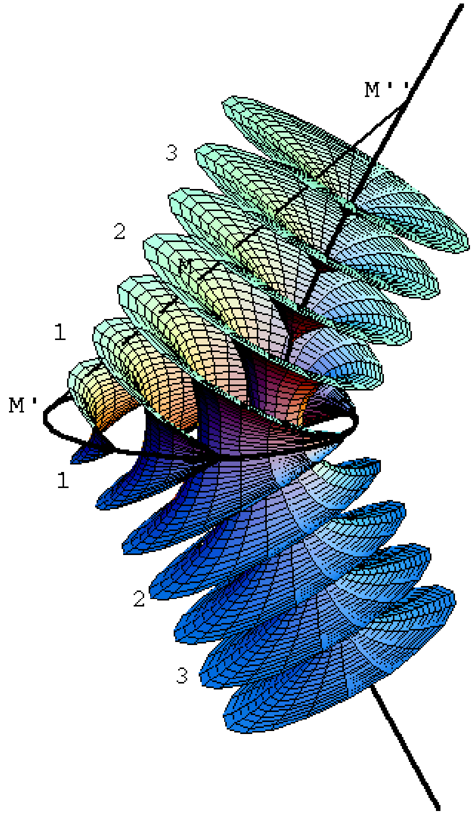




$$f_{curv} = \tfrac{1}{2}K\left(\frac{1}{R_1}+\frac{1}{R_2}\right)^2 + \bar{K}\,\frac{1}{R_1R_2}$$

At the line of contact of two FCDs,
the curvature energy densities are equal
since the radii of curvature are the same; there
is **no line energy** at the line of contact

Curvature energy of FCD-I

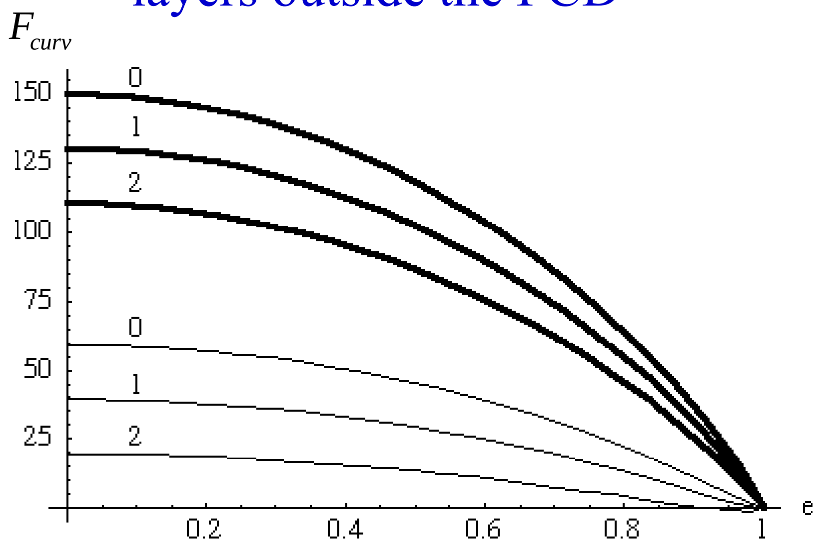


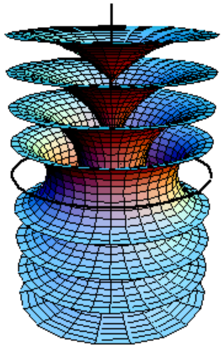
$$F_{curv} = 4\pi a\left(1-e^2\right)\mathbf{K}\left(e^2\right)\left[K\left(\ln\frac{2a\sqrt{1-e^2}}{r_c}-2\right)-\overline{K}\right]+F_{core}$$

$$F_{core} \approx 8\,a\,K\,\mathbf{E}\left(e^2\right)$$

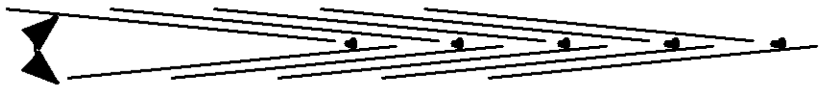
valid for any $0 \le e < 1$

Energy decreases as eccentricity increases. However eccentricity is not a minimization parameter as it is often fixed by the geometry of layers outside the FCD





