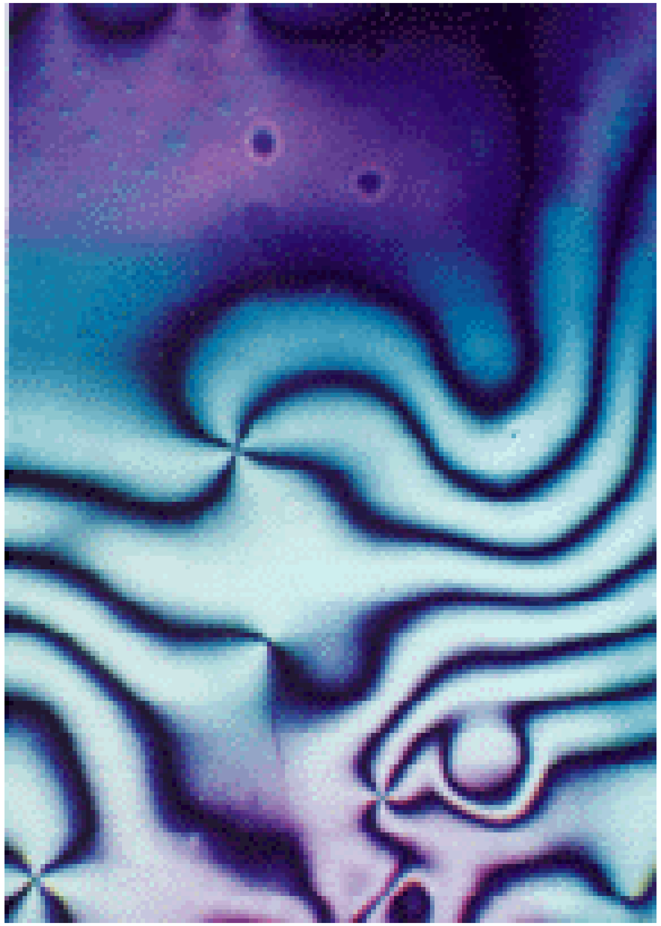
Cambridge CCA course
13-17 February 2012

# The Mathematics of Liquid Crystals



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# Liquid crystals

A multi-billion dollar industry.

An intermediate state of matter between liquids and solids.


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

The mathematics of liquid crystals involves modelling, variational methods, PDE, algebra, topology, probability, scientific computation ...

Most mathematical work has been on the *Oseen-Frank theory*, in which the mean orientation of the rod-like molecules is described by a vector field. However, more popular among physicists is the *Landau - de Gennes theory*, in which the order parameter describing the orientation of molecules is a matrix, the so-called $Q$-tensor.

Both the Oseen-Frank and Landau - de Gennes theories give rise in statics to variational problems of the form:
Minimize

$$I(u) = \int_\Omega f(x, u(x), \nabla u(x))\, dx$$

among suitable maps $u : \Omega \to \mathbf{R}^m$, where $\Omega \subset \mathbf{R}^n$ is bounded and open ($n = 2$ or 3).

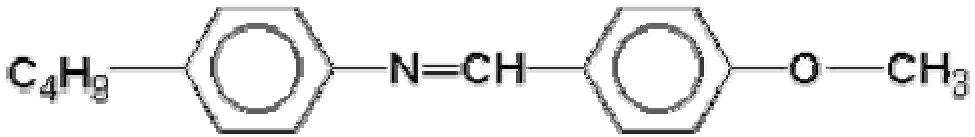
The same is true for *nonlinear elasticity*, and so at a superficial level the mathematics of elasticity and liquid crystals is similar. However, nonlinear elasticity has need of more of the special structure of the multi-dimensional calculus of variations (e.g. $f$ is quasiconvex rather than convex in $\nabla u$ whereas for liquid crystals it seems adequate to assume that $f$ is convex and even quadratic in $\nabla u$). For liquid crystals there is an important dependence of $f$ on $u$ (whereas for elasticity $f$ is independent of $u$) and topology plays a much greater role for liquid crystals than for elasticity.

# Liquid crystals (contd)

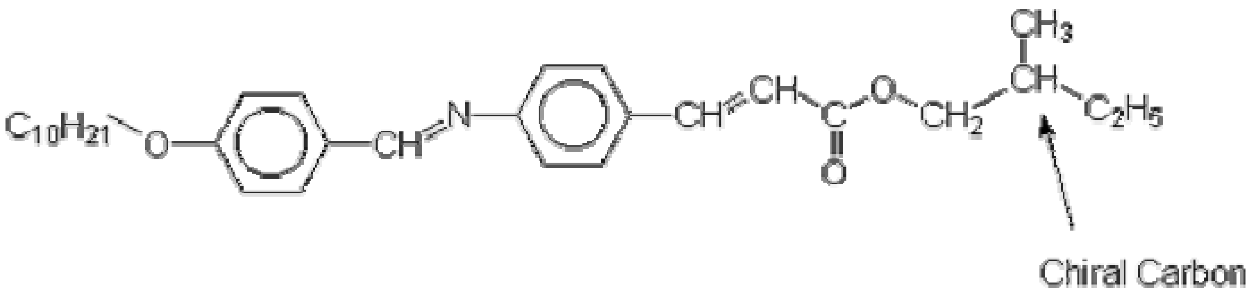
Liquid crystals are of many different types, the main classes being nematics, cholesterics and smectics

Nematics consist of rod-like molecules.

Length 2-3 nm

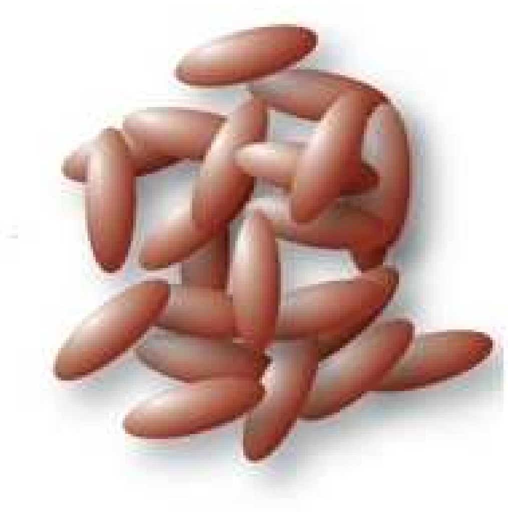



Methoxybenzilidene Butylanaline ("MBBA")

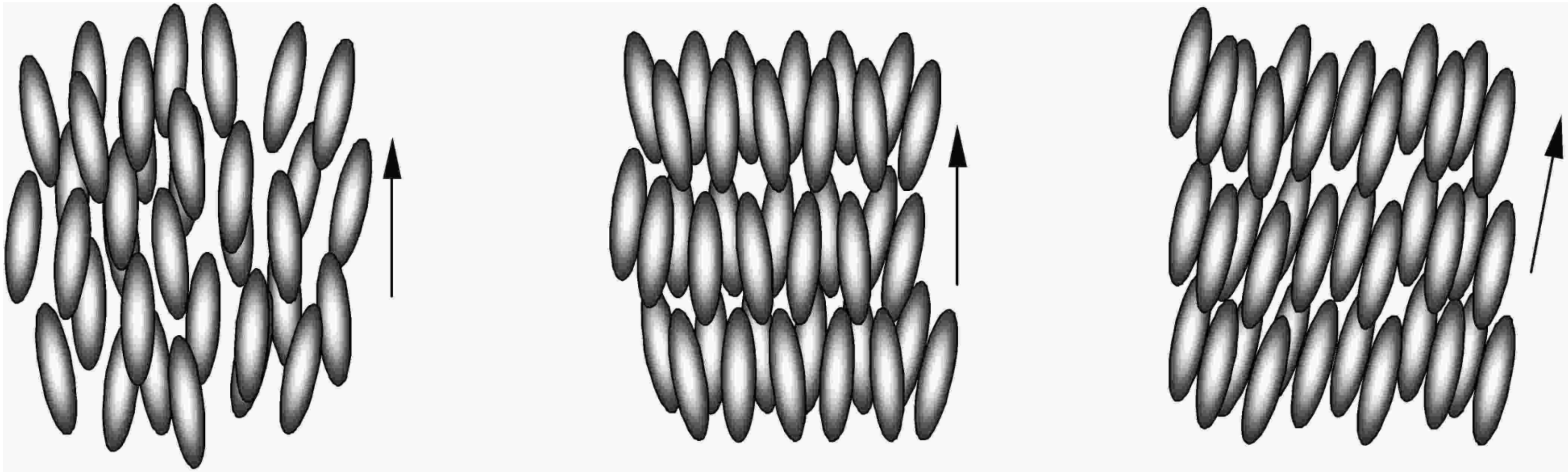



p-decyloxybenzylidene p'-amino 2-methylbutylcinnamate ("DOBAMBC")

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

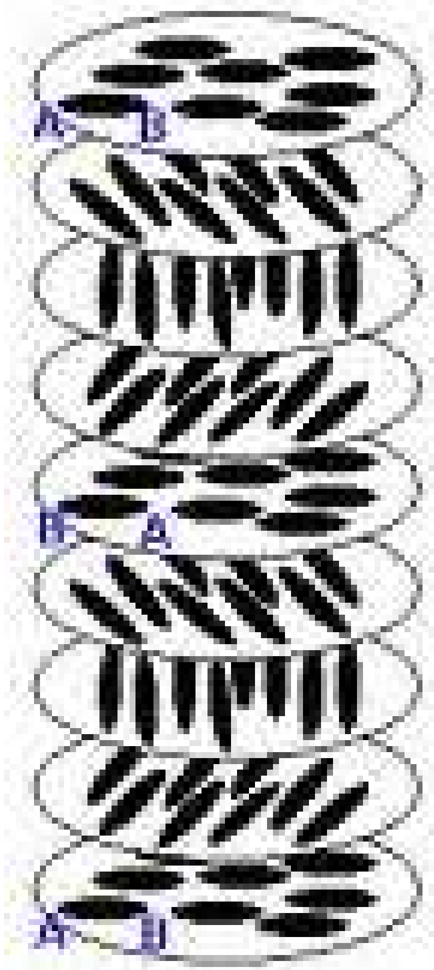
The molecules have time-varying orientations due to thermal motion.

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 $\theta_c$ by a phase transformation from a high temperature isotropic phase.

$\theta_m$ $\qquad\qquad\qquad$ $\theta_c$

| | | |
|---|---|---|
| $\theta < \theta_m$ | $\theta_m < \theta < \theta_c$ | $\theta > \theta_c$ |
| other LC or solid phase | nematic | isotropic |

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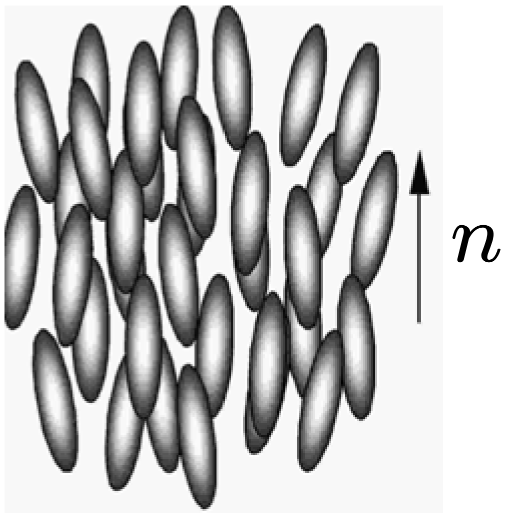
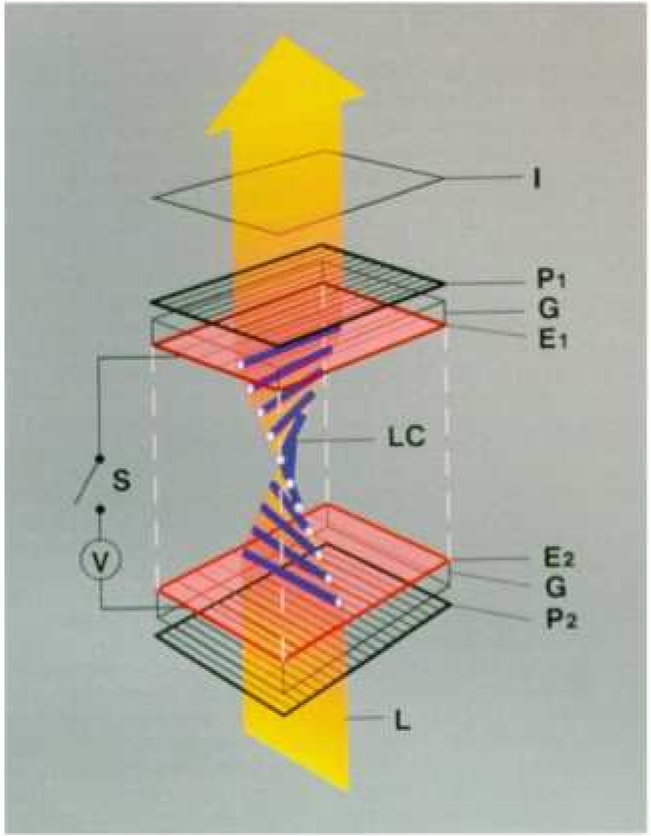
# The director

