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Analysis of liquid crystals and their defects

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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 and Oseen - Frank theories.
3. The singular bulk potential.
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

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

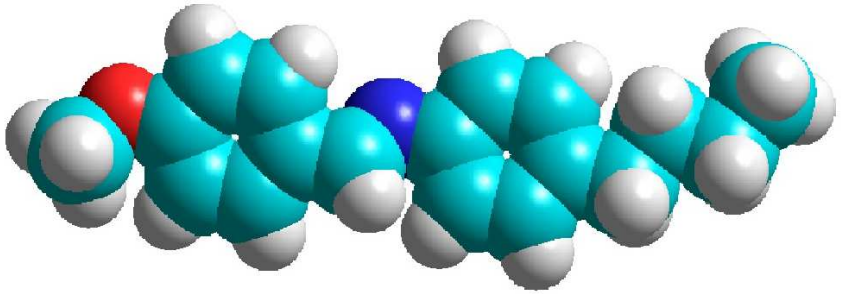
Classes of liquid crystals

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

Many liquid crystals consist of rod-like molecules.

Length 2-3 nm

Oxygen
Carbon
Nitrogen
Hydrogen



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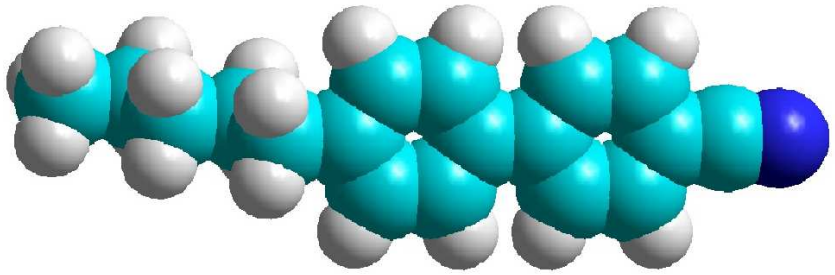
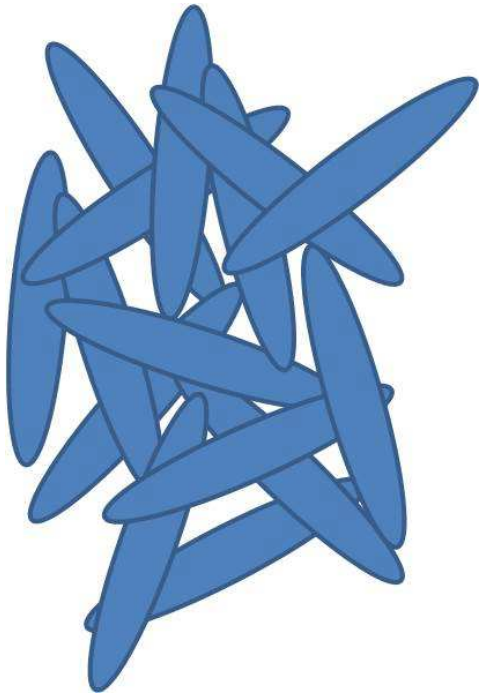


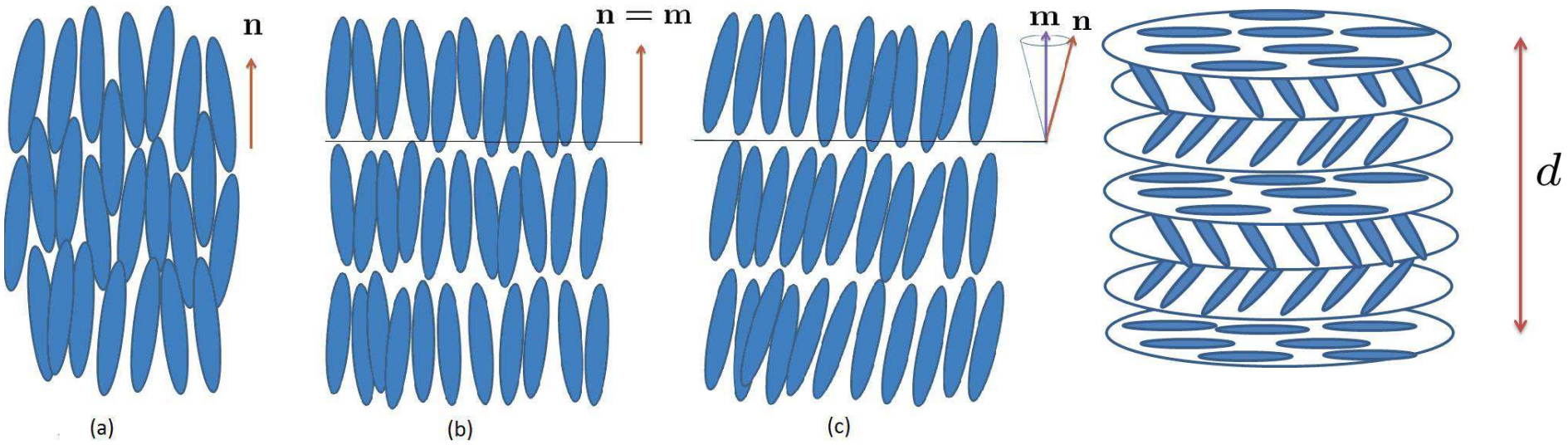
5CB

Space-filling models courtesy Claudio Zannoni.

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

Cholesteric 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

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

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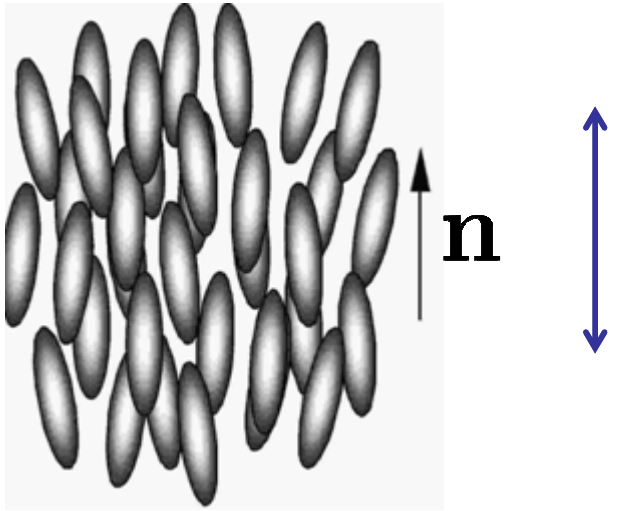
DoITPoMS,
Cambridge

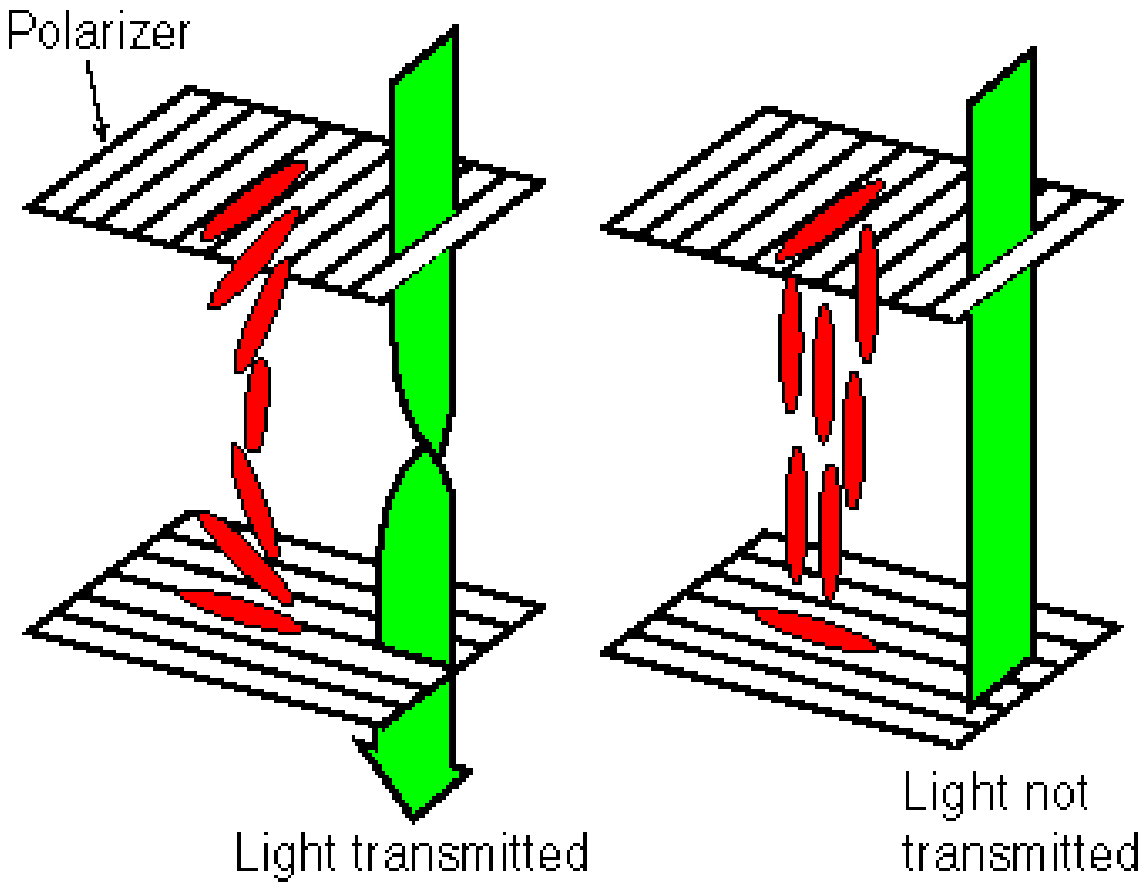
The director

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



But note that for most liquid crystals $\mathbf{n}$ is equivalent to $-\mathbf{n}$, 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.

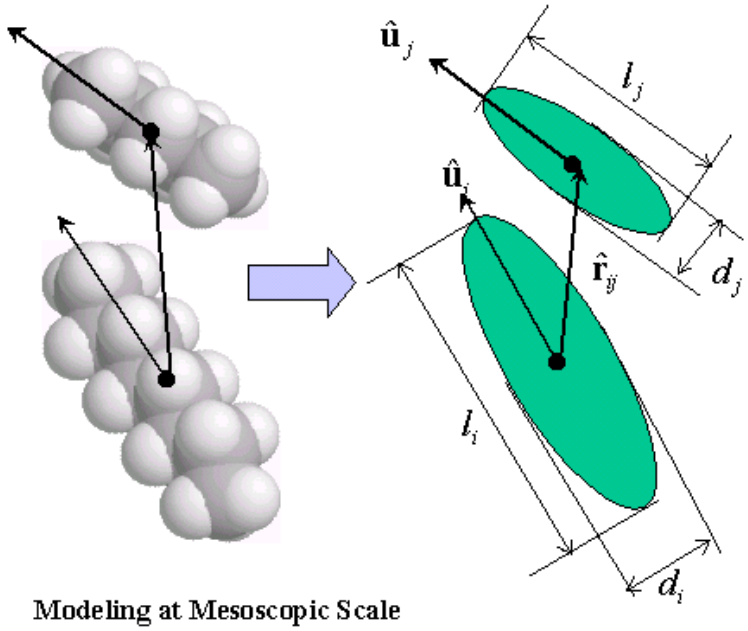
The twisted nematic display



(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

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

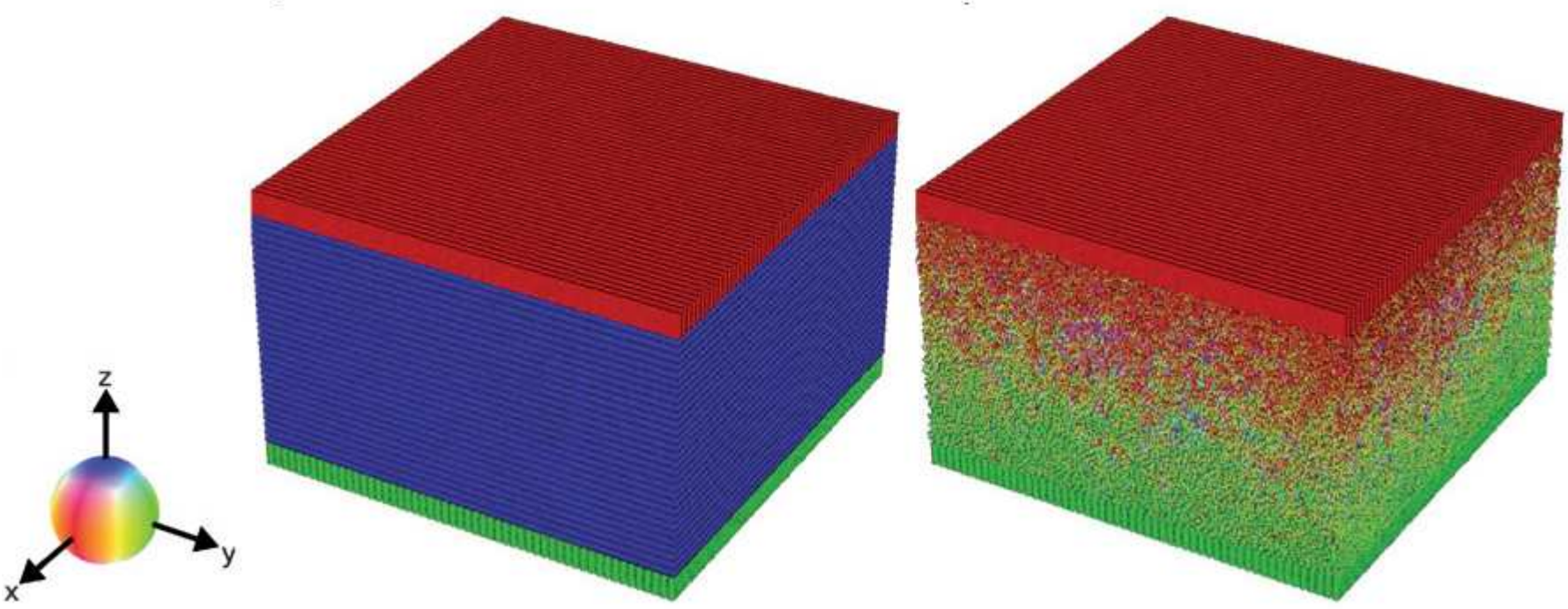
where

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

$r_{ij} = |\hat{\mathbf{r}}_{ij}|$, 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

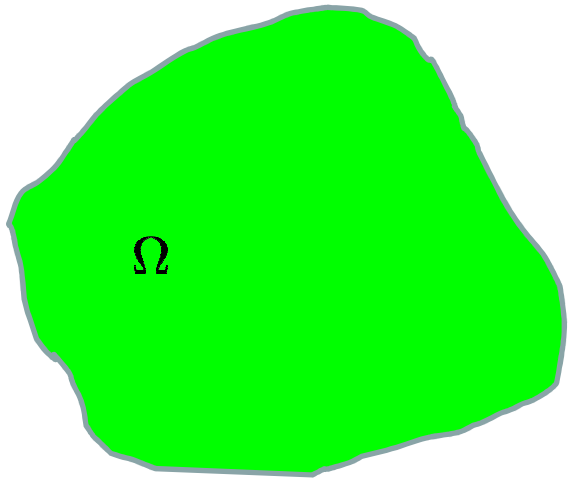
944,784 molecules, including 157,464 fixed in layers near the boundaries to prescribe the orientation there.



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

Continuum models

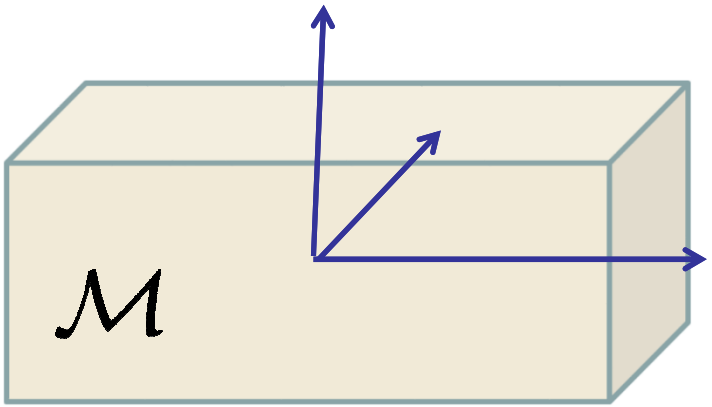
Consider a nematic liquid crystal filling a container $\Omega \subset \mathbb{R}^3$, where Ω is assumed bounded, open, with Lipschitz boundary.



