Winter school
Nonlinear Function Spaces in Mathematics and Physical Sciences
Lyon, 14-18 December 2015

Function spaces for liquid crystals

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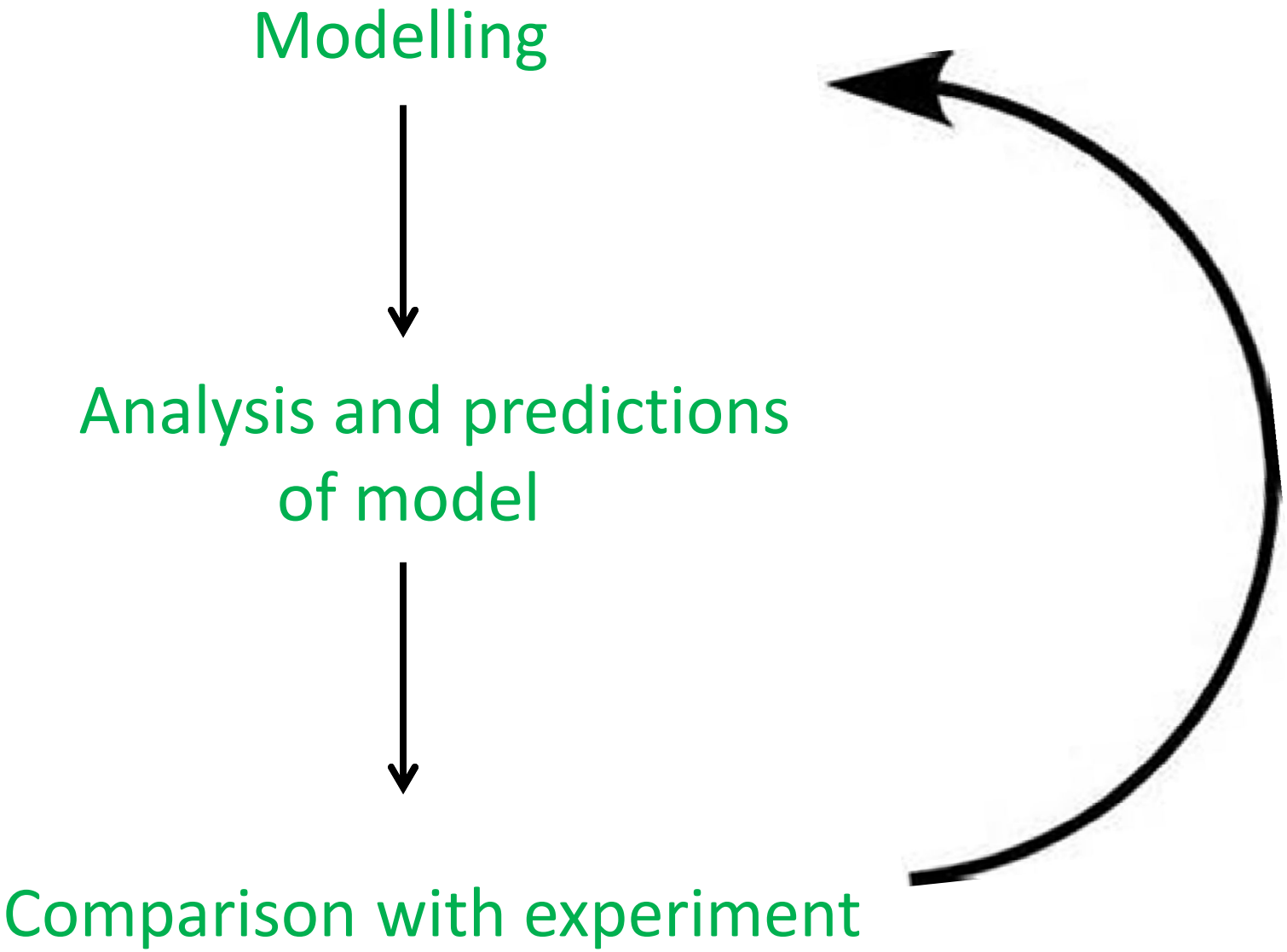
Notes at http://people.maths.ox.ac.uk/ball/teaching.shtml

Topics

1. Liquid crystals, phase transitions and order parameters.
2. The Landau – de Gennes, Oseen – Frank and Ericksen theories.
3. Onsager theory.
4. The description of defects.

Some themes

- Function spaces as a part of models in physics
- Relation between different levels of description (e.g. molecular vs continuum, order parameters of different dimensions)
- Lessons from solid mechanics
- Constraints (equality and inequality) on unknowns in variational problems


Modelling
Analysis and predictions of model
Comparison with experiment

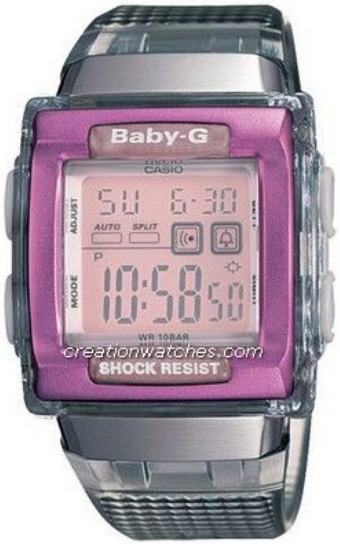
1. Liquid crystals, phase transitions and order parameters

What are liquid crystals?

An intermediate state of matter between liquids and solids.

Liquid crystals flow like liquids, but the constituent molecules retain orientational order.

A multi-billion dollar industry.



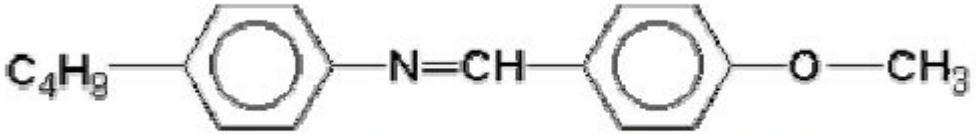
HP bistable display

Molecular structure

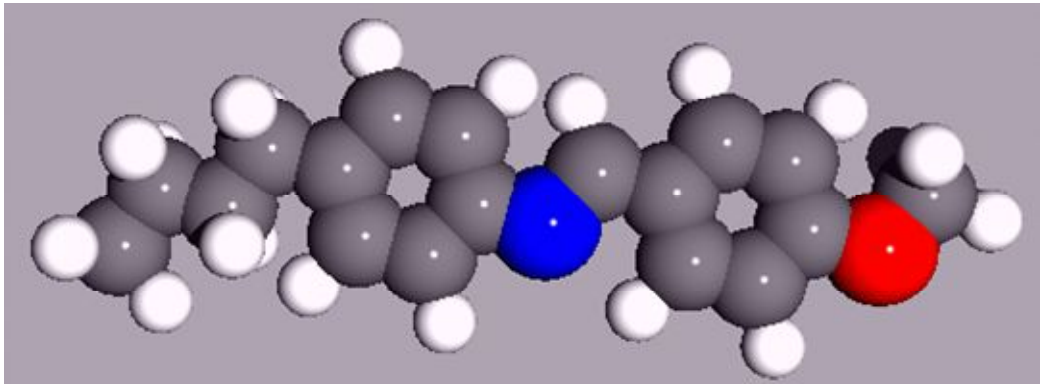
Liquid crystals are of many different types, the main classes being nematics, cholesterics and smectics

Nematics consist of rod-like molecules.

Length 2-3 nm



Methoxybenzilidene Butylanaline ("MBBA")

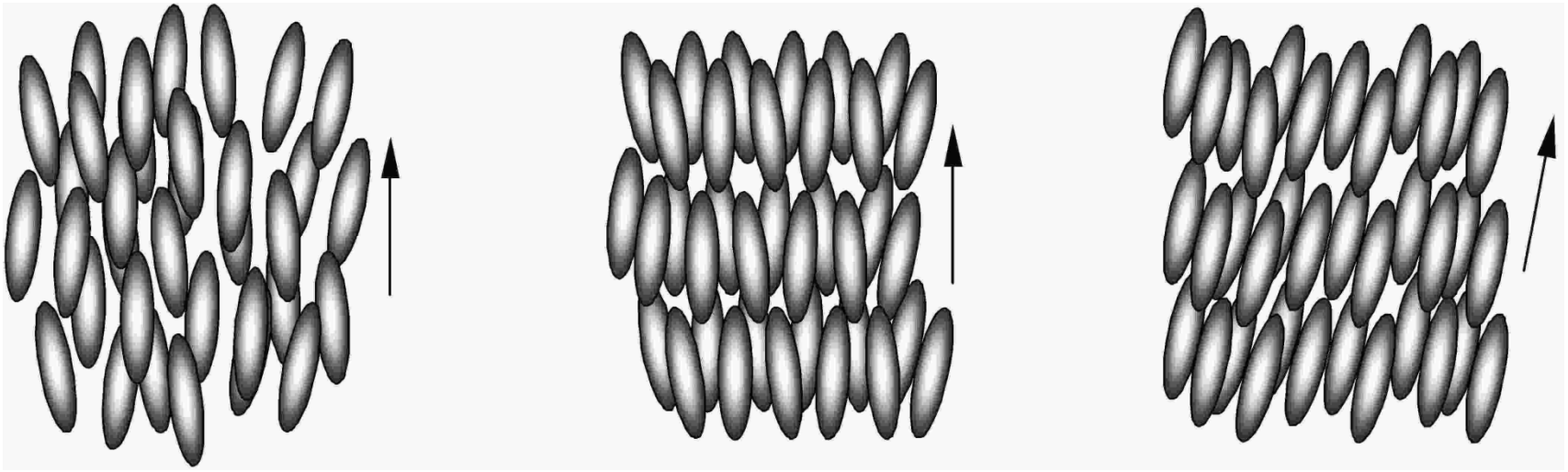


Prof. Dr. Wolfgang Muschik
TU Berlin
http://wwwitp.physik.tu-berlin.de/muschik/

Commercial liquid crystal displays use a mixture of several different fluids.

Depending on the nature of the molecules, the interactions between them and the temperature the molecules can arrange themselves in different phases.

Isotropic fluid – no orientational or positional order



Nematic phase orientational but no positional order

Smectic A phase

Smectic C phase

Orientational and some positional order

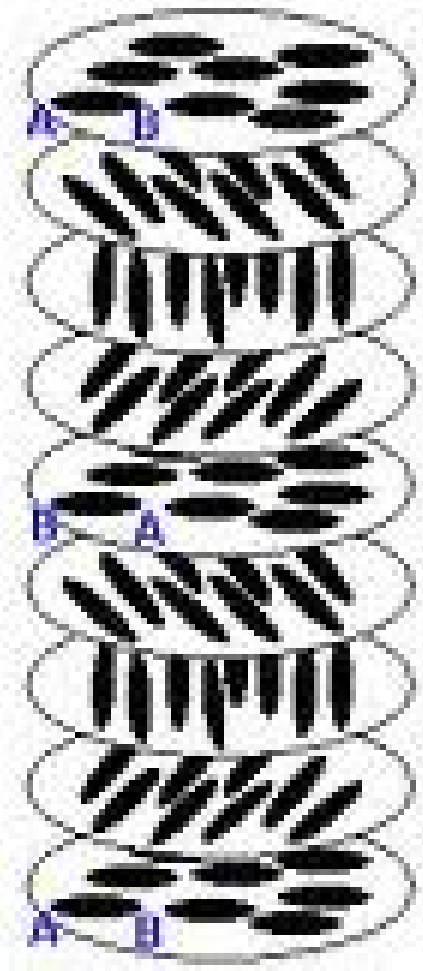
The molecules have time-varying orientations due to thermal motion.

Electron micrograph
of nematic phase

http://www.netwalk.com/~laserlab/lclinks.html

Cholesterics

If a chiral dopant is added the molecules can form a cholesteric phase in which the mean orientation of the molecules rotates in a helical fashion.



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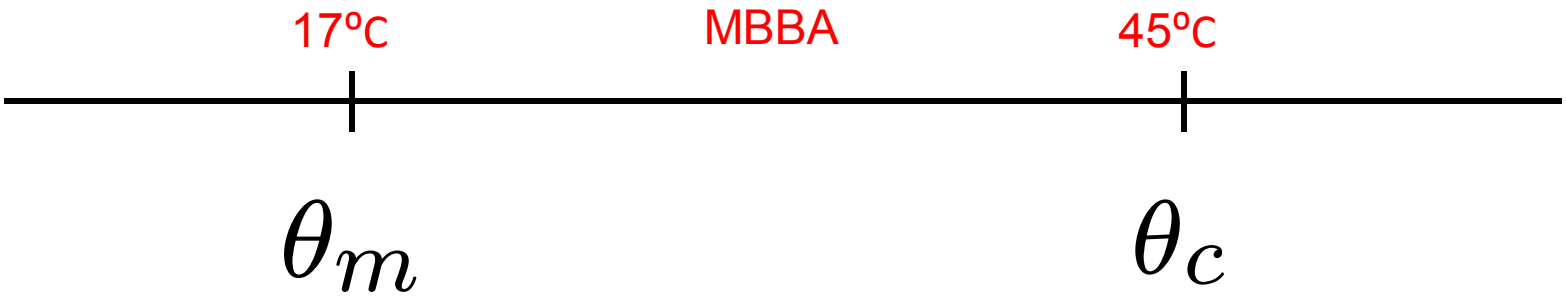
Isotropic to nematic phase transition

The nematic phase typically forms on cooling through a critical temperature θ_c by a phase transformation from a high temperature isotropic phase.



$\theta < \theta_m$
other LC or solid phase

$\theta_m < \theta < \theta_c$
nematic

$\theta > \theta_c$
isotropic

MBBA

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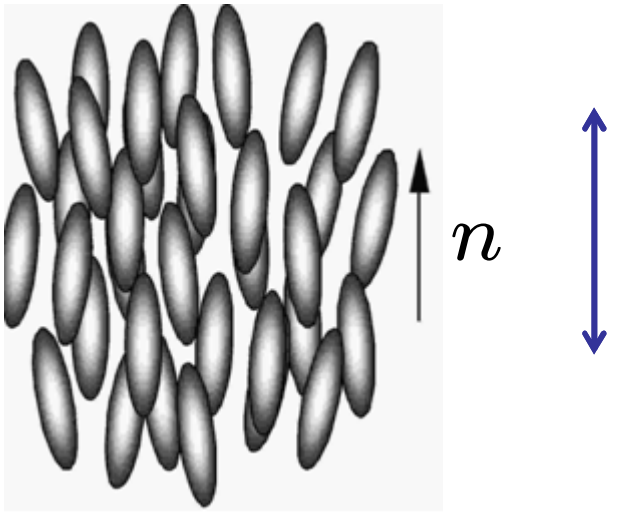
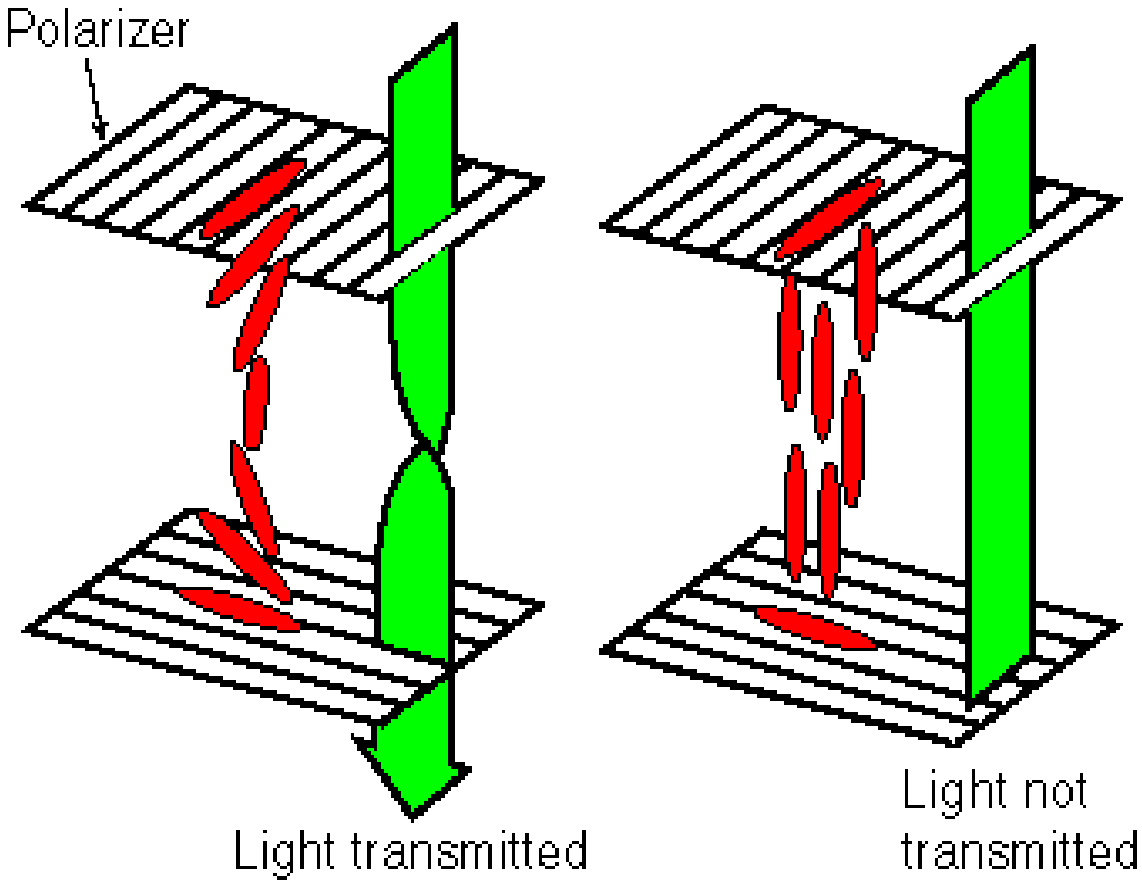
The director

A first mathematical description of the nematic phase is to represent the mean orientation of the molecules by a unit vector $n = n(x, t)$.



But note that for most liquid crystals n is equivalent to $-n$, so that a better description is via a *line field* in which we identify the mean orientation by the line through the origin parallel to it.

The twisted nematic display

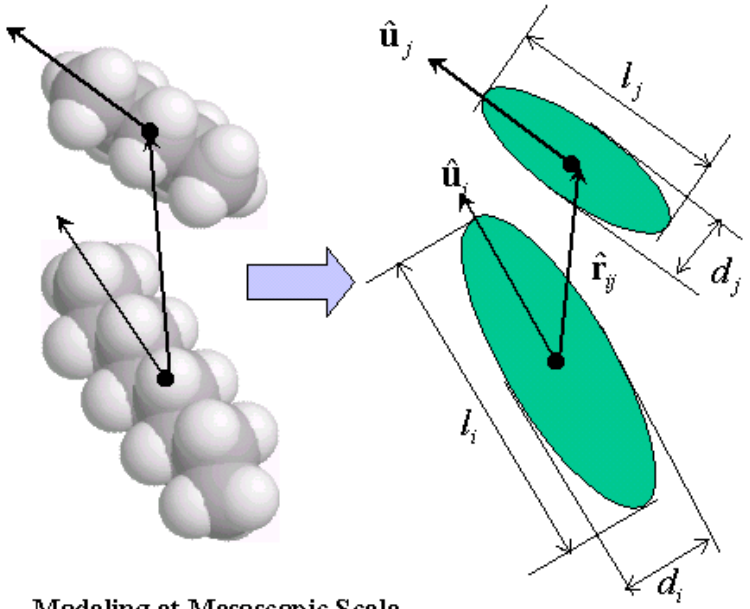


(a) Voltage **OFF**

(b) Voltage **ON**

Modelling via molecular dynamics

Monte-Carlo simulation using Gay-Berne potential to model the interaction between molecules, which are represented by ellipsoids.