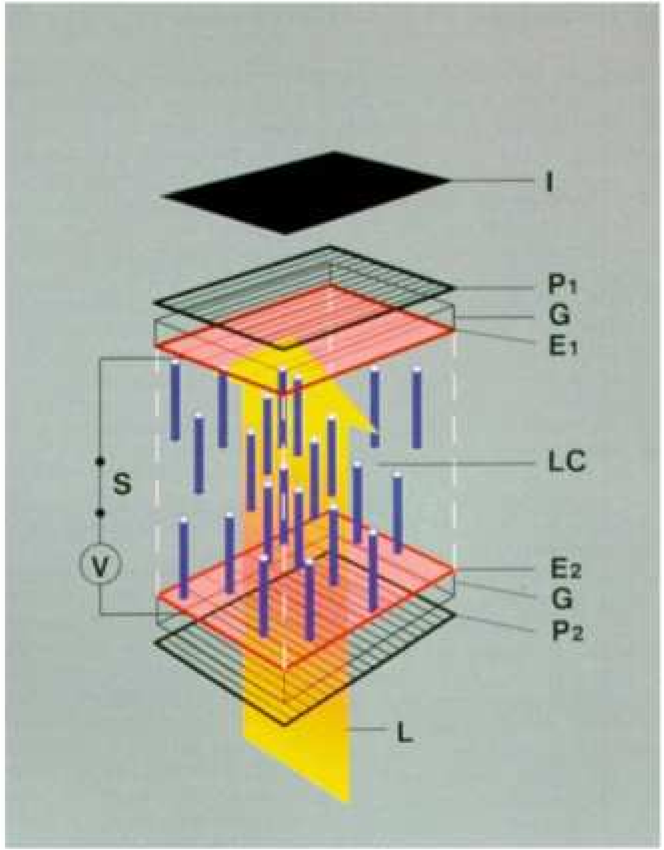
A first mathematical description of the nematic phase is to represent the mean orientation of the molecules by a unit vector $n = n(x, t)$.




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

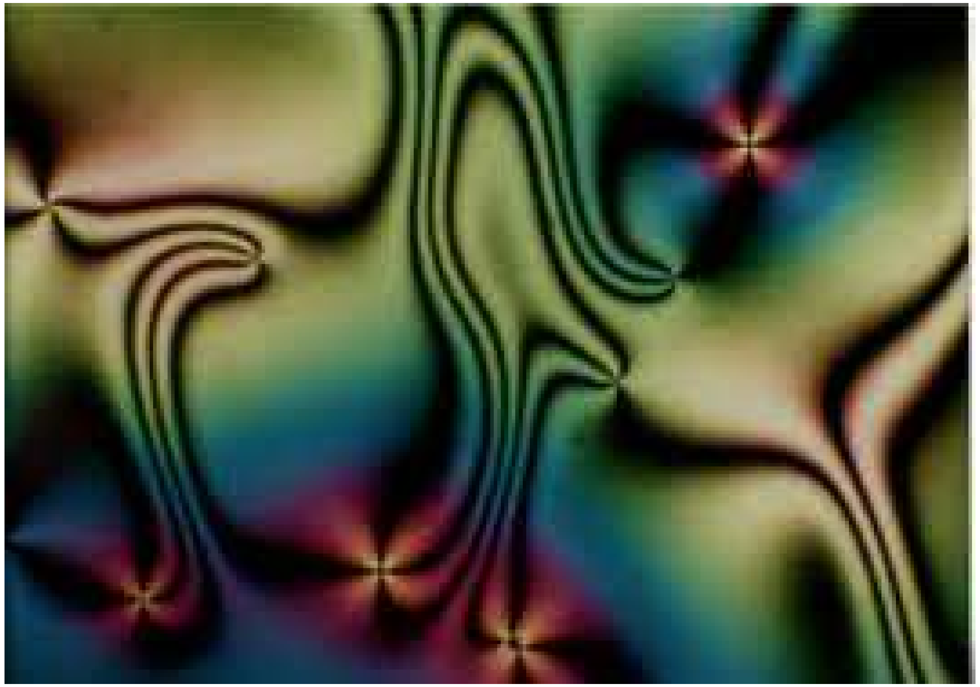


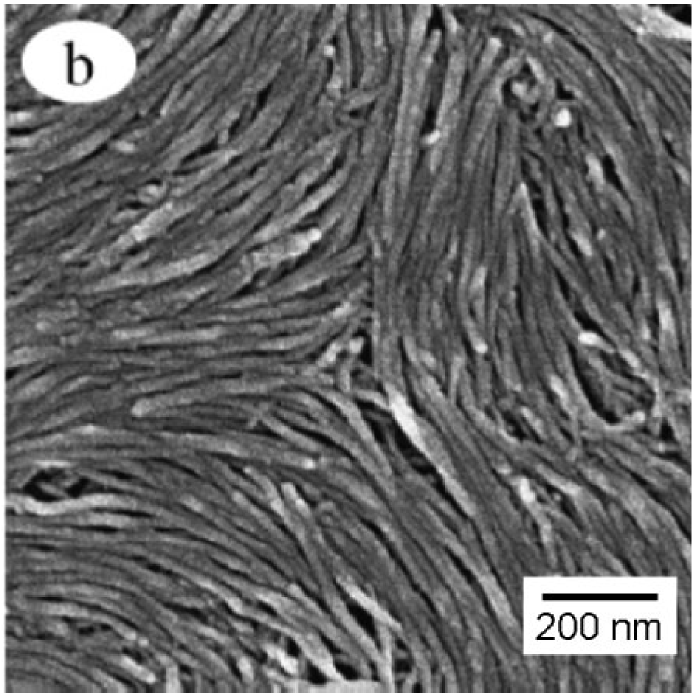

Wikipedia

# Defects

Roughly these can be thought of as (point or line) discontinuities in the director or line field.



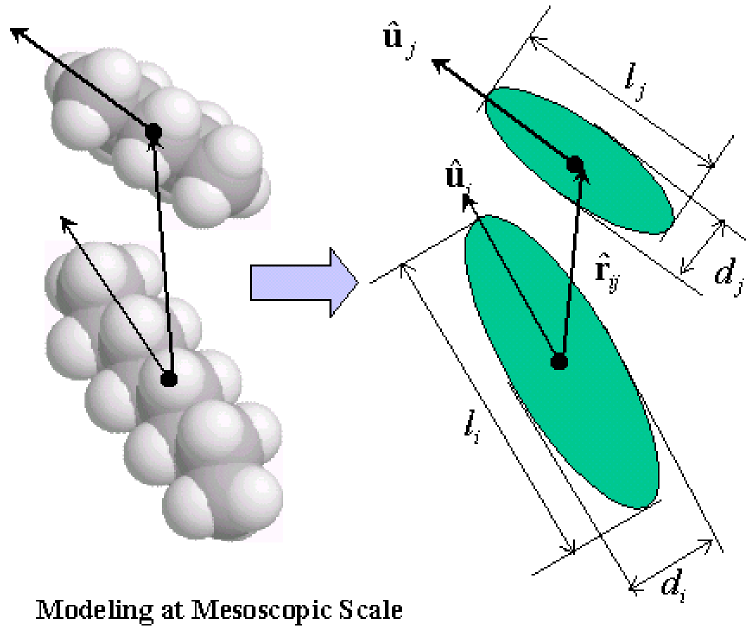
Schlieren texture of a nematic film
with surface point defects (boojums).
Oleg Lavrentovich (Kent State)




Zhang/Kumar 2007
Carbon nano-tubes as liquid crystals

# Modelling via molecular dynamics

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




http://mw.concord.org

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

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

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 $\varepsilon_0, \sigma_c$ are empirical parameters.

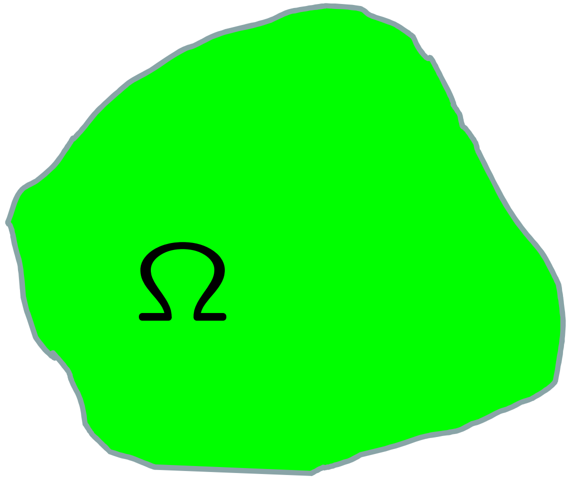
# Twisted nematic display simulation

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 (courtesy Claudio Zannoni)

# Continuum models

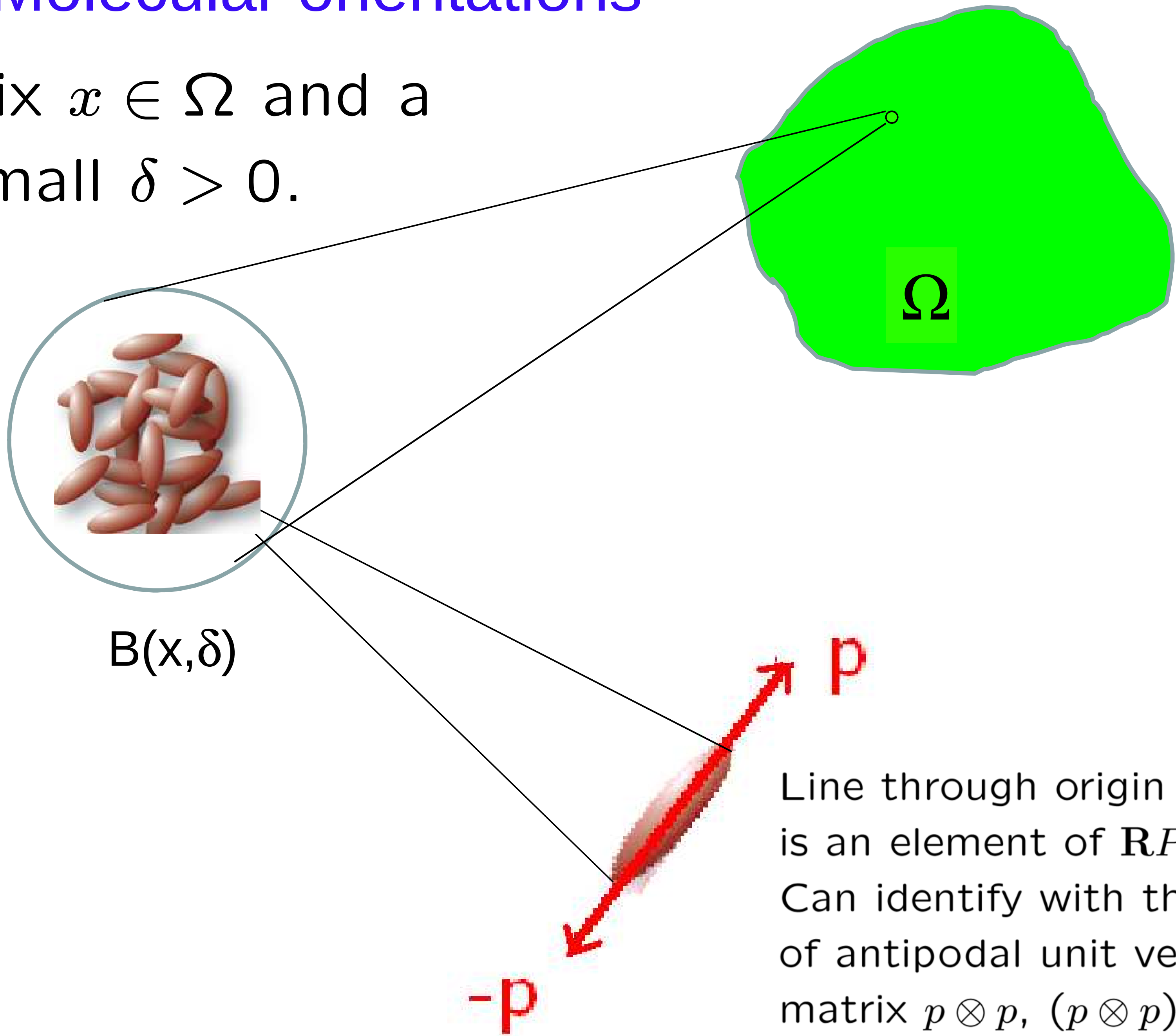
Consider a nematic liquid crystal filling a container $\Omega \subset \mathbb{R}^3$.




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

# Molecular orientations

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




Line through origin parallel to $p$ is an element of $\mathbf{R}P^2$.
Can identify with the pair $\{p, -p\}$ of antipodal unit vectors or the matrix $p \otimes p$, $(p \otimes p)_{ij} = p_i p_j$.