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 $\mathcal{M}$ (rod, ellipsoid, parallepiped ...) of approximately the same shape and symmetry. We place $\mathcal{M}$ in a standard position with centroid at the origin, e.g.



and define the isotropy groups

$$G_{\mathcal{M}} = \{\mathbf{R} \in O(3) : \mathbf{R}\mathcal{M} = \mathcal{M}\}$$
$$G^{+}_{\mathcal{M}} = \{\mathbf{R} \in SO(3) : \mathbf{R}\mathcal{M} = \mathcal{M}\}$$

If $G_{\mathcal{M}} = G^+_{\mathcal{M}}$ then the molecule is said to be *chiral* (as in cholesterics).

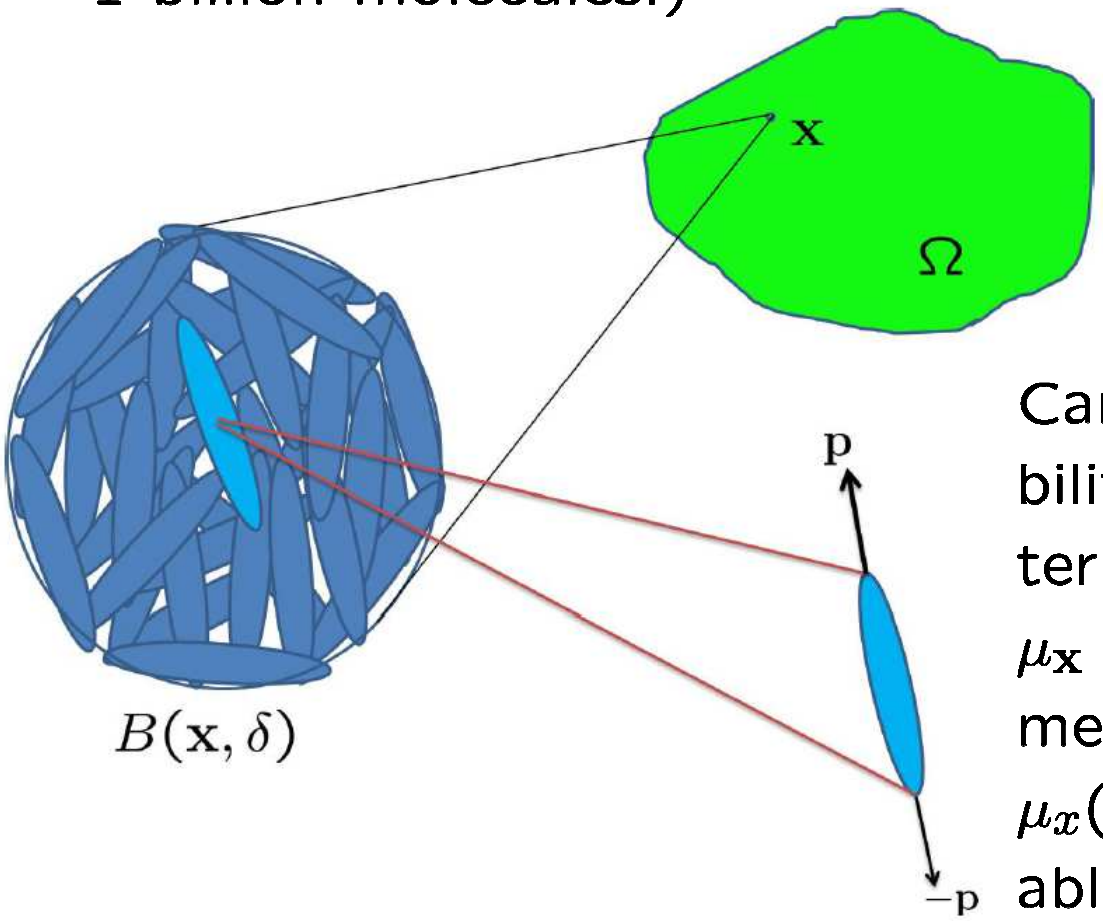
$\mathbf{R}\mathcal{M} = \tilde{\mathbf{R}}\mathcal{M}$ for $\mathbf{R}, \tilde{\mathbf{R}} \in SO(3)$ iff $\tilde{\mathbf{R}}^T\mathbf{R} \in G^+_{\mathcal{M}}$. Hence the orientation of a molecule can be represented by an element of the space of cosets $SO(3)/G^+_{\mathcal{M}}$ (cf Mermin 1979).

For $\mathcal{M}$ a cylindrical rod or ellipsoid of revolution

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

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

(If $\delta = 1\mu$m $B(\mathbf{x}, \delta)$ contains ~ 1 billion molecules.)



For E symmetric, i.e. $E = -E$, let $\mu_{\mathbf{x}}(E)$ be the probability that a molecule drawn at random from $B(\mathbf{x}, \delta)$ has orientation $\pm\mathbf{p} \in E$.

Can think of $\mu_{\mathbf{x}}$ as a probability measure on $\mathbb{R}P^2$. Alternatively we can extend $\mu_{\mathbf{x}}$ uniquely to a probability measure on S^2 that satisfies $\mu_x(E) = \mu_x(-E)$ for measurable $E \subset S^2$ by defining

$$\mu_{\mathbf{x}}(E) = \mu_{\mathbf{x}}(E \cap -E) + \frac{1}{2}\mu_{\mathbf{x}}(E \triangle -E).$$

Might also want to average over a small time interval.

Example:

$\mu_{\mathbf{x}} = \frac{1}{2}(\delta_{\mathbf{e}} + \delta_{-\mathbf{e}})$ represents a state of perfect alignment parallel to the unit vector $\mathbf{e}$.

We will almost always assume that $\mu_{\mathbf{x}}$ is continuously distributed, so that

$$d\mu_{\mathbf{x}}(\mathbf{p}) = \rho(\mathbf{x}, \mathbf{p}) d\mathbf{p},$$

where $d\mathbf{p}$ is the element of surface area on S^2 and

$$\begin{aligned} \rho(\mathbf{x}, \mathbf{p}) &\geq 0 \\ \rho(\mathbf{x}, \mathbf{p}) &= \rho(\mathbf{x}, -\mathbf{p}) \\ \int_{S^2} \rho(\mathbf{x}, \mathbf{p})\, d\mathbf{p} &= 1 \end{aligned}$$

If the orientation of molecules is equally distributed in all directions, we say that the distribution is *isotropic*, and then $\rho = \rho_0$, where

$$\rho_0(\mathbf{x}, \mathbf{p}) = \frac{1}{4\pi}.$$

A natural idea would be to use as an order parameter the probability density $\rho = \rho(\mathbf{x}, \mathbf{p})$. However this represents an infinite-dimensional state variable at each point $\mathbf{x}$, and if we use as an approximation an order parameter consisting of a finite number of moments of ρ then we have instead a finite-dimensional state variable.

Because $\rho(\mathbf{x}, \mathbf{p}) = \rho(\mathbf{x}, -\mathbf{p})$ the first moment

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

The second moment tensor

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

satisfies $\mathbf{M}(\mathbf{x}) = \mathbf{M}(\mathbf{x})^T$, $\operatorname{tr} \mathbf{M}(\mathbf{x}) = 1$. Also $\mathbf{M}(\mathbf{x}) > \mathbf{0}$ since

$$\mathbf{M}(\mathbf{x})\mathbf{e} \cdot \mathbf{e} = \int_{S^2} (\mathbf{p} \cdot \mathbf{e})^2 \rho(\mathbf{x}, \mathbf{p})\, d\mathbf{p} \geq 0$$

with equality iff $\rho(\mathbf{x}, \mathbf{p}) = 0$ whenever $\mathbf{p} \cdot \mathbf{e} = 0$, contradicting $\int_{S^2} \rho(\mathbf{x}, \mathbf{p})\, d\mathbf{p} = 1$.

The second moment tensor of the isotropic distribution $\rho_0(\mathbf{x}, \mathbf{p}) = \frac{1}{4\pi}$, is

$$\mathbf{M}_0 = \frac{1}{4\pi} \int_{S^2} \mathbf{p} \otimes \mathbf{p}\, d\mathbf{p} = \frac{1}{3}\mathbf{1}$$

(since $\int_{S^2} p_1 p_2\, d\mathbf{p} = 0$, $\int_{S^2} p_1^2\, d\mathbf{p} = \int_{S^2} p_2^2\, d\mathbf{p}$ etc and $\operatorname{tr} \mathbf{M}_0 = 1$.)

The *de Gennes* $\mathbf{Q}$*-tensor*

$$\mathbf{Q}(\mathbf{x}) = \mathbf{M}(\mathbf{x}) - \mathbf{M}_0 = \int_{S^2} \left(\mathbf{p} \otimes \mathbf{p} - \frac{1}{3}\mathbf{1} \right) \rho(\mathbf{x}, \mathbf{p})\, d\mathbf{p}$$

thus measures the deviation of $\mathbf{M}(\mathbf{x})$ from its isotropic value.

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

Let

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

Since $\mathbf{Q} = \mathbf{Q}(\mathbf{x}) \in \mathcal{E}$,

$$\mathbf{Q} = \lambda_1 \mathbf{e}_1 \otimes \mathbf{e}_1 + \lambda_2 \mathbf{e}_2 \otimes \mathbf{e}_2 + \lambda_3 \mathbf{e}_3 \otimes \mathbf{e}_3,$$

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

We can order the eigenvalues as

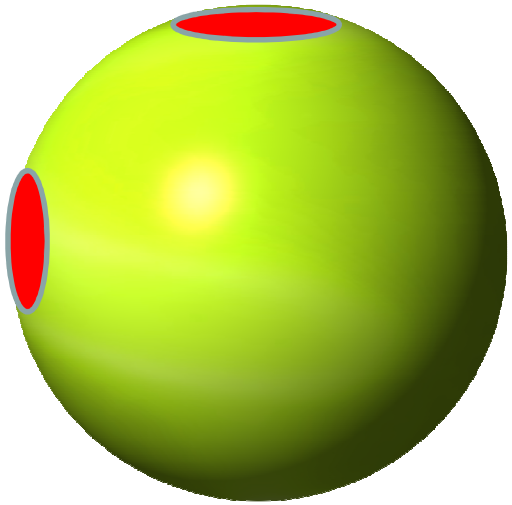
$$\lambda_{\mathsf{min}}(\mathbf{Q}) \leq \lambda_{\mathsf{mid}}(\mathbf{Q}) \leq \lambda_{\mathsf{max}}(\mathbf{Q}),$$

and since $\mathbf{Q} > -\frac{1}{3}\mathbf{1}$ we have that

$$-\frac{1}{3} < \lambda_{\mathsf{min}}(\mathbf{Q}) \leq \lambda_{\mathsf{mid}}(\mathbf{Q}) \leq \lambda_{\mathsf{max}}(\mathbf{Q}) < \frac{2}{3}. \quad (*)$$

Conversely, if (*) holds then $\mathbf{Q}$ is the normalized second moment tensor for some ρ. Such a ρ can be constructed by approximating the singular measure

$$\mu = \sum_{i=1}^{3} \left(\lambda_i + \frac{1}{3}\right) \frac{1}{2}(\delta_{\mathbf{e}_i} + \delta_{-\mathbf{e}_i}).$$



For each eigenvector $\mathbf{e}_i$ define

$$\phi_i^{\varepsilon}(\mathbf{p}) = \begin{cases} 0 & \text{if } |\mathbf{p}\cdot\mathbf{e}_i| < 1-\varepsilon \\ \frac{1}{4\pi\varepsilon} & \text{if } |\mathbf{p}\cdot\mathbf{e}_i| \geq 1-\varepsilon \end{cases}$$

where $0 < \varepsilon < 1 - \frac{1}{\sqrt{2}}$, so that the six spherical caps $\{\mathbf{p} \in S^2 : \pm\mathbf{p}\cdot\mathbf{e}_i \geq 1-\varepsilon\}$ are disjoint.

Then set

$$\rho(\mathbf{p}) = \frac{1}{(1-\frac{\varepsilon}{2})(1-\varepsilon)} \sum_{i=1}^{3} \left[\lambda_i + \frac{1}{3}\left(1-\frac{\varepsilon}{2}\right)(1-\varepsilon)\right] \phi_i^{\varepsilon}(\mathbf{p}).$$

Note that $\lambda^2_{\mathrm{min}}(\mathbf{Q}) - \lambda^2_{\mathrm{mid}}(\mathbf{Q}) = (\lambda_{\mathrm{mid}}(\mathbf{Q}) - \lambda_{\mathrm{min}}(\mathbf{Q}))\lambda_{\mathrm{max}}(\mathbf{Q})$ and so

$$\lambda^2_{\mathrm{mid}}(\mathbf{Q}) \leq \lambda^2_{\mathrm{min}}(\mathbf{Q}).$$

Hence $|\mathbf{Q}|^2 < \frac{2}{3}$.

The limiting cases $\lambda_{\mathrm{max}}(\mathbf{Q}) = \frac{2}{3}$, $\lambda_{\mathrm{min}}(\mathbf{Q}) = -\frac{1}{3}$ correspond to singular measures. If $\lambda_{\mathrm{max}}(\mathbf{Q}) = \frac{2}{3}$ then for the corresponding eigenvector $\mathbf{e}_{\mathrm{max}}$ we have

$$\mathbf{M}\mathbf{e}_{\mathrm{max}} \cdot \mathbf{e}_{\mathrm{max}} = \int_{S^2} (\mathbf{p} \cdot \mathbf{e}_{\mathrm{max}})^2 \, d\mu(\mathbf{p}) = 1,$$

and hence

$$\int_{S^2} |\mathbf{p} \otimes \mathbf{p} - \mathbf{e}_{\mathrm{max}} \otimes \mathbf{e}_{\mathrm{max}}|^2 \, d\mu(\mathbf{p}) = 0,$$

and so $\mu = \frac{1}{2}(\delta_{\mathbf{e}_{\mathrm{max}}} + \delta_{-\mathbf{e}_{\mathrm{max}}})$.

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

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

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

If two eigenvalues of $\mathbf{Q}$ are equal, say $\lambda_1 = \lambda_2 = \lambda$, $\lambda_3 = -2\lambda$, then $\mathbf{Q}$ is said to be *uniaxial* and has the form

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

where $\mathbf{n} = \mathbf{e}_3$ and the *scalar order parameter* $s = -3\lambda \in (-\frac{1}{2}, 1)$. Otherwise $\mathbf{Q}$ is *biaxial*.

In fact it is extremely difficult to find $\mathbf{Q}$ 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.

If $\mathbf{Q}$ is uniaxial and $s > 0$ then $\lambda_{\max}(\mathbf{Q}) = \frac{2}{3}s$ and $\mathbf{n} = \mathbf{e}_{\max}(\mathbf{Q})$. For general biaxial $\mathbf{Q}$ the director is often identified with $\mathbf{e}_{\max}(\mathbf{Q})$.

Proposition. The tensor $\mathbf{Q} \in \mathcal{E}$ is uniaxial with scalar order parameter s if and only if

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

Proof. Necessity:

$$\begin{aligned} |\mathbf{Q}|^2 &= s^2 \left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{1}\right) \cdot \left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{1}\right) \\ &= s^2(1 + \frac{1}{3} - \frac{2}{3}) = \frac{2s^2}{3}, \end{aligned}$$

while by the formula $\det(\mathbf{1} + \mathbf{a}\otimes\mathbf{b}) = 1 + \mathbf{a}\cdot\mathbf{b}$ we get

$$\det \mathbf{Q} = -\frac{s^3}{27}(1-3) = \frac{2s^3}{27}.$$

Sufficiency: The eigenvalues λ_i of $\mathbf{Q}$ satisfy

$$\begin{aligned}\lambda_1+\lambda_2+\lambda_3 &= 0,\\ \lambda_1^2+\lambda_2^2+\lambda_3^2 &= \frac{2s^2}{3},\\ \lambda_1\lambda_2\lambda_3 &= \frac{2s^3}{27},\end{aligned}$$

from which it follows that

$$\lambda_1\lambda_2+\lambda_2\lambda_3+\lambda_3\lambda_1 = -\frac{1}{2}(\lambda_1^2+\lambda_2^2+\lambda_3^2) = -\frac{s^2}{3}.$$

Thus the characteristic equation for $\mathbf{Q}$ is

$$\lambda^3-\frac{s^2}{3}\lambda-\frac{2s^3}{27} = \left(\lambda+\frac{s}{3}\right)^2\left(\lambda-\frac{2s}{3}\right) = 0.$$

Letting $\mathbf{n}$ be the eigenvector corresponding to the eigenvalue $\frac{2s}{3}$ we obtain $\mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n}-\frac{1}{3}\mathbf{1}\right)$ as required.