Modeling at Mesoscopic Scale

This interaction potential is an anisotropic version of the Lennard-Jones potential between pairs of atoms or molecules.

http://mw.concord.org

$$U_{\mathrm{GB}} = 4\varepsilon_0 \varepsilon(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)[u(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)^{12} - u(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)^{6}],$$

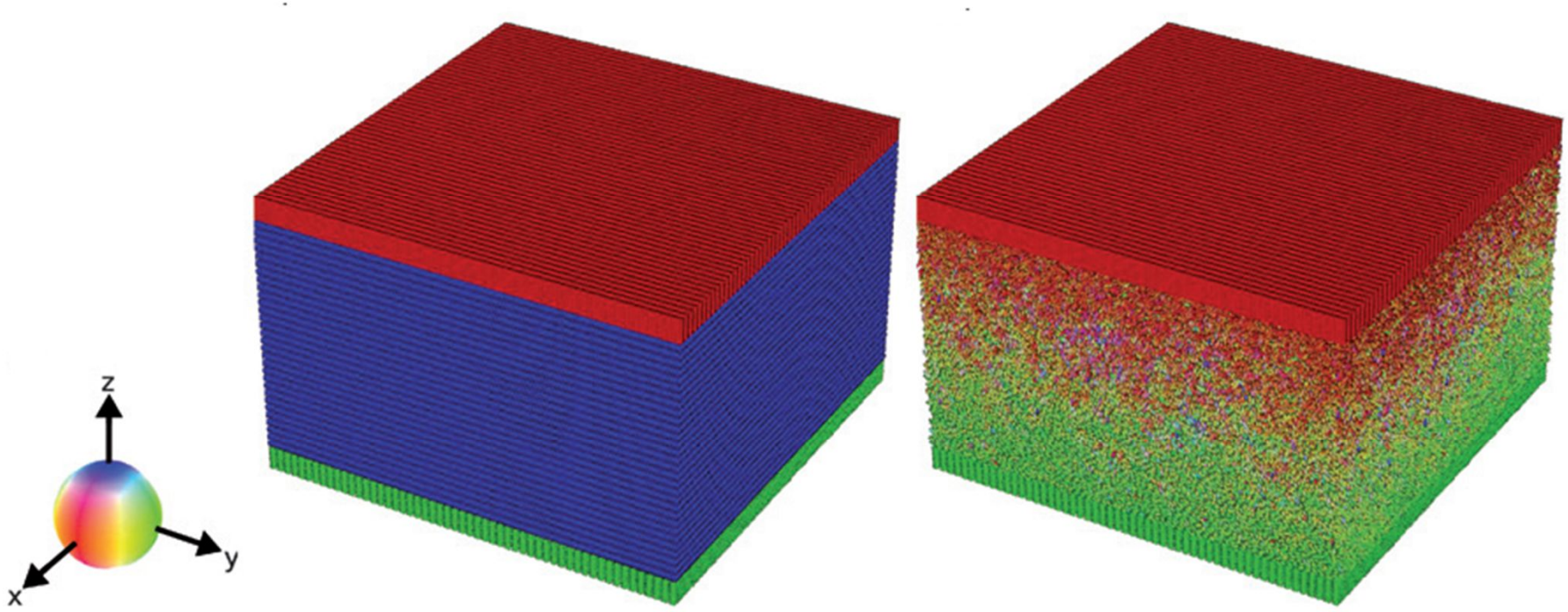
where

$$u(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j) = \frac{\sigma_c}{r_{ij} - \sigma(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j) + \sigma_c},$$

$r_{ij} = |\hat{\mathbf{r}}_{ij}|$, and where the functions $\sigma(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)$ and $\varepsilon(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j)$ measure the contact distance between the ellipsoids and the attractive well depth respectively (depending in particular on the ellipsoid geometry) and ε_0, σ_c are empirical parameters.

Twisted nematic display simulation

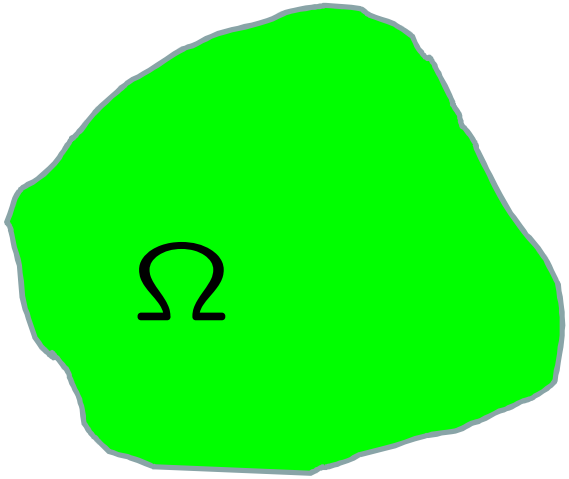
944,784 molecules, including 157,464 fixed in layers near the boundaries to prescribe the orientation there.



M. Ricci, M. Mazzeo, R. Berardi, P. Pasini, C. Zannoni, 2009 (courtesy Claudio Zannoni)

Continuum models

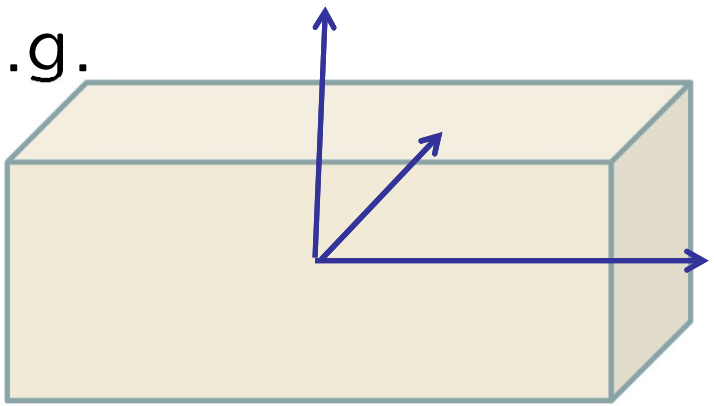
Consider a nematic or cholesteric liquid crystal filling a container $\Omega \subset \mathbb{R}^3$.



To keep things simple consider only static configurations, for which the fluid velocity is zero.

Microscopic state variables

We represent a typical liquid crystal molecule by a 3D region M (rod, ellipsoid, parallepiped ...) of approximately the same shape and symmetry. We place M in a standard position with centroid at the origin, e.g.



and define the isotropy groups

$$G_M = \{R \in O(3) : RM = M\}$$
$$G_M^+ = \{R \in SO(3) : RM = M\}$$

If $G_M = G_M^+$ then the molecule is said to be *chiral* (as in cholesterics).

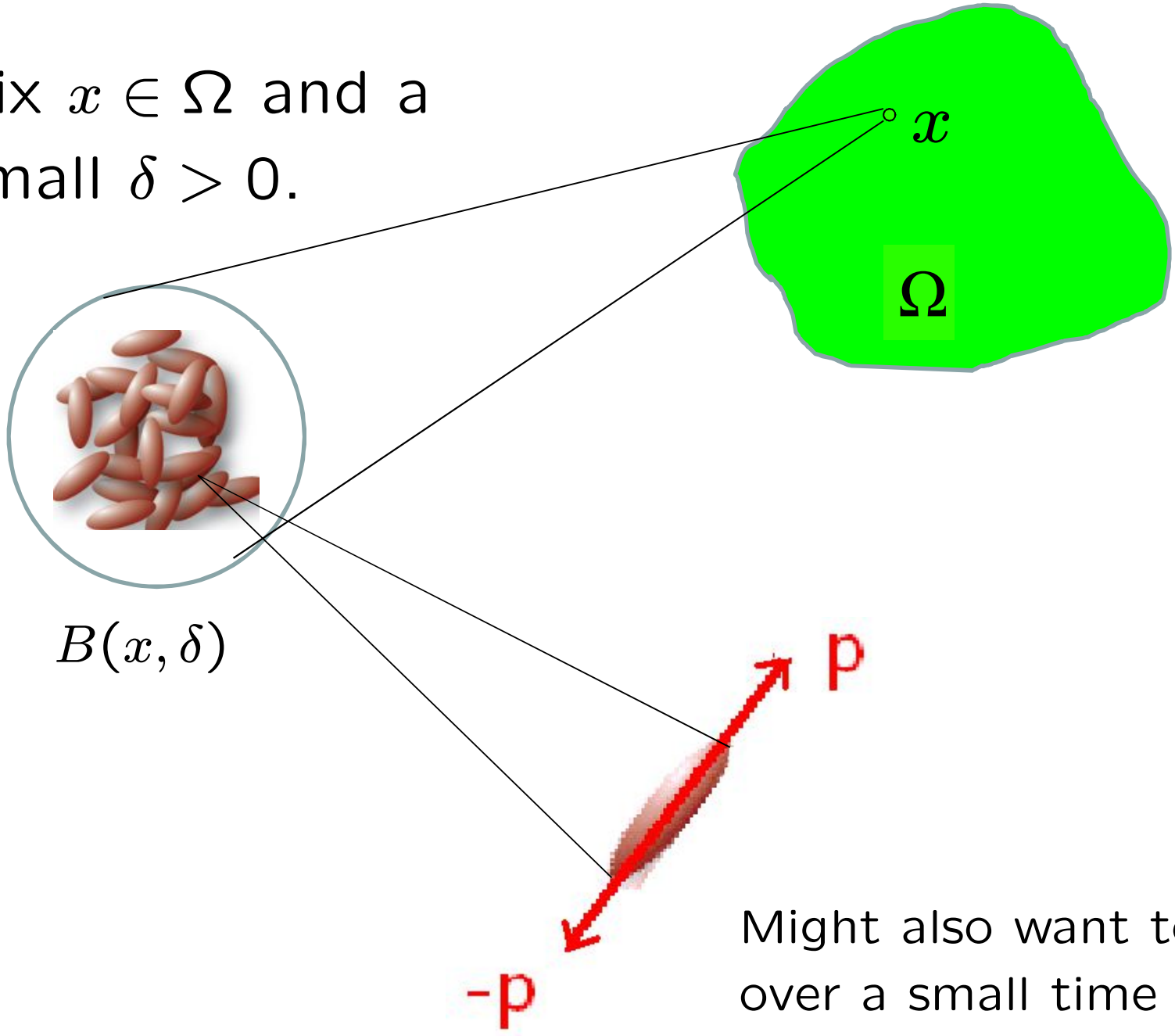
$RM = \tilde{R}M$ for $R, \tilde{R} \in SO(3)$ iff $\tilde{R}^T R \in G_M^+$. Hence the orientation of a molecule can be represented by an element of the space of cosets $SO(3)/G_M^+$ (cf Mermin 1979).

For M a cylindrical rod or ellipsoid of revolution

we can identify $SO(3)/G_M^+$ with $\mathbb{R}P^2$, that is with lines through the origin parallel to the long axis, or equivalently with matrices $p \otimes p, p \in S^2$.

Molecular orientations of nematics

Fix $x \in \Omega$ and a small $\delta > 0$.



Might also want to average over a small time interval.

The distribution of orientations of molecules in $B(x, \delta)$ can be represented by a probability measure on $\mathbb{R}P^2$, that is by a probability measure $\mu = \mu_x$ on the unit sphere S^2 satisfying $\mu(E) = \mu(-E)$ for $E \subset S^2$.

(In fact nematic and cholesteric liquid crystal molecules do not have exact head-to-tail symmetry and they are typically polarized. So the assumption $\mu(E) = \mu(-E)$ is a statistical one, that equal numbers have direction p and $-p$.)

We want δ to be sufficiently small for $B(x, \delta)$ to be macroscopically close to a point x, yet large enough to contain a large number of molecules and allow a statistical description.

Take the molecule to be a circular cylinder of length d and radius a, and assume the molecules to fill a fraction θ of $B(x, \delta)$. Then the number of molecules in $B(x, \delta)$ is $\theta \frac{4}{3} \pi \delta^3 / \pi a^2 d$.

Setting $\theta = \frac{1}{2}$, $a = d/4$, $d = 3\text{nm}$, this number is 1 billion for $\delta \sim 10^{-6}\text{m} = \frac{1}{1000}\text{mm}$.

Example:
$\mu = \frac{1}{2}(\delta_e + \delta_{-e})$ represents a state of perfect alignment parallel to the unit vector e.

For a continuously distributed measure $d\mu(p) = \rho(p)dp$, where dp is the element of surface area on S^2 and $\rho \geq 0, \int_{S^2} \rho(p)dp = 1$, $\rho(p) = \rho(-p)$.

If the orientation of molecules is equally distributed in all directions, we say that the distribution is *isotropic*, and then $\mu = \tilde{\mu}$, where

$$d\tilde{\mu}(p) = \frac{1}{4\pi} dp,$$

for which $\rho(p) = \frac{1}{4\pi}$.

A natural idea would be to use as an order parameter the probability measure $\mu = \mu_x$. However this represents an infinite-dimensional state variable at each point x, and if we use as an approximation an order parameter consisting of a finite number of moments of μ then we have instead a finite-dimensional state variable.

Because $\mu(E) = \mu(-E)$ the first moment

$$\int_{S^2} p \, d\mu(p) = 0.$$

The second moment

$$M = \int_{S^2} p \otimes p \, d\mu(p)$$

is a symmetric non-negative 3×3 matrix satisfying $\mathrm{tr} M = 1$.

The second moment tensor of the isotropic distribution $\tilde{\mu}$, $d\tilde{\mu} = \frac{1}{4\pi} dp$, is

$$\tilde{M} = \frac{1}{4\pi} \int_{S^2} p \otimes p \, dp = \frac{1}{3} \mathbf{1}$$

(since $\int_{S^2} p_1 p_2 \, dp = 0$, $\int_{S^2} p_1^2 \, dp = \int_{S^2} p_2^2 \, dp$ etc and $\operatorname{tr} \tilde{M} = 1$.)

The *de Gennes Q-tensor*

$$Q = M - \tilde{M} = \int_{S^2} \left(p \otimes p - \frac{1}{3} \mathbf{1} \right) d\mu(p)$$

thus measures the deviation of M from its isotropic value.

Note that $Q = Q^T$, $\operatorname{tr} Q = 0$, $Q \geq -\frac{1}{3} \mathbf{1}$.

Since Q is symmetric and $\operatorname{tr} Q = 0$,

$$Q = \lambda_1 n_1 \otimes n_1 + \lambda_2 n_2 \otimes n_2 + \lambda_3 n_3 \otimes n_3,$$

where $\{n_i\}$ is an orthonormal basis of eigenvectors of Q with corresponding eigenvalues $\lambda_i = \lambda_i(Q)$ satisfying $\lambda_1 + \lambda_2 + \lambda_3 = 0$.

Since $Q \geq -\frac{1}{3}\mathbf{1}$, each $\lambda_i \geq -\frac{1}{3}$ and hence $-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3}$.

Conversely, if each $\lambda_i \geq -\frac{1}{3}$ then M is the second moment tensor for some μ, e.g. for

$$\mu = \sum_{i=1}^{3} (\lambda_i + \frac{1}{3}) \frac{1}{2} (\delta_{n_i} + \delta_{-n_i}).$$

If $\lambda_{\max}(Q) = \frac{2}{3}$ then for the corresponding eigenvector $e_{\max}$ we have

$$Me_{\max} \cdot e_{\max} = \int_{S^2} (p \cdot e_{\max})^2 dp = 1,$$

and hence

$$\int_{S^2} |p \otimes p - e_{\max} \otimes e_{\max}|^2 d\mu = 0,$$

and so $\mu = \frac{1}{2}(\delta_{e_{\max}} + \delta_{-e_{\max}})$.

If $\lambda_{\min}(Q) = -\frac{1}{3}$ then for the corresponding eigenvector $e_{\min}$ we have $Qe_{\min} \cdot e_{\min} = -\frac{1}{3}$, and hence

$$\int_{S^2} (p \cdot e_{\min})^2 d\mu(p) = 0,$$

and so μ is supported on the great circle of S^2 perpendicular to $e_{\min}$.

Remark. $Q = 0$ does not imply $\mu = \tilde{\mu}$.
For example we can take

$$\mu = \frac{1}{6} \sum_{i=1}^{3} (\delta_{e_i} + \delta_{-e_i}).$$

If two eigenvalues of Q are equal then Q is said to be *uniaxial* and has the form

$$Q = s\left(n \otimes n - \frac{1}{3}1\right),$$

where $n \in S^2$ and the *scalar order parameter* $s \in [-\frac{1}{2}, 1]$. Otherwise Q is *biaxial*.

In fact it is extremely difficult to find Q that are not very close to uniaxial with a constant value of s (typically 0.6-0.7). We will see why this is to be expected later.

Note that

$$\begin{aligned} Qn \cdot n &= \frac{2s}{3} \\ &= \langle (p \cdot n)^2 - \frac{1}{3} \rangle \\ &= \langle \cos^2 \theta - \frac{1}{3} \rangle, \end{aligned}$$

where θ is the angle between p and n. Hence

$$s = \frac{3}{2} \langle \cos^2 \theta - \frac{1}{3} \rangle.$$

If Q is uniaxial and $s > 0$ then $\lambda_{\max}(Q) = \frac{2}{3}s$ and $n = n_{\max}(Q)$, the corresponding eigenvector of Q. For general biaxial Q the director is often identified with $n_{\max}(Q)$.

If $Q = s(n \otimes n - \frac{1}{3}\mathbf{1})$ is uniaxial then

$$|Q|^2 = \frac{2s^2}{3}, \det Q = \frac{2s^3}{27}.$$

Proposition.
Given $Q = Q^T$, $\operatorname{tr} Q = 0$, Q *is uniaxial iff*

$$|Q|^6 = 54(\det Q)^2.$$

Proof. The characteristic equation of Q is

$$\det(Q - \lambda 1) = \det Q - \lambda \operatorname{tr} \operatorname{cof} Q + 0\lambda^2 - \lambda^3.$$

But $2\operatorname{tr} \operatorname{cof} Q = 2(\lambda_2\lambda_3 + \lambda_3\lambda_1 + \lambda_1\lambda_2) = (\lambda_1 + \lambda_2 + \lambda_3)^2 - (\lambda_1^2 + \lambda_2^2 + \lambda_3^2) = -|Q|^2$. Hence the characteristic equation is

$$\lambda^3 - \frac{1}{2}|Q|^2\lambda - \det Q = 0,$$

and the condition that $\lambda^3 - p\lambda + q = 0$ has two equal roots is that $p \geq 0$ and $4p^3 = 27q^2$.

Thus for nematic and cholesteric liquid crystals we have various choices for the order parameter:

the probability density function ρ (∞-dimensional, Onsager-type theories)

Q (5-dimensional, Landau - de Gennes theory)

(s, n) (3-dimensional, Ericksen theory)

n (2-dimensional, Oseen-Frank theory)

For smectics we will add an extra order parameter, the molecular number density $r = r(x)$, the number of molecules in $B(x, \delta)$ divided by the volume of $B(x, \delta)$.

2. The Landau – de Gennes, Oseen – Frank and Ericksen theories

Landau – de Gennes theory

For simplicity we work at a constant temperature θ. Let Ω be a bounded domain in $\mathbb{R}^3$. At each point $x \in \Omega$, we have a corresponding order parameter tensor $Q(x)$. We suppose that the material is described by a free-energy density $\psi(Q, \nabla Q, \theta)$, so that the total free energy is given by

$$I_\theta(Q) = \int_\Omega \psi(Q(x), \nabla Q(x), \theta)\, dx.$$

We write $\psi = \psi(Q, D, \theta)$, where D is a third order tensor.

Frame-indifference

We consider two observers, one using the Cartesian coordinates $x = (x_1, x_2, x_3)$ and the second using translated and rotated coordinates $z = \bar{x} + R(x - \bar{x})$, where $R \in SO(3)$, and we require that

$$\psi(Q^*(\bar{x}), \nabla_z Q^*(\bar{x}), \theta) = \psi(Q(\bar{x}), \nabla_x Q(\bar{x}), \theta),$$

where $Q^*(\bar{x})$ is the value of Q measured by the second observer.

Then

$$\begin{aligned} Q^*(\bar{x}) &= \int_{S^2}(q \otimes q - \frac{1}{3}\mathbf{1})d\mu_{\bar{x}}(R^T q) \\ &= \int_{S^2}(Rp \otimes Rp - \frac{1}{3}\mathbf{1})d\mu_{\bar{x}}(p) \\ &= R\int_{S^2}(p \otimes p - \frac{1}{3}\mathbf{1})d\mu_{\bar{x}}(p)R^T. \end{aligned}$$

Hence $Q^*(\bar{x}) = RQ(\bar{x})R^T$.