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

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 $\mu = \mu_0$, where

$$d\mu_0(p) = \frac{1}{4\pi} dp,$$

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

A natural idea would be to use as a state variable 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 moments of $\mu$ 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 $3 \times 3$ matrix satisfying $\mathrm{tr} M = 1$.

Let $e \in S^2$. Then

$$\begin{aligned} e \cdot Me &= \int_{S^2} (e \cdot p)^2 d\mu(p) \\ &= \langle \cos^2\theta \rangle, \end{aligned}$$

where $\theta$ is the angle between $p$ and $e$.

The second moment tensor of the isotropic distribution $\mu_0$, $d\mu_0 = \frac{1}{4\pi} dp$, is

$$M_0 = \frac{1}{4\pi} \int_{S^2} p \otimes p \, dS = \frac{1}{3}\mathbf{1}$$

(since $\int_{S^2} p_1 p_2 \, dS = 0$, $\int_{S^2} p_1^2 \, dS = \int_{S^2} p_2^2 \, dS$ etc and $\mathrm{tr}\, M_0 = 1$.)

The *de Gennes Q-tensor*

$$Q = M - M_0$$

measures the deviation of $M$ from its isotropic value.

Note that

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

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

*Remark.* $Q = 0$ does not imply $\mu = \mu_0$. For example we can take

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

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 eigen-vectors of $Q$ with corresponding eigenvalues $\lambda_1, \lambda_2, \lambda_3$ with $\lambda_1 + \lambda_2 + \lambda_3 = 0$.

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 $\mu$, e.g. for

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

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

$$\int_{S_2} (p \cdot e)^2 d\mu(p) = 0,$$

and so $\mu$ is supported on the great circle perpendicular to $e$.

If the eigenvalues $\lambda_i$ of $Q$ are distinct then $Q$ is said to be *biaxial*, and if two $\lambda_i$ are equal *uniaxial*.

In the uniaxial case we can suppose $\lambda_1 = \lambda_2 = -\frac{s}{3}$, $\lambda_3 = \frac{2s}{3}$, and setting $n_3 = n$ we get

$$Q = -\frac{s}{3}(\mathbf{1} - n \otimes n) + \frac{2s}{3} n \otimes n.$$

Thus

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

where $-\frac{1}{2} \leq s \leq 1$.

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 $\theta$ is the angle between $p$ and $n$. Hence

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

$$s = -\frac{1}{2} \;\Leftrightarrow\; \int_{S^2} (p \cdot n)^2 d\mu(p) = 0$$

(all molecules perpendicular to $n$).

$$s = 0 \;\Leftrightarrow\; Q = 0$$

(which occurs when $\mu$ is isotropic).

$$s = 1 \;\Leftrightarrow\; \int_{S^2} (p \cdot n)^2 d\mu(p) = 1$$

$$\Leftrightarrow\; \mu = \frac{1}{2}(\delta_n + \delta_{-n})$$

(perfect ordering parallel to $n$).

In practice $Q$ is observed to be very nearly uniaxial except possibly very near defects, with a constant value of $s$ (typical values being in the range $0.6-0.8$).

We will provide an explanation for this later.

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 if and only if

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

*Proof.* The characteristic equation of $Q$ is

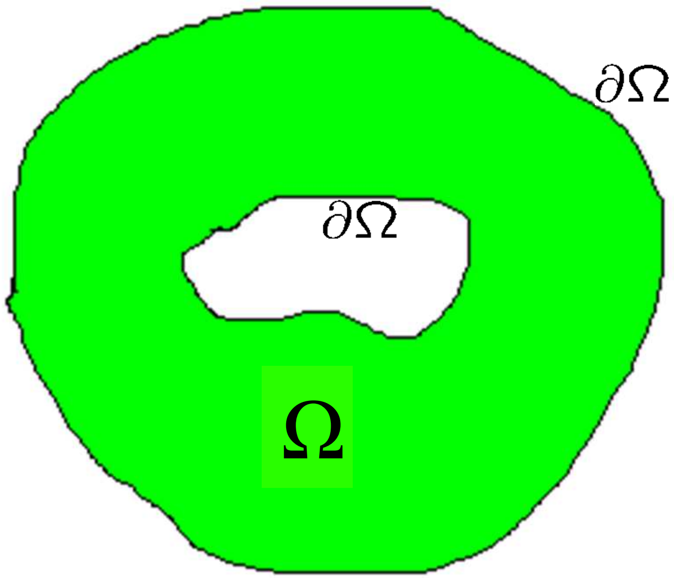
$$\det(Q - \lambda\mathbf{1}) = \det Q - \lambda \operatorname{tr} \operatorname{cof} Q + 0\lambda^2 - \lambda^3.$$

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 $4p^3 = 27q^2$.

# Energetics




Consider a liquid crystal material filling a container $\Omega \subset \mathbf{R}^3$. We suppose that the material is incompressible, homogeneous (same material at every point) and that the temperature is constant.

At each point $x \in \Omega$ we have a corresponding measure $\mu_x$ and order parameter tensor $Q(x)$. We suppose that the material is described by a free-energy density $\psi(Q, \nabla Q)$, so that the total free energy is given by

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

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

# The domain of $\psi$

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

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

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

Then note that

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

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

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

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

Thus we can assume that $\psi$ satisfies for $(Q, D) \in \operatorname{dom}\psi$

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

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

# Frame-indifference

Fix $\bar{x} \in \Omega$, 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 $R \in SO(3)$. We require that both observers see the same free-energy density, that is

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

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

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

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

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

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

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

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

# Material symmetry

The requirement that

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

when $z = \bar{x} + \widehat{R}(x - \bar{x})$, where $\widehat{R} = -\mathbf{1} + 2e \otimes e$, $|e| = 1$, 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 $\widehat{R}\tilde{R}$, where $\tilde{R} \in SO(3)$ and $\widehat{R}$ is a reflection, for a nematic

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

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

# Bulk and elastic energies

We can decompose $\psi$ as

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

Thus, putting $D=0$,

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

which holds if and only if $\psi_B$ is a function of the principal invariants of $Q$, that is, since $\operatorname{tr} Q=0$,

$$\psi_B(Q)=\bar{\psi}_B(|Q|^2, \det Q).$$

# The bulk energy

Following de Gennes, Schophol & Sluckin PRL 59(1987), Mottram & Newton, *Introduction to $Q$-tensor theory*, we consider the example

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

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

Then

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

$\psi_B$ attains a minimum subject to $\sum_{i=1}^{3} \lambda_i = 0$. A calculation shows that the critical points have two $\lambda_i$ 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 $\psi_B$ is $Q = 0$.
If $\theta < \theta_{\mathrm{NI}}$ then the minimizers are

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

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

# The elastic energy

Examples of isotropic functions quadratic in $\nabla Q$ :

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

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

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

where the $L_i$ are material constants.

# The constrained theory

If the $L_i$ are small, it is reasonable to consider the *constrained theory* in which $Q$ is required to be uniaxial with a constant scalar order parameter $s > 0$, so that

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

(For recent rigorous work justifying this see Majumdar & Zarnescu, Nguyen & Zarnescu.) In this theory the bulk energy is constant and so we only have to consider the elastic energy

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

# Oseen-Frank energy

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

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

where

$K_1 = 2L_1 s^2 + L_2 s^2 + L_3 s^2 - \frac{2}{3} L_4 s^3,$
$K_2 = 2L_1 s^2 - \frac{2}{3} L_4 s^3,$
$K_3 = 2L_1 s^2 + L_2 s^2 + L_3 s^2 + \frac{4}{3} L_4 s^3,$
$K_4 = L_3 s^2.$

# Boundary conditions

(a) In the constrained/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

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

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

Likewise, corresponding to conical anchoring we can choose

$$w(x, n) = K[(n(x) \cdot \nu(x))^2 - \alpha(x)^2]^2.$$

Weak anchoring conditions are appealing physically because they try to model the interaction between the liquid crystal and the confining boundary. They also allow for changes in topology of the director field which may not be possible with strong anchoring.

# Boundary conditions contd

(b) Landau - de Gennes

(i) Strong anchoring:

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

(ii) Weak anchoring: add surface energy term

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

(iii) Conical: ?? perhaps

$$Q(x)\nu(x) \cdot \nu(x) = \sqrt{\frac{3}{2}}|Q(x)|(\alpha(x)^2 - \frac{1}{3}), \; x \in \partial\Omega.$$

# Function Spaces
# (part of the mathematical model)

## Landau – de Gennes theory

We are interested in equilibrium configurations of finite energy

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

satisfying suitable boundary conditions. (Here we ignore electromagnetic contributions to the energy and surface terms.)

We use the Sobolev space $W^{1,p}(\Omega; M^{3\times 3})$. Since usually we assume

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

$$I_1 = Q_{ij,j} Q_{ik,k},\ I_2 = Q_{ik,j} Q_{ij,k},$$

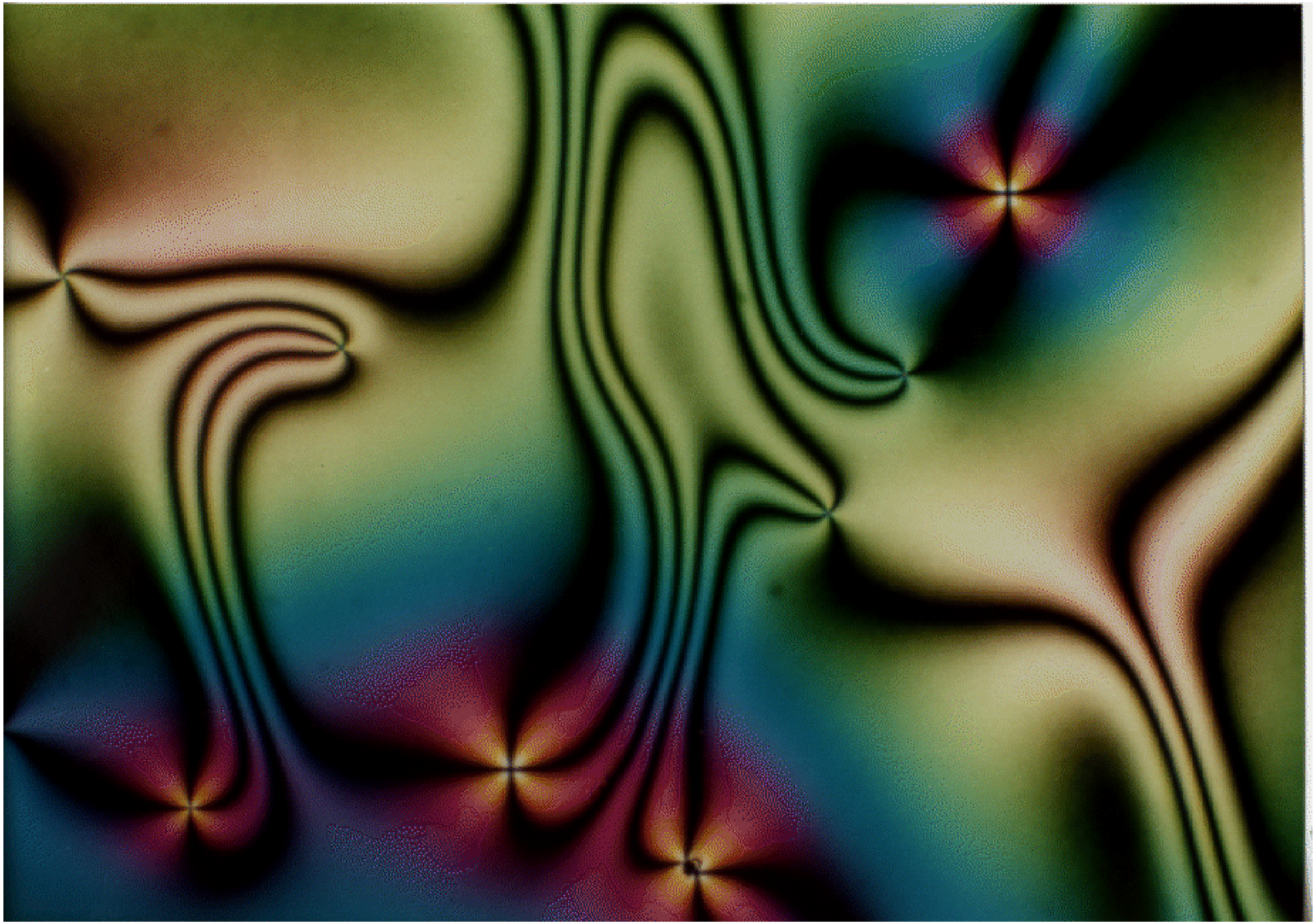
$$I_3 = Q_{ij,k} Q_{ij,k},\ I_4 = Q_{lk} Q_{ij,l} Q_{ij,k},$$

we typically take $p = 2$.

# Constrained theory.

Similarly we use the Sobolev space $W^{1,p}(\Omega, \mathbf{R}P^2)$, $1 \leq p < \infty$, which is the set of $Q = s(n \otimes n - \frac{1}{3}\mathbf{1})$ with weak derivative $\nabla Q$ satisfying $\int_\Omega |\nabla Q(x)|^p dx < \infty$.