Corollary. Necessary and sufficient conditions for $\mathbf{Q}\in\mathcal{E}$ to be uniaxial with scalar order parameter $s\in(-\frac{1}{2},1)$ are that

$$|\mathbf{Q}|^6 = 54(\det\mathbf{Q})^2,\ \det\mathbf{Q}\in\frac{2}{27}(-\tfrac{1}{8},1).$$

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

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

$\mathbf{Q}$ (5-dimensional, Landau - de Gennes theory)

$(s, \mathbf{n})$ (3-dimensional, Ericksen theory)

$\mathbf{n}$ (2-dimensional, Oseen-Frank theory)

The Landau - de Gennes and Oseen-Frank theories

Landau - de Gennes theory

For simplicity we work at a constant temperature θ, and assume that there are no electromagnetic fields. At each point $\mathbf{x} \in \Omega$, we have a corresponding order parameter tensor $\mathbf{Q}(\mathbf{x})$.

We suppose that the material is described by a free-energy density $\psi(\mathbf{Q}, \nabla\mathbf{Q}, \theta)$, so that the total free energy is given by

$$I_\theta(\mathbf{Q}) = \int_\Omega \psi(\mathbf{Q}(\mathbf{x}), \nabla\mathbf{Q}(\mathbf{x}), \theta)\, d\mathbf{x}.$$

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

Frame-indifference

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

$$\psi(\mathbf{Q}^*(\bar{\mathbf{x}}), \nabla_{\mathbf{z}}\mathbf{Q}^*(\bar{\mathbf{x}}), \theta) = \psi(\mathbf{Q}(\bar{\mathbf{x}}), \nabla_{\mathbf{x}}\mathbf{Q}(\bar{\mathbf{x}}), \theta),$$

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

$$\begin{aligned}
\text{Then} \quad \mathbf{Q}^*(\bar{\mathbf{x}}) &= \int_{S^2} \left(\mathbf{q}\otimes\mathbf{q} - \frac{1}{3}\mathbf{1}\right) \rho(\bar{\mathbf{x}}, \mathbf{R}^T\mathbf{q})\, d\mathbf{q} \\
&= \int_{S^2} \left(\mathbf{Rp}\otimes\mathbf{Rp} - \frac{1}{3}\mathbf{1}\right) \rho(\bar{\mathbf{x}}, \mathbf{p})\, d\mathbf{p} \\
&= \mathbf{R}\int_{S^2} \left(\mathbf{p}\otimes\mathbf{p} - \frac{1}{3}\mathbf{1}\right) \rho(\bar{\mathbf{x}}, \mathbf{p})\, d\mathbf{p}\, \mathbf{R}^T \\
&= \mathbf{RQ}(\bar{\mathbf{x}})\mathbf{R}^T.
\end{aligned}$$

Therefore

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

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

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

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

Material symmetry

The requirement that

$$\psi(\mathbf{Q}^*(\bar{\mathbf{x}}), \nabla_{\mathbf{z}}\mathbf{Q}^*(\bar{\mathbf{x}}), \theta) = \psi(\mathbf{Q}(\bar{\mathbf{x}}), \nabla_{\mathbf{x}}\mathbf{Q}(\bar{\mathbf{x}}), \theta)$$

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

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

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

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

Bulk and elastic energies

We can decompose ψ as

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

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

By frame-indifference $\psi_B(\cdot, \theta)$ is isotropic, i.e.

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

Isotropic functions of $\mathbf{Q}$ have a standard representation in terms of the invariants of $\mathbf{Q}$.

Lemma. A function $f(\mathbf{Q})$ of a real, symmetric, 3×3 tensor $\mathbf{Q}$ is isotropic, that is

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

if and only if $f(\mathbf{Q}) = g(\mathrm{tr}\,\mathbf{Q}, \mathrm{tr}\,\mathbf{Q}^2, \mathrm{tr}\,\mathbf{Q}^3)$ for some function g, and if f is a polynomial so is g.

Proof. Suppose f is isotropic. Choosing $\mathbf{R}$ to diagonalize $\mathbf{Q}$ we see that

$$f(\mathbf{Q}) = f(\mathrm{diag}\,(\lambda_1, \lambda_2, \lambda_3)) := h(\lambda_1, \lambda_2, \lambda_3)$$

for a function h of the eigenvalues λ_i of $\mathbf{Q}$, and choosing $\mathbf{R}$ so as to permute these eigenvalues we deduce that h is symmetric with respect to permutations of the λ_i.

Since the eigenvalues are the roots of the characteristic equation

$$\lambda^3 - (\mathrm{tr}\,\mathbf{Q})\lambda^2 + (\mathrm{tr\,cof}\,\mathbf{Q})\lambda - \det\mathbf{Q} = 0,$$

where $\mathrm{cof}\,\mathbf{Q}$ denotes the cofactor matrix of $\mathbf{Q}$, and since the coefficients determine the roots up to an arbitrary permutation, it follows that h is a function of these coefficients, namely

$$\begin{aligned} \mathrm{tr}\,\mathbf{Q} &= \lambda_1 + \lambda_2 + \lambda_3, \\ \mathrm{tr\,cof}\,\mathbf{Q} &= \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1, \\ \det\mathbf{Q} &= \lambda_1\lambda_2\lambda_3, \end{aligned}$$

and hence, on account of the formulae

$$\begin{aligned} \mathrm{tr\,cof}\,\mathbf{Q} &= \frac{1}{2}\left((\mathrm{tr}\,\mathbf{Q})^2 - \mathrm{tr}\,\mathbf{Q}^2\right), \\ \det\mathbf{Q} &= \mathrm{tr}\,\mathbf{Q}^3 - \frac{3}{2}\mathrm{tr}\,\mathbf{Q}\,\mathrm{tr}\,\mathbf{Q}^2 + \frac{1}{2}(\mathrm{tr}\,\mathbf{Q})^3, \end{aligned}$$

f is a function of $\mathrm{tr}\,\mathbf{Q}, \mathrm{tr}\,\mathbf{Q}^2, \mathrm{tr}\,\mathbf{Q}^3$. The converse is obvious since each of $\mathrm{tr}\,\mathbf{Q}, \mathrm{tr}\,\mathbf{Q}^2, \mathrm{tr}\,\mathbf{Q}^3$ is isotropic.

If f is a polynomial, then so is h, and by the fundamental theorem of symmetric polynomials h is a polynomial in its coefficients, so that g is a polynomial.

Corollary. The bulk energy ψ_B satisfies the frame-indifference condition if and only if

$$\psi_B(\mathbf{Q}, \theta) = g(\operatorname{tr} \mathbf{Q}^2, \operatorname{tr} \mathbf{Q}^3, \theta)$$

for some function g. If, for a given temperature θ, $\psi_B(\mathbf{Q}, \theta)$ is a polynomial in $\mathbf{Q}$ then $g(\operatorname{tr} \mathbf{Q}^2, \operatorname{tr} \mathbf{Q}^3, \theta)$ is a polynomial in $\operatorname{tr} \mathbf{Q}^2, \operatorname{tr} \mathbf{Q}^3$.

Proof. Apply the lemma to the function

$$\hat{\psi}_B(\mathbf{Q}, \theta) = \psi_B(\mathbf{Q} - \frac{1}{3}(\operatorname{tr} \mathbf{Q})\mathbf{1}, \theta),$$

which is isotropic.

Note that $\mathrm{tr}\,\mathbf{Q}^4 = \frac{1}{2}(\mathrm{tr}\,\mathbf{Q}^2)^2$ for $\mathbf{Q} \in \mathcal{E}$. Hence the most general frame-indifferent ψ_B that is a quartic polynomial in $\mathbf{Q}$ is a linear combination of $1, \mathrm{tr}\,\mathbf{Q}^2, \mathrm{tr}\,\mathbf{Q}^3$ and $\mathrm{tr}\,\mathbf{Q}^4$ with coefficients depending on θ.

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

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

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

(So we dropped the constant term, which doesn't affect minimizers of ψ_B, as well as the dependence of b, c on θ. In fact, later we give reasons for assuming b, c are proportional to θ, but this will only affect the value of the critical temperature θ_{NI} calculated below.)

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

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

$$\lambda(a + b\lambda + 6c\lambda^2) = 0.$$

Hence $\lambda = 0$ or $\lambda = \lambda_\pm = \frac{-b\pm\sqrt{b^2-24ac}}{12c}$.

For $\lambda = \lambda_\pm$ we have that $\psi_B = 6a\lambda^2 + 4b\lambda^3 + 18c\lambda^4$, which is negative when

$$6a + 4b\lambda + 18c\lambda^2 = 3a + b\lambda < 0.$$

A short calculation then shows that $3a + b\lambda_- < 0$ if and only if $a < \frac{b^2}{27c}$.

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

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

where $s_{\mathrm{min}} = \frac{b + \sqrt{b^2 - 24ac}}{4c} > 0$.

Form of the elastic energy

Usually it is assumed that $\psi_E(\mathbf{Q}, \nabla\mathbf{Q}, \theta)$ is quadratic in $\nabla\mathbf{Q}$. Examples of isotropic functions quadratic in $\nabla\mathbf{Q}$ are the invariants $I_i = I_i(\mathbf{Q}, \nabla\mathbf{Q})$ given by:

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

The first three linearly independent invariants I_1, I_2, I_3 span the possible isotropic quadratic functions of $\nabla\mathbf{Q}$. The invariant I_4 is one of 6 possible linearly independent cubic terms that are quadratic in $\nabla\mathbf{Q}$ (see e.g. L. Longa, D. Monselesan, H. Trebin, An extension of the Landau-Ginzburg-de Gennes theory for liquid crystals. Liq. Cryst. 2, 769-796 (1987).)

Note that

$$I_2 - I_3 = (Q_{ij}Q_{ik,k})_{,j} - (Q_{ij}Q_{ik,j})_{,k}$$

is a *null Lagrangian*, that is its integral over Ω depends only on the boundary values $\mathbf{Q}|_{\partial\Omega}$.

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

$$\psi_E(\mathbf{Q}, \nabla\mathbf{Q}, \theta) = \frac{1}{2}\sum_{i=1}^{4\,\text{or}\,5} L_i I_i(\mathbf{Q}, \nabla\mathbf{Q}),$$

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 the free energy is given by

$$I_\theta(\mathbf{Q}) = \int_\Omega \psi(\mathbf{Q}, \nabla\mathbf{Q}, \theta)\, d\mathbf{x},$$

where

$$\psi(\mathbf{Q}, \nabla\mathbf{Q}, \theta) = \psi_B(\mathbf{Q}, \theta) + \frac{1}{2} \sum_{i=1}^{4 \text{ or } 5} L_i I_i(\mathbf{Q}, \nabla\mathbf{Q}),$$

where $\psi_B(\mathbf{Q}, \theta) = g(\operatorname{tr}\mathbf{Q}^2, \operatorname{tr}\mathbf{Q}^3, \theta)$, 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 $\mathbf{Q}$ to be uniaxial with a constant scalar order parameter $s = s(\theta) > 0$, so that

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

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

$$I_\theta(\mathbf{Q}) = \int_\Omega \psi_E(\mathbf{Q}, \nabla\mathbf{Q}, \theta)\, d\mathbf{x}.$$

Remarks. 1. The L_i are not dimensionless, so care has to be taken in interpreting what it means for them to be small (see Gartland 2015). Roughly speaking L_i small corresponds to a large body limit.

2. For studies concerning when and how the constrained theory is valid in the limit $L_i \to 0$ see Majumdar & Zarnescu, Nguyen & Zarnescu, Bauman, Phillips & Park, Canevari ...)

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

$$I_\theta(\mathbf{n}) = \frac{1}{2}\int_\Omega [K_1(\operatorname{div}\mathbf{n})^2 + K_2(\mathbf{n}\cdot\operatorname{curl}\mathbf{n}+q_0)^2 + K_3|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 + (K_2+K_4)(\operatorname{tr}(\nabla\mathbf{n})^2 - (\operatorname{div}\mathbf{n})^2)]\, d\mathbf{x},$$

where

$$\begin{aligned} K_1 &= 2L_1s^2 + L_2s^2 + L_3s^2 - \frac{2}{3}L_4s^3, \\ K_2 &= 2L_1s^2 - \frac{2}{3}L_4s^3, \\ K_3 &= 2L_1s^2 + L_2s^2 + L_3s^2 + \frac{4}{3}L_4s^3, \\ K_4 &= L_3s^2, \\ q_0 &= -\frac{L_5s^2}{2K_2}, \end{aligned}$$

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

Boundary conditions

(a) Constrained LdG/Oseen-Frank theory.

(i) Strong anchoring

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

Special cases:

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

$\boldsymbol{\nu}(\mathbf{x}) =$ unit outward normal

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

(ii) Conical anchoring:

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

where $\boldsymbol{\nu}(\mathbf{x})$ is the unit outward normal.

Special cases:

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

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

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

where $w(\mathbf{x}, \mathbf{n}) = w(\mathbf{x}, -\mathbf{n})$.

For example, corresponding to strong anchoring we can choose

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

formally recovering the strong anchoring condition in the limit $K \to \infty$. The case $\bar{\mathbf{n}}(\mathbf{x}) = \boldsymbol{\nu}(\mathbf{x})$ is the *Rapini-Papoular* anchoring energy.

(b) Landau - de Gennes

(i) Strong anchoring:

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

(ii) Weak anchoring: add surface energy term

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

But is the derivation of the Oseen-Frank theory from Landau - de Gennes correct? The constrained Landau - de Gennes theory is invariant to changing $\mathbf{n}$ to $-\mathbf{n}$, 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 $\mathbf{n} \in S^2$ let

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

and set

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

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

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

$$\mathbf{Q}(\mathbf{x}) = P(\mathbf{n}(\mathbf{x})),$$

where $\mathbf{n} \in W^{1,p}(\Omega, S^2)$. In topological language this means that $\mathbf{Q}$ has a *lifting* to $W^{1,p}(\Omega, S^2)$.

Relating the $\mathbf{Q}$ and $\mathbf{n}$ descriptions

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

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

Theorem. An orientable $\mathbf{Q}$ has exactly two orientations.

Proof

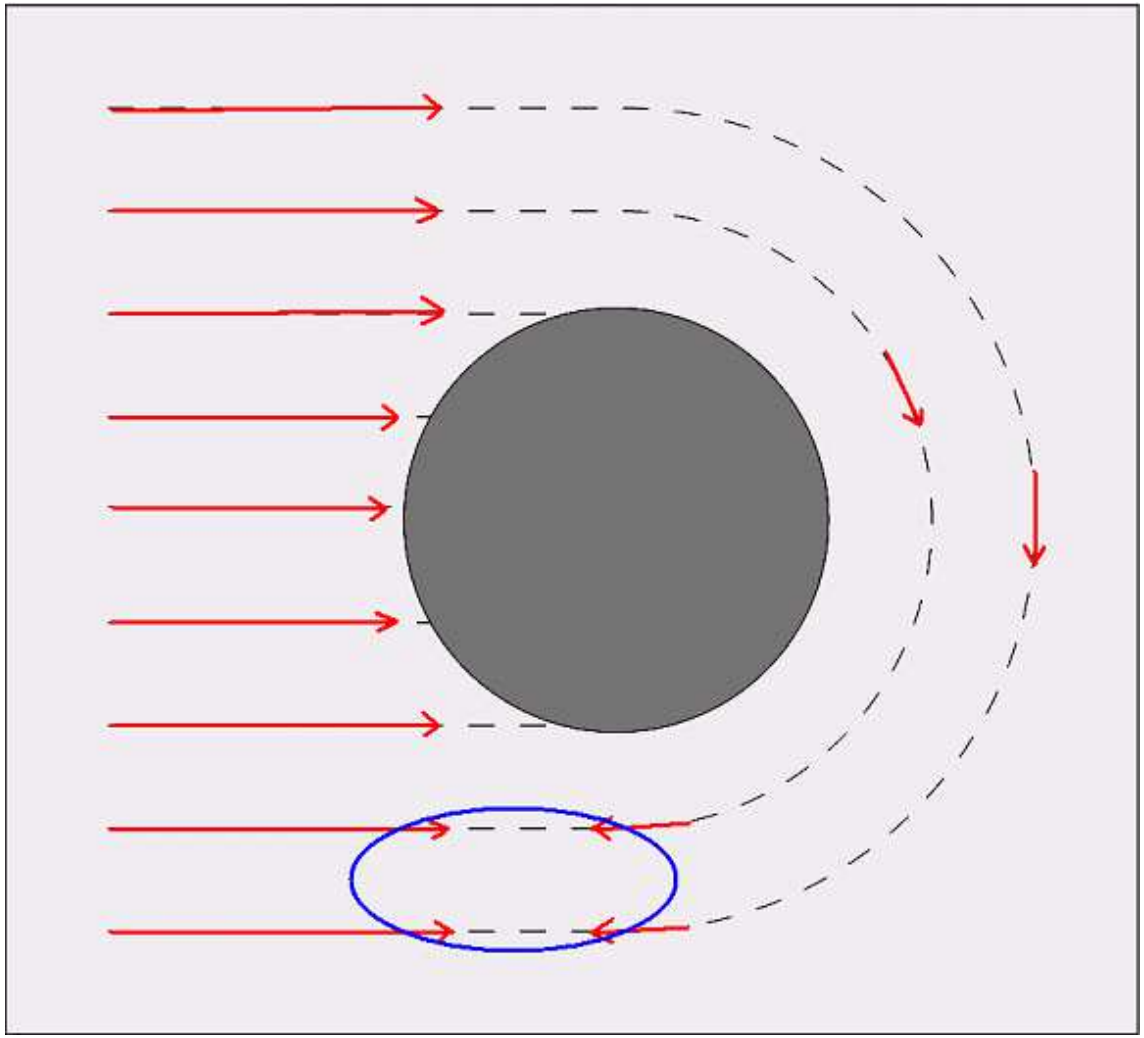
Suppose that $\mathbf{n}$ and $\tau\mathbf{n}$ both generate $\mathbf{Q}$ and belong to $W^{1,1}(\Omega, S^2)$, where $\tau^2(x) = 1$ a.e.. Let $C \subset \Omega$ be a cube with sides parallel to the coordinate axes. Let x_2, x_3 be such that the line $x_1 \mapsto (x_1, x_2, x_3)$ intersects C. Let $L(x_2,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

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

$$\int_C \tau\varphi_{,1} d\mathbf{x} = \int_C (\tau\varphi)_{,1} d\mathbf{x} = 0,$$

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 $\mathbf{Q} \in W^{1,p}$, $p \geq 2$, then $\mathbf{Q}$ is orientable.*

(There is a related topologically more general lifting result of Bethuel and Chiron 2007.)