Therefore

$$\begin{aligned}\frac{\partial Q^*_{ij}}{\partial z_k}(\bar{x}) &= \frac{\partial}{\partial z_k}(R_{il}Q_{lm}(\bar{x})R_{jm}) \\ &= \frac{\partial}{\partial x_p}(R_{il}Q_{lm}R_{jm})\frac{\partial x_p}{\partial z_k} \\ &= R_{il}R_{jm}R_{kp}\frac{\partial Q_{lm}}{\partial x_p}.\end{aligned}$$

Thus, for every $R \in SO(3)$,

$$\psi(Q^*, D^*, \theta) = \psi(Q, D, \theta),$$

where $Q^* = RQR^T$, $D^*_{ijk} = R_{il}R_{jm}R_{kp}D_{lmp}$.
Such ψ are called *hemitropic*.

Material symmetry

The requirement that

$$\psi(Q^*(\bar{x}), \nabla_z Q^*(\bar{x}), \theta) = \psi(Q(\bar{x}), \nabla_x Q(\bar{x}), \theta)$$

when $z = \bar{x} + \hat{R}(x - \bar{x})$, where $\hat{R} = 1 - 2e \otimes e$, $|e| = 1$, is a *reflection* is a condition of material symmetry satisfied by nematics, but not cholesterics, whose molecules have a chiral nature.

Since any $R \in O(3)$ can be written as $\hat{R}\tilde{R}$, where $\tilde{R} \in SO(3)$ and $\hat{R}$ is a reflection, for a nematic

$$\psi(Q^*, D^*, \theta) = \psi(Q, D, \theta)$$

where $Q^* = RQR^T$, $D^*_{ijk} = R_{il}R_{jm}R_{kp}D_{lmp}$ and $R \in O(3)$. Such ψ are called *isotropic*.

Bulk and elastic energies

We can decompose ψ as

$$\begin{aligned}\psi(Q,\nabla Q,\theta) &= \psi(Q,0,\theta)+(\psi(Q,\nabla Q,\theta)-\psi(Q,0,\theta))\\ &= \psi_B(Q,\theta)+\psi_E(Q,\nabla Q,\theta)\\ &= \text{ bulk } + \text{ elastic},\end{aligned}$$

so that $\psi_B(Q,\theta)=\psi(Q,0,\theta)$.

By frame-indifference we have that

$$\psi_B(RQR^T,\theta)=\psi_B(Q,\theta) \text{ for all } R\in SO(3).$$

Hence $\psi_B(Q,\theta)$ depends only on the invariants of Q, and one of these, $\operatorname{tr} Q$, is zero. Hence $\psi_B(Q,\theta)=\widehat{\psi}_B(|Q|^2,\det Q,\theta)$ for some function $\widehat{\psi}_B$.

The domain of ψ

For what Q, D should $\psi(Q, D, \theta)$ be defined?
Let $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$
$\mathcal{D} = \{D = (D_{ijk}) : D_{ijk} = D_{jik}, D_{kki} = 0\}$.
We suppose that $\psi(\cdot, \theta) : \operatorname{dom}\psi \to \mathbb{R}$, where

$$\operatorname{dom}\psi = \{(Q, D) \in \mathcal{E} \times \mathcal{D}, \lambda_i(Q) > -\frac{1}{3}\}.$$

But in order to differentiate ψ easily with respect to its arguments, it is convenient to extend $\psi(\cdot, \theta)$ to all of $M^{3\times 3}\times$(3rd order tensors). To do this first set $\psi(Q, D, \theta) = \infty$ if $(Q, D) \in \mathcal{E} \times \mathcal{D}$ with some $\lambda_i(Q) \leq -\frac{1}{3}$.

Then note that

$$PA = \frac{1}{2}(A + A^T) - \frac{1}{3}(\mathrm{tr}\, A)\mathbf{1}$$

is the orthogonal projection of $M^{3\times 3}$ onto $\mathcal{E}$. So for any Q, D we can set

$$\psi(Q, D, \theta) = \psi(PQ, PD, \theta),$$

where $(PD)_{ijk} = \frac{1}{2}(D_{ijk} + D_{jik}) - \frac{1}{3}D_{llk}\delta_{ij}$.

Thus we can assume that ψ satisfies

$$\frac{\partial \psi}{\partial Q_{ij}} = \frac{\partial \psi}{\partial Q_{ji}}, \ \frac{\partial \psi}{\partial Q_{ii}} = 0,$$

$$\frac{\partial \psi}{\partial D_{ijk}} = \frac{\partial \psi}{\partial D_{jik}}, \ \frac{\partial \psi}{\partial D_{iik}} = 0.$$

Q-tensor description of the isotropic to nematic phase transformation

Following de Gennes, Schophol & Sluckin PRL 59(1987), Mottram & Newton, *Introduction to Q-tensor theory* arXiv:1409.3542, we consider the special quartic bulk energy

$$\psi_B(Q,\theta) = a(\theta)\mathrm{tr}\,Q^2 - \frac{2b}{3}\mathrm{tr}\,Q^3 + \frac{c}{2}\mathrm{tr}\,Q^4,$$

where $b > 0, c > 0, a = \alpha(\theta - \theta^*), \alpha > 0$.

Then

$$\psi_B = a\sum_{i=1}^{3}\lambda_i^2 - \frac{2b}{3}\sum_{i=1}^{3}\lambda_i^3 + \frac{c}{2}\sum_{i=1}^{3}\lambda_i^4.$$

ψ_B attains a minimum subject to $\sum_{i=1}^{3}\lambda_i = 0$. A calculation shows that the critical points have two λ_i equal, so that $\lambda_1 = \lambda_2 = \lambda, \lambda_3 = -2\lambda$ say, and that

$$\lambda(a + b\lambda + 3c\lambda^2) = 0.$$

Hence $\lambda = 0$ or $\lambda = \lambda_\pm$, and

$$\lambda_\pm = \frac{-b \pm \sqrt{b^2 - 12ac}}{6c}.$$

For such a critical point we have that

$$\psi_B = 4a\lambda^2 + 4b\lambda^3 + 9c\lambda^4,$$

which is negative when

$$4a + 4b\lambda + 9c\lambda^2 = a + b\lambda < 0.$$

A short calculation then shows that $a + b\lambda_- < 0$ if and only if $a < \frac{2b^2}{27c}$.

Hence we find that there is a phase transformation from an isotropic fluid to a uniaxial nematic phase at the critical temperature $\theta_{\mathrm{NI}} = \theta^* + \frac{2b^2}{27\alpha c}$. If $\theta > \theta_{\mathrm{NI}}$ then the unique minimizer of ψ_B is $Q = 0$.

If $\theta < \theta_{\mathrm{NI}}$ then the minimizers are

$$Q = s_{\mathrm{min}}(n \otimes n - \frac{1}{3}1) \text{ for } n \in S^2,$$

where $s_{\mathrm{min}} = \frac{b+\sqrt{b^2-12ac}}{2c} > 0$.

Form of the elastic energy.

Usually it is assumed that $\psi_E(Q, \nabla Q, \theta)$ is quadratic in ∇Q. Examples of isotropic functions quadratic in ∇Q are:

$$I_1 = Q_{ij,j}Q_{ik,k}, \quad I_2 = Q_{ik,j}Q_{ij,k}$$
$$I_3 = Q_{ij,k}Q_{ij,k}, \quad I_4 = Q_{lk}Q_{ij,l}Q_{ij,k}$$

Note that

$I_1 - I_2 = (Q_{ij}Q_{ik,k})_{,j} - (Q_{ij}Q_{ik,j})_{,k}$

is a null Lagrangian.

An example of a hemitropic, but not isotropic, function is

$$I_5 = \varepsilon_{ijk}Q_{il}Q_{jl,k}.$$

For the elastic energy we take

$$\psi_E(Q, \nabla Q, \theta) = \sum_{i=1}^{4 \text{ or } 5} L_i I_i,$$

where the $L_i = L_i(\theta)$ are material constants, with $L_5 = 0$ for nematics.

To summarize, we assume that for nematics and cholesterics

$$\psi(Q, \nabla Q, \theta) = \psi_B(Q, \theta) + \sum_{i=1}^{4 \text{ or } 5} L_i I_i,$$

where $\psi_B(Q, \theta) = \hat{\psi}_B(|Q|^2, \det Q, \theta)$, and $L_i = L_i(\theta)$, with $L_5 = 0$ for nematics.

The constrained theory

For small L_i it is reasonable to consider a constrained theory in which we require Q to be uniaxial with a constant scalar order parameter $s = s(\theta) > 0$, so that

$$Q(x) = s\left(n(x) \otimes n(x) - \frac{1}{3}\mathbf{1}\right), \quad n(x) \in S^2.$$

(For rigorous work studying whether and when this is justified see Majumdar & Zarnescu, Nguyen & Zarnescu, Bauman, Phillips & Park, Canevari.)

Then the bulk energy just depends on θ, so we only have to consider the elastic energy

$$I_\theta(Q) = \int_\Omega \psi_E(Q, \nabla Q, \theta)\, dx.$$

Oseen-Frank energy

Formally calculating ψ_E in terms of $n, \nabla n$ we obtain the Oseen-Frank energy functional

$$I_\theta(n) = \int_\Omega [K_1(\operatorname{div} n)^2 + K_2(n \cdot \operatorname{curl} n + q_0)^2 + K_3|n \times \operatorname{curl} n|^2 + (K_2 + K_4)(\operatorname{tr}(\nabla n)^2 - (\operatorname{div} n)^2)]\, dx,$$

where

$K_1 = L_1 s^2 + L_2 s^2 + 2L_3 s^2 - \frac{2}{3} L_4 s^3,$

$K_2 = 2L_3 s^2 - \frac{2}{3} L_4 s^3,$

$K_3 = L_1 s^2 + L_2 s^2 + 2L_3 s^2 + \frac{4}{3} L_4 s^3,$

$K_4 = L_2 s^2$, $q_0 = -\frac{L_5 s^2}{2K_2}$ and

$q_0 = 0$ for nematics, $q_0 \neq 0$ for cholesterics.

Boundary conditions

(a) Constrained LdG/Oseen-Frank theory.

(i) Strong anchoring

$$n(x) = \pm \bar{n}(x),\ x \in \partial\Omega.$$

Special cases:

1. (*Homeotropic*) $\bar{n}(x) = \nu(x)$,

$\nu(x) =$ unit outward normal

2. (*Planar*) $\bar{n}(x) \cdot \nu(x) = 0$.

(ii) Conical anchoring:

$$|n(x) \cdot \nu(x)| = \alpha(x) \in [0, 1],\ x \in \partial\Omega,$$

where $\nu(x)$ is the unit outward normal.

Special cases:

1. $\alpha(x) = 1$ homeotropic .
2. $\alpha(x) = 0$ *planar degenerate* (or *tangent*), director parallel to boundary but preferred direction not prescribed.

(iii) No anchoring: no condition on n on $\partial\Omega$. This is natural mathematically but seems difficult to realize in practice.

(iv) Weak anchoring. No boundary condition is explicitly imposed, but a surface energy term is added, of the form

$$\int_{\partial\Omega} w(x,n)\,dS$$

where $w(x,n) = w(x,-n)$.

For example, corresponding to strong anchoring we can choose

$$w(x,n) = K(1-(n(x)\cdot\bar{n}(x))^2),$$

formally recovering the strong anchoring condition in the limit $K \to \infty$.

(b) Landau - de Gennes

(i) Strong anchoring:

$$Q(x) = \bar{Q}(x),\ x \in \partial\Omega.$$

(ii) Weak anchoring: add surface energy term

$$\int_{\partial\Omega} w(x, Q)\, dS.$$

Ericksen theory

Similarly, if we use the uniaxial ansatz

$$Q(x) = s(x)\left(n(x) \otimes n(x) - \frac{1}{3}\mathbf{1}\right)$$

we get the *Ericksen theory*, for which the order parameter is the pair $(s, \mathbf{n})$, $|\mathbf{n}| = 1$, with corresponding energy

$$I_E(s, \mathbf{n}) = \int_\Omega W(s, \nabla s, \mathbf{n}, \nabla \mathbf{n})\, d\mathbf{x}.$$

But is the derivation of the Oseen-Frank theory from Landau - de Gennes correct? The constrained Landau - de Gennes theory is invariant to changing n to $-n$, but is Oseen-Frank?

The issue here is whether a line field can be oriented, i.e. turned into a vector field by assigning an orientation at each point. If we don't care about the regularity of the vector field this can always be done by choosing an arbitrary orientation at each point.

For s a nonzero constant and $n \in S^2$ let

$$\Pi(n) = s\left(n \otimes n - \frac{1}{3}\mathbf{1}\right),$$

and set

$$\mathcal{Q} = \left\{Q \in M^{3\times 3} : Q = \Pi(n) \text{ for some } n \in S^2\right\}.$$

Thus $\Pi : S^2 \to \mathcal{Q}$. The operator Π provides us with a way of 'unorienting' an S^2-valued vector field.

Given $Q \in W^{1,p}(\Omega, \mathcal{Q})$ we say Q is *orientable* if we can write

$$Q(x) = \Pi(n(x)),$$

where $n \in W^{1,p}(\Omega, S^2)$. That is Q has a *lifting* to $W^{1,p}(\Omega, S^2)$.

Relating the Q and n descriptions

Proposition (JB/Zarnescu 2011)
Let $Q = s(n \otimes n - \frac{1}{3}\mathbf{1})$, s a nonzero constant, $|n| = 1$ a.e., belong to $W^{1,p}(\Omega; \mathbb{R}P^2)$ for some p, $1 \leq p < \infty$. If n is continuous along almost every line parallel to the coordinate axes, then $n \in W^{1,p}(\Omega, S^2)$ (in particular n is orientable), and

$$n_{i,k} = Q_{ij,k} n_j.$$

Theorem.(JB/Zarnescu 2011) *An orientable Q has exactly two orientations.*

Proof

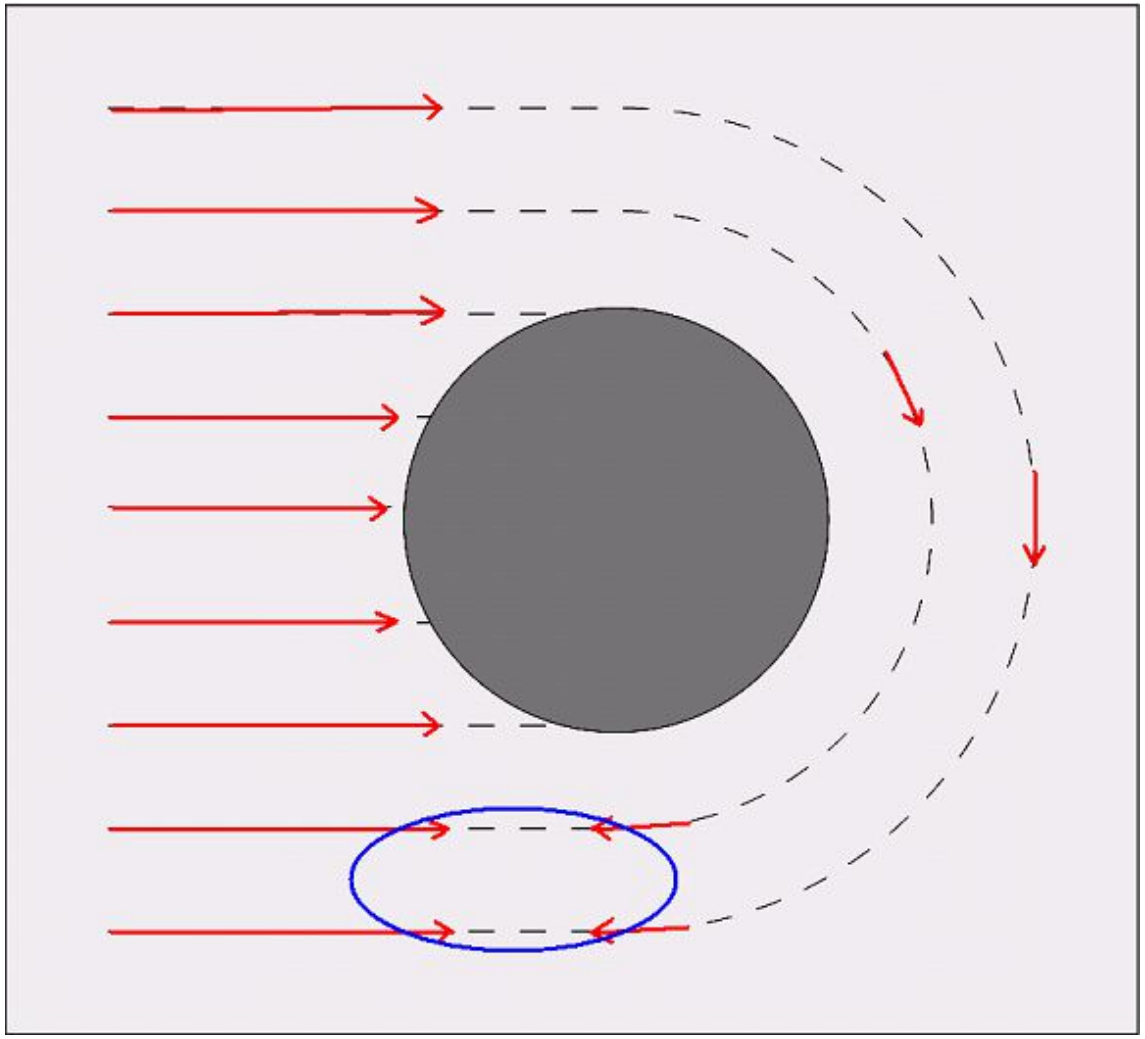
Suppose that n and τn both generate Q and belong to $W^{1,1}(\Omega, S^2)$, where $\tau^2(x) = 1$ a.e.. Let $C \subset \Omega$ be a cube with sides parallel to the coordinate axes. Let x_2, x_3 be such that the line $x_1 \mapsto (x_1, x_2, x_3)$ intersects C. Let $L(x_2, x_3)$ denote the intersection. For a.e. such x_2, x_3 we have that $n(x)$ and $\tau(x)n(x)$ are absolutely continuous in x_1 on $L(x_2, x_3)$. Hence $n(x) \cdot \tau(x)n(x) = \tau(x)$ is continuous in x_1, so that $\tau(x)$ is constant on $L(x_2, x_3)$.

Let $\varphi \in C_0^\infty(C)$. Then by Fubini's theorem

$$\int_C \tau \varphi_{,1} dx = \int_C (\tau\varphi)_{,1} dx = 0,$$

so that the weak derivative $\tau_{,1}$ exists in C and is zero. Similarly the weak derivatives $\tau_{,2}, \tau_{,3}$ exist in C and are zero. Thus $\nabla\tau = 0$ in C and hence τ is constant in C. Since Ω is connected, τ is constant in Ω, and thus $\tau \equiv 1$ or $\tau \equiv -1$ in Ω.

A smooth nonorientable line field in a non simply connected region.



Theorem (JB/Zarnescu 2011) *If Ω is simply-connected and $Q \in W^{1,p}$, $p \geq 2$, then Q is orientable.*

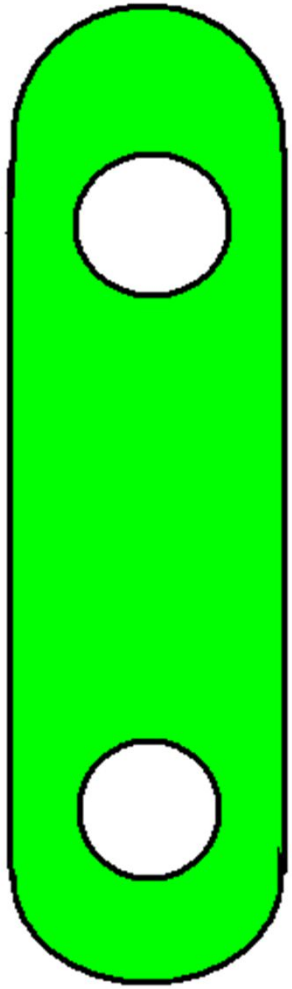
(There is a related topologically more general lifting result of Bethuel and Chiron 2007. Some details of the proof are given in the 2015 Oxford thesis of C. Hopper.)

Thus in a simply-connected region the uniaxial de Gennes and Oseen-Frank theories are equivalent.