Grain Boundaries in SmA

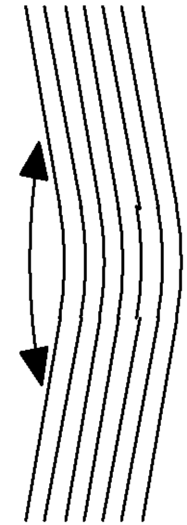


$\omega \to 0$ dislocation wall

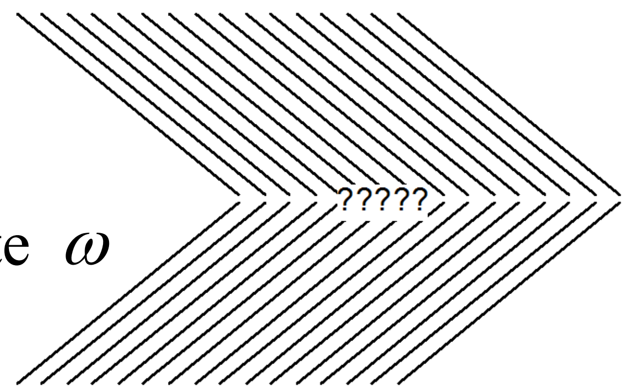
curvature wall

$\omega \to \pi/2$

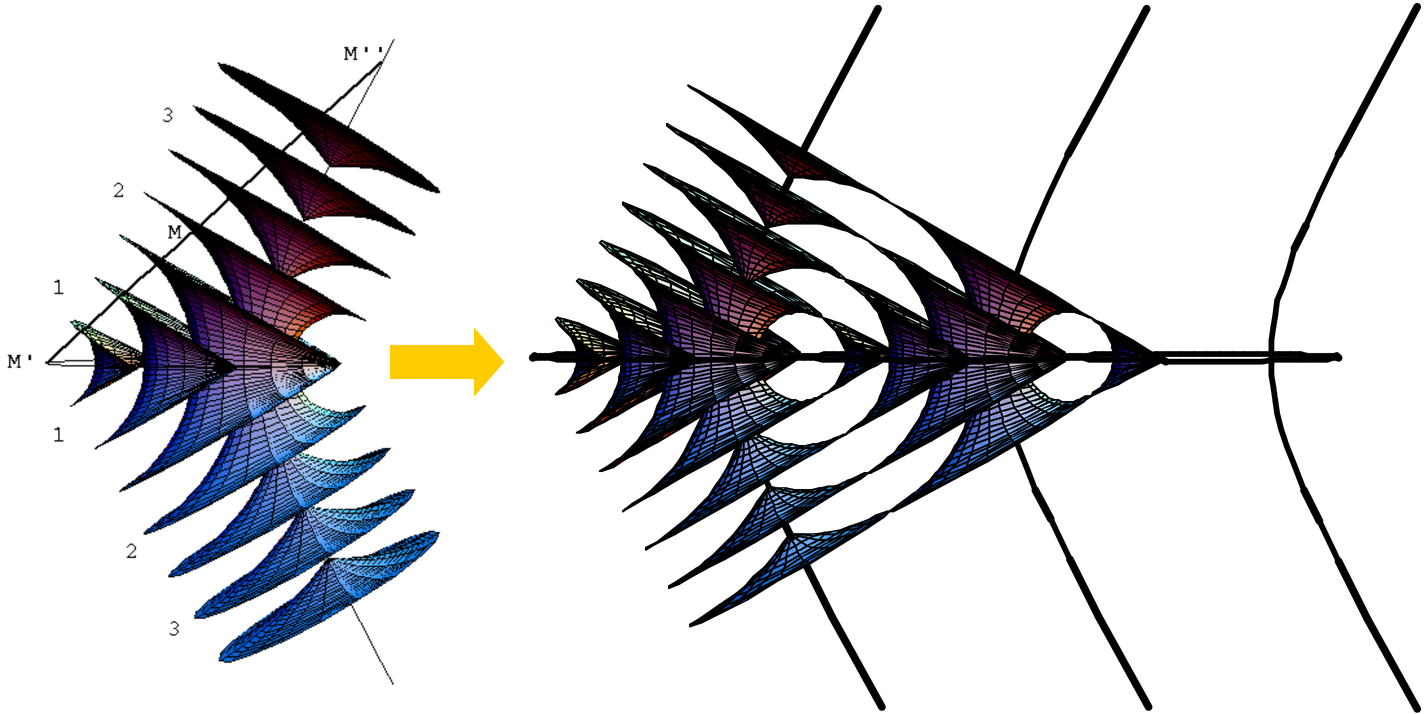
de Gennes, 1970



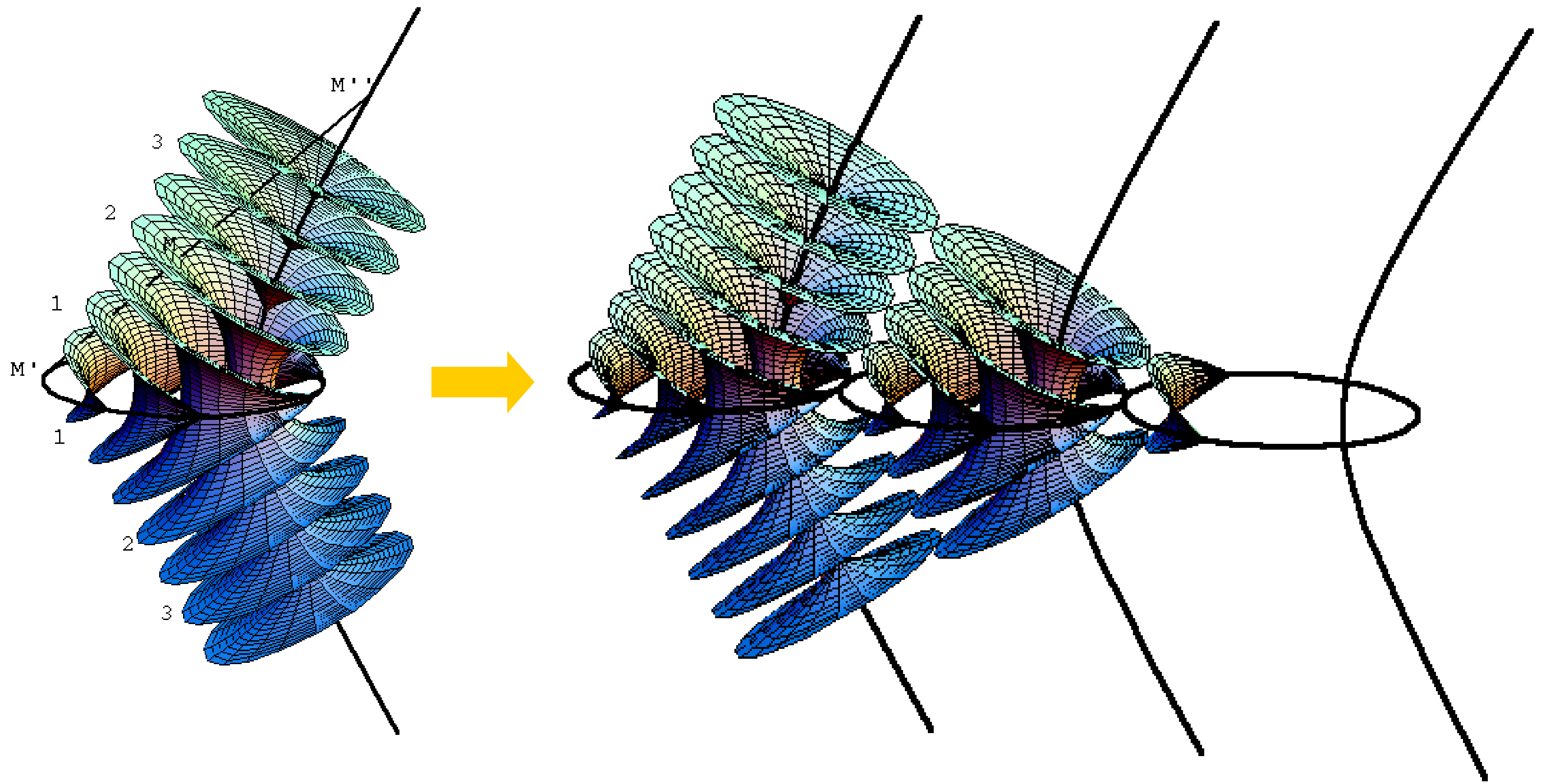
FCDs:
intermediate ω

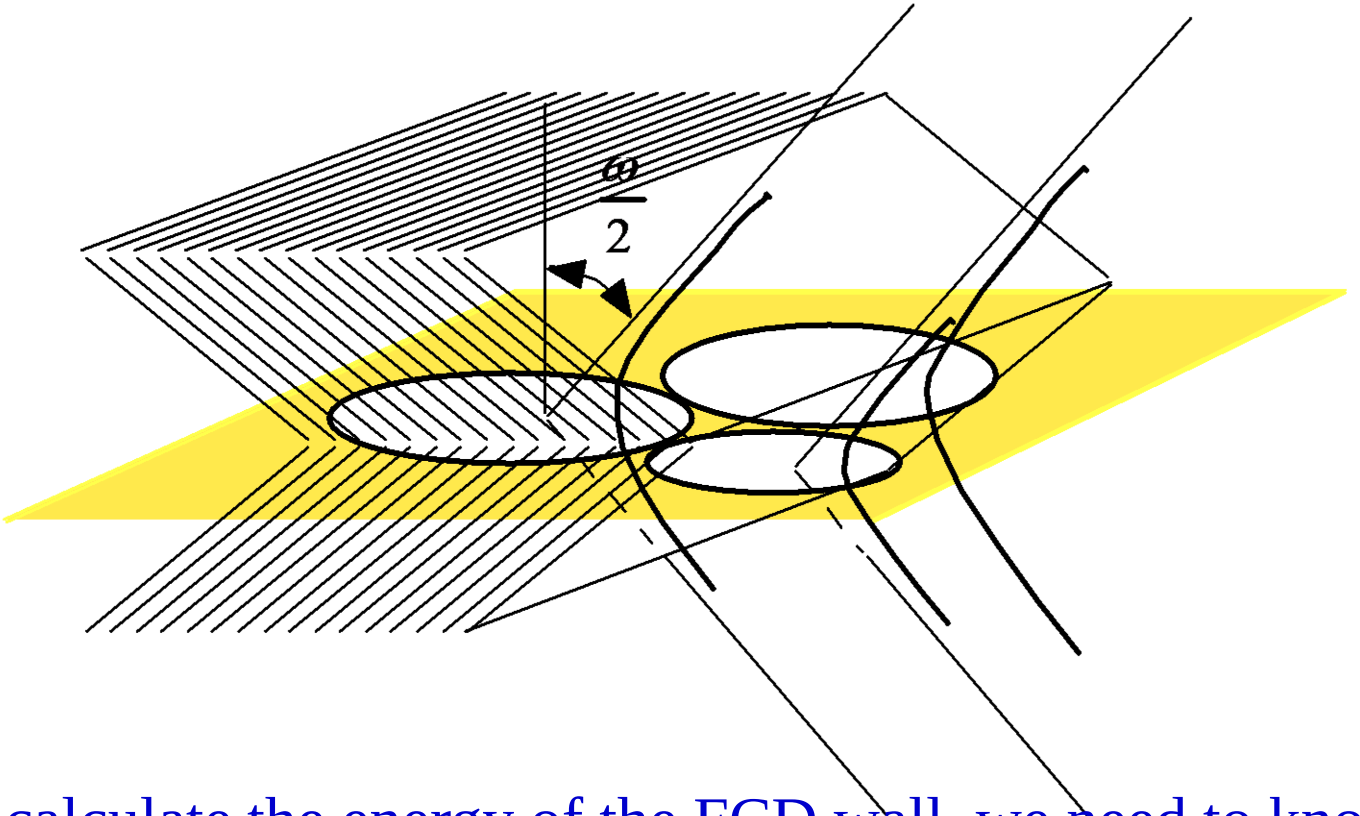


FCD-filled Grain Boundary-Ist hint



FCD-filled Grain Boundary-Ist hint



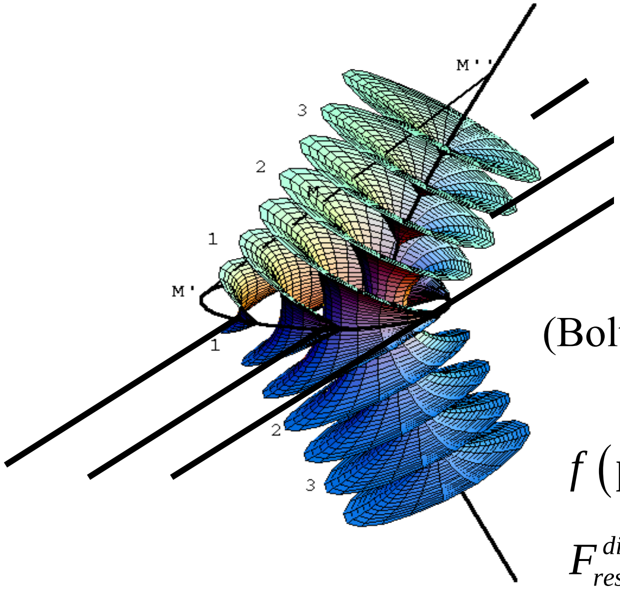


To calculate the energy of the FCD wall, we need to know:

- FCD energy (curvatures and defect cores)
- Spatial filling pattern, size distribution
- The energy of residual areas

M. Kleman et al, Eur. Phys. J E **2**, 47 (2000)

Residual Areas with Dislocations

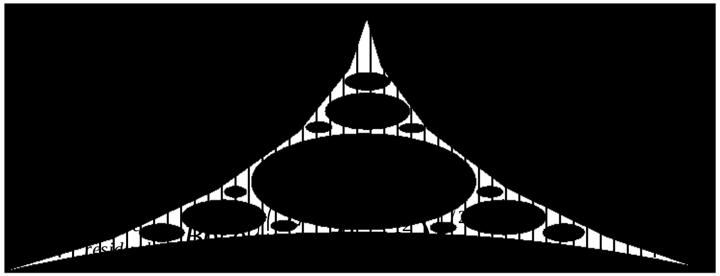


Dislocations with total Burgers vector $b_u = 2ae$

(Boltenhagen et al, J. Physique (1991))