Since the natural energy space for the Oseen-Frank energy is $W^{1,2}(\Omega; S^2)$ it follows that in a simply-connected region the constrained Landau - de Gennes and Oseen-Frank theories are equivalent.

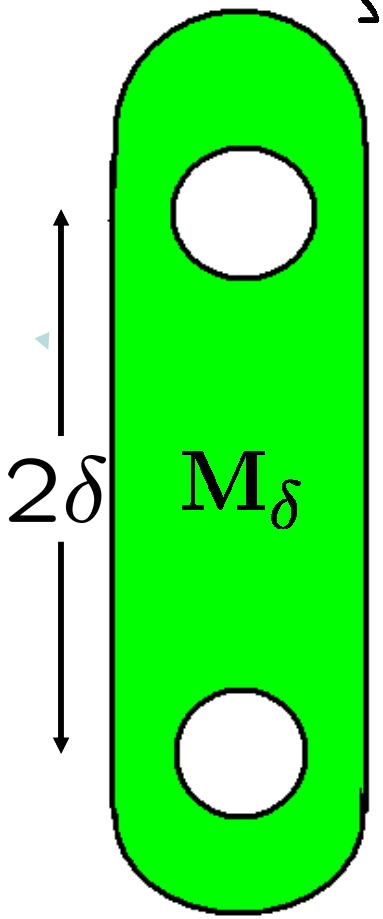
Ingredients of proof

- Lifting possible if $\mathbf{Q}$ 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 $\mathbf{Q}^{(j)} : \Omega \to \mathbb{R}P^2$ converging weakly to $\mathbf{Q}$ 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. (This 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 domain

(modification of a 2D example in JB/Zarnescu (2011))

$$\Omega_\delta = \{\mathbf{x} = (x_1, x_2, x_3) : (x_1, x_2) \in M_\delta, |x_3| < 1\}$$



Boundary conditions on $\partial\Omega_\delta$: On the curved outer boundary the line-field is tangent to the boundary and lies in the (x_1, x_2) plane.

On the two flat parts of $\partial\Omega_\delta$ the line-field also lies in the (x_1, x_2) plane.

On the inner two curved parts C_δ of the boundary there is weak anchoring of Rapini-Papoular type.

The one-constant Landau - de Gennes energy

$$I(\mathbf{Q}) = \frac{1}{2}L_1 \int_{\Omega_\delta} |\nabla \mathbf{Q}|^2 d\mathbf{x} - \frac{1}{2}K \int_{C_\delta} (\mathbf{n} \cdot \boldsymbol{\nu})^2 dS$$

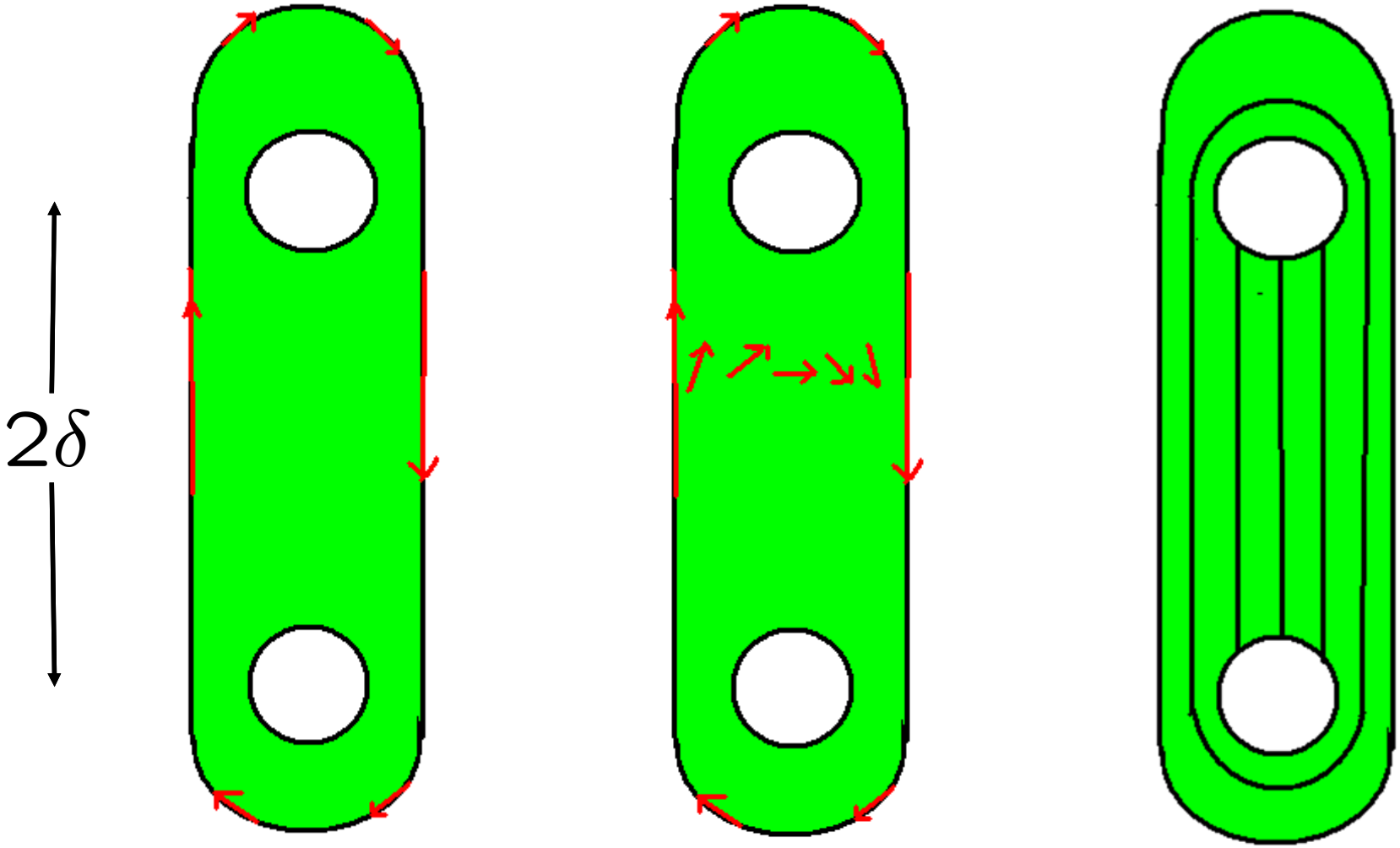
attains a minimum in $W^{1,2}(\Omega_\delta; \mathcal{Q})$ subject to the boundary conditions on the outer boundary $\partial\Omega_\delta \setminus C_\delta$.

The corresponding Oseen-Frank energy

$$I(\mathbf{n}) = s^2 L_1 \int_{\Omega_\delta} |\nabla \mathbf{n}|^2 d\mathbf{x} - \frac{1}{2}K \int_{C_\delta} (\mathbf{n} \cdot \boldsymbol{\nu})^2 dS$$

also attains a minimum subject to the boundary conditions $\mathbf{n} \cdot \mathbf{e}_3 = 0$ on $\partial\Omega_\delta \setminus C_\delta$.

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



For details see JB, Liquid crystals and their defects, CIME lecture notes, Springer 2017.

Existence in Landau - de Gennes theory

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

$$I_\theta(\mathbf{Q}) = \int_\Omega [\psi_B(\mathbf{Q},\theta) + \frac{1}{2}\sum_{i=1}^{3} L_i I_i(\nabla\mathbf{Q})]\, d\mathbf{x}$$

attains a minimum on

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

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

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

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

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

so that for a subsequence (not relabelled)

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

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

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

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

by Fatou's lemma and the convexity in $\nabla\mathbf{Q}$. Hence $\mathbf{Q}^*$ is a minimizer.

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

But what if $L_4 \neq 0$?

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

$$I_\theta(\mathbf{Q}) = \int_\Omega \left(\psi_B(\mathbf{Q}, \theta) + \frac{1}{2} \sum_{i=1}^{4} L_i I_i(\nabla \mathbf{Q}) \right) dx$$

is unbounded below.

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

$$J(\mathbf{Q}) = \int_B \left(\psi_B(\mathbf{Q}, \theta) + \sum_{i=1}^{4} L_i I_i \right) d\mathbf{x}$$

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

Choose

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

where $r = |\mathbf{x}|$. Then

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

and

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

Hence

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

where C is a constant.

Provided h is bounded, all the terms are bounded except

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

Choose

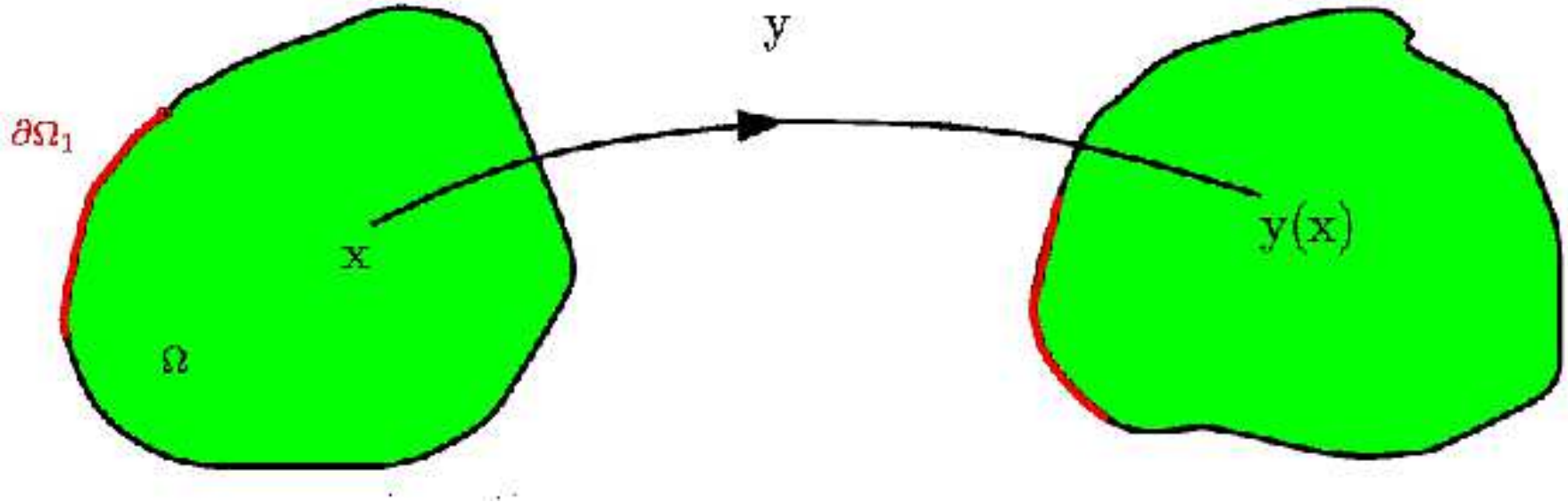
$$h(r) = \begin{cases} h_0(2 + \sin kr) & 0 < r < \frac{1}{2} \\ 2h_0(2 + \sin \frac{k}{2})(1 - r) & \frac{1}{2} < r < 1 \end{cases}$$

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

$$4\pi \int_0^{\frac{1}{2}} r^2 \left(\frac{2}{3} C + \frac{4}{9} L_4 h_0 (2 + \sin kr) \right) h_0^2 k^2 \cos^2 kr \, dr,$$

which tends to $-\infty$ as $k \to \infty$ if $L_4 h_0$ is sufficiently negative.

Analogy with nonlinear elasticity



Minimize

$$I(\mathbf{y}) = \int_\Omega \psi(\nabla \mathbf{y}(\mathbf{x}))\, d\mathbf{x}$$

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

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

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

To ensure this can assume that

$$\psi(\mathbf{A}) \to \infty \text{ as } \det \mathbf{A} \to 0+ .$$

But then it is a difficult open problem to prove that a minimizer $\mathbf{y}^*$ satisfies

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

Correspondingly, it is natural to suppose that

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

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 $L_4 \neq 0$.

The singular bulk potential (JB/Majumdar)

The Maier-Saupe theory

In the Maier-Saupe model the bulk free-energy at temperature $\theta > 0$ of a homogeneous nematic liquid crystal has the form

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

where $\rho = \rho(\mathbf{p})$ and the entropy is given by

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

and k_B is Boltzmann's constant.

(Here and below we define $t \ln t = 0$ for $t = 0$.)

Consider an interaction potential $U(\rho)$ of the form

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

We assume that K is frame-indifferent, so that

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

which holds iff

$$K(\mathbf{p}, \mathbf{q}) = k(\mathbf{p} \cdot \mathbf{q})$$

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

In the Maier-Saupe theory k is given by

$$k(\mathbf{p}\cdot\mathbf{q}) = \kappa\left(\frac{1}{3} - (\mathbf{p}\cdot\mathbf{q})^2\right),$$

where $\kappa > 0$ is independent of θ.

Denoting by

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

the corresponding $\mathbf{Q}$-tensor, we have that

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

Hence

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

Theorem (Fatkullin & Slastikov 2005, Liu, Zhang & Zhang 2005)
For the Maier-Saupe potential all critical points of $I_\theta(\rho)$ 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, 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, Vollmer (2015) has established a similar bifurcation picture for a class of potentials k including the Onsager potential $k(\mathbf{p}\cdot\mathbf{q}) = \kappa\sqrt{1-(\mathbf{p}\cdot\mathbf{q})^2}$.

Given $\mathbf{Q} \in \mathcal{E}$ with $\lambda_{\min}(\mathbf{Q}) > -\frac{1}{3}$ define

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

(cf. Katriel, Kventsel, Luckhurst & Sluckin (1986))

Thus we just need to understand how to minimize

$$E(\rho) = \int_{S^2} \rho(\mathbf{p}) \ln \rho(\mathbf{p}) \, d\mathbf{p}$$

subject to $\mathbf{Q}(\rho) = \mathbf{Q}$.

Given $\mathbf{Q} \in \mathcal{E}$ with $\lambda_{\min}(\mathbf{Q}) > -1/3$ we seek to minimize

$$E(\rho) = \int_{S^2} \rho(\mathbf{p}) \ln \rho(\mathbf{p})\, d\mathbf{p}$$

on

$$\mathcal{A}_{\mathbf{Q}} = \{\rho \in L^1(S^2) : \rho \geq 0, \int_{S^2} \rho(\mathbf{p})\, d\mathbf{p} = 1, \mathbf{Q}(\rho) = \mathbf{Q}, E(\rho) < \infty\}.$$

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

Theorem. E attains a minimum at a unique $\rho_{\mathbf{Q}} \in \mathcal{A}_{\mathbf{Q}}$.

Proof. We already showed that $\mathcal{A}_{\mathbf{Q}}$ is nonempty. Let $\rho^{(j)}$ be a minimizing sequence for E in $\mathcal{A}_{\mathbf{Q}}$. By the de la Vallée Poussin criterion and the superlinear growth of $\rho \ln \rho$, we may assume that $\rho^{(j)} \rightharpoonup \rho_{\mathbf{Q}}$ in $L^1(S^2)$ for some $\rho_{\mathbf{Q}}$, and $\rho_{\mathbf{Q}} \geq 0$, $\mathbf{Q}(\rho_{\mathbf{Q}}) = \mathbf{Q}$.