Ingredients of proof

- Lifting possible if Q is smooth and Ω is simply connected.
- Pakzad-Rivière theorem (2003) implies that if $\partial\Omega$ is smooth, then there is a sequence of smooth $Q^{(j)} : \Omega \to \mathbb{R}P^2$ converging weakly to Q in $W^{1,2}$.
- We can approximate a simply-connected domain with boundary of class C^0 by ones that are simply-connected with smooth boundary. In JB/Zarnescu (2014) it is shown that a bounded domain with boundary of class C^0 can always be approximated from the inside and out by diffeomorphic domains with smooth boundary. (This step can be avoided using an argument of Bedford (2015).)
- Orientability is preserved under weak convergence.

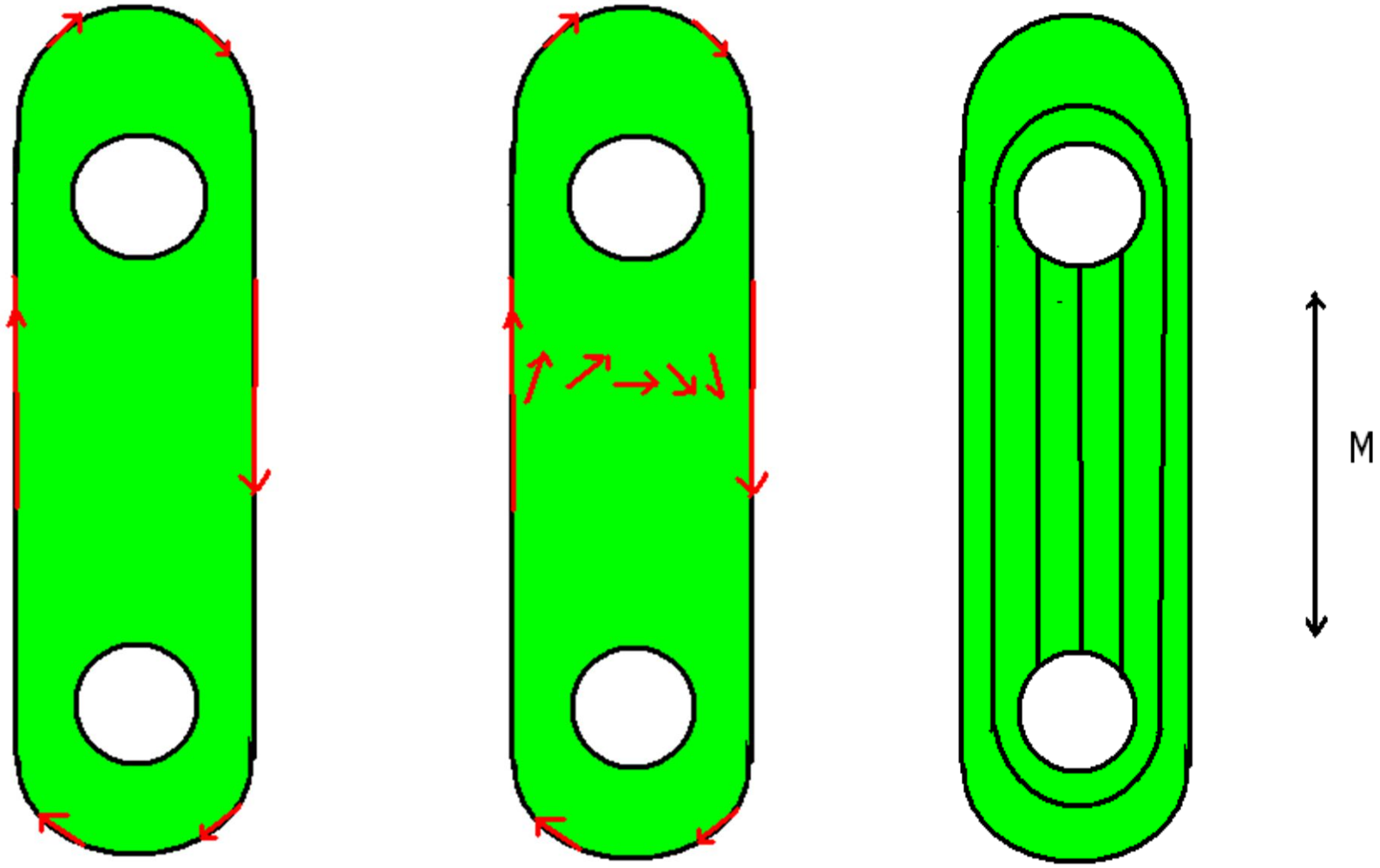
Non-equivalence of Oseen-Frank and constrained LdG in non simply-connected 2D domain (JB/Zarnescu 2011)

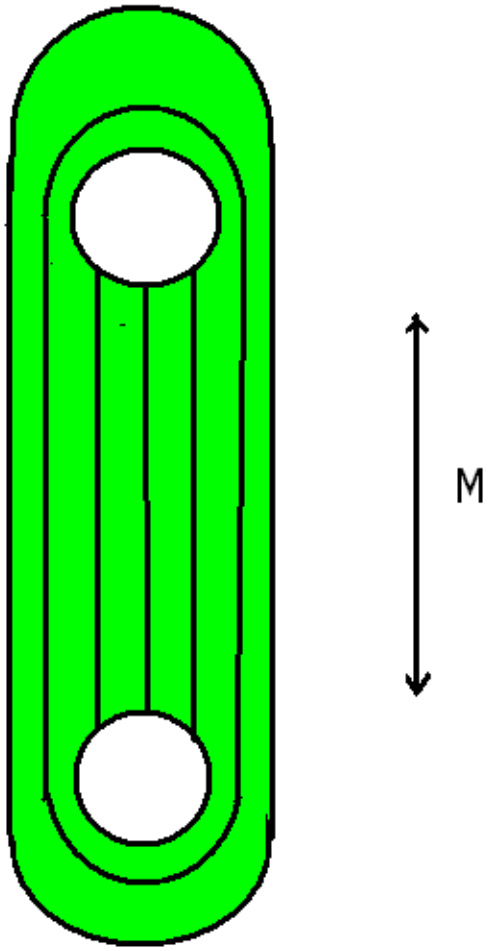


Tangent boundary conditions on outer boundary. No (free) boundary conditions on inner circles.

$$I(Q) = \int_\Omega |\nabla Q|^2 dx$$

$$I(n) = 2s^2 \int_\Omega |\nabla n|^2 dx$$


M



For M large enough the minimum energy configuration is unoriented, even though there is a minimizer among oriented maps. (In fact this is true whatever M is.)

If the boundary conditions correspond to the Q-field shown, then there is no orientable Q that satisfies them.

Existence in Landau – de Gennes theory

Let $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$.

Theorem (Davis & Gartland 1998)
Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with smooth boundary $\partial\Omega$. Let $\psi_B(\cdot,\theta)$ be continuous and bounded below, $L_4 = L_5 = 0$ and

$$L_3 > 0, -L_3 < L_2 < 2L_3, -\frac{3}{5}L_3 - \frac{1}{10}L_2 < L_1.$$

Let $\bar{Q} : \partial\Omega \to \mathcal{E}$ be smooth. Then

$$I_\theta(Q) = \int_\Omega [\psi_B(Q,\theta) + \sum_{i=1}^{3} L_i I_i(\nabla Q)]\, dx$$

attains a minimum on

$$\mathcal{A} = \{Q \in W^{1,2}(\Omega;\mathcal{E}) : Q|_{\partial\Omega} = \bar{Q}\}.$$

Proof

By the direct method of the calculus of variations. Let $Q^{(j)}$ be a minimizing sequence in $\mathcal{A}$. the inequalities on the L_i imply that

$$\sum_{i=1}^{3} L_i I_i(\nabla Q) \geq \mu |\nabla Q|^2$$

for all Q (in particular $\sum_{i=1}^{3} I_i(\nabla Q)$ is convex in ∇Q). By the Poincaré inequality we have that

$$Q^{(j)} \text{ is bounded in } W^{1,2}$$

so that for a subsequence (not relabelled)

$$Q^{(j)} \rightharpoonup Q^* \text{ in } W^{1,2}$$

for some $Q^* \in \mathcal{A}$.

We may also assume, by the compactness of the embedding of $W^{1,2}$ in L^2, that $Q^{(j)} \to Q$ a.e. in Ω. But

$$I(Q^*) \leq \liminf_{j \to \infty} I(Q^{(j)})$$

by Fatou's lemma and the convexity in ∇Q. Hence Q^* is a minimizer.

In the quartic case we can use elliptic regularity (Davis & Gartland) to show that any minimizer Q^* is smooth.

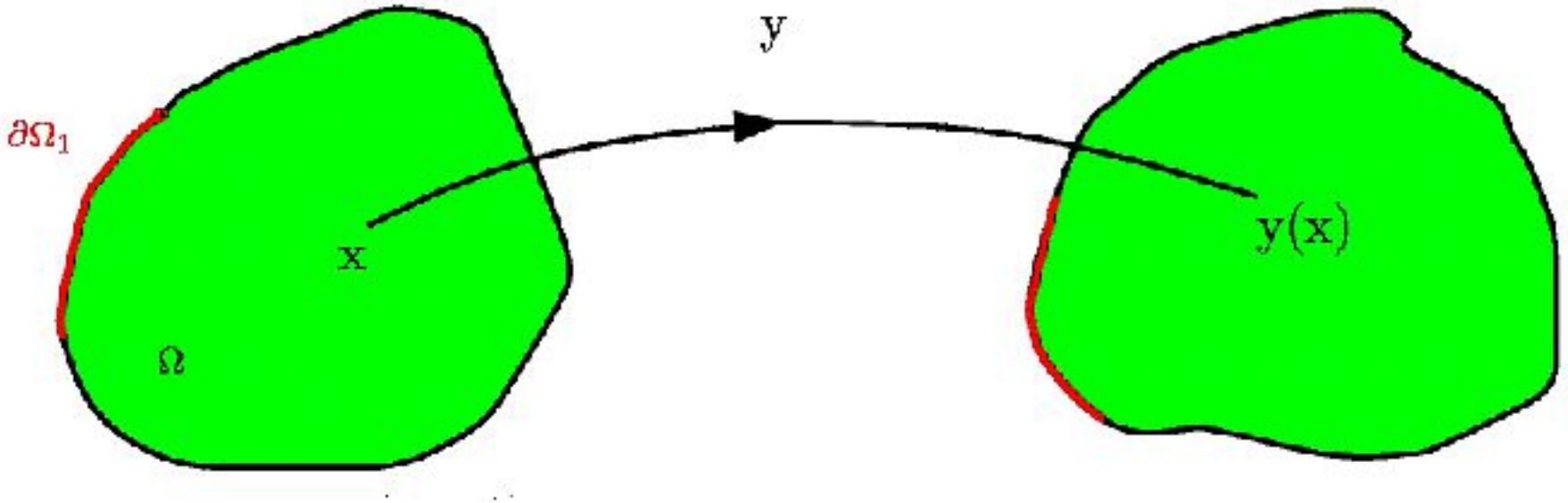
But what if $L_4 \neq 0$?

Proposition (JB/Majumdar) *For any boundary conditions, if* $L_4 \neq 0$ *then*

$$I_\theta(Q) = \int_\Omega [\psi_B(Q,\theta) + \sum_{i=1}^{4} L_i I_i]\, dx$$

is unbounded below.

Analogy with nonlinear elasticity



Minimize

$$I(y) = \int_\Omega W(Dy(x))\,dx$$

subject to suitable boundary conditions, e.g. $y|_{\partial\Omega_1} = \bar{y}$.

To prevent interpenetration of matter we required that y is invertible, and in particular that

$$\det Dy(x) > 0 \text{ a.e. } x \in \Omega.$$

To help ensure this we assumed that

$$W(A) \to \infty \text{ as } \det A \to 0+$$

Correspondingly, it is natural to suppose that

$$\psi_B(Q,\theta) \to \infty \text{ as } \lambda_{\min}(Q) \to -\frac{1}{3}+ .$$

Such a suggestion was made by Ericksen in the context of his model of nematic liquid crystals.

We show how such an ψ_B can be constructed on the basis of a microscopic model, the interpretation being that perfectly aligned states have entropy $-\infty$.

This will also allow us to get existence of a minimizer when $L_4 \neq 0$.

3. Onsager theory (JB/Majumdar).

In the Onsager model the probability measure μ is assumed to be continuous with density $\rho = \rho(p)$, and the bulk free-energy at temperature $\theta > 0$ has the form

$$I_\theta(\rho) = U(\rho) - \theta\eta(\rho),$$

where the entropy is given by

$$\eta(\rho) = -k_B \int_{S^2} \rho(p) \ln \rho(p)\, dp,$$

where k_B is Boltzmann's constant.

We suppose that U is given by

$$U(\rho) = \int_{S^2} \int_{S^2} K(p,q)\rho(p)\rho(q)\, dp\, dq.$$

We assume that K is frame-indifferent, so that

$$K(Rp, Rq) = K(p,q) \text{ for all } R \in SO(3),$$

which holds iff

$$K(p,q) = k(p \cdot q)$$

for some $k : [-1,1] \to \mathbb{R}$.

Two important examples of the potential k are:

(i) $k(p \cdot q) = \kappa(\frac{1}{3} - (p \cdot q)^2)$ (Maier-Saupe)

(ii) $k(p \cdot q) = \kappa\sqrt{1 - (p \cdot q)^2}$ (Onsager),

where $\kappa > 0$ is a coupling constant.

We will assume that κ is independent of θ. If κ depends on θ (due to steric effects) then the analysis is similar.

Denoting by

$$Q(\rho) = \int_{S^2} (p \otimes p - \frac{1}{3}\mathbf{1})\rho(p)\, dp$$

the corresponding Q-tensor, we have that

$$\begin{aligned} |Q(\rho)|^2 &= \int_{S^2}\int_{S^2} (p \otimes p - \frac{1}{3}\mathbf{1}) \cdot (q \otimes q - \frac{1}{3}\mathbf{1})\rho(p)\rho(q) dp\, dq \\ &= \int_{S^2}\int_{S^2} [(p \cdot q)^2 - \frac{1}{3}]\rho(p)\rho(q)\, dp\, dq. \end{aligned}$$

Hence for the Maier-Saupe potential $U(\rho) = -\kappa|Q(\rho)|^2$ and

$$I_\theta(\rho) = k_B\theta \int_{S^2} \rho(p) \ln \rho(p)\, dp - \kappa|Q(\rho)|^2.$$

Theorem (Fatkullin & Slastikov 2005, Liu, Zhang & Zhang 2005)
For the Maier-Saupe potential all critical points of ρ can be explicitly determined and are uniaxial. The isotropic state $\bar{\rho} = \frac{1}{4\pi}$ is a critical point for all θ. At the largest bifurcation point θ_c there is a transcritical bifurcation to a uniaxial state, so that $\bar{\rho}$ is stable for $\theta > \theta_c$, and unstable for $\theta < \theta_c$.

Using equivariant bifurcation theory and an analysis involving spherical harmonics, Michaela Vollmer (2015) has established a similar bifurcation picture for a class of potentials k including the Onsager potential (see also related work of Wachsmuth 2006).

For the Maier-Saupe potential, given Q we define (here and below we follow JB/Majumdar 2012)

$$\begin{aligned}\psi_B(Q,\theta) &= \inf_{\{\rho:Q(\rho)=Q\}} U(\rho) - \theta\eta(\rho) \\ &= k_B\theta \inf_{\{\rho:Q(\rho)=Q\}} \int_{S^2} \rho \ln \rho \, dp - \kappa|Q|^2.\end{aligned}$$

(cf. Katriel, J., Kventsel, G. F., Luckhurst, G. R. and Sluckin, T. J.(1986))

Thus we just need to understand how to minimize

$$I(\rho) = \int_{S^2} \rho(p) \ln \rho(p) \, dp$$

subject to $Q(\rho) = Q$.

Given Q with $Q = Q^T, \operatorname{tr} Q = 0$ and satisfying $\lambda_i(Q) > -1/3$ we seek to minimize $I(\rho) = \int_{S^2} \rho(p) \ln \rho(p)\, dp$ on

$$\mathcal{A}_Q = \{\rho \in L^1(S^2) : \rho \geq 0, \int_{S^2} \rho(p)\, dp = 1, Q(\rho) = Q\}.$$

Remark: We do not impose the condition $\rho(p) = \rho(-p)$, since it turns out that the minimizer in $\mathcal{A}_Q$ satisfies this automatically.

Lemma. $\mathcal{A}_Q$ is nonempty.

Sketch of proof. We can suppose that $Q = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$. The singular measure

$$\mu(p) = \frac{1}{2} \sum_{i=1}^{3} \left(\lambda_i + \frac{1}{3} \right) (\delta_{e_i} + \delta_{-e_i})$$

satisfies $\int_{S^2} \left(p \otimes p - \frac{1}{3}\mathbf{1} \right) d\mu(p) = Q$ and can be approximated by an L^1 function ρ satisfying $Q(\rho) = Q$.

Theorem. I attains a minimum at a unique $\rho_Q \in \mathcal{A}_Q$.

Proof. Let $\rho^{(j)}$ be a minimizing sequence for I in $\mathcal{A}_Q$. By the de la Vallée Poussin criterion and the superlinear growth of $\rho \ln \rho$, we may assume that $\rho^{(j)} \rightharpoonup \rho_Q$ in $L^1(S^2)$ for some ρ_Q, and $\rho_Q \geq 0$, $Q(\rho_Q) = Q$.

Since $\rho \ln \rho$ is convex,
$I(\rho_Q) \leq \liminf_{j\to\infty} I(\rho^{(j)})$,
so that ρ_Q is a minimizer, which is unique since $\rho \ln \rho$ is strictly convex.

The Euler-Lagrange equation for I

Theorem. Let $Q = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$. Then

$$\rho_Q(p) = \frac{\exp(\mu_1 p_1^2 + \mu_2 p_2^2 + \mu_3 p_3^2)}{Z(\mu_1, \mu_2, \mu_3)},$$

where

$$Z(\mu_1, \mu_2, \mu_3) = \int_{S^2} \exp(\mu_1 p_1^2 + \mu_2 p_2^2 + \mu_3 p_3^2)\, dp.$$

The μ_i (unique up to adding a constant to each) solve the equations

$$\frac{\partial \ln Z}{\partial \mu_i} = \lambda_i + \frac{1}{3}, \quad i = 1, 2, 3.$$

To show that ρ_Q satisfies the corresponding Euler-Lagrange equation, the μ_i appearing as Lagrange multipliers, is a bit tricky because of the possibility that ρ_Q is not bounded away from zero. A quicker proof is to use a 'dual' variational principle for $\mu = (\mu_1, \mu_2, \mu_3)$ (cf Mead & Papanicolaou 1984), from which the existence of a minimizer ρ_Q also follows.

Let $f(Q) = I(\rho_Q) = \inf_{\rho \in \mathcal{A}_Q} I(\rho)$, so that

$$\psi_B(Q, \theta) = \theta k_B f(Q) - \kappa |Q|^2.$$

Hence the bulk free energy has the form

$$\psi_B(Q, \theta) = k_B \theta \left(\sum_{i=1}^{3} \mu_i (\lambda_i + \frac{1}{3}) - \ln Z(\mu) \right) - \kappa \sum_{i=1}^{3} \lambda_i^2.$$

Theorem

f is strictly convex in Q and

$$\lim_{\lambda_{\min}(Q)\to -\frac{1}{3}+} f(Q) = \infty.$$

Proof

The strict convexity of f follows from that of $\rho \ln \rho$. Suppose that $\lambda_{\min}(Q^{(j)}) \to -\frac{1}{3}$ but $f(Q^{(j)})$ remains bounded. Then

$$Q^{(j)} e^{(j)} . e^{(j)} + \frac{1}{3}|e^{(j)}|^2 = \int_{S^2} \rho_{Q^{(j)}}(p)(p \cdot e^{(j)})^2 dp \to 0,$$

where $e^{(j)}$ is the eigenvector of $Q^{(j)}$ corresponding to $\lambda_{\min}(Q^{(j)})$.

But we can assume that $\rho_{Q^{(j)}} \rightharpoonup \rho$ in $L^1(S^2)$, where $\int_{S^2} \rho(p)\, dp = 1$ and that $e^{(j)} \to e$, $|e| = 1$. Passing to the limit we deduce that

$$\int_{S^2} \rho(p)(p \cdot e)^2 dp = 0.$$

But this means that $\rho(p) = 0$ except when $p \cdot e = 0$, contradicting $\int_{S^2} \rho(p)\, dp = 1$. $\square$

Asymptotics

Theorem

$$C_1 - \frac{1}{2}\ln(\lambda_{\min}(Q) + \frac{1}{3}) \leq f(Q) \leq C_2 - \ln(\lambda_{\min}(Q) + \frac{1}{3})$$

for constants C_1, C_2.