Thus for the Landau - de Gennes energy density, the space of $Q$ with finite elastic energy is $W^{1,2}(\Omega, \mathbf{R}P^2)$.



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

# Possible defects in constrained theory

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

Hedgehog $\quad n(x) = \dfrac{x}{|x|}$

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

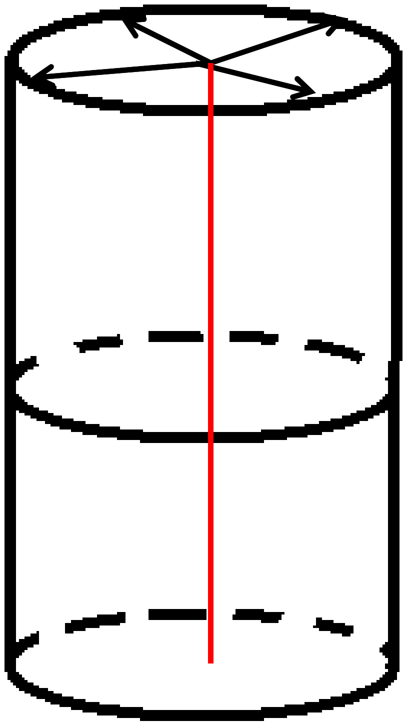
$$|\nabla n(x)|^2 = \tfrac{2}{|x|^2}$$

$$\textstyle\int_0^1 r^{2-p} dr < \infty$$

$Q, n \in W^{1,p},\ 1 \le p < 3$

Finite energy

# Disclinations



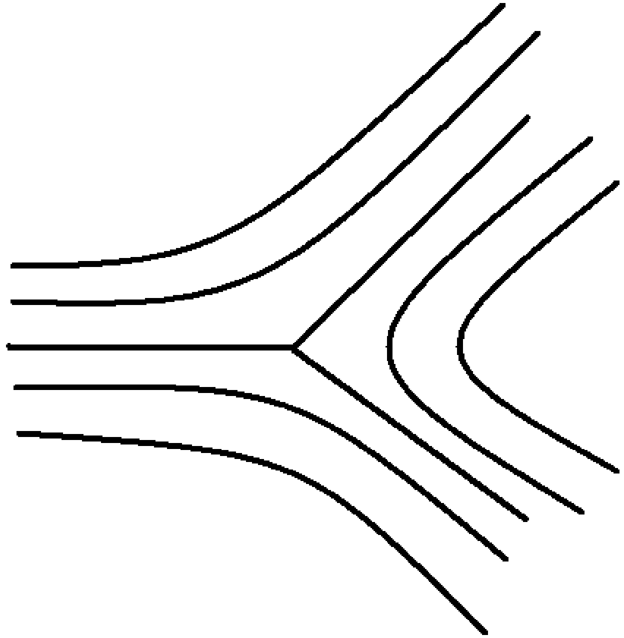
$$n(x) = \left(\frac{x_1}{r}, \frac{x_2}{r}, 0\right) \quad r = \sqrt{x_1^2 + x_2^2}$$

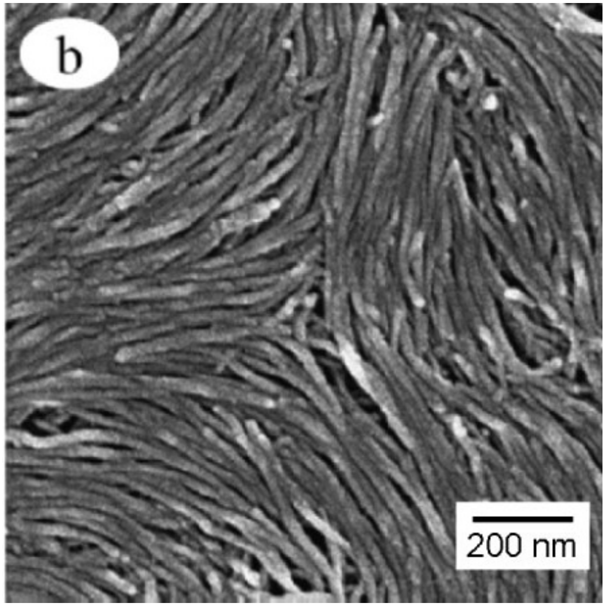
$$|\nabla n(x)|^2 = \frac{1}{r^2}$$

$$n, Q \in W^{1,p} \Leftrightarrow 1 \leq p < 2$$

infinite energy for quadratic models

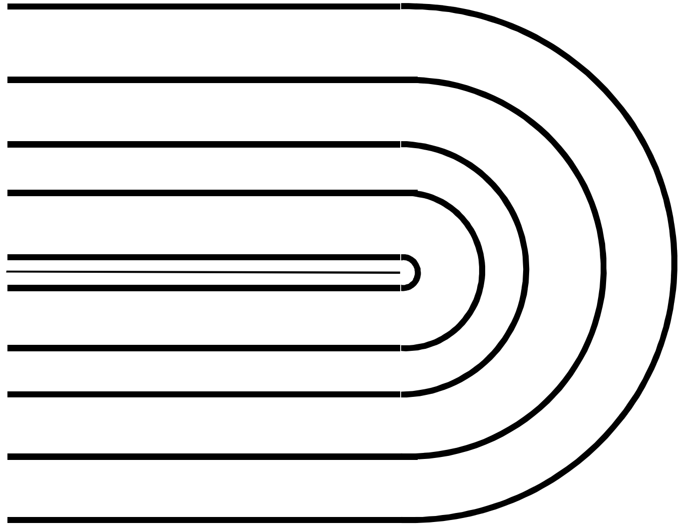
# Index one half singularities






Zhang/Kumar 2007
Carbon nano-tubes
as liquid crystals

$$Q \notin W^{1,2}$$



# Existence in Landau – de Gennes theory

We have to minimize

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

subject to suitable boundary conditions.

Suppose we take $\psi_B : \mathcal{E} \to \mathbf{R}$ to be continuous and bounded below, $\mathcal{E} = \{Q \in M^{3\times 3} : Q = Q^T, \mathrm{tr}\, Q = 0\}$, (e.g. of the quartic form considered previously) and

$$\psi_E(Q, \nabla Q) = \sum_{i=1}^{4} L_i I_i.$$

Theorem (Davis & Gartland 1998)
Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with smooth boundary $\partial\Omega$. Let $L_4 = 0$ 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

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

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 $\nabla Q$). 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 $\Omega$. But

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

by Fatou's lemma and the convexity in $\nabla Q$. 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

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

is unbounded below.

*Proof.* Choose any $Q$ satisfying the boundary conditions, and multiply it by a smooth function $\varphi(x)$ which equals one in a neighbourhood of $\partial\Omega$ and is zero in some ball $B \subset \Omega$, which we can take to be $B(0,1)$. We will alter $Q$ in $B$ so that

$$J(Q) = \int_B [\psi_B(Q) + \sum_{i=1}^{4} L_i I_i]\, dx$$

is unbounded below subject to $Q|_{\partial B} = 0$.

Choose

$$Q(x) = \theta(r)\left[\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}\mathbf{1}\right], \; \theta(1) = 0,$$

where $r = |x|$. Then

$$|\nabla Q|^2 = \frac{2}{3}\theta'^2 + \frac{4}{r^2}\theta^2,$$

and

$$I_4 = Q_{kl}Q_{ij,k}Q_{ij,l} = \frac{4}{9}\theta(\theta'^2 - \frac{3}{r^2}\theta^2).$$

Hence

$$J(Q) \leq 4\pi \int_0^1 r^2 \left[\psi_B(Q) + C\left(\frac{2}{3}\theta'^2 + \frac{4}{r^2}\theta^2\right) + L_4\frac{4}{9}\theta\left(\theta'^2 - \frac{3}{r^2}\theta^2\right)\right] dr,$$

where $C$ is a constant.

Provided $\theta$ is bounded, all the terms are bounded except

$$4\pi \int_0^1 r^2 \left(\frac{2}{3}C + \frac{4}{9}L_4\theta\right)\theta'^2 \, dr.$$

Choose

$$\theta(r) = \begin{cases} \theta_0(2 + \sin kr) & 0 < r < \frac{1}{2} \\ 2\theta_0(2 + \sin \frac{k}{2})(1 - r) & \frac{1}{2} < r < 1 \end{cases}$$

The integrand is then bounded on $(\frac{1}{2}, 1)$ and we need to look at

$$4\pi \int_0^{\frac{1}{2}} r^2 \left(\frac{2}{3}C + \frac{4}{9}L_4\theta_0(2 + \sin kr)\right) \theta_0^2 k^2 \cos^2 kr \, dr,$$

which tends to $-\infty$ if $L_4\theta_0$ is sufficiently negative.

# Existence of minimizers in the constrained theory

Similar. In fact, since in the constrained theory $|Q|$ is bounded we can allow $L_4 \neq 0$ under appropriate inequalities on the $L_i$. The only difference from the unconstrained case is how to handle the constraint.

But this can be written as

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

and if $Q^{(j)}$ satisfy the constraint with $Q^{(j)} \rightharpoonup Q^*$ in $W^{1,2}$ then by the compactness of the embedding of $W^{1,2}$ in $L^2$ we may assume that $Q^{(j)} \to Q^*$ a.e., so that $Q^*$ also satisfies the constraint.

# Can we orient the director? (JB/Zarnescu, ARMA 2011)

We say that $Q = Q(x)$ is *orientable* if we can write

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

where $n \in W^{1,p}(\Omega, S^2)$.
This means that for each $x$ we can make a choice of the unit vector $n(x) = \pm\tilde{n}(x) \in S^2$ so that $n(\cdot)$ has some reasonable regularity, sufficient to have a well-defined gradient $\nabla n$ (in topological jargon such a choice is called a *lifting*).

# Relating the Q and n descriptions

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

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

and set

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

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

Proposition

If $n \in W^{1,p}(\Omega, S^2)$, $1 \leq p \leq \infty$, then $Q = P(n)$ belongs to $W^{1,p}(\Omega, \mathcal{Q})$. Conversely, let $Q \in W^{1,p}(\Omega, \mathcal{Q})$, $1 \leq p \leq \infty$, and $n$ be a measurable function on $\Omega$ with values in $S^2$ such that $P(n) = Q$. If $n$ is continuous along almost every line parallel to the coordinate axes and intersecting $\Omega$, then $n \in W^{1,p}(\Omega, S^2)$ (so that $Q$ is orientable). Moreover

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

Proof

For $g, h \in W^{1,1}(\Omega) \cap L^\infty(\Omega)$ we have $gh \in W^{1,1}(\Omega) \cap L^\infty(\Omega)$ and $(gh)_{,i} = gh_{,i} + g_{,i}h$. Hence, if $n \in W^{1,p}$, we have $Q \in W^{1,1}$ and $Q_{ij,k} = s(n_i n_{j,k} + n_{i,k} n_j)$ from which we obtain $\nabla Q \in L^p$ and then $Q \in W^{1,p}$. Also

$$\begin{aligned} Q_{ij,k} n_j &= s\left[n_i (n_{j,k} n_j) + n_{i,k}\right] \\ &= s[\frac{n_i}{2} \underbrace{(n_j n_j)}_{=1}{}_{,k} + n_{i,k}] = s n_{i,k}. \end{aligned}$$

Conversely, suppose that $Q \in W^{1,p}$. Let $x \in \Omega$ with $n$ continuous along the line $(x + \mathbf{R}e_k) \cap \Omega$. Let $x + te_k \in \Omega$. As $Q \in W^{1,1}$ we can suppose that $Q$ is differentiable at $x$ in the direction $e_k$. Then

$$\frac{Q_{ij}(x + te_k) - Q_{ij}(x)}{t}$$

$$= s\left[\frac{n_i(x+te_k)n_j(x+te_k) - n_i(x)n_j(x)}{t}\right]$$

$$= s \cdot n_i(x + te_k)\left[\frac{n_j(x+te_k) - n_j(x)}{t}\right]$$

$$+ s \cdot \left[\frac{n_i(x+te_k) - n_i(x)}{t}\right] n_j(x).$$

Multiply both sides by $\frac{1}{2}\Big[n_j(x+te_k)+n_j(x)\Big]$. Then, since

$$\Big[n_j(x+te_k)-n_j(x)\Big]\Big[n_j(x+te_k)+n_j(x)\Big]$$
$$= n_j(x+te_k)n_j(x+te_k)-n_j(x)n_j(x) = 1-1 = 0$$

we have that

$$\frac{Q_{ij}(x+te_k)-Q_{ij}(x)}{t}\cdot\frac{1}{2}\Big[n_j(x+te_k)+n_j(x)\Big]$$
$$= s\cdot\left[\frac{n_i(x+te_k)-n_i(x)}{t}\right]n_j(x)\frac{1}{2}\Big[n_j(x+te_k)+n_j(x)\Big].$$

Letting $t \to 0$ and using the assumed continuity of $n$ we deduce that

$$s \cdot \lim_{t \to 0} \frac{n_i(x + te_k) - n_i(x)}{t} = Q_{ij,k}(x) n_j(x).$$

Hence the partial derivatives of $n$ exist almost everywhere in $\Omega$ and satisfy

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

and since $\nabla Q \in L^p$ it follows that $n \in W^{1,p}(\Omega, \mathbb{S}^2)$ as required.