Since $\rho \ln \rho$ is convex,

$$I(\rho_{\mathbf{Q}}) \leq \liminf_{j \to \infty} I(\rho^{(j)}),$$

so that $\rho_{\mathbf{Q}}$ is a minimizer, which is unique since $\rho \ln \rho$ is strictly convex.

In fact $\rho_{\mathbf{Q}}$ can be given semi-explicitly as a Gaussian on the sphere.

Theorem. Let $\mathbf{Q} \in \mathcal{E}$ with $\lambda_{\min}(\mathbf{Q}) > -\frac{1}{3}$ have spectral decomposition $\mathbf{Q} = \sum_{i=1}^{3} \lambda_i \mathbf{e}_i \otimes \mathbf{e}_i$. Then in the basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ the unique minimizer $\rho_{\mathbf{Q}}$ of $E(\rho)$ in $\mathcal{A}_{\mathbf{Q}}$ is given by

$$\rho_{\mathbf{Q}}(\mathbf{p}) = \frac{\exp\left(\mu_1 p_1^2 + \mu_2 p_2^2 + \mu_3 p_3^2\right)}{Z(\mu_1, \mu_2, \mu_3)},$$

where $\mathbf{p} = (p_1, p_2, p_3)$, $\boldsymbol{\mu} = (\mu_1, \mu_2, \mu_3)$,

$$Z(\boldsymbol{\mu}) = \int_{S^2} \exp\left(\mu_1 p_1^2 + \mu_2 p_2^2 + \mu_3 p_3^2\right) d\mathbf{p}$$

is the *partition function*, and

$$\nabla_{\boldsymbol{\mu}} \ln Z(\boldsymbol{\mu}) = \boldsymbol{\gamma},$$

with $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \gamma_3)$ and $\gamma_i = \lambda_i + \frac{1}{3}$. The μ_i are unique up to an additive constant.

To show that $\rho_{\mathbf{Q}}$ satisfies the corresponding Euler-Lagrange equation, the μ_i appearing as Lagrange multipliers, is a bit tricky because of the possibility that $\rho_{\mathbf{Q}}$ is not bounded away from zero. A quicker proof is via the following 'dual' variational principle (cf Mead & Papanicolaou 1984, Borwein & Lewis 1991), from which the existence of a minimizer $\rho_{\mathbf{Q}}$ also follows.

Theorem. $\boldsymbol{\mu}$ maximizes

$$H(\mathbf{v}) = \boldsymbol{\gamma} \cdot \mathbf{v} - \ln Z(\mathbf{v})$$

over $\mathbf{v} \in \mathbb{R}^3$, and

$$\min_{\mathcal{A}_{\mathbf{Q}}} E(\rho) = \max_{\mathbf{v} \in \mathbb{R}^3} H(\mathbf{v}),$$

so that $E(\rho_{\mathbf{Q}}) = H(\boldsymbol{\mu})$.

Note that if $\mathbf{m} = (1, 1, 1)$ then for any $\tau \in \mathbb{R}$

$$\begin{aligned} H(\mathbf{v} + \tau\mathbf{m}) &= \boldsymbol{\gamma} \cdot \mathbf{v} + \tau - \ln \int_{S^2} \exp\left(\sum_{i=1}^{3} v_i p_i^2 + \tau \right) d\mathbf{p} \\ &= \boldsymbol{\gamma} \cdot \mathbf{v} - \ln Z(\mathbf{v}) = H(\mathbf{v}), \end{aligned}$$

so that it is sufficient to consider $H(\mathbf{v})$ for $\mathbf{v} \in \mathbf{m}^{\perp}$, where

$$\mathbf{m}^{\perp} = \{\mathbf{v} \in \mathbb{R}^3 : \mathbf{v} \cdot \mathbf{m} = 0\}.$$

Lemma. $H(\mathbf{n})$ is a strictly concave function on $\mathbf{m}^{\perp}$ with $H(\mathbf{n}) \to -\infty$ as $|\mathbf{n}| \to \infty$, and hence attains a unique maximum on $\mathbf{m}^{\perp}$.

Proof. If $\mathbf{a}, \mathbf{v} \in \mathbf{m}^{\perp}$ with $\mathbf{a} \neq \mathbf{0}$ then a calculation shows that

$$\frac{\partial^2 \ln Z(\mathbf{v})}{\partial v_i \partial v_j} a_i a_j = \frac{1}{2Z(\mathbf{v})^2} \int_{S^2} \int_{S^2} \left(\sum_{i=1}^{3} a_i (p_i^2 - q_i^2) \right)^2 \exp\left(\sum_{k=1}^{3} v_k (p_k^2 + q_k^2) \right) d\mathbf{p}\, d\mathbf{q} > 0,$$

so that $H(\mathbf{v})$ is strictly concave.

To prove that $H(\mathbf{v}) \to -\infty$ as $|\mathbf{v}| \to \infty$ it suffices to prove that $\exp(-H(\mathbf{v})) \to \infty$. But

$$\exp(-H(\mathbf{v})) = \int_{S^2} \exp\left(\sum_{i=1}^{3} v_i(p_i^2 - \gamma_i)\right) d\mathbf{p}$$

and

$$\begin{aligned}\sum_{i=1}^{3} v_i(p_i^2 - \gamma_i) &= v_1(2p_1^2 + p_2^2 - 2\gamma_1 - \gamma_2) \\ &\quad + v_2(2p_2^2 + p_1^2 - 2\gamma_2 - \gamma_1).\end{aligned}$$

The result follows by examining the sets of $\mathbf{p} \in S^2$ where the two quantities in brackets are positive and negative.

Given a maximizer $\boldsymbol{\mu}$ of H we have that $\nabla_{\boldsymbol{\mu}} H(\boldsymbol{\mu}) = \mathbf{0}$, that is

$$\frac{\nabla_{\boldsymbol{\mu}} Z(\boldsymbol{\mu})}{Z(\boldsymbol{\mu})} = \boldsymbol{\gamma},$$

expressing the fact that

$$\rho_{\mathbf{Q}}(\mathbf{p}) = \frac{\exp\left(\sum_{i=1}^{3} \mu_i p_i^2\right)}{Z(\boldsymbol{\mu})}$$

satisfies $\mathbf{Q}(\rho_{\mathbf{Q}}) = \mathbf{Q}$.

Now let $\rho \in \mathcal{A}_{\mathbf{Q}}$, $\rho \neq \rho_{\mathbf{Q}}$. Then by the strict convexity of $\rho \ln \rho$ we have that

$$\begin{aligned} E(\rho) &= \int_{S^2} \rho \ln \rho \, d\mathbf{p} \\ &> \int_{S^2} \left(\rho_{\mathbf{Q}} \ln \rho_{\mathbf{Q}} + (\rho - \rho_{\mathbf{Q}}) \left(1 + \sum_{i=1}^{3} \mu_i p_i^2 - \ln Z(\boldsymbol{\mu}) \right) \right) d\mathbf{p} \\ &= I(\rho_{\mathbf{Q}}), \end{aligned}$$

so that $\rho_{\mathbf{Q}}$ is the unique global minimizer.

Let $f(\mathbf{Q}) = E(\rho_{\mathbf{Q}}) = \inf_{\rho \in \mathcal{A}_{\mathbf{Q}}} E(\rho)$, so that

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

Hence the bulk free energy has the form

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

Theorem. f is strictly convex in $\mathbf{Q}$ and

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

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

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

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

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

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

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

The blow-up is logarithmic.

Theorem

$$\frac{1}{2}\ln\left(\frac{1}{(2\pi)^3 e\gamma_{\min}(\mathbf{Q})}\right) \leq f(\mathbf{Q}) \leq \ln\left(\frac{1}{\gamma_{\min}(\mathbf{Q})}\right),$$

$$\frac{1}{2}\sqrt{\frac{3}{2}}\ln\left(\frac{2}{\pi e\gamma_{\min}(\mathbf{Q})}\right) \leq |\nabla f(\mathbf{Q})| \leq \frac{1}{\gamma_{\min}(\mathbf{Q})}\ln\left(\frac{1}{2\pi^3 e\,\gamma_{\min}(\mathbf{Q})}\right),$$

where $\gamma_{\min}(\mathbf{Q}) = \lambda_{\min}(\mathbf{Q}) + \frac{1}{3}$.

The proof uses our initial construction of a function $\rho \in \mathcal{A}_{\mathbf{Q}}$ 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 $\mathbf{Q}$ of $\psi_B(\mathbf{Q}, \theta)$. 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, using the estimates

$$-\frac{1}{3}|\nabla \mathbf{Q}|^2 \leq Q_{lk}Q_{ij,l}Q_{ij,k} \leq \frac{2}{3}|\nabla \mathbf{Q}|^2.$$

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

$$\frac{1}{\theta k_B}\psi_B(\mathbf{Q},\theta) = \ln 4\pi + \left(\frac{15}{4} - \frac{\kappa}{\theta k_B}\right)\mathrm{tr}\,\mathbf{Q}^2 - \frac{75}{14}\mathrm{tr}\,\mathbf{Q}^3 + \frac{3825}{784}\left(\mathrm{tr}\,\mathbf{Q}^2\right)^2 - \\ -\frac{280125}{15092}\mathrm{tr}\,\mathbf{Q}^2\mathrm{tr}\,\mathbf{Q}^3 + \frac{14728}{6000}\left(\mathrm{tr}\,\mathbf{Q}^2\right)^3 + \frac{51246}{600}\left(\mathrm{tr}\,\mathbf{Q}^3\right)^2 + \ldots$$

In particular the expansion gives that the coefficients b, c in the quartic form should be proportional to θ and satisfy $\frac{b}{c} = \frac{14}{17} \simeq .82$, while experimental values reported in the literature are for MBBA 1.19, and for 5CB 0.82.

Given appropriate boundary conditions, do minimizers of

$$I_\theta(\mathbf{Q}) = \int_\Omega [\psi_B(\mathbf{Q}, \theta) + \psi_E(\mathbf{Q}, \nabla\mathbf{Q}, \theta)]\, d\mathbf{x}$$

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

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

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

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.

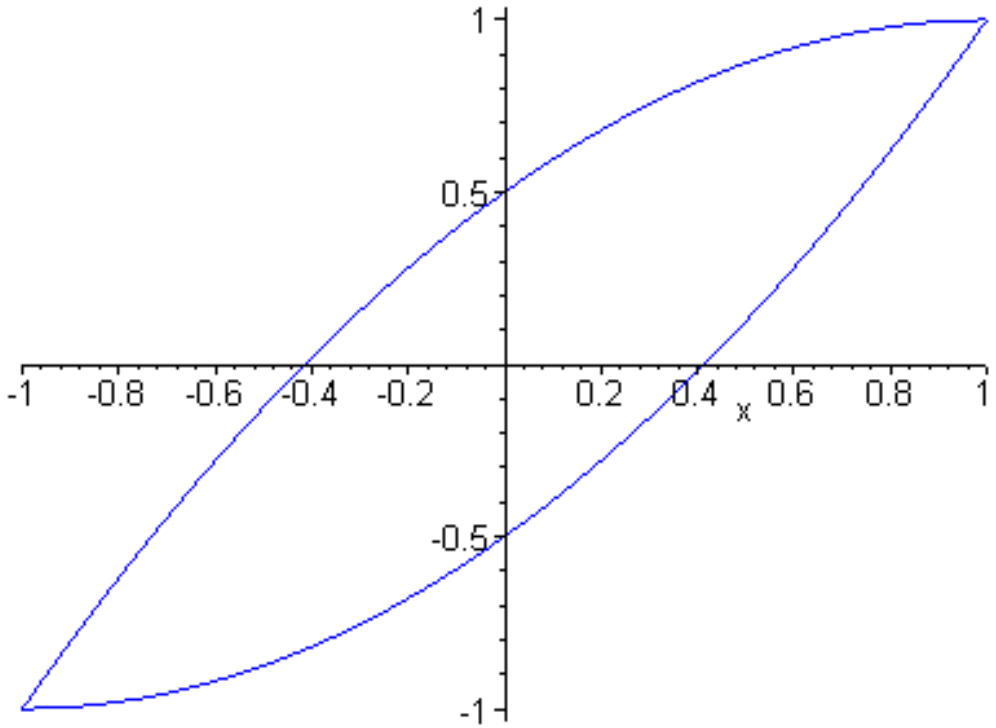
Example. (JB & Mizel)
Minimize

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

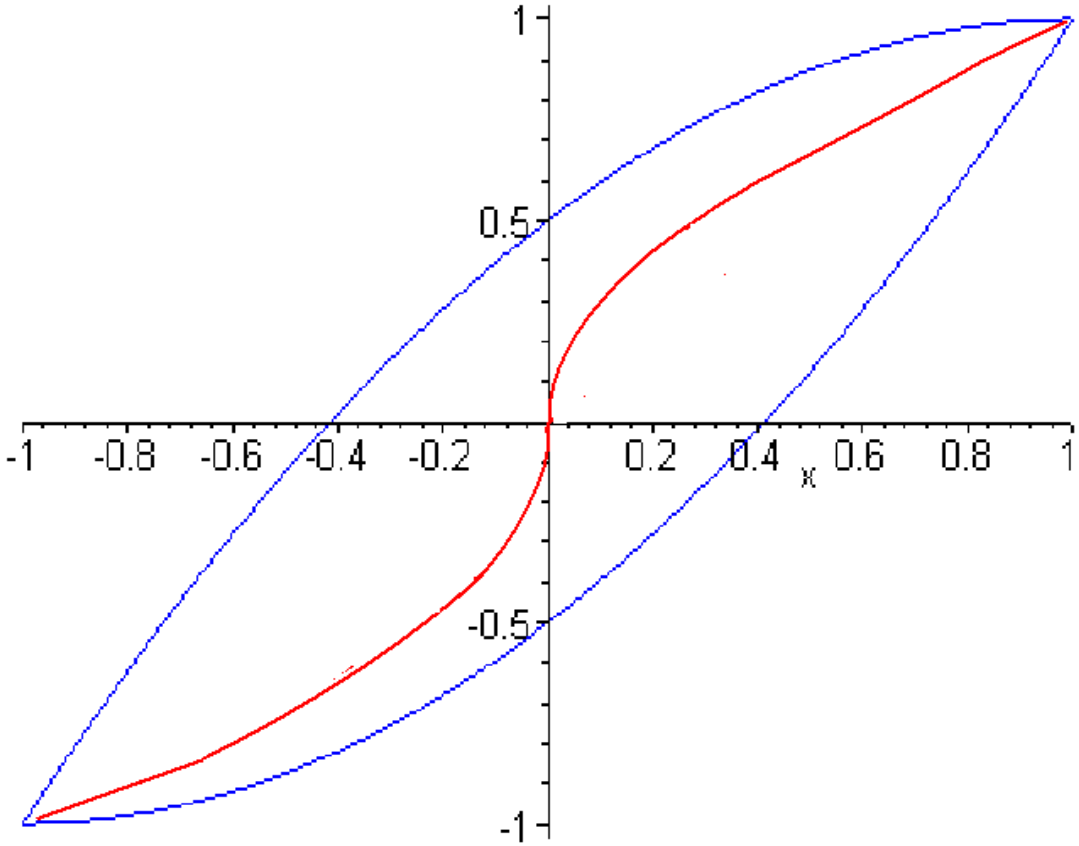
subject to

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

with $0 < \varepsilon < \varepsilon_0 \approx \cdot 001$.



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 $\mathbf{Q}$ minimize

$$I_\theta(\mathbf{Q}) = \int_\Omega [\psi_B(\mathbf{Q}, \theta) + K(\theta)|\nabla \mathbf{Q}|^2]\, d\mathbf{x},$$

subject to $\mathbf{Q}(\mathbf{x}) = \mathbf{Q}_0(\mathbf{x})$ for $\mathbf{x} \in \partial\Omega$, where $K(\theta) > 0$ and $\mathbf{Q}_0(\cdot)$ is sufficiently smooth with $\lambda_{\min}(\mathbf{Q}_0(x)) > -\frac{1}{3}$. Then

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

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

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

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

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. Tthere are partial results in 2D of Bauman & Phillips (2016), and a related partial regularity result in 3D of Evans, Kneuss & Tran (2016).