The proof uses our initial construction of a function $\rho \in \mathcal{A}_Q$ to get the upper bound, and the dual variational principle to get the lower bound.

Other predictions

1. All stationary points uniaxial and phase transition predicted from isotropic to uniaxial nematic phase just as in the quartic model.

2. Minimizers ρ^* of $U(\rho) - \theta\eta(\rho)$ correspond to minimizers over Q of $\psi_B(Q, \theta)$. As already mentioned, these ρ^* were calculated and shown to be uniaxial by Fatkullin and Slastikov (2005), and by Liu, Zhang & Zhang (2005).

3. Existence when $L_4 \neq 0$ under suitable inequalities on the L_i, because $I_4 = Q_{lk}Q_{ij,l}Q_{ij,k} \geq -\frac{1}{3}|\nabla Q|^2$.

4. Near $Q = 0$ we have (see also Katriel *et al*) the expansion

$$\frac{1}{\theta k_B}\psi_B(Q,\theta) = \ln 4\pi + \left(\frac{15}{4} - \frac{\kappa}{2\theta k_B}\right)\mathrm{tr}\, Q^2 - \frac{225}{42}\mathrm{tr}\, Q^3 + \frac{225}{112}(\mathrm{tr}\, Q^2)^2 + \ldots$$

The ratio of the coefficients of the last two terms gives $\frac{b}{c} = 2$, while experimental values reported in the literature are for MBBA 1.19, and for 5CB 0.82.

Given appropriate boundary conditions, do minimizers of

$$I_\theta(Q) = \int_\Omega [\psi_B(Q,\theta) + \psi_E(Q, \nabla Q, \theta)]\, dx$$

have eigenvalues which are *bounded away from* $-\frac{1}{3}$, i.e. for some $\varepsilon > 0$

$$-\frac{1}{3}+\varepsilon \leq \lambda_{\mathsf{min}}(Q(x)) \leq \lambda_{\mathsf{max}}(Q(x)) < \frac{2}{3}-\varepsilon \text{ for a.e. } x \in \Omega?$$

If not, this would mean that a minimizer of I would have an unbounded integrand. Surely this is inconsistent with being a minimizer ....

Similar nonlinear elasticity problem: Do minimizers for suitable boundary conditions of

$$I(y) = \int_\Omega W(Dy)\,dx$$

with $W(A) \to \infty$ as $\det A \to 0+$ satisfy

$$\det Dy(x) \geq \varepsilon > 0 \text{ a.e. } x \in \Omega$$

for some $\varepsilon > 0$?

This seems to be very difficult.

One might think that for a minimizer to have the integrand infinite somewhere is some kind of contradiction, but in fact this is a common phenomenon in the calculus of variations, even in one dimension.

Example (B & Mizel)

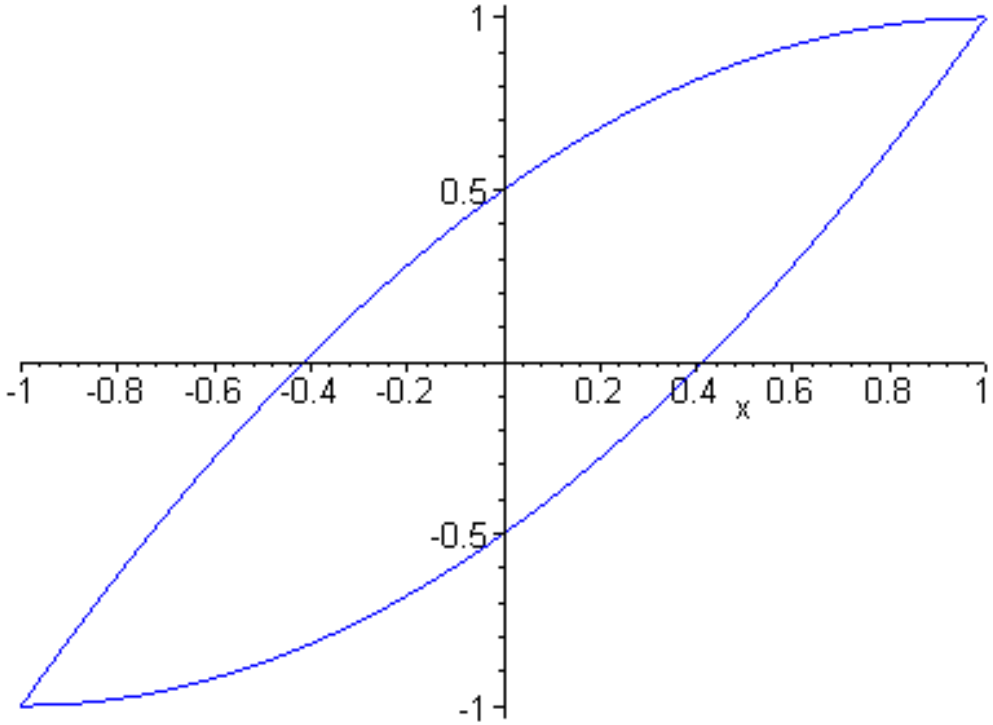
Minimize

$$I(u) = \int_{-1}^{1} [(x^4 - u^6)^2 u_x^{28} + \epsilon u_x^2]\, dx$$

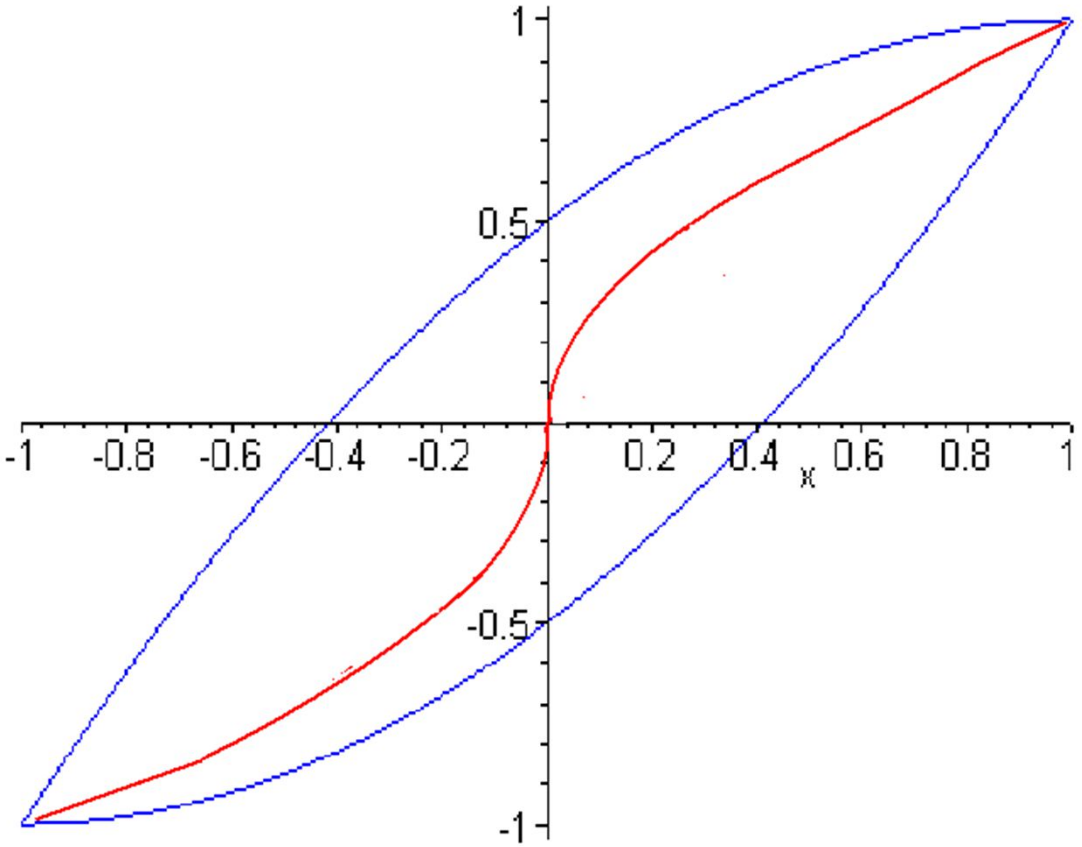
subject to

$$u(-1) = -1,\ u(1) = 1,$$

with $0 < \epsilon < \epsilon_0 \approx \cdot 001$.



Result of finite-element minimization, minimizing $I(u_h)$ for a piecewise affine approximation u_h to u on a mesh of size h, when h is very small. The method converges and produces two curves $u^{\pm}$.



However the real minimizer is u^*, which has a singularity

$$u^*(x) \sim |x|^{\frac{2}{3}} \text{sign}\, x \text{ as } x \sim 0.$$

Theorem (JB/Majumdar) *Let Q minimize*

$$I_\theta(Q) = \int_\Omega [\psi_B(Q,\theta) + K(\theta)|\nabla Q|^2]\, dx,$$

subject to $Q(x) = Q_0(x)$ for $x \in \partial\Omega$, where $K(\theta) > 0$ and $Q_0(\cdot)$ is sufficiently smooth with $\lambda_{\min}(Q_0(x)) > -\frac{1}{3}$. Then

$$\lambda_{\min}(Q(x)) > -\frac{1}{3} + \varepsilon,$$

for some $\varepsilon > 0$ and Q is a smooth solution of the corresponding Euler-Lagrange equation.

Proof: Project using the nearest point projection onto the convex set

$$K = \{Q : f(Q) \leq M\}$$

for large M. It can be shown that this reduces *both* terms in the integral.

Open problem. Prove this for the case of three or more elastic constants. The above method does not work. In the three elastic constant case Evans, Kneuss & Tran prove partial regularity, but not $\lambda_{\min}(Q(x)) > -\frac{1}{3} + \varepsilon$. See also recent results in 2D of Bauman & Phillips.

Developments.

1. Jamie Taylor (2015) has generalized the construction of the singular potential to a broad class of moment problems, with various applications.

2. For studies of dynamics using the singular potential see
E. Feireisl, E. Rocca, G. Schimperna and A. Zarnescu 2013, 2014, M. Wilkinson 2015

4. The description of defects

Summary of LC models

For simplicity we drop the explicit dependence on the temperature θ.

Landau - de Gennes

$$I_{LdG}(Q) = \int_\Omega \left(\psi_B(Q) + \sum_{i=1}^{4 \text{ or } 5} L_i I_i \right) dx,$$

where $\psi_B(Q)$ has one of the forms discussed,

$$I_1 = Q_{ij,j}Q_{ik,k}, \quad I_2 = Q_{ik,j}Q_{ij,k},$$
$$I_3 = Q_{ij,k}Q_{ij,k}, \quad I_4 = Q_{lk}Q_{ij,l}Q_{ij,k},$$
$$I_5 = \varepsilon_{ijk}Q_{il}Q_{jl,k},$$

and the L_i are constants with $L_5 = 0$ for nematics.

Uniaxial ansatz $Q = s(n \otimes n - \frac{1}{3}\mathbf{1})$ for constant $s > 0$ leads to the

Oseen-Frank energy

$$I_{OF}(n) = \int_\Omega W(n, \nabla n)\, dx,$$

The work of Lamy (2014) shows/suggests that few equilibrium solutions of LdG are uniaxial (whereas most are nearly uniaxial).

where

$$W(n, \nabla n) = K_1(\operatorname{div} n)^2 + K_2(n \cdot \operatorname{curl} n + q_0)^2 + K_3|n \times \operatorname{curl} n|^2 + (K_2 + K_4)(\operatorname{tr}(\nabla n)^2 - (\operatorname{div} n)^2),$$

and the K_i and q_0 are constants with $q_0 = 0$ for nematics.

If $s = s(x)$ we get the Ericksen energy

$$I_E(s, n) = \int_\Omega W(s, \nabla s, n, \nabla n)\, dx.$$

Natural function spaces.

Landau - de Gennes: $Q \in W^{1,2}(\Omega, \mathcal{E})$, where $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$.

Oseen-Frank: $n \in W^{1,2}(\Omega, S^2)$. Indeed if $q_0 = 0$ then under the Ericksen inequalities

$$2K_1 > K_2 + K_4, \quad K_2 > |K_4|, \quad K_3 > 0$$

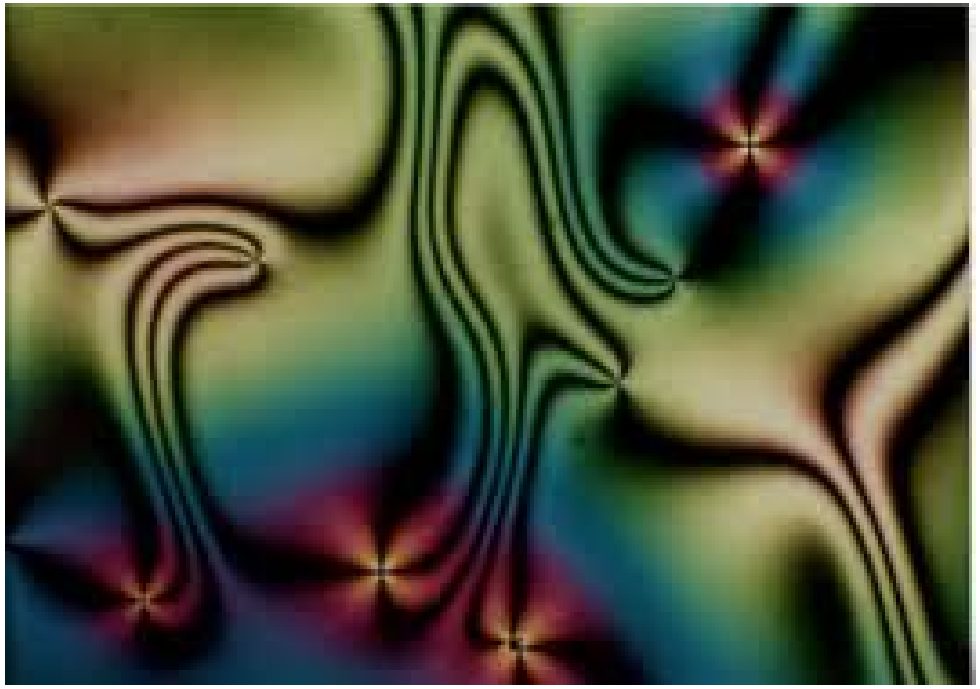
we have that

$$C'|\nabla n|^2 \leq W(n, \nabla n) \leq C|\nabla n|^2.$$

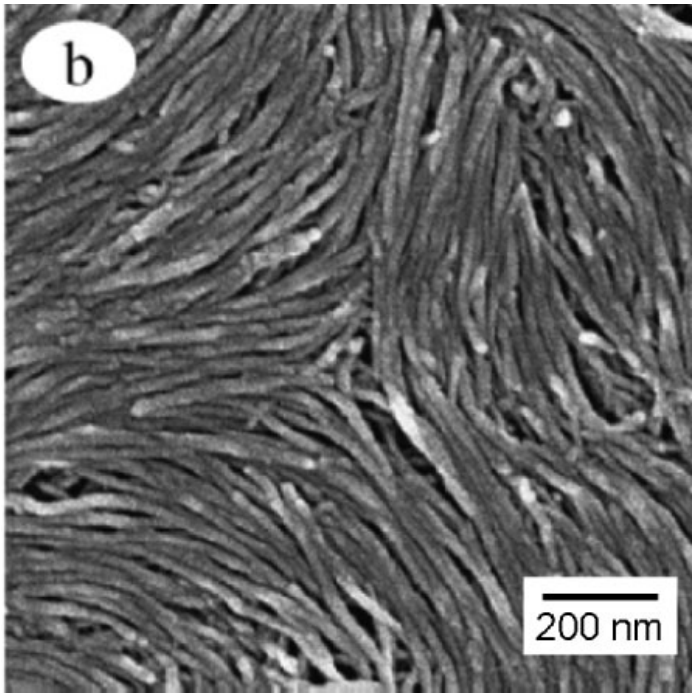
Ericksen: $(s, n) \in W^{1,2}(\Omega, \mathbb{R}) \times W^{1,2}(\Omega, S^2)$.

Defects

Roughly these can be thought of as regions of sharp change in the director or line field.

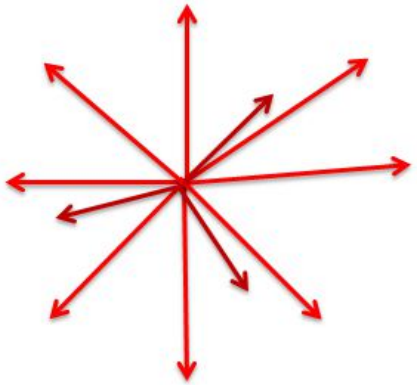


Schlieren texture of a nematic film
with surface point defects (boojums).
Oleg Lavrentovich (Kent State)



Zhang/Kumar 2007
Carbon nano-tubes as liquid crystals

Point defects



The Euler-Lagrange equation for

$$I_{OF} = \int_\Omega W(n, \nabla n)\, dx$$

has solutions representing point defects, e.g.

$$\tilde{n}(x) = \frac{x}{|x|} \quad \text{(radial hedgehog)}$$

$$\nabla \tilde{n}(x) = \tfrac{1}{|x|}(1 - n \otimes n)$$

$$|\nabla \tilde{n}(x)|^2 = \tfrac{2}{|x|^2}$$

$\int_0^1 r^{2-p} dr < \infty$ for $1 \leq p < 3$.

$\tilde{n} \in W^{1,p}$ for $1 \leq p < 3$ finite energy for quadratic models

If $q_0 = 0, K_1 = K_2 = K_3 = K,\ K_4 = 0$ (the *one constant approximation*) then $\tilde{\mathbf{n}}$ is the unique minimizer of $I_{OF} = K \int_\Omega |\nabla n|^2 d\mathbf{x}$ subject to its own boundary conditions (Brezis, Coron, Lieb 1986). In this case any minimizer is smooth except for a finite number of point defects (Schoen & Uhlenbeck 1982) at points $x(i)$ such that

$$n(x) \sim \pm R(i) \frac{x - x(i)}{|x - x(i)|} \text{ as } x \to x(i),$$

for some $R(i) \in SO(3)$.

Much less is known about point defects in the Oseen-Frank theory for the general case of unequal elastic constants. For example it is not known if a minimizer can have infinitely many point defects.

Helein (1987) proved that $\tilde{n}$ is not a minimizer if $8(K_1 - K_2) > K_3$, this condition being sharp (Cohen & Taylor (1990)).

Why is one-constant approximation easier?

Remark: for Oseen-Frank the Euler-Lagrange equation is

$$\frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial n_{i,j}}\right) - \frac{\partial W}{\partial n_i} = \lambda(x) n_i,$$

where the Lagrange multiplier $\lambda(x)$ is given by

$$\lambda(x) = \left(\frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial n_{k,j}}\right) - \frac{\partial W}{\partial n_k}\right) n_k.$$

$= 2K|\nabla n|^2$

for the one-constant approximation, but in general depends on second derivatives of n.

$\Delta n \cdot n = -|\nabla n|^2$

for $n \in S^2$

Description of defects in the Landau – de Gennes theory

Since weak solutions in Landau - de Gennes are smooth, modulo difficulties with the eigenvalue constraints, defects are not represented by singularities in Q. Rather they can be seen as singularities in the eigenvectors of Q, which can occur when eigenvalues coincide. (cf de Gennes, Biscari ...)

The situation might be different for free-energy densities $\psi(Q, \nabla Q)$ which are convex but not quadratic in ∇Q. For such integrands there is a counterexample of Šverák & Yan which has a singular minimizer of the form

$$Q(x) = |x| \left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} \mathbf{1} \right).$$

Point defects in the Ericksen and Landau - de Gennes theories

Since weak solutions in Landau - de Gennes are smooth, point defects are not represented by point singularities in Q. In both the Landau - de Gennes and Ericksen theories there are solutions to the Euler-Lagrange equations representing *melting hedgehogs*, of the form

$$Q(x) = s(|x|)\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}\mathbf{1}\right),$$

where $s(0) = 0$.