$$f\left(\text{per unit length}\right) \sim Bb_u\lambda \sim Bae\lambda$$

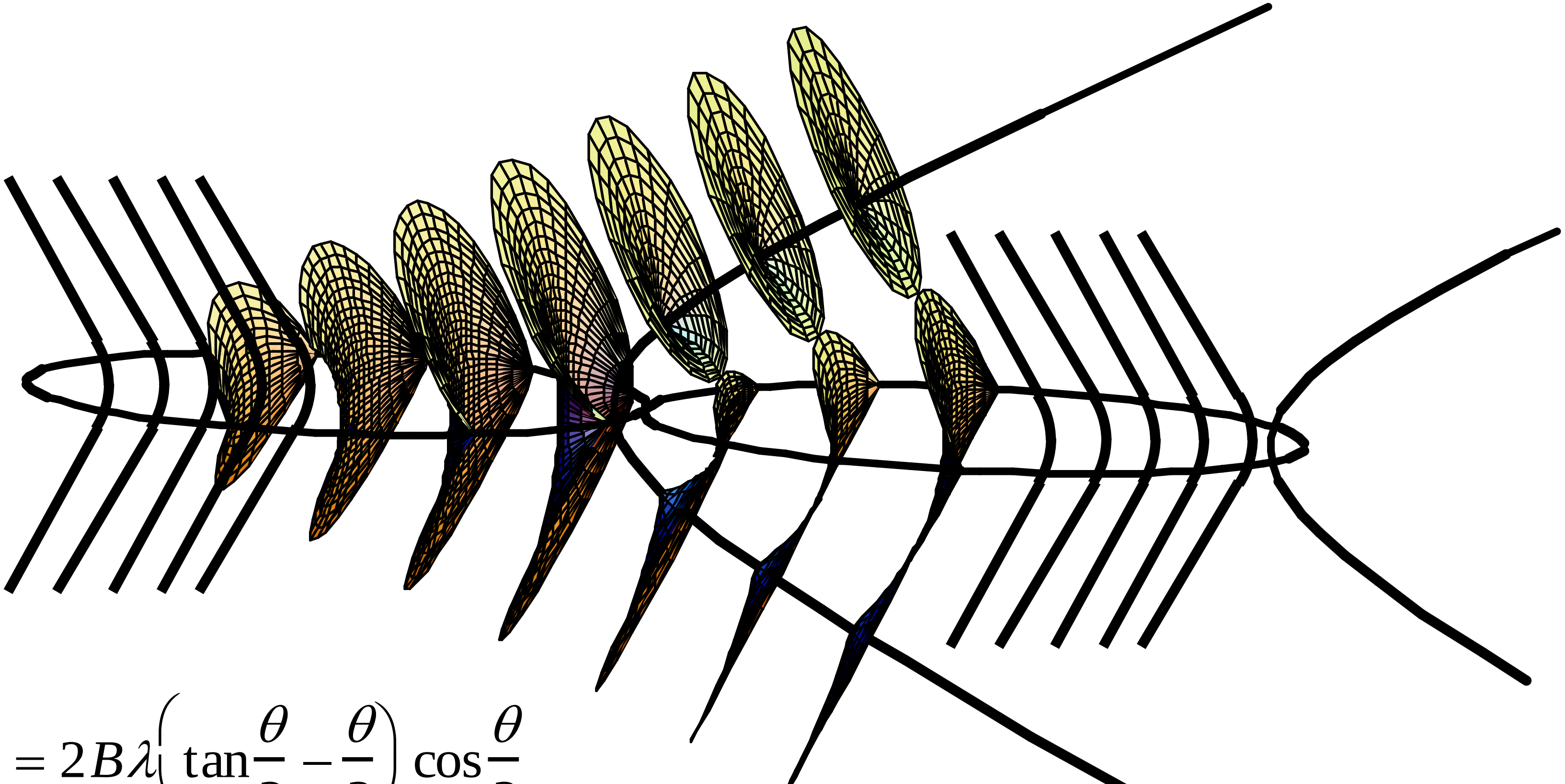
$$F_{residual}^{disloc} = f \times b \times Number\ of\ gaps \sim Bae\lambda \times b \times \frac{\Sigma(b)}{ab} \sim Be\lambda\Sigma(b)$$



$$F_{residual}^{disloc} \sim Be\lambda b^2\left(\frac{L}{b}\right)^n\left(1-e^2\right)^{-1/2}$$

M. Kleman et al, Eur. Phys. J E **2**, 47 (2000)

Residual Areas with Curvatures



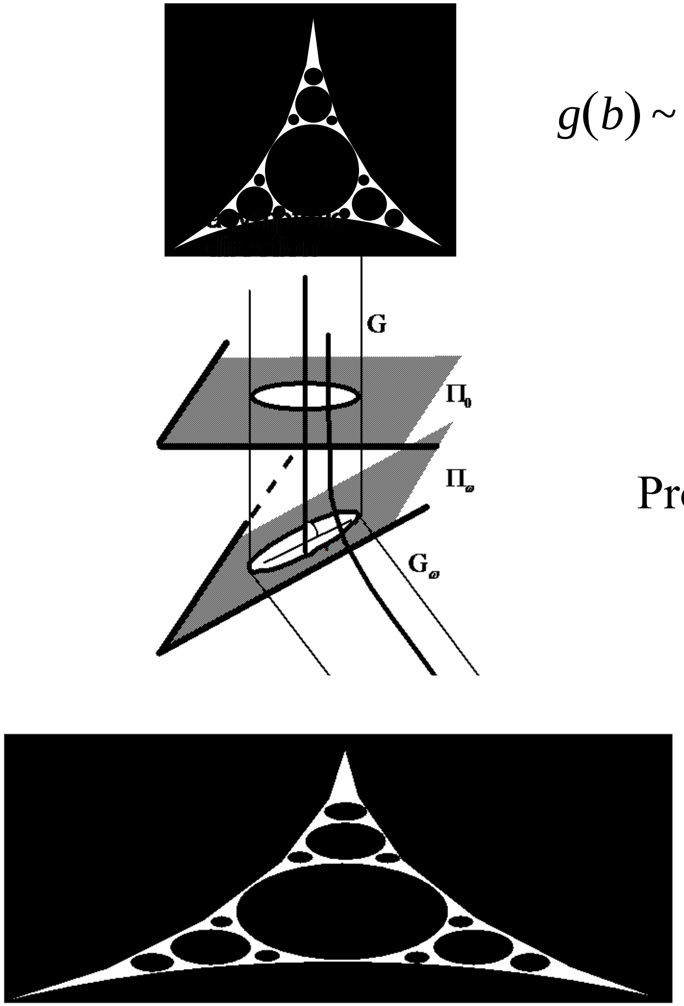
$$\sigma_{curv} = 2B\lambda\left(\tan\frac{\theta}{2} - \frac{\theta}{2}\right)\cos\frac{\theta}{2}$$