Proposition

Orientability is preserved by weak convergence: if $Q^{(k)} \in W^{1,p}(\Omega; \mathbf{R}P^2)$, $1 \leq p \leq \infty$, is a sequence of orientable maps with $Q^{(k)}$ converging weakly to $Q$ in $W^{1,p}$ (weak* if $p = \infty$), then $Q$ is orientable.

Proof

If $Q^{(k)} = P(n^{(k)})$ where $n^{(k)} \in W^{1,1}$ then by the previous result $n^{(k)}$ is bounded in $W^{1,p}$ (equi-integrable if $p = 1$) and so we may assume that $n^{(k)} \rightharpoonup n$ in $W^{1,p}$ and $n^{(k)} \to n$ a.e., which implies that $P(n) = Q$.

*Theorem*

An orientable $Q$ has exactly two orientations.

Proof

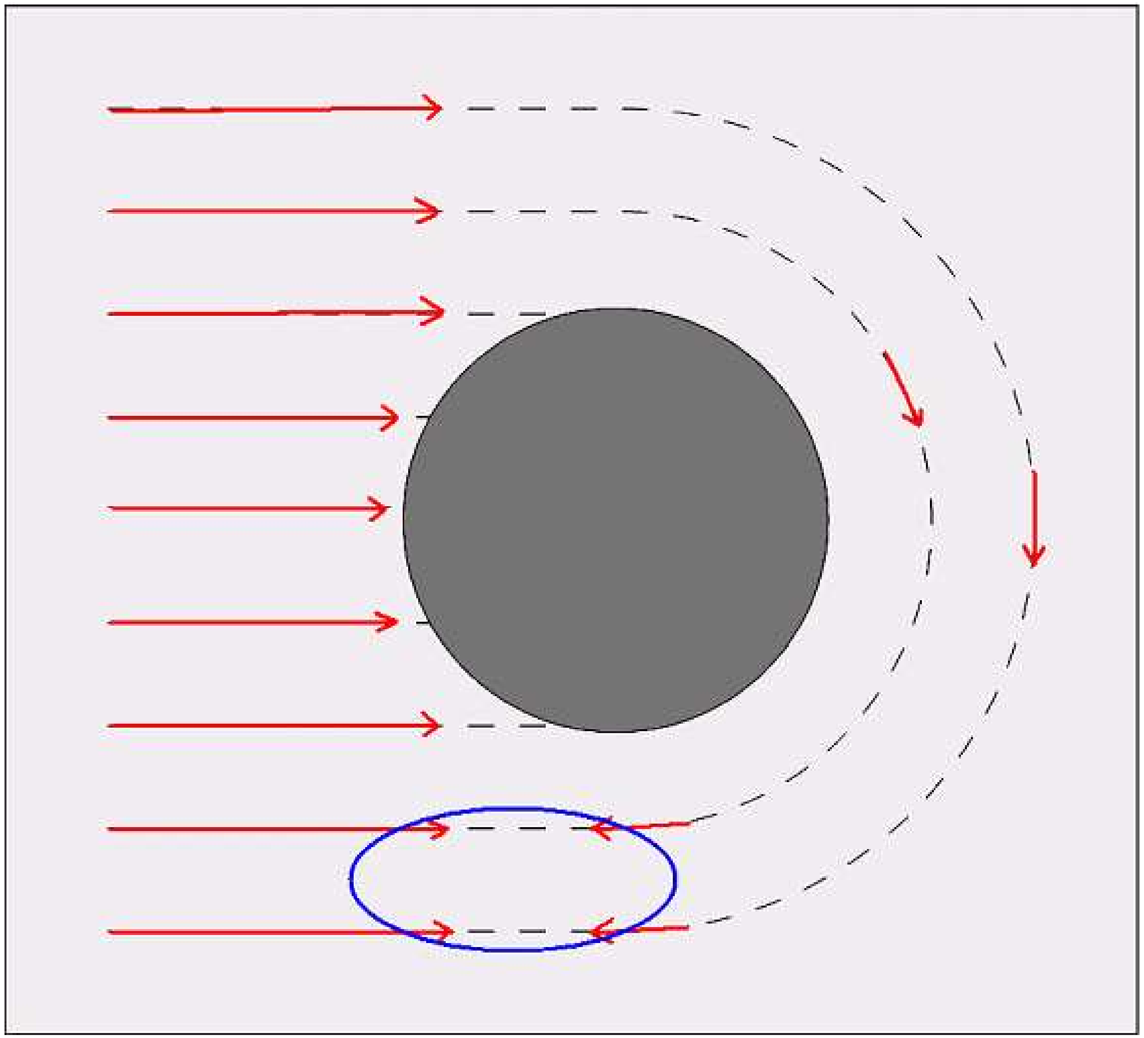
Suppose that $n$ and $\tau n$ both generate $Q$ and belong to $W^{1,1}(\Omega, S^2)$, where $\tau^2(x) = 1$ a.e.. Let $Q \subset \Omega$ be a cube with sides parallel to the coordinate axes. Let $x_2, x_3$ be such that the line $x_1 \mapsto (x_1, x_2, x_3)$ intersects $Q$. Let $L(x_2, x_3)$ denote the 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 $\varphi \in C_0^\infty(Q)$. Then by Fubini's theorem

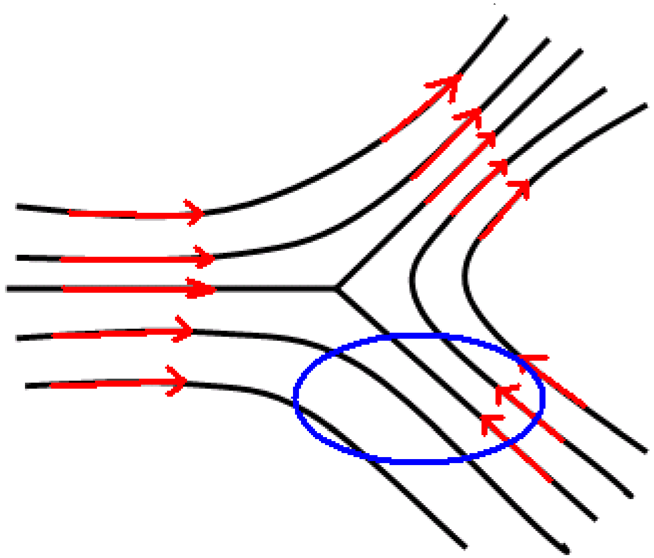
$$\int_Q \tau\varphi_{,1} dx = \int_Q (\tau\varphi)_{,1} dx = 0,$$

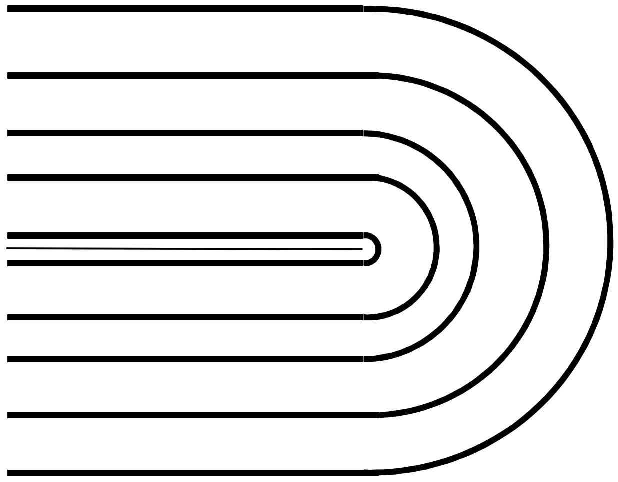
so that the weak derivative $\tau_{,1}$ exists in $Q$ and is zero. Similarly the weak derivatives $\tau_{,2}, \tau_{,3}$ exist in $Q$ and are zero. Thus $\nabla\tau = 0$ in Q and hence $\tau$ is constant in $Q$. Since $\Omega$ is connected, $\tau$ is constant in $\Omega$, and thus $\tau \equiv 1$ or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

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



The index one half singularities are non-orientable



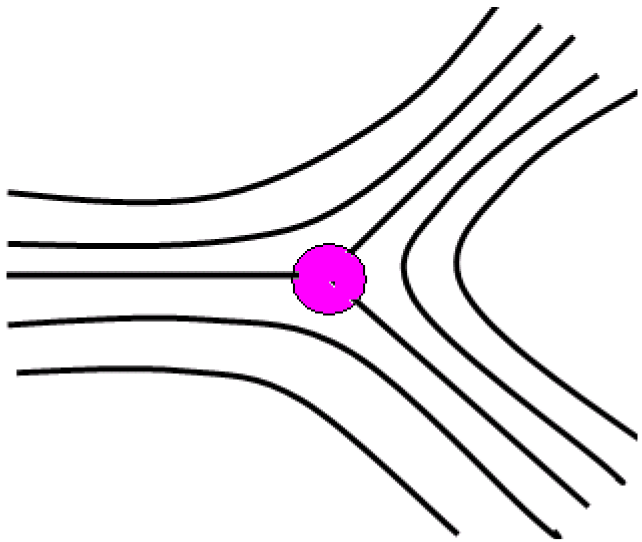


*Theorem 2*

If $\Omega$ is simply-connected and $Q \in W^{1,p}$, $p \geq 2$, then $Q$ is orientable.

(See also a recent topologically more general lifting result of Bethuel and Chiron for maps u:Ω→N.)

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



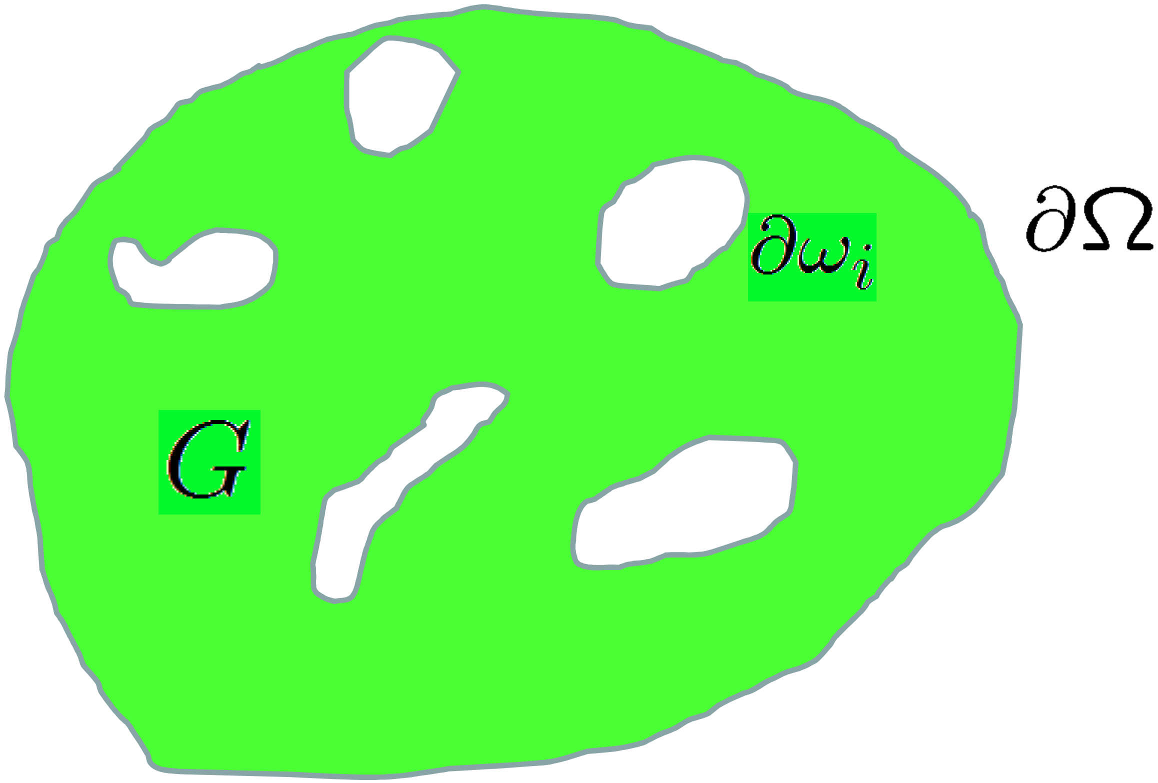
Another consequence is that it is impossible to modify this Q-tensor field in a core around the singular line so that it has finite Landau-de Gennes energy.