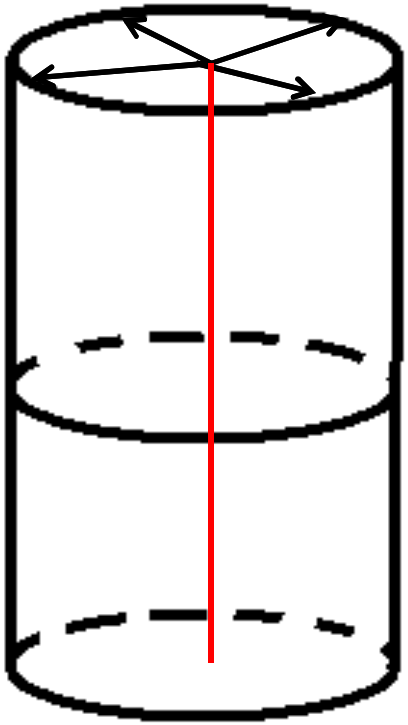
For the quartic bulk energy ψ_B and the one constant elastic energy such a solution is shown by Ignat, Nguyen, Slastikov & Zarnescu (2014) to be a local minimizer for $\Omega = \mathbb{R}^3$ subject to the condition at infinity

$$Q(x) \to s_{\text{min}} \left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}\mathbf{1} \right) \text{ as } |x| \to \infty,$$

where $s_{\text{min}} = \frac{b+\sqrt{b^2-12ac}}{2c} > 0$, for temperatures close to the nematic initiation temperature.

However for lower temperatures the melting hedgehog is not a minimizer (Gartland & Mkaddem (1999)) and numerical evidence suggests a biaxial torus structure for the defect without melting. Majumdar, Pisante & Henao (2015) show the existence biaxiality near defects in the low temperature limit.

Line defects

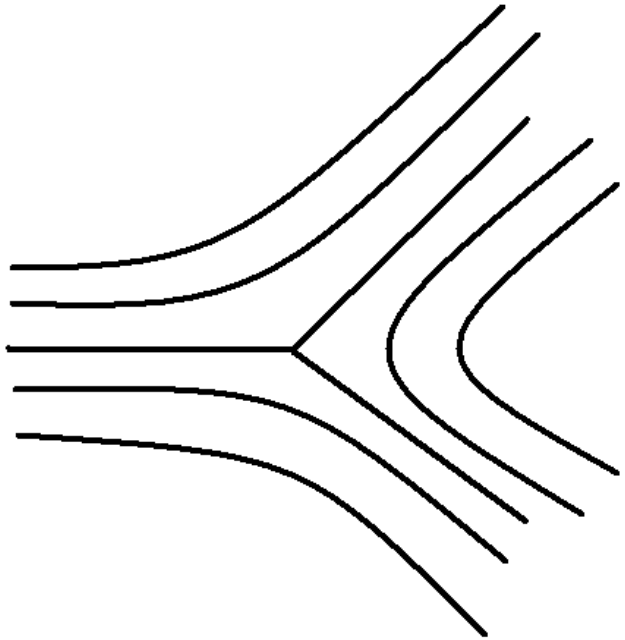


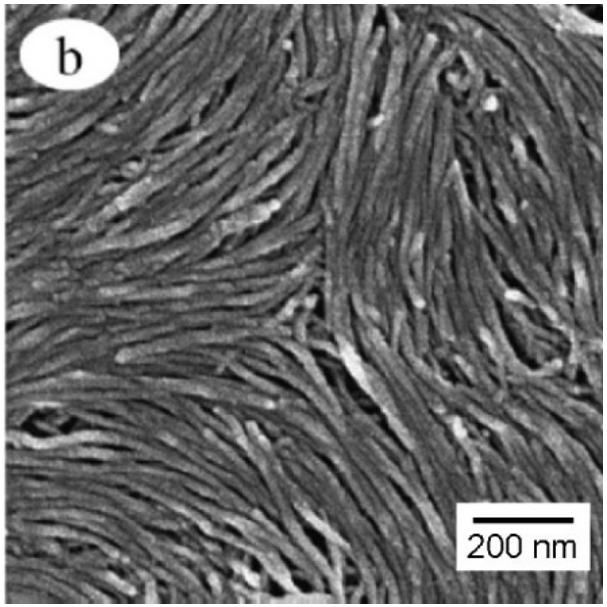
$$\hat{n}(x) = (\frac{x_1}{r}, \frac{x_2}{r}, 0) \quad r = \sqrt{x_1^2 + x_2^2}$$
$$|\nabla \hat{n}(x)|^2 = \frac{1}{r^2}$$

$$\hat{n}, \hat{Q} = s\left(\hat{n} \otimes \hat{n} - \frac{1}{3}\mathbf{1}\right) \in W^{1,p} \Leftrightarrow 1 \leq p < 2$$

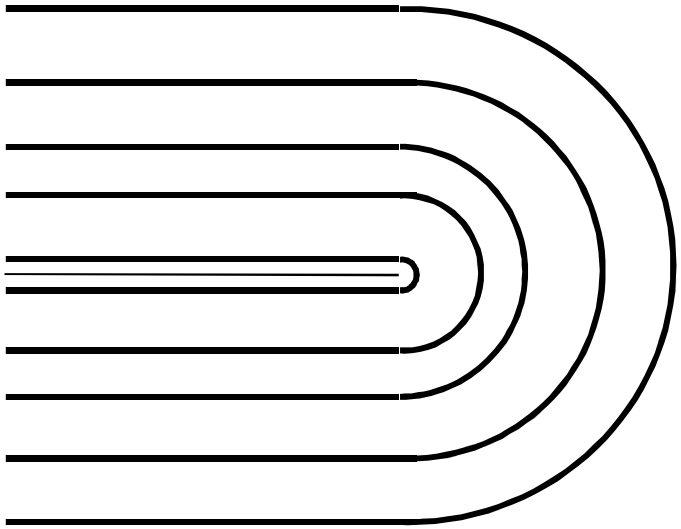
infinite energy for Oseen-Frank and constrained Landau-de Gennes quadratic models

Index one half defects

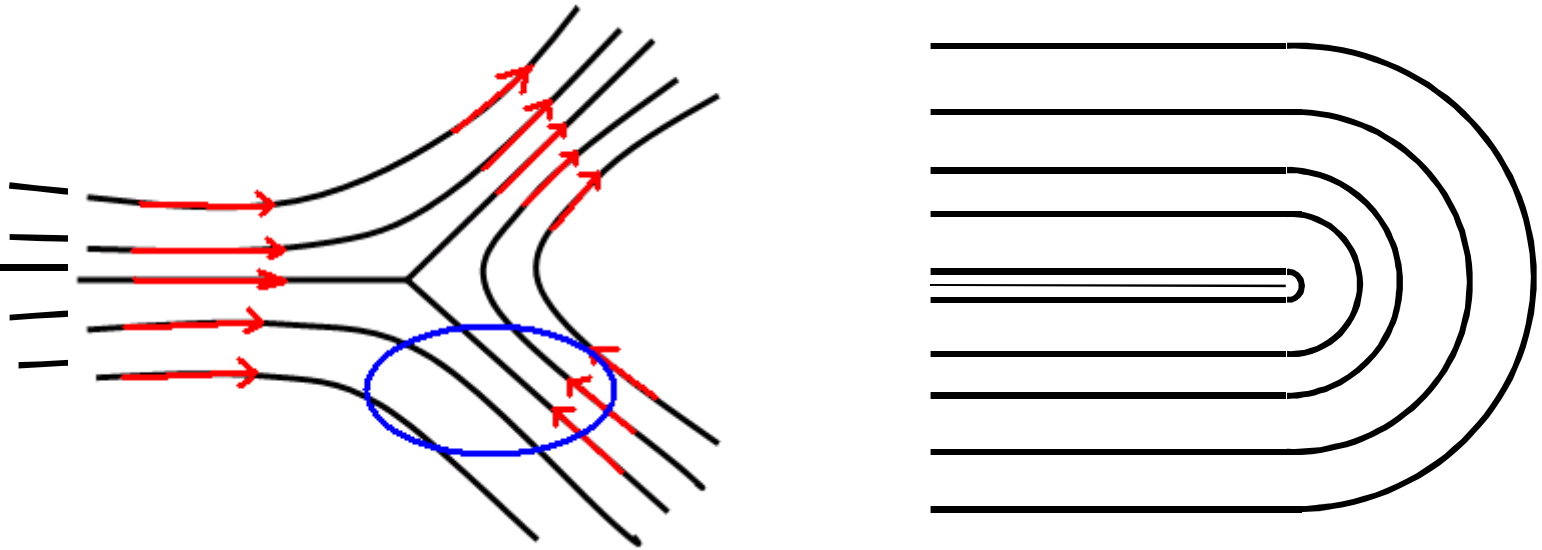




Zhang/Kumar 2007
Carbon nano-tubes
as liquid crystals



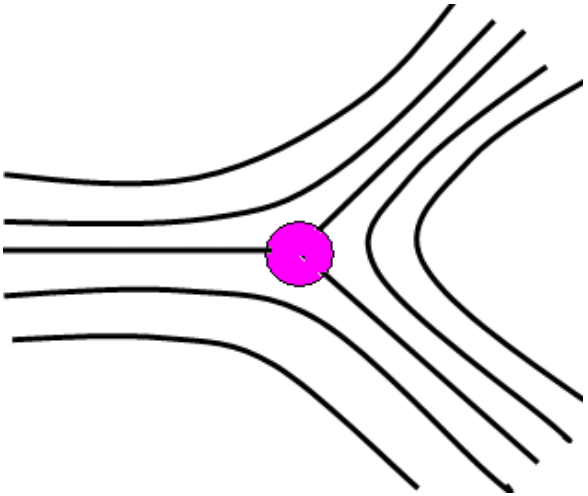
The index one half singularities are non-orientable



$Q \notin W^{1,2}$ since otherwise orientable

Can one change Q (while remaining uniaxial) in a core around the defect in such a way that the energy becomes finite?

Yes for the cylindrical hedgehog by 'escape into the third dimension'.



No for the index $\frac{1}{2}$ defects because then Q would be nonorientable and in $W^{1,2}$, contradicting the orientability result for simply-connected domains.

Lessons from solid mechanics

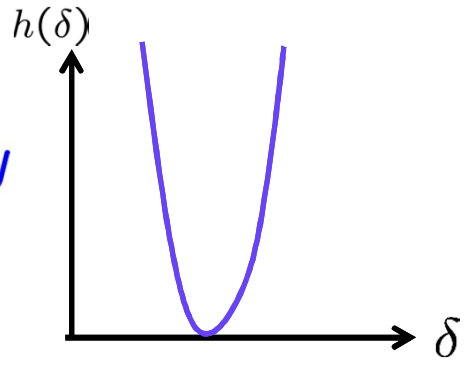
For nonlinear elasticity, with free-energy functional

$$I(y) = \int_\Omega W(Dy(x))\,dx,$$

minimizers can have singularities, and the predictions of the model depend on the function space.

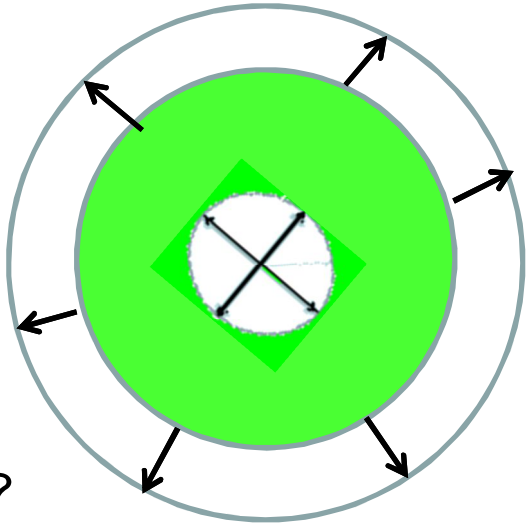
e.g. cavitation: given $\lambda > 0$ the minimizer of

$$I(y) = \int_{B(0,1)} [|Dy|^2 + h(\det Dy)]\, dx \quad + \kappa \text{ area } S_y$$

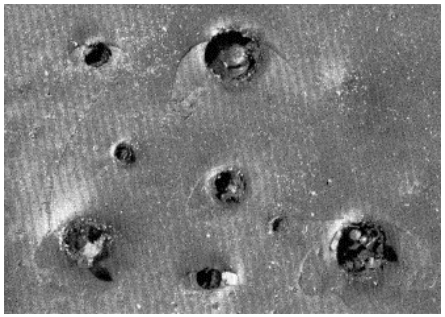


among smooth y subject to $y(x) = \lambda x$ for $|x| = 1$ is $y^*(x) = \lambda x$.

But among radial deformations $y(x) = \frac{r(|x|)}{|x|}x$ in $W^{1,2}$ the minimizer for large enough λ satisfies $r(0) > 0$.

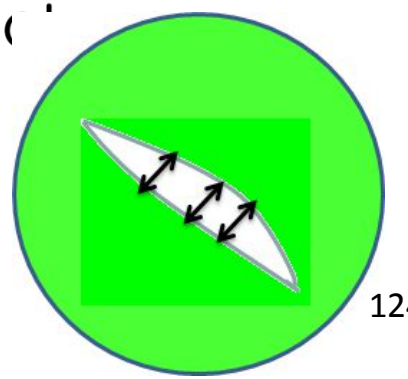


(Lavrentiev phenomenon)

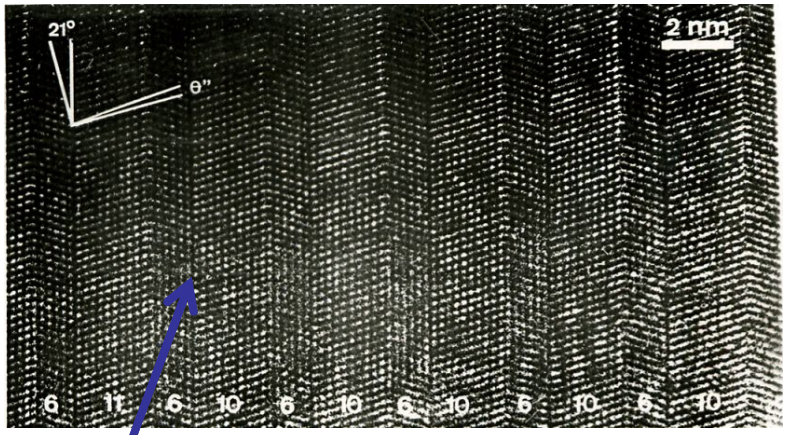


But is $W^{1,2}$ the largest such function space?

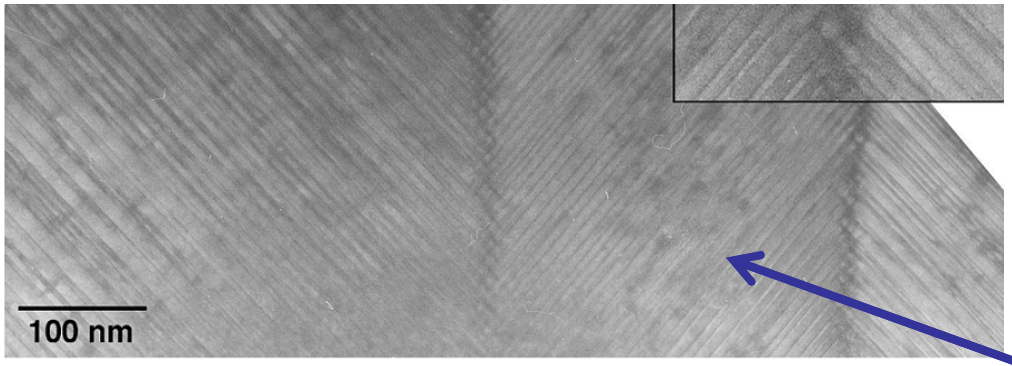
No, because the body could develop fra
surfaces across which y is discontinuous.
Francfort-Marigo theory of fracture.
$y \in SBV$ (special functions of bounded variation), jump set S_y



As we have seen, there can also be planar discontinuities in Dy representing phase boundaries.

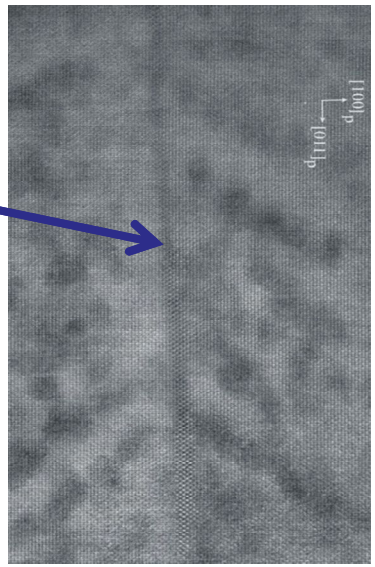


NiMn, Baele, van Tenderloo, Amelinckx



Macrotwins in $Ni_{65}Al_{35}$ single crystal (D. Schryvers)

Sharp, and diffuse interfaces



Perovskite. Salje.

And there are models similar to Landau - de Gennes allowing both sharp and diffuse interfaces, e.g.

$$I(y) = \int_\Omega [\psi(Dy) + \varepsilon |D^2 y|^2]\, dx + \kappa \,\text{area}\, S_{Dy}.$$

(Ball & Mora-Corral 2009)

The important conclusion to draw for liquid crystals is that the function space is part of the model. (Proof. Change the function space and the predictions change.)

Indeed the Lavrentiev phenomenon (the infimum of the total free energy is different in different function spaces is different) occurs in the Oseen-Frank theory. In fact we have that for the unit ball B

$$\inf_{n\in X,\, n|_{\partial B}=x} \int_B K|\nabla n|^2\,dx \begin{cases} = \infty & \text{if } X = C^1 \\ < \infty & \text{if } X = W^{1,2} \end{cases}$$

(Hardt & Lin 1986 give an example with smooth degree zero boundary data for which both infima are finite but that in $W^{1,2}$ is lower.)

Director modeling of line defects with finite energy

That these defects have infinite energy arises from the quadratic growth in ∇n of $W(n, \nabla n)$, which results in turn from the quadratic dependence of $\psi(Q, \nabla Q)$ on ∇Q.

One option is to live with this and study the appearance of line defects with infinite energy as the elastic coefficients in the Landau - de Gennes theory tend to zero, as done in the interesting recent work of Canevari (2015).

Alternatively one can take the view that there is no reason to suppose that $W(n, \nabla n)$ is quadratic for large $|\nabla n|$ (such as near defects).

So a possible remedy would be to assume that $W(n, \nabla n)$ has *subquadratic* growth, i.e.

$$W(n, \nabla n) \leq C(|\nabla n|^p + 1),$$

where $1 \leq p < 2$, which would make line defects have finite energy.

For example, we can let

$$W_\alpha(n, \nabla n) = \frac{2}{p\alpha}\left((1 + \alpha W(n, \nabla n))^{\frac{p}{2}} - 1\right),$$

where $\alpha > 0$ is small. Then $W_\alpha(n, \nabla n) \to W(n, \nabla n)$ as $\alpha \to 0$. Also, assuming the Ericksen inequalities, W_α satisfies the growth conditions

$$C'_\alpha(|\nabla n|^p - 1) \leq W_\alpha(n, \nabla n) \leq C_\alpha |\nabla n|^p,$$

for positive constants C_α, C'_α. Setting

$$I_\alpha(n) = \int_\Omega W_\alpha(n, \nabla n)\, dx,$$

we obtain that $I_\alpha(\hat{n}) < \infty$ as desired. Also $W_\alpha(n, \cdot)$ is convex.