C. Blanc, M. Kleman, 1999

$$F_{resid}^{curv} \sim 2Bb^2\lambda\left[1 - \frac{e\ \mathrm{Arc}\cos e}{\sqrt{1-e^2}}\right]\left(\frac{L}{b}\right)^n$$

M. Kleman et al, Eur. Phys. J E **2**, 47 (2000)

From Circles to Ellipses



$$g(b) \sim \left(\frac{L}{b}\right)^n \qquad P(b) \sim \left(\frac{L}{b}\right)^n b \qquad \Sigma(b) \sim \left(\frac{L}{b}\right)^n b^2 \qquad n \approx 1.32$$

Projective properties of conic sections lead to:

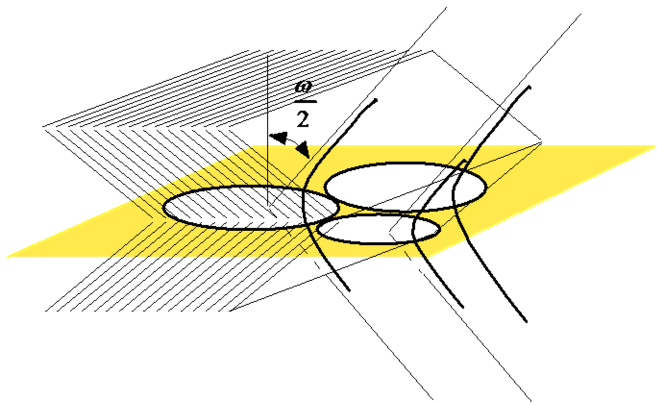
$$g(b) \sim \left(\frac{L}{b}\right)^n \qquad n \approx 1.32$$

$$P(b) \sim \frac{\mathbf{E}\left(e^2\right)}{\sqrt{1-e^2}} \times \left(\frac{L}{b}\right)^n b$$

$$\Sigma(b) \sim \frac{1}{\sqrt{1-e^2}} \times \left(\frac{L}{b}\right)^n b^2$$

M. Kleman et al, Eur. Phys. J E **2**, 47 (2000)

FCD wall with Dislocations



$$F = F_{bulk} + F_{core} + F_{residual}^{disloc}$$

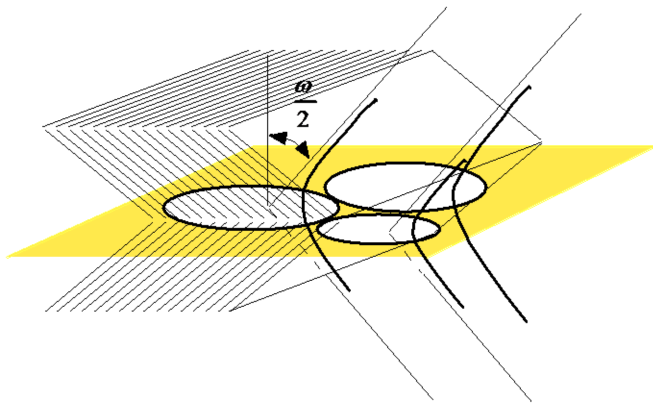
$$F_{bulk} = -\int_{x=b}^{L} dg(x)\, f_{bulk}(x) \sim \alpha_b K_1 \left(1-e^2\right)^{1/2} \mathbf{K}\left(e^2\right) \int_b^L n \left[\ln 2\frac{x}{\lambda} - 2\right] \left(\frac{L}{x}\right)^n dx$$

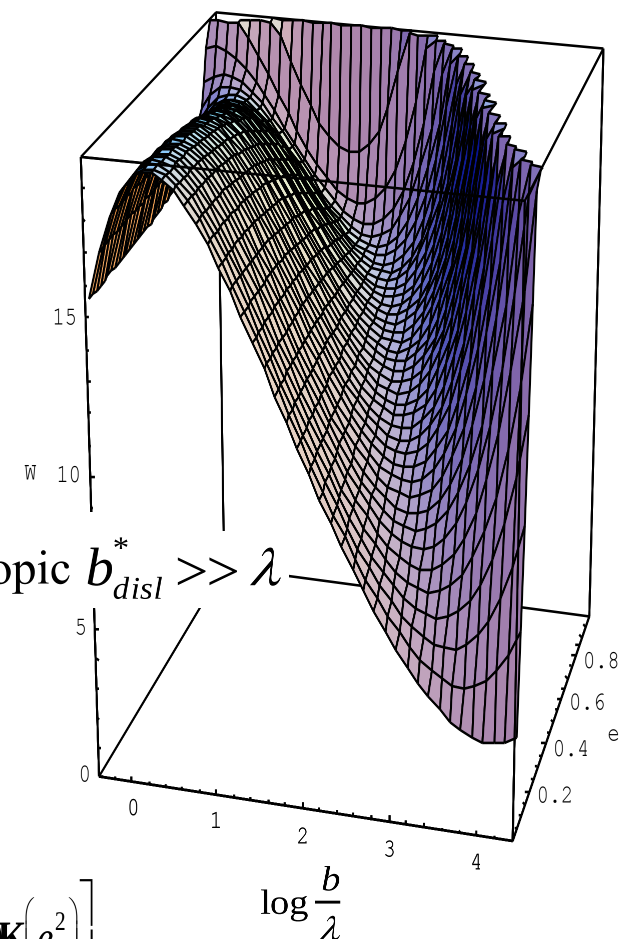
$$F_{core} = -\int_{x=b}^{L} dg(x)\, f_{core}(x) \sim \alpha_c K_1 \left(1-e^2\right)^{-1/2} \mathbf{E}\left(e^2\right) \int_b^L n \left(\frac{L}{x}\right)^n dx$$