# Ingredients of Proof of Theorem 2

- Lifting possible if $Q$ is smooth and $\Omega$ is simply connected
- Pakzad-Rivière theorem (2003) implies that if $\partial\Omega$ is smooth, then there is a sequence of smooth $Q^{(j)} : \Omega \to \mathbf{R}P^2$ 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
- Orientability is preserved under weak convergence

# 2D examples and results for non simply-connected regions

Let $\Omega \subset \mathbb{R}^2$, $\omega_i \subset \mathbb{R}^2, i = 1, \ldots, n$ be bounded, open and simply connected, with $C^1$ boundary, such that $\bar{\omega}_i \subset \Omega$, $\bar{\omega}_i \cap \bar{\omega}_j \neq \emptyset$ for $i \neq j$, and set $G = \Omega \backslash \bigcup_{i=1}^{n} \bar{\omega}_i$.



$$\mathcal{Q}_2 = \{Q = s(n \otimes n - \frac{1}{3}\mathbf{1}) : n = (n_1, n_2, 0)\}$$

Given $Q \in W^{1,2}(G; \mathcal{Q}_2)$ define the auxiliary complex-valued map

$$A(Q) = \frac{2}{s} Q_{11} - \frac{1}{3} + i\frac{2}{s} Q_{12}.$$

Then $A(Q) = Z(n)^2$,
where $Z(n) = n_1 + in_2$.

$A : Q_2 \to S^1$ is bijective.

Let $C = \{C(s) : 0 \leq s \leq 1\}$ be a smooth Jordan curve in $\mathbb{R}^2 \simeq \mathbb{C}$.

If $Z : C \to S^1$ is smooth then the degree of $Z$ is the integer

$$\deg(Z, C) = \frac{1}{2\pi i} \int_C \frac{Z_s}{Z} ds.$$

Writing $Z(s) = e^{i\theta(s)}$ we have that

$$\deg(Z, C) = \frac{1}{2\pi i} \int_0^1 i\theta_s ds = \frac{\theta(1) - \theta(0)}{2\pi}.$$

If $Z \in H^{\frac{1}{2}}(C; S^1)$ then the degree may be defined by the same formula

$$\deg(Z, C) = \frac{1}{2\pi i} \int_C \frac{Z_s}{Z} ds.$$

interpreted in the sense of distributions (L. Boutet de Monvel).

Theorem

Let $Q \in W^{1,2}(G;Q_2)$. The following are equivalent:

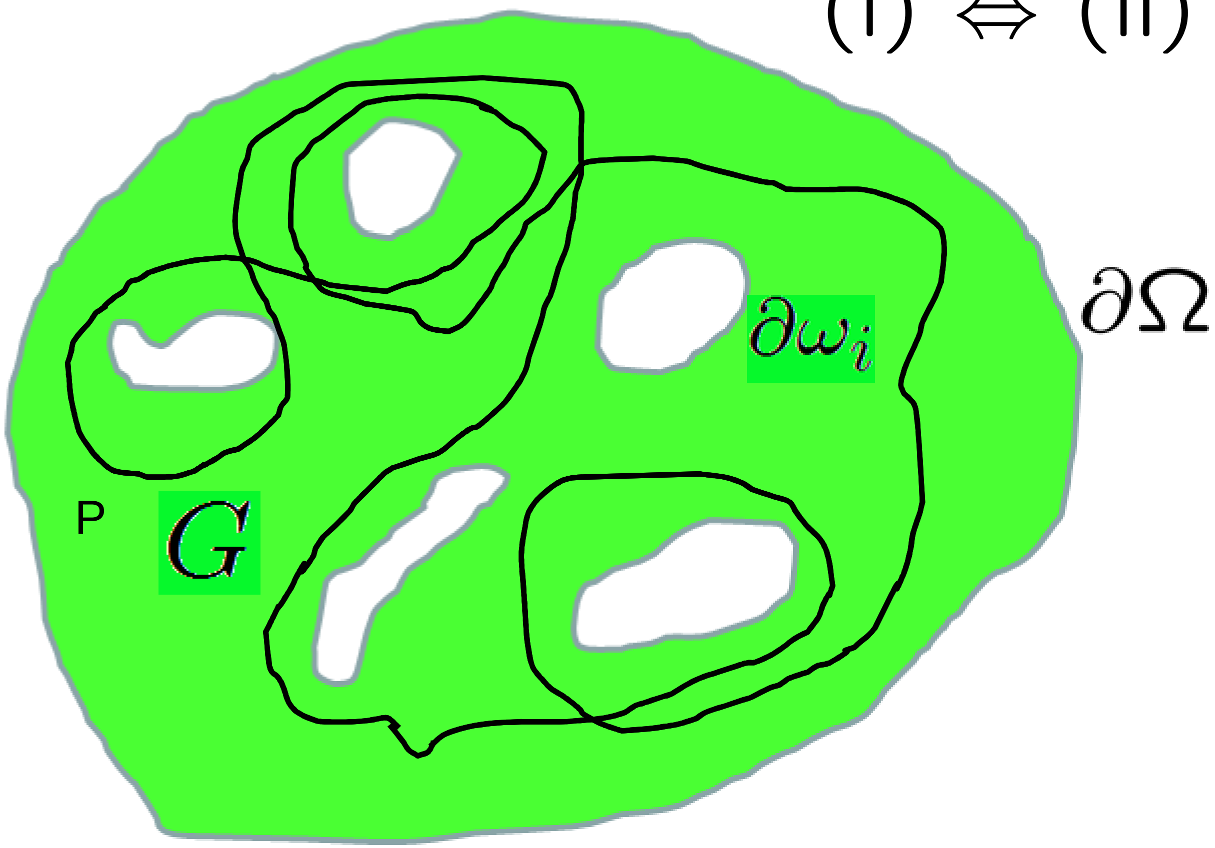
(i) $Q$ is orientable.

(ii) $\operatorname{Tr} Q \in H^{\frac{1}{2}}(C;Q_2)$ is orientable for every component $C$ of $\partial G$.

(iii) $\deg(A(\operatorname{Tr} Q), C) \in 2\mathbb{Z}$ for each component $C$ of $\partial G$.

We sketch the proof, which is technical.

(i) $\Leftrightarrow$ (ii) for continuous $Q$




The orientation at the beginning and end of the loop are the same since we can pass the loop through the holes using orientability on the boundary.

(ii) $\Leftrightarrow$ (iii). If $\mathrm{Tr}\, Q$ is orientable on $C$ then

$$\begin{aligned} \deg\left(A(\mathrm{Tr}\, Q), C\right) &= \deg\left(Z^2(n), C\right) \\ &= \frac{1}{2\pi i}\int_C \frac{(Z^2)_s}{Z^2} ds \\ &= \frac{1}{2\pi i}\int_C 2\frac{Z_s}{Z} ds \\ &= 2\deg\left(Z(n), C\right) \end{aligned}$$

Conversely, if $A(\mathrm{Tr}\, Q(s)) = e^{i\theta(s)}$ and

$$\deg(A(\mathrm{Tr}\, Q), C) = \frac{\theta(1) - \theta(0)}{2\pi} \in 2\mathbb{Z}$$

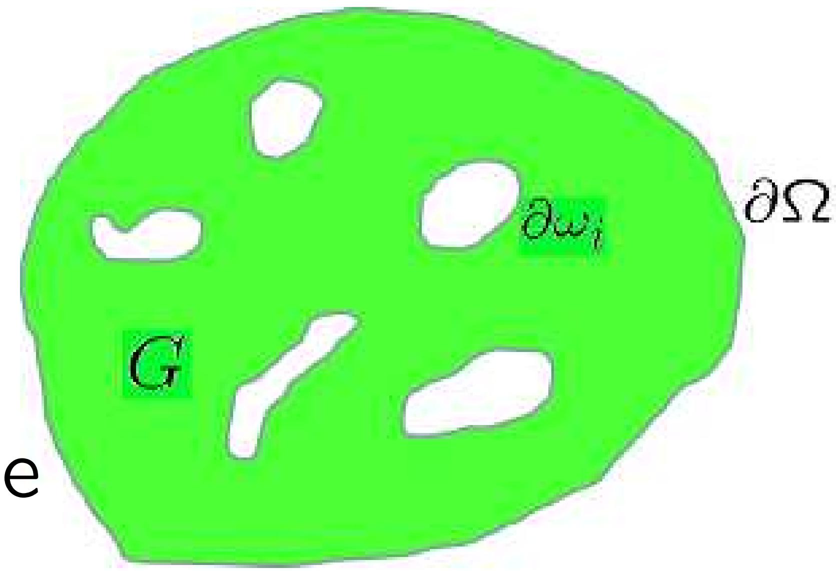
then $Z(s) = e^{\frac{i\theta(s)}{2}} \in H^{\frac{1}{2}}(C, S^1)$ and so $\mathrm{Tr}\, Q$ is orientable.

We have seen that the (constrained) Landau-de Gennes and Oseen-Frank theories are equivalent in a simply-connected domain. Is this true in 2D for domains with holes?

If we specify $Q$ on each boundary component then by the Theorem either all $Q$ satisfying the boundary data are orientable (so that the theories are equivalent), or no such $Q$ are orientable, so that the Oseen Frank theory cannot apply and the Landau- de Gennes theory must be used.

More interesting is to apply boundary conditions which allow both the Landau - de Gennes and Oseen-Frank theories to be used and compete energetically.

$$G = \Omega \setminus \bigcup_{i=1}^{n} \bar{\omega}_i$$




So we consider the problem of minimizing

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

subject to $Q|_{\partial\Omega} = g$ orientable with the boundaries $\partial\omega_i$ free.

Since $A$ is bijective and

$$I(Q) = \frac{2}{s^2} \int_G |\nabla A(Q)|^2 dx$$

our minimization problem is equivalent to minimizing

$$\widehat{I}(m) = \frac{2}{s^2} \int_G |\nabla m|^2 dx$$

in $W^{1,2}_{A(g)}(G; S^1) =$

$$\{m \in W^{1,2}(G; S^1) : m|_{\partial\Omega} = A(g)\}.$$

In order that $Q$ is orientable on $\partial\Omega$ we need that

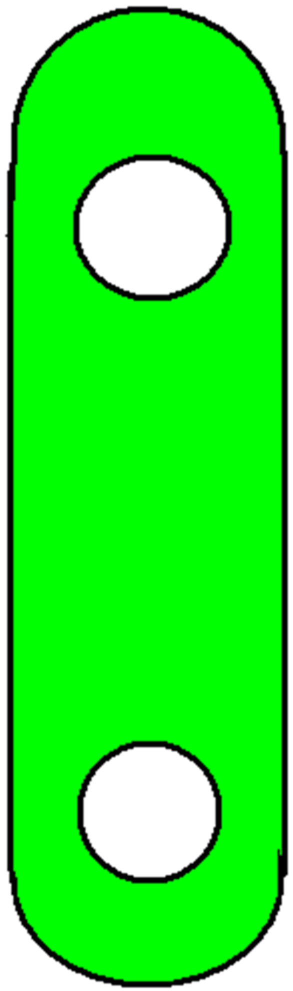
$$\deg(m, \partial\Omega) \in 2\mathbb{Z}.$$

We always have that

$$\deg(m, \partial\Omega) = \sum_{i=1}^{n} \deg(m, \partial\omega_i).$$

Hence if there is only one hole ($n = 1$) then $\deg(m, \partial\omega_1)$ is even and so every $Q$ is orientable.

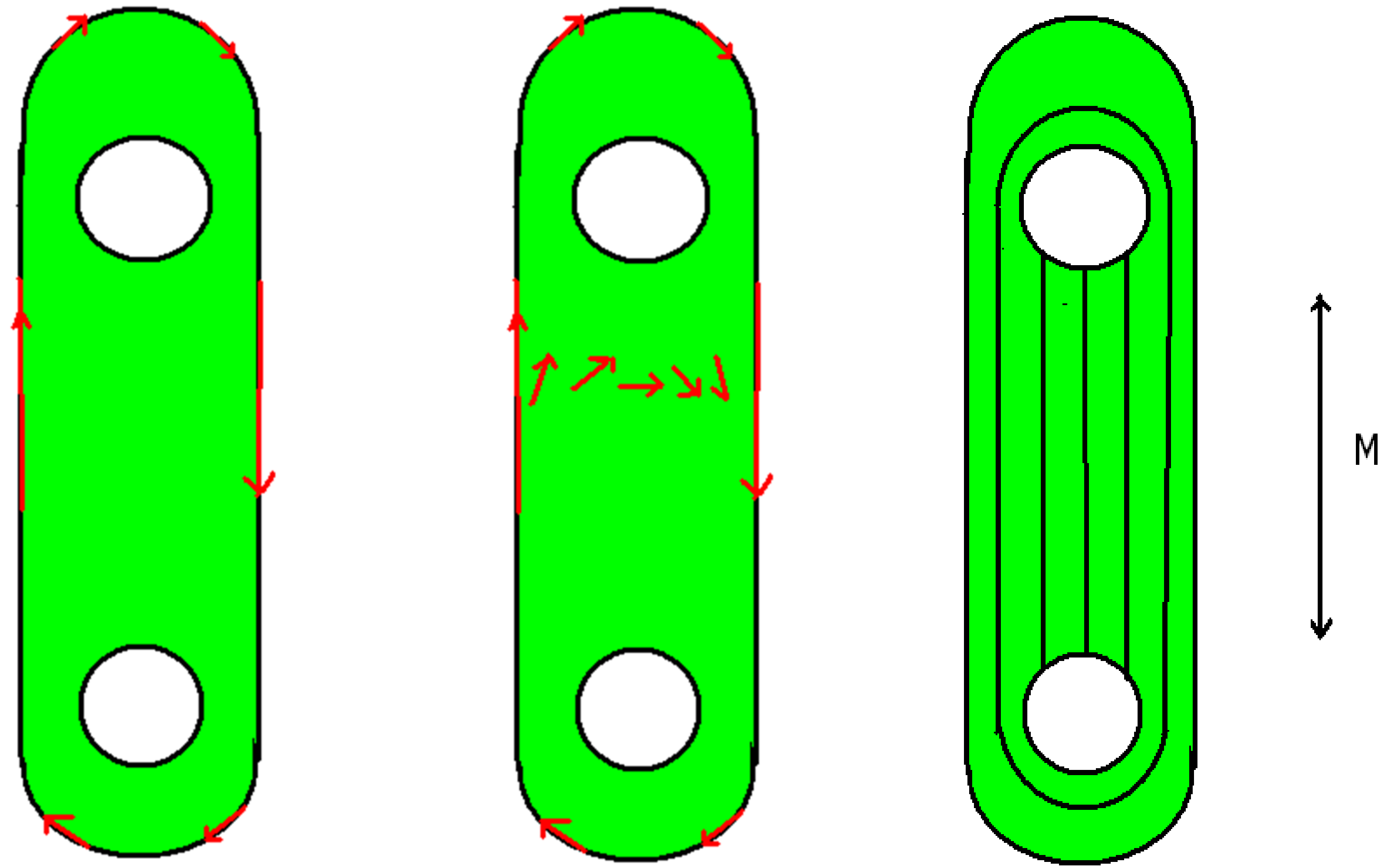
So to have both orientable and non-orientable $Q$ we need at least two holes.