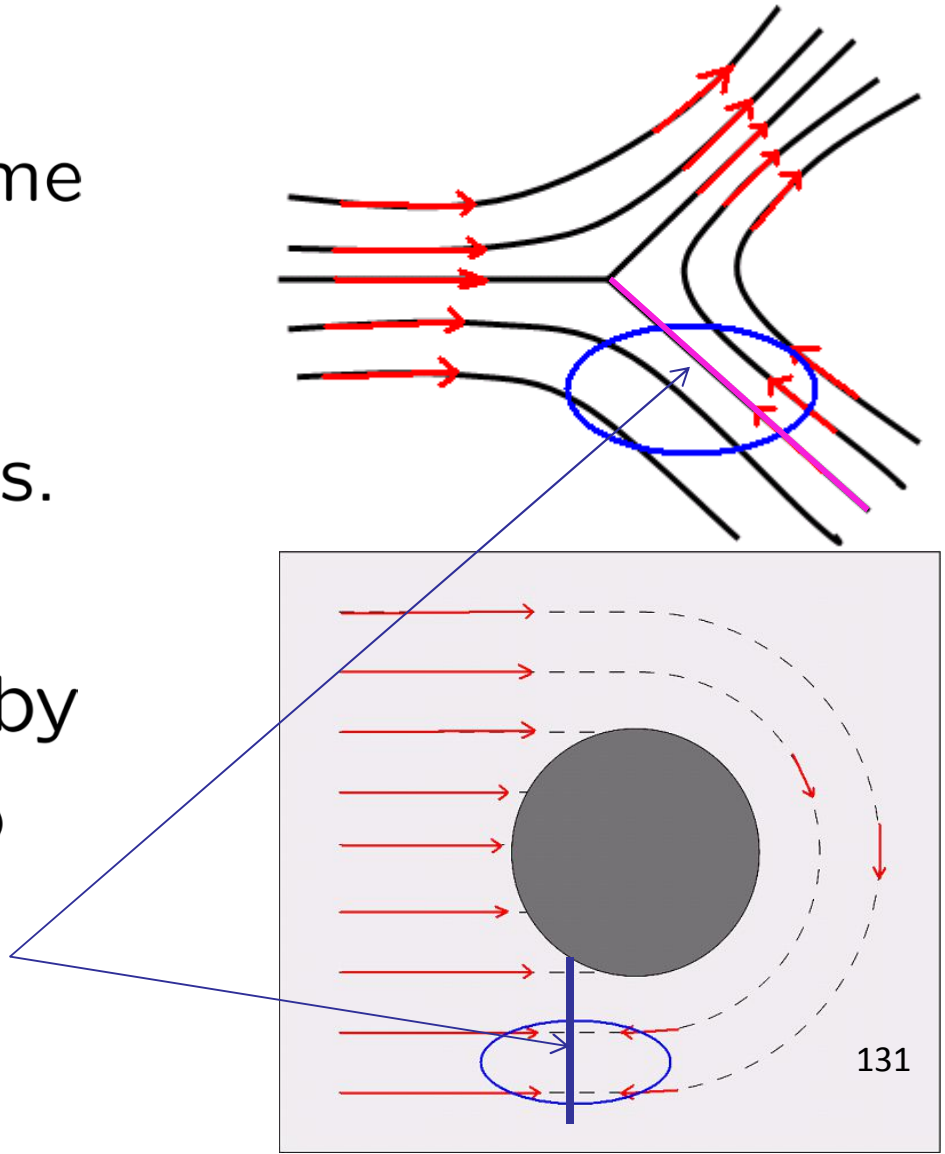
Boundary conditions:

If $\Omega \subset \mathbb{R}^3$ has smooth boundary and a sufficiently smooth unit vector field N is given on the boundary $\partial\Omega$, then it is known (Hardt & Lin 1987) that there is a unit vector field $n \in W^{1,2}(\Omega; S^2)$ with $n = N$ on $\partial\Omega$.

However, if, for example, $\Omega = (0,1)^3$ is a cube and N is the inward normal to the boundary, then (Bedford) there is no such n. Thus the Oseen-Frank theory does not apply to homeotropic boundary conditions on a cube, although a theory with subquadratic growth would be OK.

But the index $\frac{1}{2}$ singularities cannot be modelled this way because they are not *orientable.*

As we have seen the same issue arises for smooth line fields in non simply-connected regions.



This can be handled by allowing n to jump to $-n$ across suitable surfaces.

Theorem (Bedford). *Let* $\mathbf{Q} = s\left(n \otimes n - \frac{1}{3}\mathbf{1}\right) \in W^{1,2}(\Omega; M^{3\times 3})$, *where* $s \neq 0$ *is constant. Then there exists a unit vector field* $m \in SBV$ *such that* $m \otimes m = n \otimes n$, *and* $m_+ = -m_-$ *across any jump.*

This applies to the second situation above but not to index $\frac{1}{2}$ defects, for which an extension to $W^{1,p}$, $1 < p < 2$, would be required.

Ericksen theory. Here we can model point and line defects by finite energy configurations in which n is discontinuous and $s = 0$ at the defect (melting core). In this case there is no need to change the growth rate at infinity.

For example, if we consider the special case when

$$I_{LdG}(Q) = \int_\Omega [\psi_B(Q) + K|\nabla Q|^2]\, dx,$$

then the uniaxial ansatz

$$Q(x) = s(x)\left(n(x) \otimes n(x) - \frac{1}{3}\mathbf{1}\right)$$

gives the functional

$$I_E(s,n) = \int_\Omega [\psi_B(s) + K(|\nabla s|^2 + 2s^2|\nabla n|^2)]\, dx,$$

where $\psi_b(s) = \widehat{\psi}(\frac{2s^2}{3}, \frac{2s^3}{27})$.

Then n can have a singularity at a point or curve which has finite energy because s can tend to zero sufficiently fast as the point or curve is approached to make $I_E(s, n)$ finite. However for non simply-connected domains or index $\frac{1}{2}$ defects there is the same orientability problem as in the Oseen-Frank theory, which can be 'cured' by allowing jumps from n to $-n$ across surfaces.

Theorem [Bedford] *Let* $Q \in W^{1,2}(\Omega; M^{3\times 3})$ *be uniaxial with* $s \in C(\Omega)$. *Then* $s \in W^{1,2}(\Omega)$ *and there exists a vector field*

$$m \in SBV_{\text{loc}}(\Omega \setminus \{s = 0\}; S^2)$$

such that $m \otimes m = n \otimes n$.

There is also the possibility of 'genuine' planar defects in this theory (see later).

Planar defects (JB/Bedford)

Let's explore whether it might be reasonable to consider a free-energy functional for nematic and cholesteric liquid crystals of free-discontinuity type

$$I(n) = \int_\Omega W(n, \nabla n)\, dx + \int_{S_n} f(n_+, n_-, \nu)\, d\mathcal{H}^2,$$

for $n \in SBV(\Omega, S^2)$, where ν is the normal to the jump set S_n. Here $W(n, \nabla n)$ is assumed to have the Oseen-Frank form or be modified so as to have subquadratic growth as suggested previously.

Admissible interfacial energies

Suppose that $f : S^2 \times S^2 \times S^2 \to [0, \infty)$ is continuous and frame-indifferent, i.e.

$$f(Rn_+, Rn_-, R\nu) = f(n_+, n_-, \nu) \qquad (1)$$

for all $R \in SO(3), n_+, n_-, \nu \in S^2$, and that f is invariant to reversing the signs of n_+, n_-, reflecting the statistical head-to-tail symmetry of nematic and cholesteric molecules, so that

$$f(-n_+, n_-, \nu) = f(n_+, -n_-, \nu) = f(n_+, n_-, \nu). \qquad (2)$$

Theorem. *A necessary and sufficient condition that a continuous* $f : S^2 \times S^2 \times S^2 \to [0, \infty)$ *satisfies* (1) *and* (2) *is that*

$$f(n_+, n_-, \nu) = \\ g((n_+ \cdot n_-)^2, (n_+ \cdot \nu)^2, (n_- \cdot \nu)^2, (n_+ \cdot n_-)(n_+ \cdot \nu)(n_- \cdot \nu))$$

for a continuous function $g : D \to [0, \infty)$*, where*

$$D = \{(\alpha, \beta, \gamma, \delta) : \alpha, \beta, \gamma \in [0, 1], \delta^2 = \alpha\beta\gamma, \alpha+\beta+\gamma-2\delta \leq 1\}.$$

An equivalent representation is in terms of the matrices $M_+ = n_+ \otimes n_+, M_- = n_- \otimes n_-,\ N = \nu \otimes \nu$, namely

$$f(n_+, n_-, \nu) = g(M_+ \cdot M_-, M_+ \cdot N, M_- \cdot N, \mathrm{tr}\,(M_+ M_- N)).$$

In fact the theorem, though without the characterization of the domain of g, follows from a representation theorem (Smith 1971) for isotropic functions of symmetric matrices.

Possible candidates for planar defects.

1. Nematic elastomers

The energy functional for nematic elastomers proposed by Bladon, Terentjev, Warner (1993) is given by

$$I(y,n) = \int_\Omega \frac{\mu}{2}\left(Dy(Dy)^T \cdot L_{a,n}^{-1} - 3\right)\, dx,$$

where

$$L_{a,n} = a^{\frac{2}{3}} n \otimes n + a^{-\frac{1}{6}}(\mathbf{1} - n \otimes n)$$

and $\mu > 0, a > 0$ are material parameters.

The material is assumed incompressible, so that $\mathbf{y}$ is subjected to the constraint $\det Dy = 1$.

Stripe domains in nematic elastomer
Kundler & Finkelmann
Mathematical theory due to De Simone & Dolzmann

By minimizing the integrand over $n \in S^2$ we obtain the purely elastic energy

$$I(y) = \int_\Omega W(Dy)\, dx, \qquad (1)$$

where

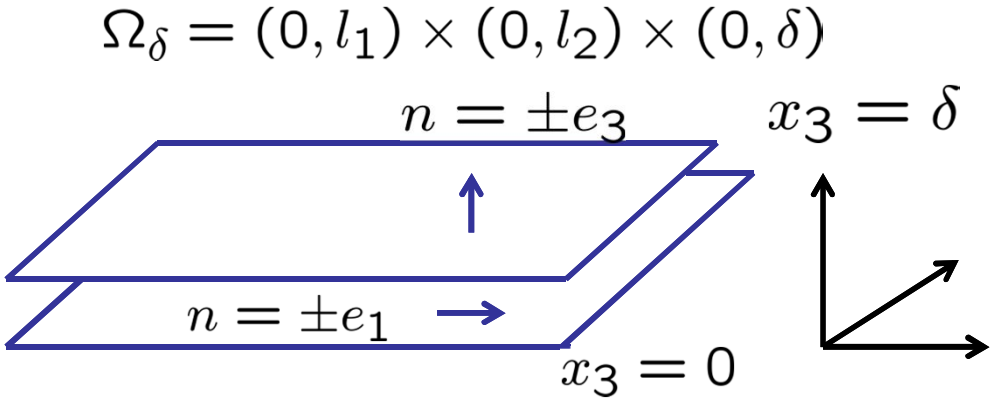
$$W(A) = \frac{\mu}{2}\left(a^{-\frac{2}{3}} v_1^2(A) + a^{\frac{1}{3}}(v_2^2(A) + v_3^2(A))\right),$$

and $v_1(A) \geq v_2(A) \geq v_3(A) > 0$ denote the singular values of A, that is the eigenvalues of $\sqrt{A^T A}$.

As discussed by De Simone & Dolzmann (2002) the free-energy function (1) is not quasiconvex, and admits minimizers in which ∇y jumps across planar interfaces, so that the minimizing n of the integrand also jumps. Of course the functional ignores Frank elasticity, i.e. terms in ∇n, but the experimental observations might suggest that even with such terms allowing jumps in n may be a useful approximation.

Order reconstruction

Barbero & Barberi (1983)
Palffy-Muhoray, Gartland & Kelly (1994)
Lamy (2015)



(a) Analysis using Landau - de Gennes

Boundary conditions:

$Q(x_1, x_2, 0) = Q^{(0)}, \;\; Q(x_1, x_2, \delta) = Q^{(1)},$

for a.e. $(x_1, x_2) \in (0, l_1) \times (0, l_2)$, where

$Q^{(0)} = s_1 \left(e_1 \otimes e_1 - \frac{1}{3}\mathbf{1} \right), \;\; Q^{(1)} := s_2 \left(e_3 \otimes e_3 - \frac{1}{3}\mathbf{1} \right),$

and Q periodic in x_1, x_2.

Assume that $L_4 = 0$ with the Longa inequalities

$$L_3 > 0, \;\; -L_3 < L_2 < 2L_3, \;\; -\frac{3}{5}L_3 - \frac{1}{10}L_2 < L_1,$$

which imply that

$$\psi_E(\nabla Q) \geq \alpha |\nabla Q|^2$$

for some $\alpha > 0$.

Rescale, defining

$$P(x_1, x_2, x_3) = Q(x_1, x_2, \delta x_3),$$

so that $I_{LdG}(Q) = \delta^{-1} E^{\delta}(P)$, where

$$E^{\delta}(P) = \int_D [\delta^2 \psi_B(P) + \psi_E(\delta P_{,1}, \delta P_{,2}, P_{,3})] \, dx$$

and $D = (0, l_1) \times (0, l_2) \times (0, 1)$.

Theorem. *Let P^δ be a minimizer of E^δ. Then as $\delta \to 0$*

$$P^\delta \to \bar{P},\ P^\delta_{,3} \to \bar{P}_{,3},\ \delta P^\delta_{,1} \to 0,\ \delta P^\delta_{,2} \to 0 \ \ \textit{in}\ L^2(D;S),$$

where

$$\bar{P}(x) = (1 - x_3)Q^{(0)} + x_3 Q^{(1)},$$

and $S = \{Q \in M^{3\times 3} : Q = Q^T, \operatorname{tr} Q = 0\}$.

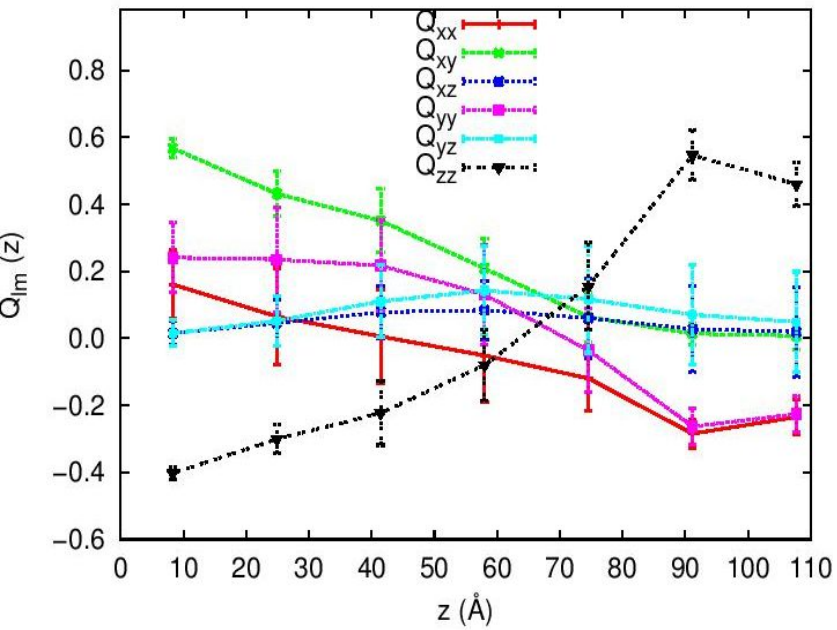
So for sufficiently small δ, Q is given approximately by

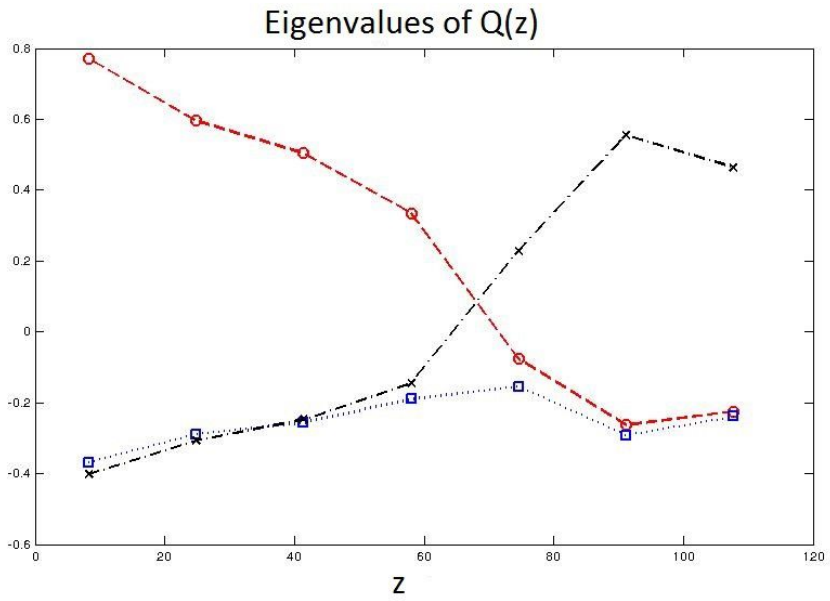
$$Q(x) = (1 - \delta^{-1}x_3)Q^{(0)} + \delta^{-1}x_3 Q^{(1)},$$

for which the director (the eigenvector of Q corresponding to the largest eigenvalue)

$$n(x) = \begin{cases} e_1 & \text{if } 0 \le x_3 \le \frac{s_1}{s_1+s_2}\delta \\ e_3 & \text{if } \frac{s_1}{s_1+s_2}\delta \le x_3 \le 1. \end{cases}$$

has a discontinuity on the plane $x_3 = \frac{s_1}{s_1+s_2}\delta$.





A. Pizzirusso, R. Berardi, L. Muccioli, M. Riccia, and C. Zannoni. Predicting surface anchoring: molecular organization across a thin film of 5CB liquid crystal on silicon. Chem. Sci., 3:573–579, 2012.

(b) Analysis using director model

Consider for simplicity the functional

$$I(n) = \int_{\Omega_\delta} K'|\nabla n|^2\,dx + k' \int_{S_n} (1-(n_+\cdot n_-)^2)^{\frac{r}{2}})\,d\mathcal{H}^2,$$

where $k' > 0$ and $0 < r < 1$, with boundary conditions $n(x_1, x_2, 0) = \pm e_1$, $n(x_1, x_2, \delta) = \pm e_3$ and $l_1 = l_2 = 1$.

Formally this can be obtained from the Landau - de Gennes functional

$$I(Q) = \int_{\Omega_\delta} K|\nabla Q|^2\,dx + k \int_{S_Q} |Q_+ - Q_-|^r\,d\mathcal{H}^2,$$

by making the uniaxial ansatz

$$Q(x) = s\left(n(x) \otimes n(x) - \frac{1}{3}1\right),$$

where $|n(x)| = 1$ and $s \in (0,1)$ is constant, with $K' = 2Ks^2$, $k' = 2^{\frac{r}{2}} s^r k$.

Some care is needed when interpreting the boundary conditions and periodicity, since it is possible that Q might jump at the boundary $\partial\Omega_\delta$ of Ω_δ. This is handled by minimizing $I(Q)$ among $Q \in SBV_{\text{loc}}(\mathbb{R}^2 \times (-1, \delta+1); M^{3\times 3})$ satisfying

$$Q(x_1, x_2, x_3) = s\left(e_1 \otimes e_1 - \frac{1}{3}\mathbf{1}\right) \text{ for } -1 < x_3 < 0,$$

$$Q(x_1, x_2, x_3) = s\left(e_3 \otimes e_3 - \frac{1}{3}\mathbf{1}\right) \text{ for } \delta < x_3 < \delta+1,$$

and $Q(x_1 + l_1, x_2, x_3) = Q(x_1, x_2 + l_2, x_3) = Q(x_1, x_2, x_3)$ for all $(x_1, x_2, x_3) \in \mathbb{R}^2 \times (-1, \delta + 1)$. With this interpretation S_Q can be partly on $\partial\Omega_\delta$.

Candidates for minimizers of I are the two smooth Q given by

$$Q^{\pm}(x) = \frac{s}{2}\begin{pmatrix} \frac{1}{3} + \cos\frac{\pi x_3}{\delta} & 0 & \pm\sin\frac{\pi x_3}{\delta} \\ 0 & -\frac{2}{3} & 0 \\ \pm\sin\frac{\pi x_3}{\delta} & 0 & \frac{1}{3} - \cos\frac{\pi x_3}{\delta} \end{pmatrix},$$

which are the minimizers of $\int_{\Omega_\delta} |\nabla Q|^2 dx$ among uniaxial $Q \in W^{1,2}(\Omega_\delta; M^{3\times 3})$ satisfying the boundary conditions, and which correspond to the two Oseen-Frank solutions in which the line field rotates anticlockwise (resp. clockwise) in the (x_1, x_3) plane from horizontal to vertical.