Developments

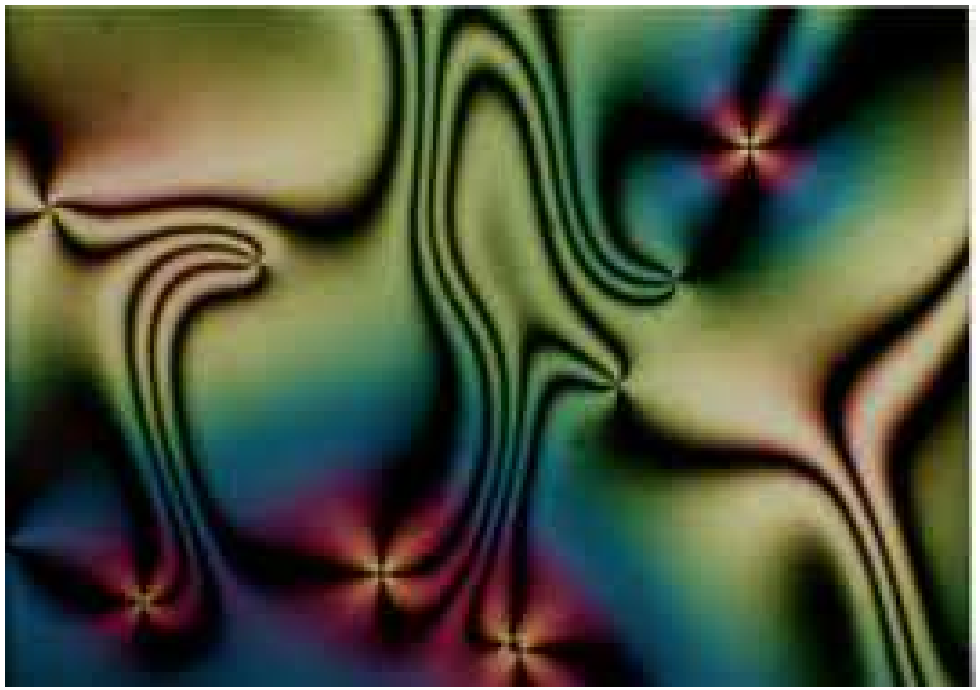
1. Jamie Taylor (2016) has generalized the construction of the singular potential to a broad class of moment problems, with various applications.

2. For studies of dynamics using the singular potential see
E. Feireisl, E. Rocca, and G. Schimperna, Annali di Matematica Pura ed Applicata (2013)
M. Wilkinson, Arch. Rat. Mech. Anal. (2015)

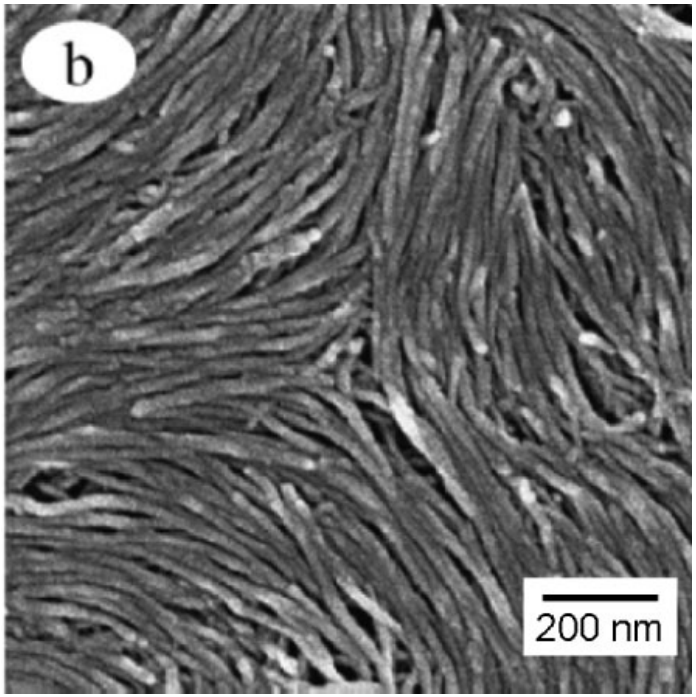
The description of defects

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

Oseen-Frank free energy

(drop explicit dependence on θ)

$$I(\mathbf{n}) = \int_\Omega W(\mathbf{n}, \nabla \mathbf{n})\, d\mathbf{x}, \qquad \mathbf{n} = \mathbf{n}(\mathbf{x}) \in S^2$$

splay twist bend

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

saddle-splay null Lagrangian

$\int_\Omega (\operatorname{tr}(\nabla \mathbf{n})^2 - (\operatorname{div} \mathbf{n})^2)\, d\mathbf{x}$ depends only on $\mathbf{n}|_{\partial\Omega}$

Ericksen (1966) inequalities. $W(\mathbf{n}, \nabla \mathbf{n}) \geq 0$ for all $\mathbf{n}$ if and only if

$$K_1 \geq 0,\ K_2 \geq 0,\ K_3 \geq 0,\ K_2 \geq |K_4|,\ 2K_1 \geq K_2 + K_4.$$

We will always assume the strict form

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

which are necessary and sufficient for $W(\mathbf{n}, \nabla \mathbf{n}) \geq \mu |\nabla \mathbf{n}|^2$ for some $\mu > 0$.

Energy minimization problem: find $\mathbf{n}$ that minimizes $I(\mathbf{n}) = \int_\Omega W(\mathbf{n}, \nabla\mathbf{n})\, d\mathbf{x}$ subject to suitable boundary conditions, for example $\mathbf{n}|_{\partial\Omega} = \bar{\mathbf{n}}$, where $\bar{\mathbf{n}}$ is given.

Important identities

$$(\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2 + |\mathbf{n} \wedge \operatorname{curl} \mathbf{n}|^2 = |\operatorname{curl} \mathbf{n}|^2$$

$$|\nabla\mathbf{n}|^2 = (\operatorname{div} \mathbf{n})^2 + (\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2 + |\mathbf{n} \wedge \operatorname{curl} \mathbf{n}|^2 + (\operatorname{tr} (\nabla\mathbf{n})^2 - (\operatorname{div} \mathbf{n})^2).$$

So if $K_1 = K_2 = K_3, K_4 = 0$ (the *one constant approximation*) then

$$I(\mathbf{n}) = \frac{K_1}{2} \int_\Omega |\nabla\mathbf{n}|^2 d\mathbf{x},$$

which is the energy functional for *harmonic maps*.

If $\mathbf{n}$ is a minimizer and $\mathbf{m} : \Omega \to \mathbb{R}^3$ is any smooth mapping with $\mathbf{m}|_{\partial\Omega} = 0$, then

$$\mathbf{n}_\varepsilon(\mathbf{x}) = \frac{\mathbf{n}(\mathbf{x}) + \varepsilon\mathbf{m}(\mathbf{x})}{|\mathbf{n}(\mathbf{x}) + \varepsilon\mathbf{m}(\mathbf{x})|}$$

satisfies $|\mathbf{n}_\varepsilon(\mathbf{x})| = 1$ and $\mathbf{n}_\varepsilon|_{\partial\Omega} = \bar{\mathbf{n}}$.

Hence formally we have that $\frac{d}{d\varepsilon} I(\mathbf{n}_\varepsilon)|_{\varepsilon=0} = 0$.

Noting that $\frac{d\mathbf{n}_\varepsilon}{d\varepsilon}|_{\varepsilon=0} = (\mathbf{1} - \mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}))\mathbf{m}(\mathbf{x})$, we obtain the weak form of the Euler-Lagrange equation, that for all such $\mathbf{m}$

$$\int_\Omega \Big(\frac{\partial W}{\partial \nabla \mathbf{n}} \cdot \nabla((\mathbf{1} - \mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}))\mathbf{m}(\mathbf{x})) + \frac{\partial W}{\partial \mathbf{n}} \cdot (\mathbf{1} - \mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}))\mathbf{m}(\mathbf{x}) \Big) \, d\mathbf{x} = 0. \qquad \text{(WEL)}$$

Hence, integrating by parts and using the arbitrariness of $\mathbf{m}$, we formally obtain the Euler-Lagrange equation

$$(\mathbf{1}-\mathbf{n}\otimes\mathbf{n})\left(\operatorname{div}\frac{\partial W}{\partial\nabla\mathbf{n}}-\frac{\partial W}{\partial\mathbf{n}}\right)=\mathbf{0}, \qquad \text{(EL)}$$

a system of second order nonlinear PDE to be solved subject to the pointwise constraint $|\mathbf{n}|=1$.

This can be written in the equivalent form

$$\operatorname{div}\frac{\partial W}{\partial\nabla\mathbf{n}}-\frac{\partial W}{\partial\mathbf{n}}=\lambda(\mathbf{x})\mathbf{n},$$

where $\lambda(\mathbf{x})$ is a Lagrange multiplier.

In the one-constant case (EL) becomes

$$\boldsymbol{\Delta}\mathbf{n}+|\nabla\mathbf{n}|^2\mathbf{n}=\mathbf{0}, \quad \text{i.e. } n_{i,jj}+(n_{j,k}n_{j,k})n_i=0\ (i=1,2,3).$$

How can we solve these equations?

Are there some exact solutions?

The question of what (smooth) $\mathbf{n}(\mathbf{x})$ can be solutions of (EL) for *all* K_1, K_2, K_3, K_4, so called *universal solutions*, was addressed by Marris (1978,1979), following Ericksen (1967).

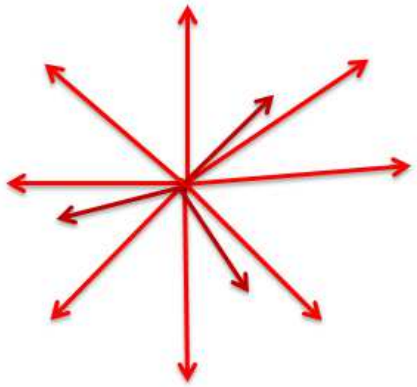
Marris showed that these consist of
(i) constant vector fields, or those orthogonal to families of concentric spheres or cylinders,
(ii) pure twists, such as

$$\mathbf{n}(\mathbf{x}) = (\cos \mu x_3, \sin \mu x_3, 0),$$

(iii) planar fields that form concentric or coaxial circles.

An example from family (i) is the *hedgehog*

$$\hat{\mathbf{n}}(\mathbf{x}) = \frac{\mathbf{x}}{|\mathbf{x}|}$$



which represents a point defect.

Of course $\hat{\mathbf{n}}$ is not even continuous at $\mathbf{0}$, but for $\mathbf{x} \neq \mathbf{0}$ it is smooth and we have

$$\nabla\hat{\mathbf{n}}(\mathbf{x}) = \frac{1}{|\mathbf{x}|}\left(1 - \frac{\mathbf{x}}{|\mathbf{x}|} \otimes \frac{\mathbf{x}}{|\mathbf{x}|}\right), \; |\nabla\hat{\mathbf{n}}(\mathbf{x})|^2 = \frac{2}{|\mathbf{x}|^2},$$

so that formally calculating its energy over the ball $B(\mathbf{0},1) = \{|\mathbf{x}| < 1\}$ we find that

$$\int_{B(\mathbf{0},1)} W(\hat{\mathbf{n}}, \nabla\hat{\mathbf{n}})\, d\mathbf{x} \leq C \int_{B(\mathbf{0},1)} |\nabla\hat{\mathbf{n}}|^2 d\mathbf{x} = 4\pi C \int_0^1 r^2 \cdot \frac{2}{r^2} dr < \infty.$$

More precisely, $\hat{\mathbf{n}}$ belongs to the Sobolev space

$$H^1(\Omega; S^2) = \{\mathbf{n} : \Omega \to S^2 : \int_\Omega |\nabla\mathbf{n}|^2\, d\mathbf{x} < \infty\},$$

where $\nabla\mathbf{n}$ is the weak or distributional derivative.

Theorem (Brezis, Coron & Lieb (1986), Lin (1987), Helein (1987), Ou (1992)) If $K_1 \leq K_2$ then $\hat{\mathbf{n}}$ is the unique minimizer of $I(\mathbf{n})$ in $H^1(\Omega; S^2)$ subject to its own boundary conditions.

Proof that $\hat{\mathbf{n}}$ is a minimizer. (JB/Virga)
Claim: if $K_1 \leq K_2$ then

$$K_1(\mathrm{div}\,\mathbf{n})^2 + K_2(\mathbf{n}\cdot\mathrm{curl}\,\mathbf{n})^2 + K_3|\mathbf{n}\wedge\mathrm{curl}\,\mathbf{n}|^2 + 2K_1[\mathrm{tr}\,(\nabla\mathbf{n})^2 - (\mathrm{div}\,\mathbf{n})^2] \geq 0.$$

Proof of claim: K_1, K_2, K_3, $K_4 = 2K_1 - K_2$ satisfy the Ericksen inequalities.

Hence, ignoring the saddle-splay term

$$\begin{aligned} I(\mathbf{n}) &= \frac{1}{2}\int_\Omega \left(K_1(\mathrm{div}\,\mathbf{n})^2 + K_2(\mathbf{n}\cdot\mathrm{curl}\,\mathbf{n})^2 + K_3|\mathbf{n}\wedge\mathrm{curl}\,\mathbf{n}|^2\right) d\mathbf{x} \\ &\geq K_1\int_\Omega \left((\mathrm{div}\,\mathbf{n})^2 - \mathrm{tr}\,(\nabla\mathbf{n})^2\right) d\mathbf{x} \\ &= K_1\int_\Omega \left((\mathrm{div}\,\hat{\mathbf{n}})^2 - \mathrm{tr}\,(\nabla\hat{\mathbf{n}})^2\right) d\mathbf{x} = I(\hat{\mathbf{n}}), \end{aligned}$$

since by direct computation $(\mathrm{div}\,\hat{\mathbf{n}})^2 = 2\mathrm{tr}\,(\nabla\hat{\mathbf{n}})^2$, $\mathrm{curl}\,\hat{\mathbf{n}} = \mathbf{0}$.

Results of Hélein 1987, Cohen & Taylor 1990, Kinderlehrer & Ou 1992 give that the second variation $\delta^2 I(\hat{\mathbf{n}}) > 0$ if and only if

$$K_2 - K_1 \geq -\frac{1}{8} K_3,$$

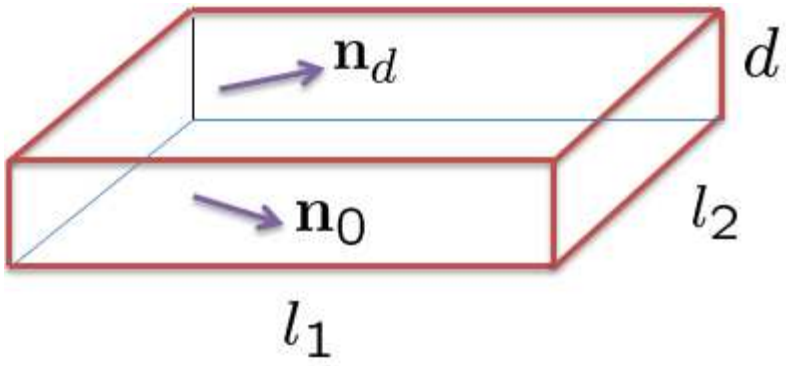
and can be negative if $K_2 - K_1 < -\frac{1}{8} K_3$, when $\hat{\mathbf{n}}$ is not a minimizer.

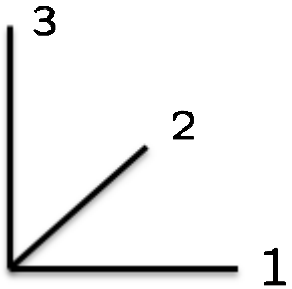
Numerical calculations of Alouges & Ghidaglia 1997 suggested that $\hat{\mathbf{n}}$ need not be a minimizer if $K_2 - K_1 > -\frac{1}{8} K_3$, but some of their examples had $K_1 = K_2$, when we know $\hat{\mathbf{n}}$ *is* a minimizer.

The same results on the second variation can be obtained (JB/Virga) within the class of twisted hedgehogs of the form $\mathbf{n} = \mathbf{R}(|\mathbf{x}|)\hat{\mathbf{n}}(\mathbf{x})$ with $\mathbf{R}(|\mathbf{x}|)\mathbf{e}_3 = \mathbf{e}_3$, and our analysis suggests that perhaps $\hat{\mathbf{n}}$ is a minimizer for $K_2 - K_1 \geq -\frac{1}{8} K_3$.

Pure twist solutions.

$\Omega = (0, l_1) \times (0, l_2) \times (0, d)$





Boundary conditions:

$$\mathbf{n}|_{x_1=0} = \mathbf{n}|_{x_1=l_1}, \qquad \mathbf{n}|_{x_2=0} = \mathbf{n}|_{x_2=l_2},$$
$$\mathbf{n}|_{x_3=0} = \mathbf{n}_0, \qquad \mathbf{n}|_{x_3=d} = \mathbf{n}_d,$$
$$\mathbf{n}_0 \cdot \mathbf{e}_3 = \mathbf{n}_d \cdot \mathbf{e}_3 = 0.$$

If $\mathbf{n} \in H^1(\Omega; S^2)$ satisfies these boundary conditions then

$$\int_\Omega \left(\mathrm{tr}\,(\nabla \mathbf{n})^2 - (\mathrm{div}\,\mathbf{n})^2 \right) d\mathbf{x} = 0.$$

Theorem. Assume $\mathbf{n}_d \neq \pm\mathbf{n}_0$. Suppose $K_2 \leq \min(K_1, K_3)$. Then there is a unique minimizer $\mathbf{n}^* \in H^1(\Omega; S^2)$ satisfying the boundary conditions, and $\mathbf{n}^*$ is a pure twist of the form

$$\mathbf{n}^*(\mathbf{x}) = (\cos(\lambda + \mu x_3), \sin(\lambda + \mu x_3), 0)$$

for constants λ, μ.