$$F_{residual}^{disloc} = Be\lambda b^2 \left(\frac{L}{b}\right)^n \left(1-e^2\right)^{-1/2}$$

M. Kleman et al, Eur. Phys. J E **2**, 47 (2000)

FCD wall with Dislocations





macroscopic $b^{*}_{disl} >> \lambda$

$$\partial\left(F_{bulk} + F_{core} + F^{disl}_{resid}\right) / \partial b = 0$$

$$\frac{b^{*}_{disl}}{\lambda} \sim \frac{1}{e}\frac{n}{2-n}\left\{\alpha_b\left(1-\ e^2\right)\mathbf{K}\left(e^2\right)\left[\ln\frac{2b^{*}_{disl}}{\lambda} - 2\right] + \alpha_c \mathbf{E}\left(e^2\right)\right\}$$

$$\sigma^{disl}_{FCD}(e) \sim \frac{1}{(n-1)L^2}\left(\frac{L}{\lambda}\right)^n B\lambda^3\left(\frac{\lambda}{b^{*}_{disl}}\right)^{n-1}\left(1-e^2\right)^{-1/2}\left[e\frac{b^{*}_{disl}}{\lambda} + \alpha_b\frac{n}{n-1}\left(1-e^2\right)\mathbf{K}\left(e^2\right)\right]$$