Theorem. *For any $\delta > 0$ there exists at least one minimizer $Q \in SBV(\Omega_\delta : M^{3\times 3})$ of I subject to the boundary conditions.*

Conjecture. *There is a small $\delta_0 > 0$ such that if $\delta > \delta_0$ then $Q^{\pm}$ are the only minimizers, while if $0 < \delta < \delta_0$ then any minimizer Q has a single jump with jump set $S_Q = \{x : x_3 = \gamma(\delta)\}$, where $0 < \gamma(\delta) < \delta$.*

That $Q^{\pm}$ are not minimisers for δ sufficiently small is easily seen. In fact, $|\nabla Q^{\pm}| = \frac{C}{\delta}$ for some $C > 0$, so that $I(Q^{\pm}) = Ks^2\frac{C^2}{\delta}$. But if

$$\hat{Q}(x) = \begin{cases} s\left(e_1 \otimes e_1 - \frac{1}{3}\mathbf{1}\right) & \text{if } 0 < x_3 < \frac{\delta}{2} \\ s\left(e_3 \otimes e_3 - \frac{1}{3}\mathbf{1}\right) & \text{if } \frac{\delta}{2} < x_3 < \delta \end{cases}$$

then $I(\hat{Q}) = ks^r 2^{\frac{r}{2}}$, so that $I(\hat{Q}) < I(Q^{\pm})$ if $s^{r-2}\frac{\delta k}{K} < 2^{-\frac{r}{2}}C^2$.

Related problems for cholesterics

Bedford (2014, 2015) considers related problems for cholesterics, for example to minimize

$$I(n) = \int_\Omega [|\nabla n|^2 + 2tn \cdot \nabla \wedge n + t^2|n|^2]\, dx$$

for $\Omega = (0, l_1) \times (0, l_2) \times (0, \delta)$, where $t \geq 0$ and

$n(x_1, x_2, 0) = e_1$, $n(x_1, x_2, \delta) = e_3$, n periodic in x_1, x_2.

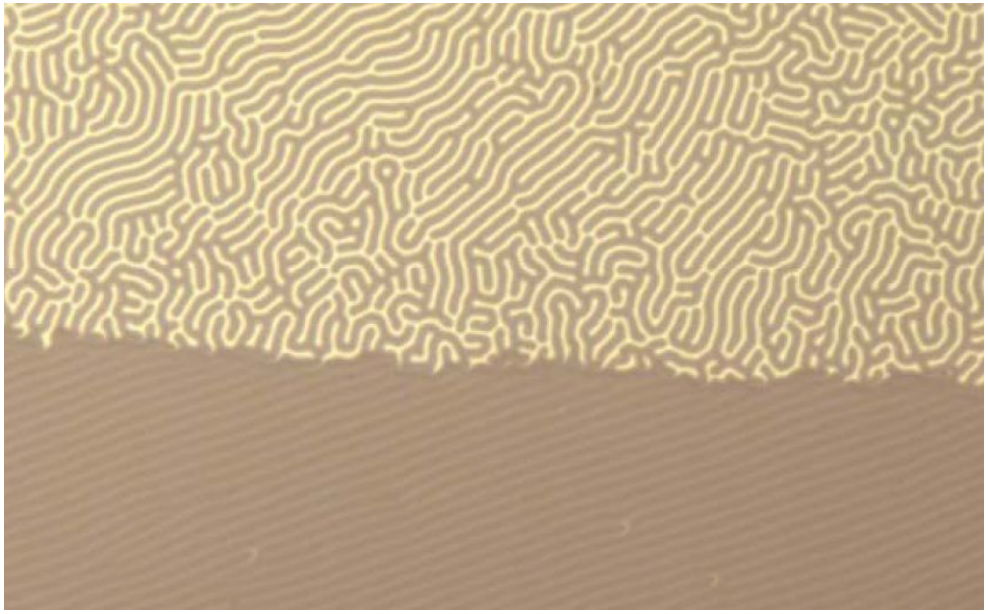
He proves that there is an explicit unique global minimizer $n^* = n^*(x_3)$ among n depending only on x_3, and there exists $\tau > 0$ such that n^* is the unique global minimizer in $W^{1,2}$ among all admissible n for $t \in [0, \tau]$.

Similarly, for the boundary conditions

$n(x_1, x_2, 0) = e_3, n(x_1, x_2, \delta) = e_3, n$ periodic in x_1, x_2,

Bedford proves that $n = e_3$ is for some $\tau > 0$ the unique minimizer in $W^{1,2}$ for $t \in [0, \tau]$, a strong local minimizer if $t \in [0, \pi)$ and not a weak local minimizer if $t > \pi$.

Cholesteric fingering (courtesy Hewlett-Packard) formed between two plates with homeotropic boundary conditions. In the lower half of the figure the bottom surface is a grating, and the effective boundary condition is planar.



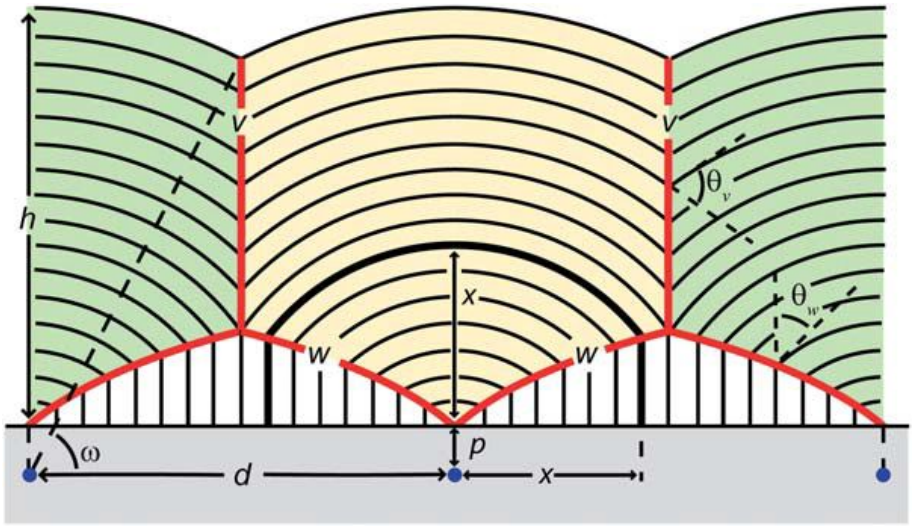
In an attempt to understand the mechanism for the origin of such patterns via energy minimization, Bedford motivated the study of the variational problem of minimizing

$$I(n) = \int_\Omega [|\nabla n|^2 + 2tn \cdot \nabla \wedge n + t^2|n|^2]\, dx + K\mathcal{H}^2(S_n)$$

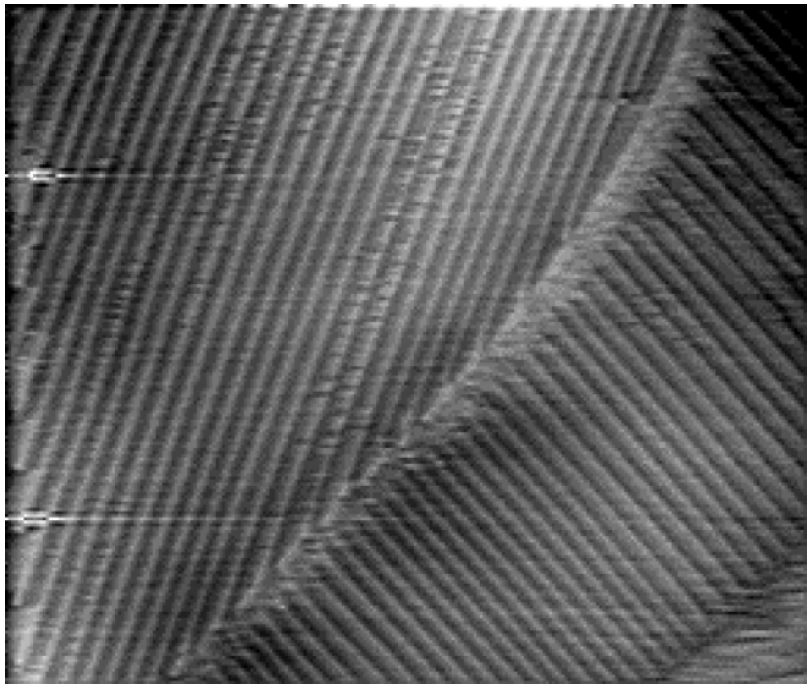
over $n \in SBV(\Omega; \{0\} \cup S^2)$ satisfying $n(x_1, x_2, 0) = e_1, n(x_1, x_2, \delta) = e_3$ and n periodic in x_1, x_2.

He proves that there exist $\bar{\tau} > 0$ and $\bar{K}$ such that the unique minimizer for $t \in [0, \bar{\tau}]$ and $\bar{K} > K$ is $n^* = n^*(x_3)$, but that if t is sufficiently large then the minimizer cannot be a function of x_3 alone. The latter statement involves a construction using a packing of double-twist cylinders involving jumps in n.

3. Smectic thin films



8CB smectic thin films
Zappone, Lacaze et al, 2010



AFM image
Michel, Lacaze
et al, 2004

Models of smectics

de Gennes approach: model using a complex order parameter $\Psi(x) = \gamma(x)e^{i\phi(x)}$, in terms of which the molecular density $r(x)$ is given by

$$r(x) = r_0 + \sigma(x) = r_0 + \mathrm{Re}\Psi(x) = r_0 + \gamma(x)\cos\phi(x),$$

where $r_0 > 0$ is a constant average density. Thus $\sigma(x)$ describes the fluctuations in the density due to the smectic layers, and $\nabla\phi$ gives the normals to the layers.

(We could define $r(x)$ as the number of molecules in $B(x, \delta)$ divided by the volume of $B(x, \delta)$, taking some care over molecules that overlap the boundary.)

Various free-energy densities for smectics have been proposed (Chen & Lubensky, Kleman & Parodi, Leslie, Stewart & Nakagawa, Mcmillan, Zhang ...). We will restrict attention to smectic A liquid crystals, for which it is often assumed that $r(x)$ is constant, with the free-energy density being expressed in terms of n and ϕ. For example, the free-energy functional proposed by Kleman & Parodi is given by

$$I(n,\phi) = \int_\Omega \left(W(n, \nabla n) + \frac{1}{2}\mathbf{B}(n - \nabla\phi) \cdot (n - \nabla\phi) \right) dx,$$

where $\mathbf{B} = B_\perp \mathbf{1} + (B_\parallel - B_\perp) n \otimes n$ and $B_\perp, B_\parallel$ are positive material constants.

E (1994) argued that a good approximation is given by

$$\int_\Omega (K_1(\operatorname{div} n)^2 + B_{\|}(|\nabla\phi| - 1)^2)\, dx,$$

together with the constraint

$$n = \frac{\nabla\phi}{|\nabla\phi|}$$

that rigidly enforces that the director points parallel to the normal.

Existence of a minimizer for the Kleman & Parodi model is easy, but for the reduced one unclear.

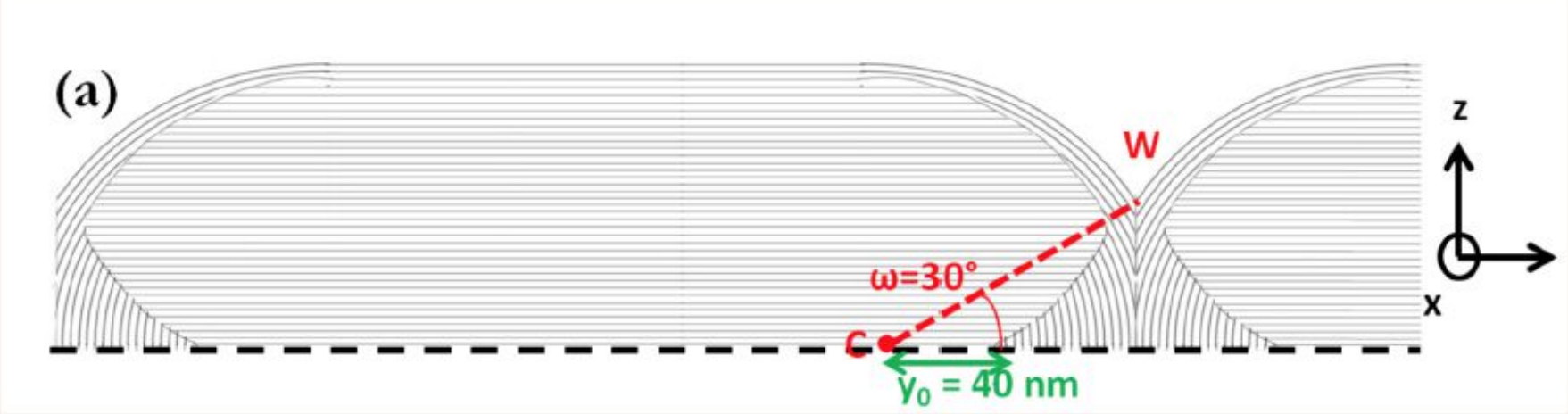
Modified Pevnyi, Selinger & Sluckin model (2014)

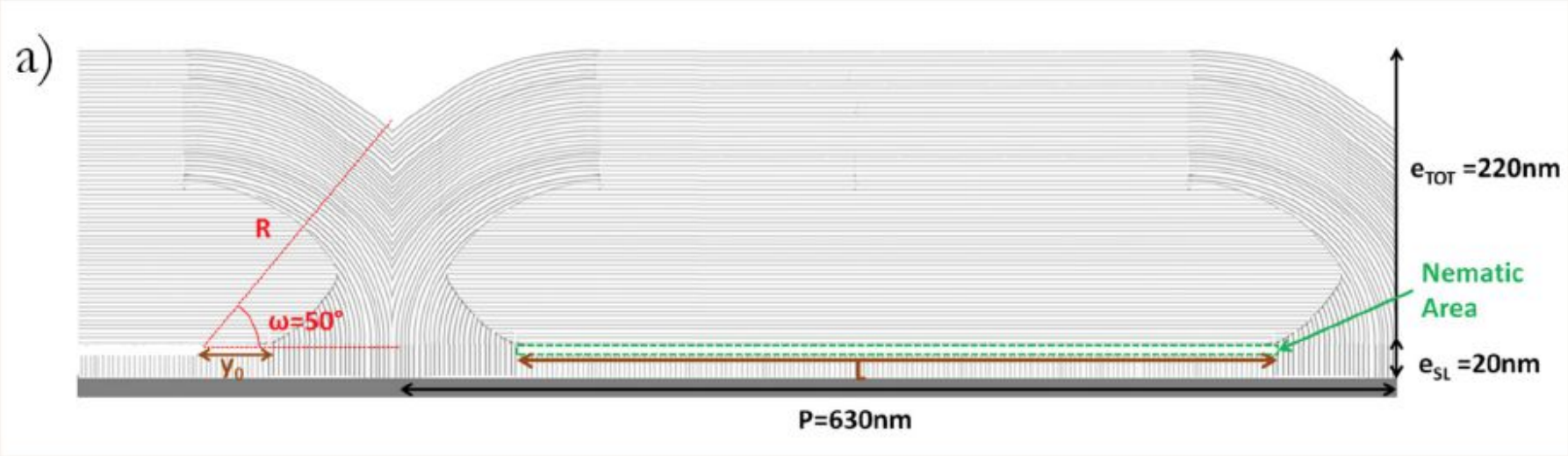
$$I(Q,\sigma)=\int_\Omega\left(\psi_E(Q,\nabla Q)+B\left|D^2\sigma+\frac{q^2}{3s}\left(3Q+s\mathbf{1}\right)\sigma\right|^2+f(\sigma)\right)\,d\mathbf{x}$$
$$+k\int_{S_Q}\left|Q_+-Q_-\right|^r\,d\mathcal{H}^2$$

$$Q(x)=s\left(n(x)\otimes n(x)-\tfrac{1}{3}\mathbf{1}\right)$$

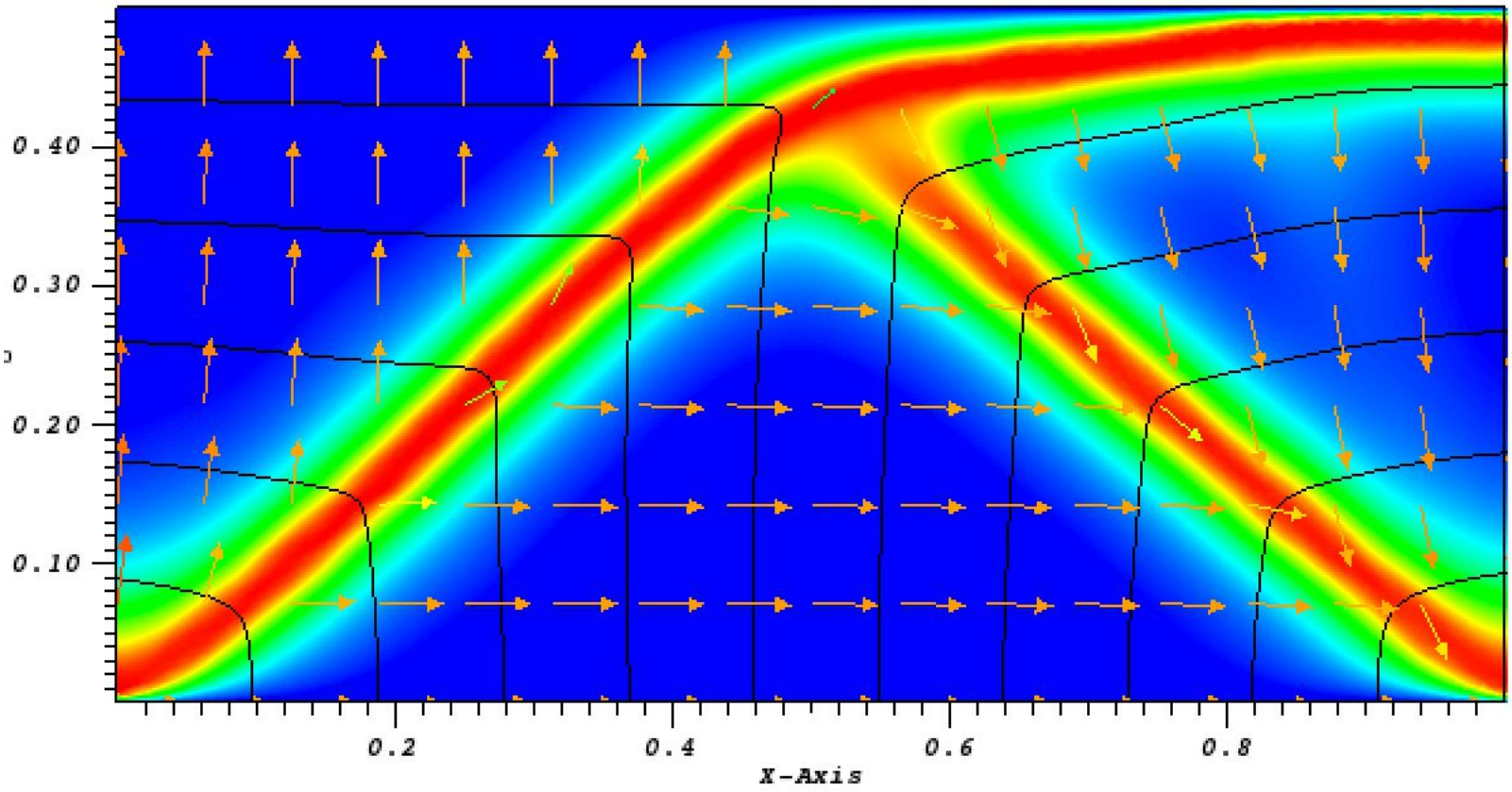
Then under suitable hypotheses on ψ_E and f one can prove the existence of a minimizing pair Q,σ in

$$\mathcal{A}:=\left\{Q\in SBV\left(\Omega,\mathbb{R}^{3\times3}\right),\sigma\in W^{2,2}\left(\Omega,\mathbb{R}\right):\right.$$
$$\left.Q=s\left(n\otimes n-\frac{1}{3}\mathbf{1}\right),\ |n|=1,\ Q|_{\partial\Omega}=\overline{Q}\right\}$$





Coursault, ... , Lacaze (2015)



Computation (A. Léon Baldelli 2015) of minimizer for functional

$$\int_\Omega \left(s^2|\nabla n|^2 + \gamma((1-s)^2 + \varepsilon^2|\nabla s|^2) + \frac{\kappa}{l^2}|\lambda\nabla\varphi - n|^2 + \frac{1}{4\eta^2}(|n|^2-1)^2 \right) dx.$$