Proof. Let $\mathbf{n}^* = \mathbf{n}^*(x_3)$ be the unique minimizer of $E(\mathbf{n}) = \int_0^d |\mathbf{n}'(x_3)|^2 dx_3$ subject to $\mathbf{n}(0) = \mathbf{n}_0, \mathbf{n}(d) = \mathbf{n}_d$, which has the given form. Then

$$\begin{aligned}
2I(\mathbf{n}) &= \int_\Omega [K_1(\operatorname{div}\mathbf{n})^2 + K_2(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + K_3|\mathbf{n}\wedge\operatorname{curl}\mathbf{n}|^2]\,d\mathbf{x} \\
&= \int_\Omega [(K_1 - K_2)(\operatorname{div}\mathbf{n})^2 + K_2|\nabla\mathbf{n}|^2 + (K_3 - K_2)|\mathbf{n}\wedge\operatorname{curl}\mathbf{n}|^2]\,d\mathbf{x} \\
&\geq \int_\Omega K_2|\nabla\mathbf{n}|^2 d\mathbf{x} \\
&\geq \int_\Omega K_2|\mathbf{n}_{,3}|^2 d\mathbf{x} = \int_0^{l_1}\int_0^{l_2} K_2\left(\int_0^d |\mathbf{n}_{,3}(x_1,x_2,x_3)|^2 dx_3\right) dx_1 dx_2 \\
&\geq \int_\Omega K_2|\mathbf{n}^*_{,3}(x_3)|^2 d\mathbf{x} = 2I(\mathbf{n}^*),
\end{aligned}$$

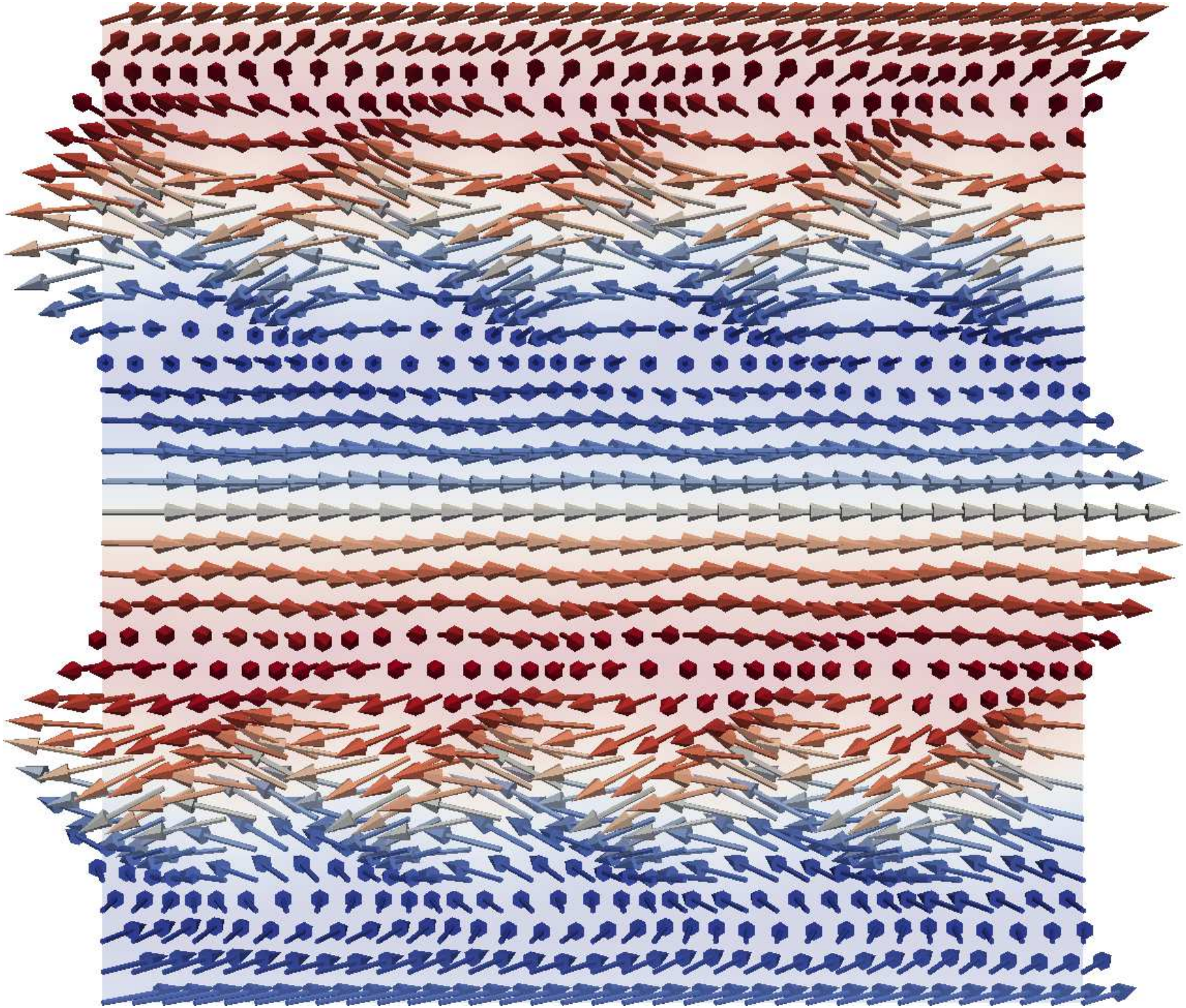
since $\operatorname{div}\mathbf{n}^* = 0$ and $\mathbf{n}^*\wedge\operatorname{curl}\mathbf{n}^* = 0$.

Numerical results of Patrick Farrell (Oxford) (see also Adler, Emerson, Farrell & Maclachlan (2016)) using his 'deflation' algorithm for finding stationary points.

In the computations $d = 1, l_1 = 1$, and only solutions independent of x_2 are sought.

For the one-constant case only the pure twist solution is found. But for a case with $K_1 = K_3 = 1, K_2 = 2.8$ he finds 74 solutions, the one with least energy being a tilt-twist configuration depending only on x_3.

Red arrows point towards you, blue arrows away.



A routine use of the direct method of the calculus of variations gives:

Theorem. If $\bar{\mathbf{n}} \in H^1(\Omega; S^2)$ then there exists $\mathbf{n}^*$ that minimizes $I(\mathbf{n})$ over all $\mathbf{n} \in H^1(\Omega; S^2)$ with $\mathbf{n}|_{\partial\Omega} = \bar{\mathbf{n}}$, and $\mathbf{n}^*$ satisfies (WEL).

Much deeper are results of Schoen & Uhlenbeck (1982), Brezis, Coron & Lieb (1986).

Theorem. In the one-constant case $\mathbf{n}^*$ is smooth except for a finite number of point defects located at points $\mathbf{x}(i) \in \Omega$, and

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

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

The best result for general Frank constants is:

Theorem (Hardt, Lin & Kinderlehrer (1986)) Any minimizer $\mathbf{n} \in H^1(\Omega; S^2)$ is analytic outside a closed set $\mathcal{S}$ whose Hausdorff dimension is less than one.

Remarks on weak solutions.

1. In the one-constant case finite energy solutions of (WEL) can be *everywhere discontinuous* (Rivière (1995)).

2. Minimizers also satisfy the identity

$$\int_\Omega \left(W\delta_{kj} - n_{i,k}\frac{\partial W}{\partial n_{i,j}} \right) \varphi_{k,j}\, d\mathbf{x} = 0 \qquad (\dagger)$$

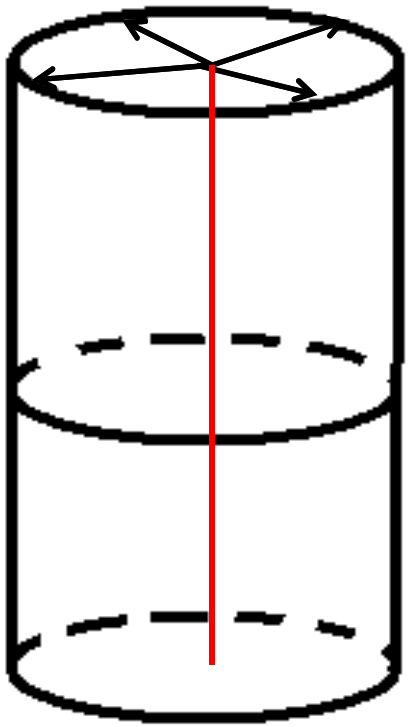
for all $\varphi \in C_0^\infty(\Omega;\mathbb{R}^3)$, obtained by considering variations of the form $\mathbf{n}(\mathbf{z}(\mathbf{x}))$ that rearrange the values of $\mathbf{n}$.

3. Smooth solutions of (EL) satisfy (†), but in general solutions of (WEL) do not.

4. In the one-constant case, solutions of (WEL) satisfying (†) are smooth outside a closed set E of zero 1D Hausdorff measure (Evans 1991), thus smoother than general solutions of (WEL).

5. Solutions of (WEL) satisfying (†) are weak equilibrium solutions to the Ericksen-Leslie dynamic equations, but the converse is not clear.

Line defects

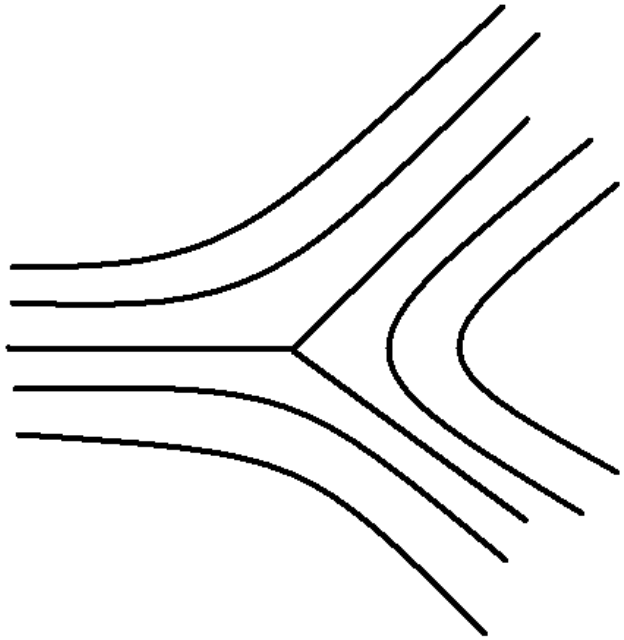


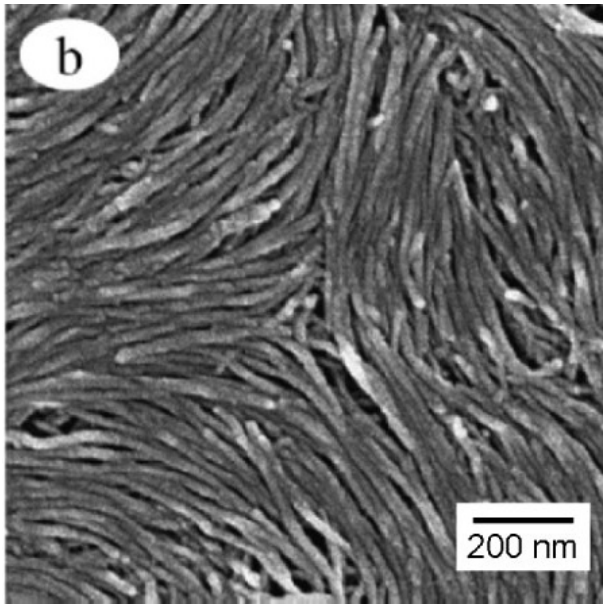
$$\hat{\mathbf{n}}(\mathbf{x}) = (\tfrac{x_1}{r}, \tfrac{x_2}{r}, 0) \quad r = \sqrt{x_1^2 + x_2^2}$$
$$|\nabla \hat{\mathbf{n}}(\mathbf{x})|^2 = \tfrac{1}{r^2}$$

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

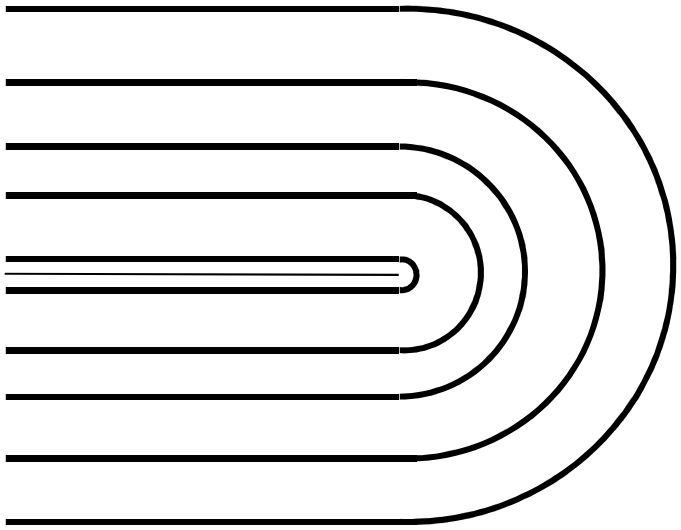
infinite energy for Oseen-Frank and constrained Landau-de Gennes quadratic models

Index one half defects

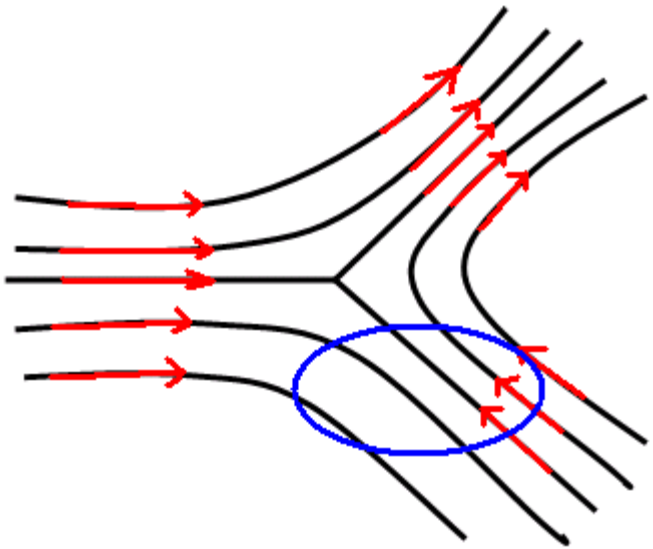


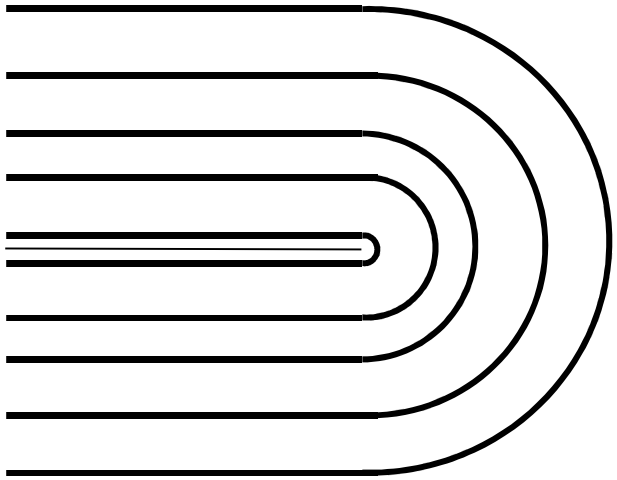


Zhang/Kumar 2007
Carbon nano-tubes
as liquid crystals



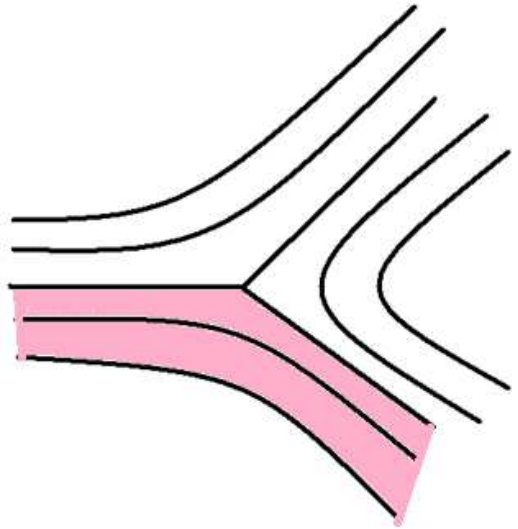
The index one half singularities are non-orientable





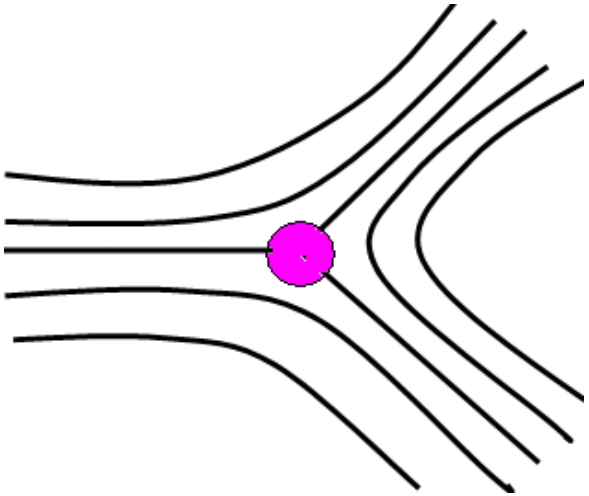
$\mathbf{Q} = s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1}\right) \notin W^{1,2}$ since otherwise orientable

In each sector $\mathbf{Q}$ is orientable but $\mathbf{Q} \notin W^{1,2}$.