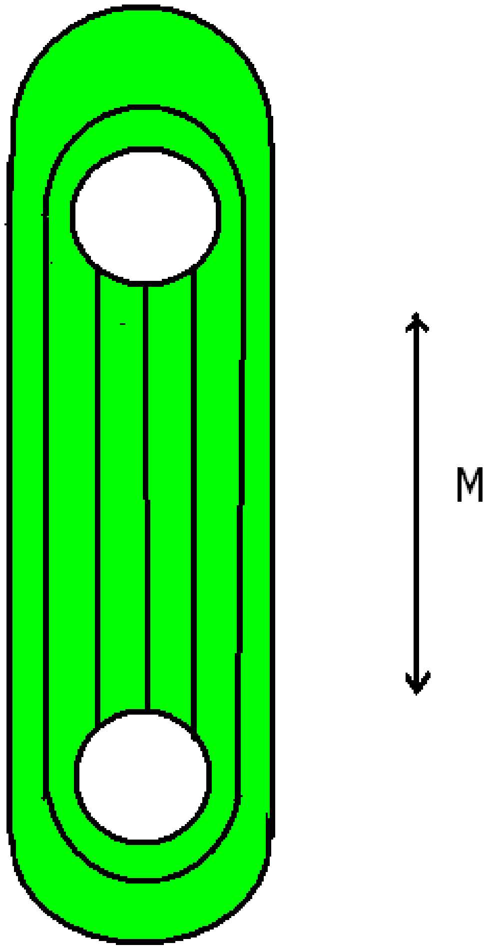


Tangent boundary conditions on outer boundary. No (free) boundary conditions on inner circles.

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

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


M




For M large enough the minimum energy configuration is unoriented, even though there is a minimizer among oriented maps.

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

# The general case of two holes ($n = 2$).

Let $h(g)$ be the solution of the problem

$$\begin{aligned} \Delta h(g) &= 0 \text{ in } G \\ \frac{\partial h(g)}{\partial \nu} &= A(g) \times \frac{\partial A(g)}{\partial \tau} \text{ on } \partial\Omega \\ h(g) &= 0 \text{ on } \partial\omega_1 \cup \partial\omega_2, \end{aligned}$$

where $\frac{\partial}{\partial \tau}$ is the tangential derivative on the boundary (cf Bethuel, Brezis, Helein).

Let $J(g) = (J(g)^1, J(g)^2)$, where $J(g)^i = \frac{1}{2\pi} \int_{\partial\omega_i} \frac{\partial h(g)}{\partial \nu} ds$.

Theorem

All global minimizers are nonorientable iff

$$\mathrm{dist}(J(g)^1, \mathbb{Z}) < \mathrm{dist}(J(g)^1, 2\mathbb{Z})$$

and all are orientable iff

$$\mathrm{dist}(J(g)^1, 2\mathbb{Z}) < \mathrm{dist}(J(g)^1, 2\mathbb{Z} + 1)$$

In the stadium example we can show that $J(g)^1 = -1$. Hence the first condition holds whatever the distance between the holes, so that the minimizer is always non-orientable.

# The eigenvalue constraints

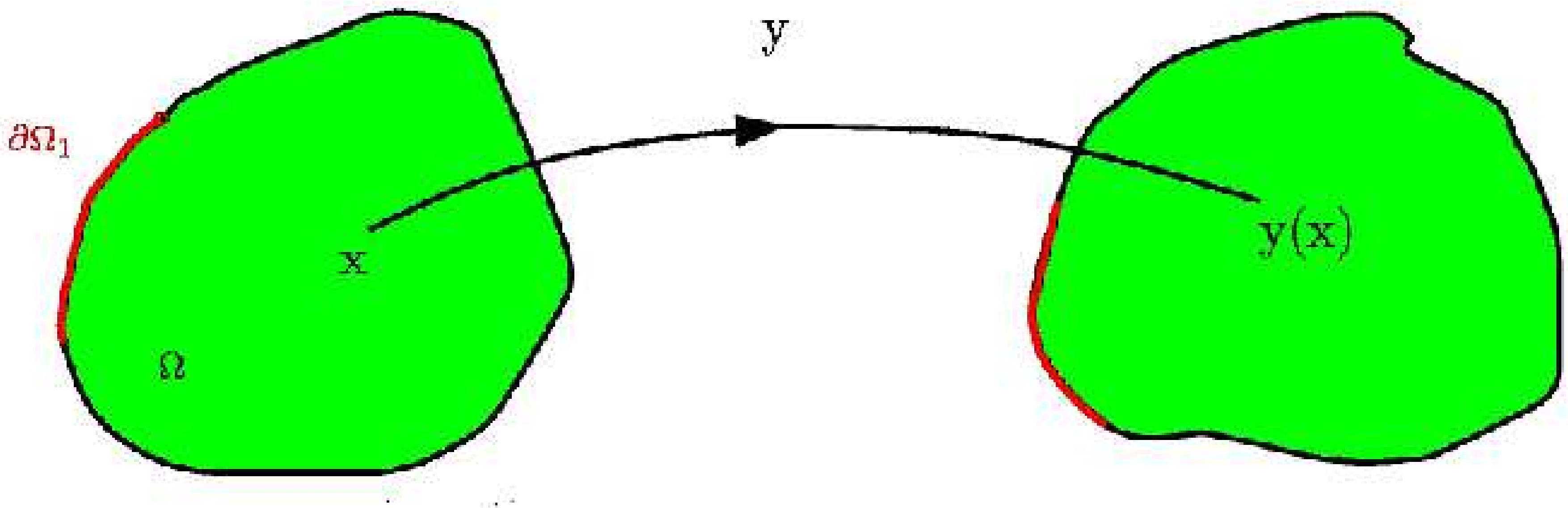
Question: how are the eigenvalue constraints

$$-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}$$

maintained in the theory?

B/ Apala Majumdar

# Nonlinear elasticity




Minimize

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

subject to suitable boundary conditions,

e.g. $y|_{\partial\Omega_1} = \bar{y}$.

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

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

To ensure this we assume that

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

Correspondingly, it is natural to suppose that

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

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

We show how such an $\psi_B$ can be constructed on the basis of a microscopic model.

# The Onsager model

In the Onsager model the probability measure $\mu$ 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

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

With the Maier-Saupe molecular interaction, the internal energy is given by

$$U(\rho) \;=\; \kappa(\theta)\int_{S^2}\int_{S^2}[\tfrac{1}{3}-(p\cdot q)^2]\rho(p)\rho(q)\,dp\,dq$$

where $\kappa(\theta)>0$ is a coupling constant.

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 $U(\rho) = -\kappa(\theta)|Q(\rho)|^2$ and

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

Given $Q$ we define

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

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

Let

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

Given $Q$ with $Q = Q^T, \operatorname{tr} Q = 0$ and satisfying $\lambda_i(Q) > -1/3$ we seek to minimize $J$ on the set of admissible $\rho$

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

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

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

(Remark: this is not true if we allow some $\lambda_i = -1/3$.)

*Proof.* A singular measure $\mu$ satisfying the constraints is

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

and a $\rho \in \mathcal{A}_Q$ can be obtained by approximating this.

For $\varepsilon > 0$ sufficiently small and $i = 1, 2, 3$ let

$$\varphi_i^\varepsilon = \begin{cases} 0 & \text{if } |p \cdot e_i| < 1 - \varepsilon \\ \frac{1}{4\pi\varepsilon} & \text{if } |p \cdot e_i| \geq 1 - \varepsilon \end{cases}$$

Then

$$\rho(p) = \frac{1}{(1 - \frac{1}{2}\varepsilon)(1 - \varepsilon)} \sum_{i=1}^{3} [\lambda_i + \frac{1}{3} - \frac{\varepsilon}{2} + \frac{\varepsilon^2}{6}] \varphi_{e_i}^\varepsilon(p)$$

works. $\square$

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

*Proof.* By the direct method, using the facts that $\rho \ln \rho$ is strictly convex and grows super-linearly in $\rho$, while $\mathcal{A}_Q$ is sequentially weakly closed in $L^1(S^2)$. $\square$

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

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

*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

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

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 $\int_{S^2} \rho(p)\,dp = 1$. $\Box$

# The Euler-Lagrange equation for J

*Theorem.* Let $Q = \text{diag}\,(\lambda_1, \lambda_2, \lambda_3)$. 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 $\mu_i$ solve the equations

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

and are unique up to adding a constant to each $\mu_i$.

*Proof.* We need to show that $\rho_Q$ satisfies the Euler-Lagrange equation. There is a small difficulty due to the constraint $\rho \geq 0$. For $\tau > 0$ let $S_\tau = \{p \in S^2 : \rho_Q(p) > \tau\}$, and let $z \in L^\infty(S^2)$ be zero outside $S_\tau$ and such that

$$\int_{S_\tau} (p \otimes p - \frac{1}{3}\mathbf{1}) z(p)\, dp = 0, \quad \int_{S_\tau} z(p)\, dp = 0.$$

Then $\rho_\varepsilon := \rho_Q + \varepsilon z \in \mathcal{A}_Q$ for all $\varepsilon > 0$ sufficiently small. Hence

$$\frac{d}{d\varepsilon} J(\rho_\varepsilon)|_{\varepsilon=0} = \int_{S_\tau} [1 + \ln \rho_Q] z(p)\, dp = 0.$$

So by Hahn-Banach

$$1 + \ln \rho_Q = \sum_{i,j=1}^{3} C_{ij}[p_i p_j - \frac{1}{3}] + C$$

for constants $C_{ij}(\tau), C(\tau)$. Since $S_\tau$ increases as $\tau$ decreases the constants are independent of $\tau$, and hence

$$\rho_Q(p) = A \exp\left(\sum_{i,j=1}^{3} C_{ij} p_i p_j\right) \text{ if } \rho_Q(p) > 0.$$

Suppose for contradiction that

$$E = \{p \in S^2 : \rho_Q(p) = 0\}$$

is such that $\mathcal{H}^2(E) > 0$. Note that since $\int_{S^2} \rho_Q dp = 1$ we also have that $\mathcal{H}^2(S^2 \backslash E) > 0$. There exists $z \in L^\infty(S^2)$ such that

$$\int_{\{\rho_Q > 0\}} (p \otimes p - \frac{1}{3}\mathbf{1}) z(p)\, dp = 0, \ \int_{\{\rho_Q > 0\}} z(p)\, dp = 4\pi.$$

Indeed if this were not true then by Hahn-Banach we would have

$$1 = \sum_{i,j=1}^{3} D_{ij}(p_i p_j - \frac{1}{3}\delta_{ij}) \text{ on } S^2 \backslash E$$

for a constant matrix $D = (D_{ij})$.
Changing coordinates we can assume that $D = \sum_{i=1}^{3} \alpha_i e_i \otimes e_i$ and so $1 = \sum_{i=1}^{3} \alpha_i (p_i^2 - \frac{1}{3})$ on $S^2 \backslash E$ for constants $\alpha_i$. If the $\alpha_i$ are equal then the right-hand side is zero, a contradiction, while if the $\alpha_i$ are not all equal it is easily shown that the intersection of $S^2$ with the set of such $p$ has 2D measure zero.