Grain boundaries with FCDs

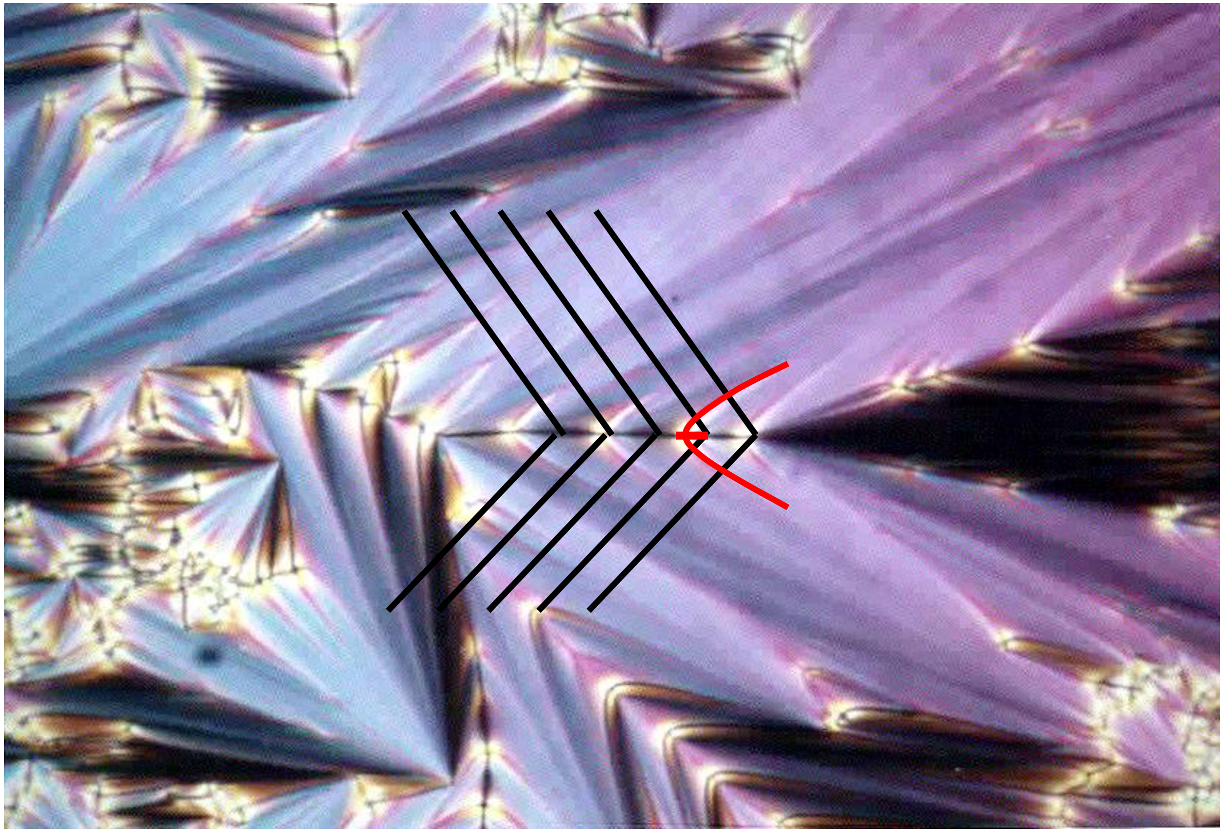
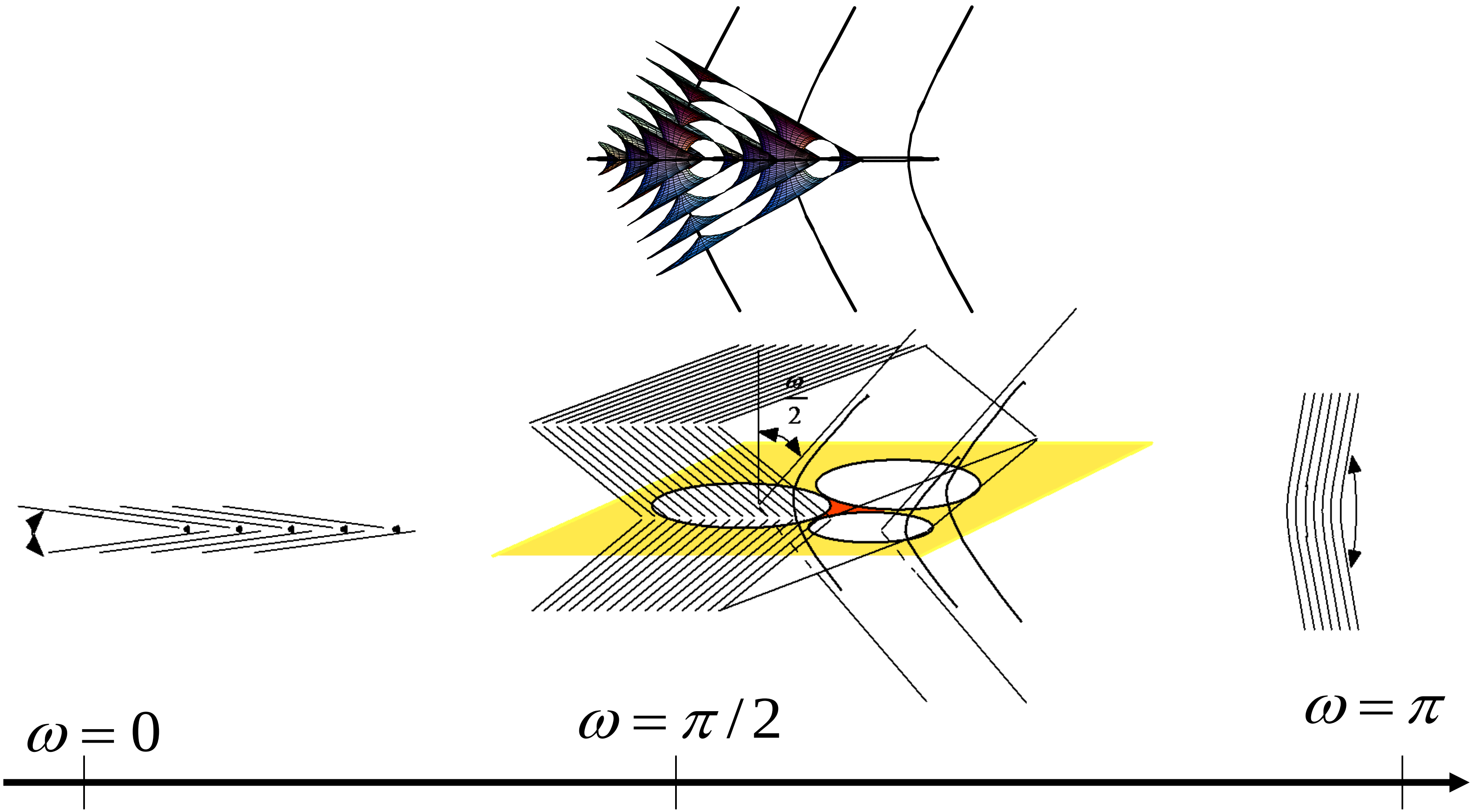


Photo: Claire Meyer

Domain walls in SmA



dislocations

FCDs, gaps with dislocations

FCDs, gaps with curvatures

curvatures

Conclusions/What have you learned

☐ Lamellar phases

- Both compressibility and curvatures are generally important in weak elastic deformation, such as dislocations, surface perturbations, undulations
- Strong deformations such as focal conic domains are described sufficiently well by the curvature term; layer thickness is preserved everywhere except at singular lines (confocal pairs) that are remnants of singular focal surfaces
- Observation of focal conic domains led to correct identification of smectics as 1D periodic stacks of fluid 2D layers
- Focal conic domains participate in relaxation of surface anchoring and grain boundaries