Define for $\varepsilon > 0$ sufficiently small

$$\rho_\varepsilon = \rho_Q + \varepsilon - \varepsilon z.$$

Then $\rho_\varepsilon \in \mathcal{A}_Q$, since $\int_{S^2}(p \otimes p - \frac{1}{3}\mathbf{1})\, dp = 0$. Hence, since $\rho_Q$ is the unique minimizer,

$$\int_E \varepsilon \ln \varepsilon + \int_{\{\rho_Q > 0\}} [(\rho_Q + \varepsilon - \varepsilon z) \ln(\rho_Q + \varepsilon - \varepsilon z) - \rho_Q \ln \rho_Q]\, dp > 0.$$

This is impossible since the second integral is of order $\varepsilon$.
Hence we have proved that

$$\rho_Q(p) = A \exp\Big(\sum_{i,j=1}^{3} C_{ij} p_i p_j\Big), \text{a.e. } p \in S^2.$$

*Lemma.* Let $R^T Q R = Q$ for some $R \in O(3)$. Then $\rho_Q(Rp) = \rho_Q(p)$ for all $p \in S^2$.

*Proof.*

$$\begin{aligned}
&\int_{S^2} (p \otimes p - \frac{1}{3}\mathbf{1}) \rho_Q(Rp)\, dp \\
&\qquad = \int_{S^2} (R^T q \otimes R^T q - \frac{1}{3}\mathbf{1}) \rho_Q(q)\, dq \\
&\qquad = R^T Q R = Q,
\end{aligned}$$

and $\rho_Q$ is unique. $\Box$

Applying the lemma with $Re_i = -e_i$, $Re_j = e_j$ for $j \neq i$, we deduce that for $Q = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$,

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

where

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

as claimed.

Finally

$$\begin{aligned} \frac{\partial \ln Z}{\partial \mu_i} &= Z^{-1} \int_{S^2} p_i^2 \exp\Big(\sum_{j=1}^{3} \mu_j p_j^2\Big)\, dp \\ &= \lambda_i + \frac{1}{3}, \end{aligned}$$

and the uniqueness of the $\mu_i$ up to adding a constant to each follows from the uniqueness of $\rho_Q$. $\square$

Hence the bulk free energy has the form

$$\begin{aligned}\psi_B(Q,\theta) &= \theta f(Q) - \kappa(\theta)|Q|^2 \\ &= \theta\left(\sum_{i=1}^{3}\mu_i(\lambda_i+\frac{1}{3}) - \ln Z\right) - \kappa(\theta)\sum_{i=1}^{3}\lambda_i^2,\end{aligned}$$

where

$$f(Q) = \int_{S^2}\rho_Q(p)\ln\rho_Q(p)\,dp.$$

# Asymptotics

In order to understand more about how $\psi_B(Q,\theta)$ blows up as $\lambda_{\min}(Q) \to -\frac{1}{3}+$ we need to study the corresponding asymptotics for

$$f(Q) = \int_{S^2} \rho_Q(p) \ln \rho_Q(p)\, dp.$$

Theorem

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

for constants $C_1, C_2$.

Proof

For the lower bound we first note that $\ln Z(\nu_1, \nu_2, \nu_3)$ is a strictly convex function of the $\nu_i$. In fact a short calculation shows that

$$\sum_{i.j=1}^{3} \frac{\partial^2 \ln Z}{\partial \nu_i \partial \nu_j} a_i a_j$$
$$= \frac{1}{2Z^2} \int_{S^2} \int_{S^2} \left( \sum p_i^2 a_i - \sum q_j^2 a_j \right)^2$$
$$\times \exp \left( \sum \nu_k (p_k^2 + q_k^2) \right) \, dp \, dq > 0$$

if $a = (a_1, a_2, a_2) \neq 0$.

Hence

$$\sum \nu_i(\lambda_i + \frac{1}{3}) - \ln Z(\nu_1, \nu_2, \nu_3)$$

is a strictly concave function of the $\nu_i$ that is maximized when $\nu_i = \mu_i$, with maximum value $f(Q)$. So we can get a lower bound by choosing any $\nu_i$ and the choice $\nu_1 = 2s, \nu_2 = \nu_3 = -s$ for $s = \lambda_{\text{min}} + \frac{1}{3}$ gives the result.

For the upper bound we can choose any probability density $\rho = \rho(p)$ with $Q(\rho) = Q$, since we know that

$$f(Q) \leq \int_{S^2} \rho(p) \ln \rho(p)\, dp.$$

The choice

$$\rho(p) = \sum_i \frac{\lambda_i + \frac{1}{3}(1 - \frac{\varepsilon}{2})(1 - \varepsilon)}{(1 - \frac{\varepsilon}{2})(1 - \varepsilon)} \varphi_i(p),$$

where $\varphi_i(p) = \frac{1}{4\pi\varepsilon}$ for $p \cdot e_i > 1 - \delta$, $\varphi_i(p) = 0$ otherwise, works.

# Other predictions

1. All critical points of $\psi_B$ are uniaxial.

2. Phase transition predicted from isotropic to uniaxial nematic phase just as in the quartic model.

3. Minimizers $\rho^*$ of $I_\theta(\rho)$ correspond to minimizers over $Q$ of $\psi_B(Q,\theta)$. These $\rho^*$ were calculated and shown to be uniaxial by Fatkullin and Slastikov (2005).

4. Near $Q = 0$ we have the expansion

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

The ratio of the coefficients of the last two terms is

$$\frac{8}{3} = 2.6666\ldots$$

while experimental values reported in the literature give the ratio 2.438.

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

Given appropriate boundary conditions, do minimizers of

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

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

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

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

Example (B & Mizel)

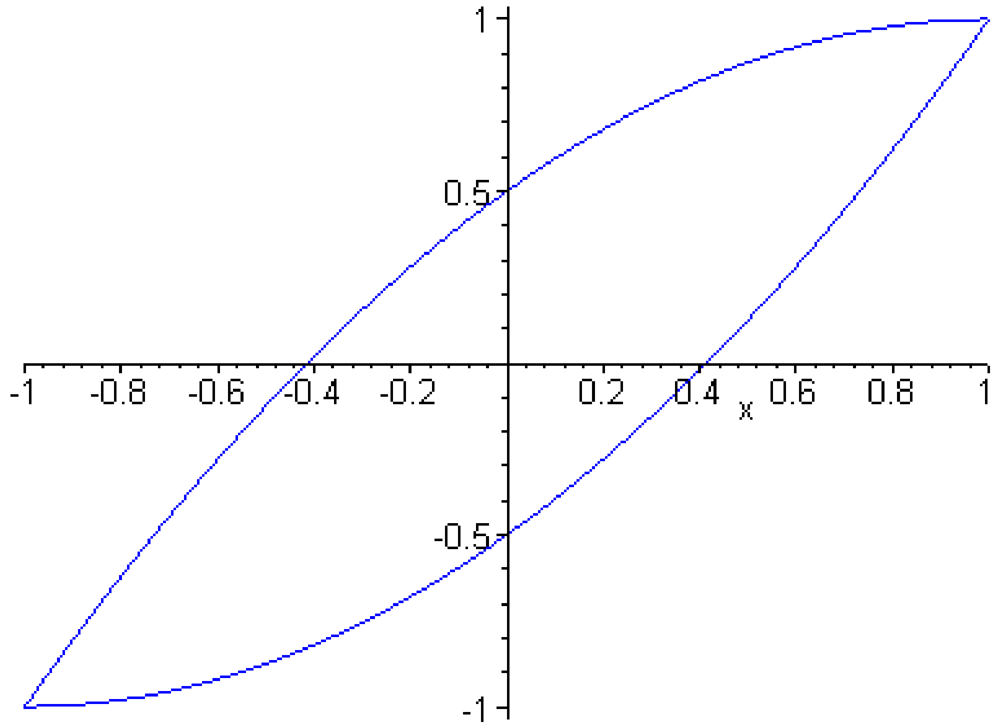
Minimize

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

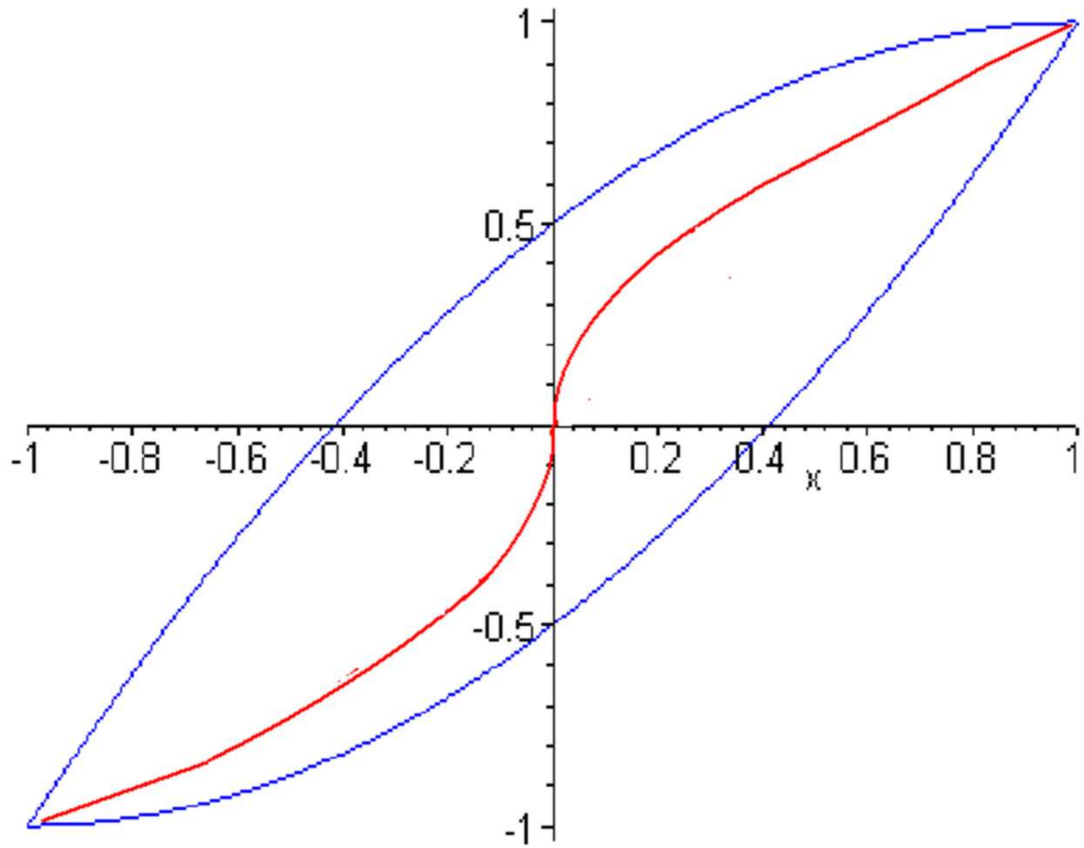
subject to

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

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

Let $Q$ minimize

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

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

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

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

Idea of Proof

Suppose not. Given the minimizer $Q$ denote by $P_\varepsilon(Q)$ the nearest point projection onto the convex set

$$K_\varepsilon = \{Q : f(Q) \leq \frac{1}{\varepsilon}\}.$$

Then if $\varepsilon > 0$ is small enough we have

$$\psi_B(P_\varepsilon(Q)) < \psi_B(Q)$$

and

$$|\nabla P_\varepsilon(Q)|^2 \leq |\nabla Q|^2.$$

Remark.

It is not clear how to prove the same result for more general elastic energies, although L.C.Evans & Hung Tran can prove partial regularity of minimizers in that case.

Nonlinear elasticity problem: Do minimizers for suitable boundary conditions of

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

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

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

for some $\varepsilon > 0$?

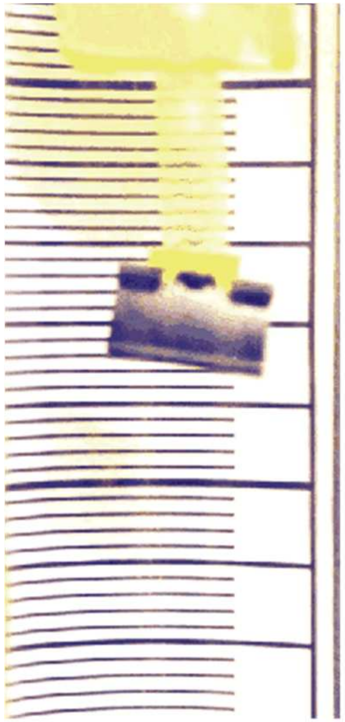
This seems to be very difficult.

# Liquid crystal elastomers

These are polymers for which the long chain molecules are liquid crystals.

Actuation by
hot and cold air
(E. Terentyev)

Courtesy M. Warner



Thermo-optical actuation
(P. Palffy-Muhoray)

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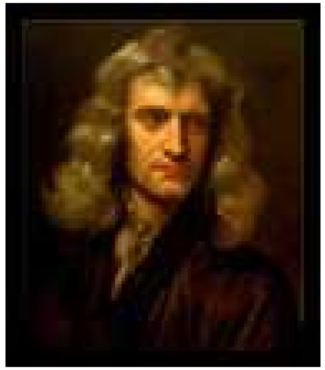

# The Mathematics of Liquid Crystals

7 January - 5 July 2013

http://www.newton.ac.uk/programmes/MLC/index.htm


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The end