Can one change $\mathbf{Q}$ (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 $\mathbf{Q}$ would be nonorientable and in $W^{1,2}$, contradicting the orientability result for simply-connected domains.

Director modeling of line defects with finite energy

That these defects have infinite energy arises from the quadratic growth in $\nabla \mathbf{n}$ of $W(\mathbf{n}, \nabla \mathbf{n})$.

But there is no reason to suppose that $W(\mathbf{n}, \nabla \mathbf{n})$ is quadratic for large $|\nabla \mathbf{n}|$ (such as near defects).

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

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

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

For example, we can let

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

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

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

for positive constants C_α, C'_α. Setting

$$I_\alpha(\mathbf{n}) = \int_\Omega W_\alpha(\mathbf{n}, \nabla \mathbf{n})\, d\mathbf{x},$$

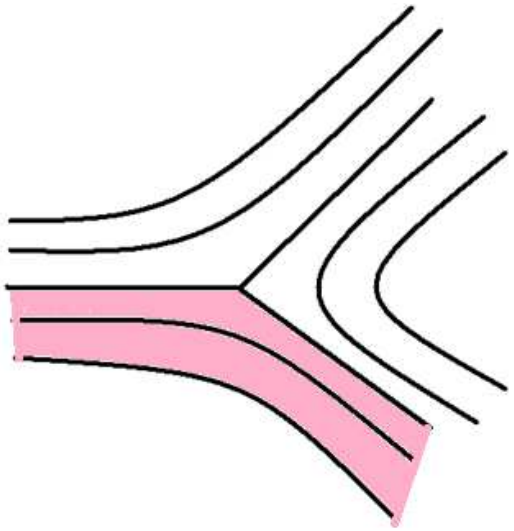
we obtain that $I_\alpha(\hat{\mathbf{n}}) < \infty$ as desired. Also $W_\alpha(\mathbf{n}, \cdot)$ is convex.

Boundary conditions:

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

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

For a subquadratic W the index-$\frac{1}{2}$ singularities have finite energy in the constrained LdG theory. However there still remains the issue of non-orientability (see later).



Canevari (2017) studies the behaviour as $K \to 0+$ of minimizers $\mathbf{Q}_K$ of the one-constant LdG energy

$$I_K(\mathbf{Q}) = \int_\Omega \left(\psi_B(\mathbf{Q}) + \frac{K}{2} |\nabla \mathbf{Q}|^2 \right) d\mathbf{x}$$

with quartic ψ_B under the logarithmic scaling

$$I_K(\mathbf{Q}_K) \leq CK|\ln K|,$$

which allows the appearance of line defects in the limit. He shows that these consist of straight line segments.

(For colloids, where curved disclinations are seen, there are other small geometric parameters. See the study of Saturn rings by Alama, Bronsard & Lamy (2016).)

Canevari & Majumdar (2018) also study defects in a subquadratic theory.

Description of defects in the full 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 $\mathbf{Q}$. Rather they can be seen as singularities in the eigenvectors of $\mathbf{Q}$, which can occur when eigenvalues coincide. (cf de Gennes, Biscari ...)

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

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

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 $\mathbf{Q}$. In both the Landau - de Gennes and Ericksen theories there are solutions to the Euler-Lagrange equations representing *melting hedgehogs*, of the form

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

where $s(\mathbf{0}) = 0$.

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 $\Omega = \mathbb{R}^3$ of

$$I(\mathbf{Q}) = \int_{\mathbb{R}^3} [\psi_B(\mathbf{Q}) + \frac{1}{2} K |\nabla \mathbf{Q}|^2] \, d\mathbf{x}$$

subject to the condition at infinity

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

where $s_{\text{min}} = \frac{b + \sqrt{b^2 - 24ac}}{4c} > 0$, 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.

Ericksen theory. Here we can model point and line defects by finite energy configurations in which $\mathbf{n}$ 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

$$I(\mathbf{Q}) = \int_\Omega [\psi_B(\mathbf{Q}) + \frac{1}{2}K|\nabla \mathbf{Q}|^2]\, d\mathbf{x},$$

then the uniaxial ansatz

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

gives the functional

$$I_E(s, \mathbf{n}) = \int_\Omega [2s^2|\nabla \mathbf{n}|^2 + \frac{1}{2}K(|\nabla s|^2) + \psi_B(s)]\, d\mathbf{x},$$

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

Then $\mathbf{n}$ 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 $I_E(s, \mathbf{n})$ finite.

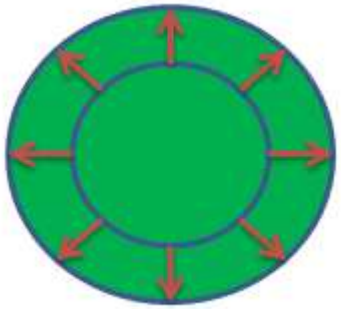
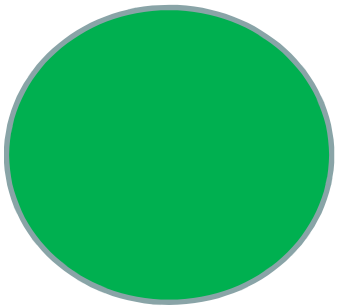
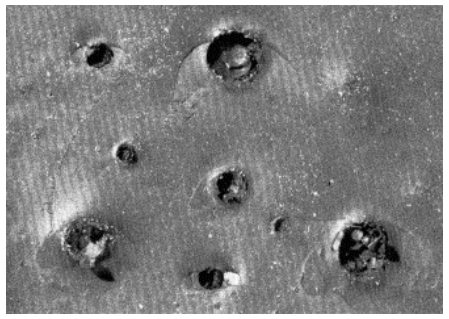
The Lavrentiev phenomenon

(Lavrentiev 1926)

Minimizers of the same energy in different function spaces can be different, and give different values for the minimum energy.

Consequence: the function space is part of the model.

Example from solid mechanics: ball of rubber subjected to outward radial boundary displacement, modelled using nonlinear elasticity.

Function space	Smooth maps	H^1	SBV
			
	Uniform dilatation	Cavitation (point defects)	Fracture (Surface defects)

The Lavrentiev phenomenon in liquid crystals.

One example is due to Hardt & Lin (1986) for the one-constant case. They show that there is a smooth map $\bar{\mathbf{n}} : B \to S^2$ such that for some $\alpha > 0$

$$\min_{\mathbf{n}\in H^1(B;S^2),\mathbf{n}|_{\partial B}=\bar{\mathbf{n}}} I(\mathbf{n}) + \alpha \leq I(\mathbf{m})$$

for all continuous $\mathbf{m} \in H^1(B; S^2)$.

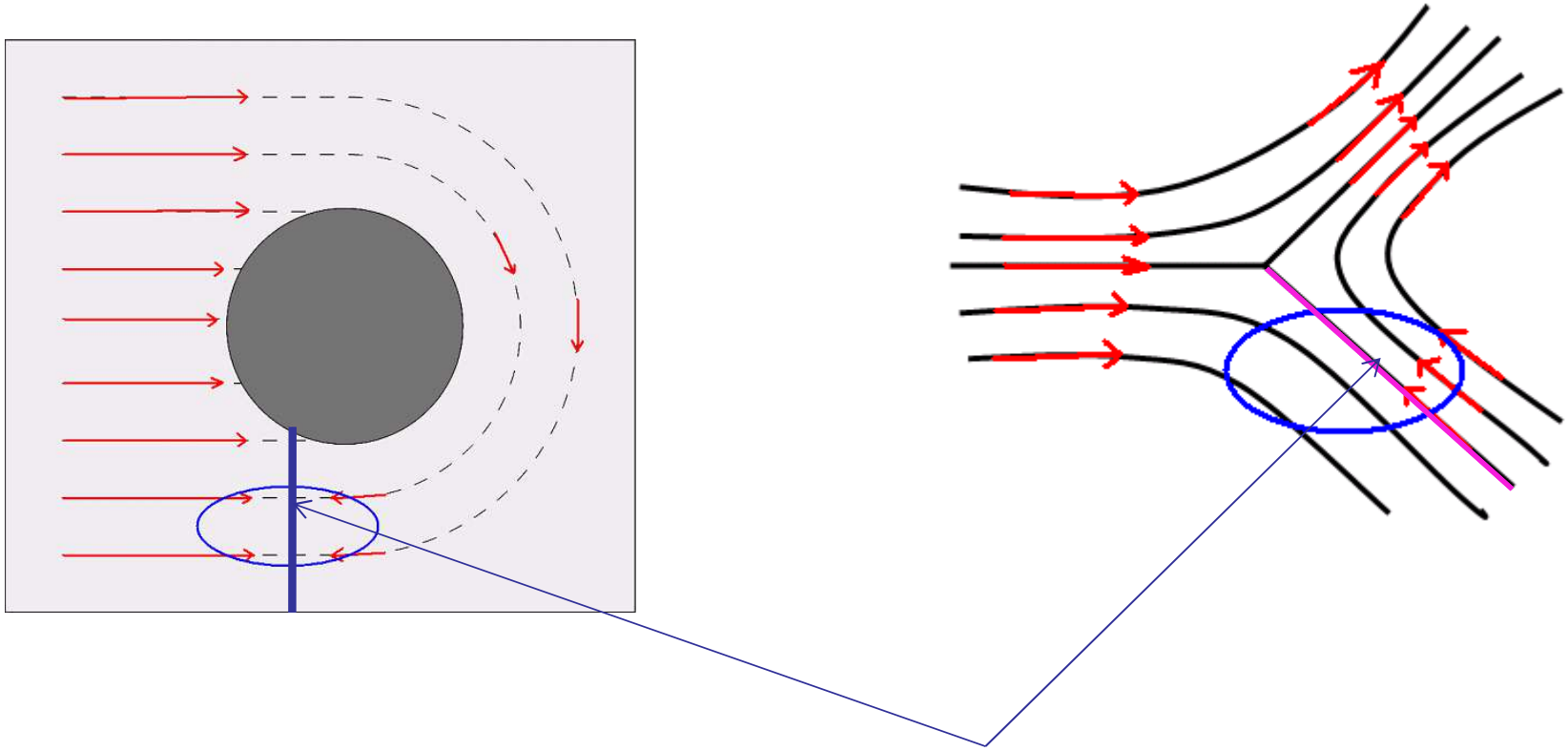
Another example is if we allow the director $\mathbf{n}$ to be discontinuous across surfaces (planar defects). In this case one should pay an energetic penalty for a jump in $\mathbf{n}$, so that we have an augmented functional defined for $\mathbf{n} \in SBV$

$$I(\mathbf{n}) = \int_\Omega W(\mathbf{n}, \nabla\mathbf{n})\, d\mathbf{x} + \int_{S_\mathbf{n}} f(\mathbf{n}_+, \mathbf{n}_-, \boldsymbol{\nu})\, dA.$$

normal to $S_\mathbf{n}$

jump set of $\mathbf{n}$

limits of $\mathbf{n}$ on either side of $S_\mathbf{n}$



One possible application is to recover orientability by allowing $\mathbf{n}$ to jump to $-\mathbf{n}$ across suitable surfaces with zero energy cost.

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

Planar defects (JB/Bedford)

Consider further a free-energy functional for nematic liquid crystals of free-discontinuity type

$$I(\mathbf{n}) = \int_\Omega W(\mathbf{n}, \nabla \mathbf{n})\, d\mathbf{x} + \int_{S_\mathbf{n}} f(\mathbf{n}_+, \mathbf{n}_-, \boldsymbol{\nu})\, d\mathcal{H}^2,$$

for $\mathbf{n} \in \mathrm{SBV}(\Omega, S^2)$, where $\boldsymbol{\nu}$ is the normal to the jump set $S_\mathbf{n}$.

Properties of f

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

$$f(\mathbf{R}\mathbf{n}_+, \mathbf{R}\mathbf{n}_-, \mathbf{R}\boldsymbol{\nu}) = f(\mathbf{n}_+, \mathbf{n}_-, \boldsymbol{\nu}) \tag{1}$$

for all $\mathbf{R} \in SO(3), \mathbf{n}_+, \mathbf{n}_-, \boldsymbol{\nu} \in S^2$, and that f is invariant to reversing the signs of $\mathbf{n}_+, \mathbf{n}_-$, reflecting the statistical head-to-tail symmetry of the molecules, so that

$$f(-\mathbf{n}_+, \mathbf{n}_-, \boldsymbol{\nu}) = f(\mathbf{n}_+, -\mathbf{n}_-, \boldsymbol{\nu}) = f(\mathbf{n}_+, \mathbf{n}_-, \boldsymbol{\nu}). \tag{2}$$

Also would like that $f(\mathbf{n}, \mathbf{n}, \boldsymbol{\nu}) = 0$, though sometimes it is easier to consider the case when $\min f > 0$.

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

$$f(\mathbf{n}_+, \mathbf{n}_-, \boldsymbol{\nu}) = g((\mathbf{n}_+ \cdot \mathbf{n}_-)^2, (\mathbf{n}_+ \cdot \boldsymbol{\nu})^2, (\mathbf{n}_- \cdot \boldsymbol{\nu})^2, (\mathbf{n}_+ \cdot \mathbf{n}_-)(\mathbf{n}_+ \cdot \boldsymbol{\nu})(\mathbf{n}_- \cdot \boldsymbol{\nu}))$$

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

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

(c.f. Smith 1971)

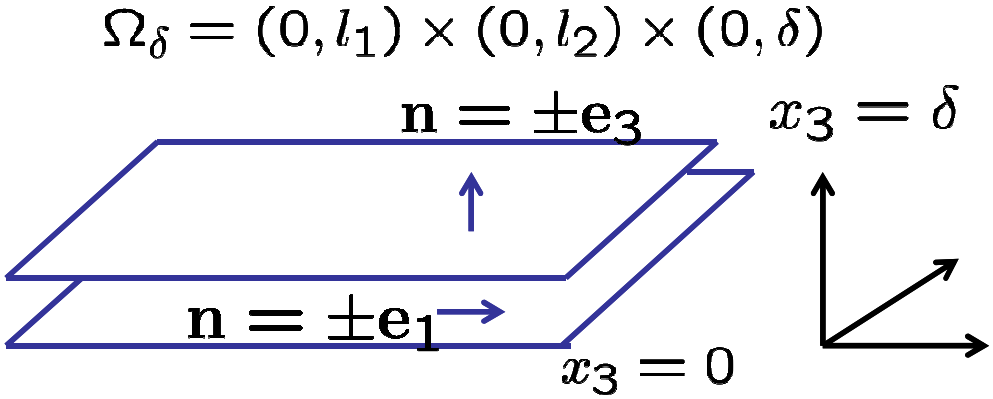
Order reconstruction

Barbero & Barberi (1983)

Ambrosio & Virga (1991)

Palffy-Muhoray, Gartland & Kelly (1994)

Lamy (2015)



(a) Analysis using Landau - de Gennes

Boundary conditions:

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

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

$\mathbf{Q}^{(0)} = s_1\left(\mathbf{e}_1\otimes\mathbf{e}_1 - \frac{1}{3}\mathbf{1}\right), \;\; \mathbf{Q}^{(1)} := s_2\left(\mathbf{e}_3\otimes\mathbf{e}_3 - \frac{1}{3}\mathbf{1}\right),$

$\mathbf{Q}$ periodic in x_1, x_2 and $s_1 > 0$, $s_2 > 0$.

Suppose that $\psi(\mathbf{Q}, \nabla\mathbf{Q}) = \psi_B(\mathbf{Q}) + \psi_E(\nabla\mathbf{Q})$ with ψ_B of standard form and

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

for some $\alpha > 0$.

Rescale, defining

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

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

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

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

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

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

where

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

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

So for sufficiently small δ, $\mathbf{Q}$ is given approximately by

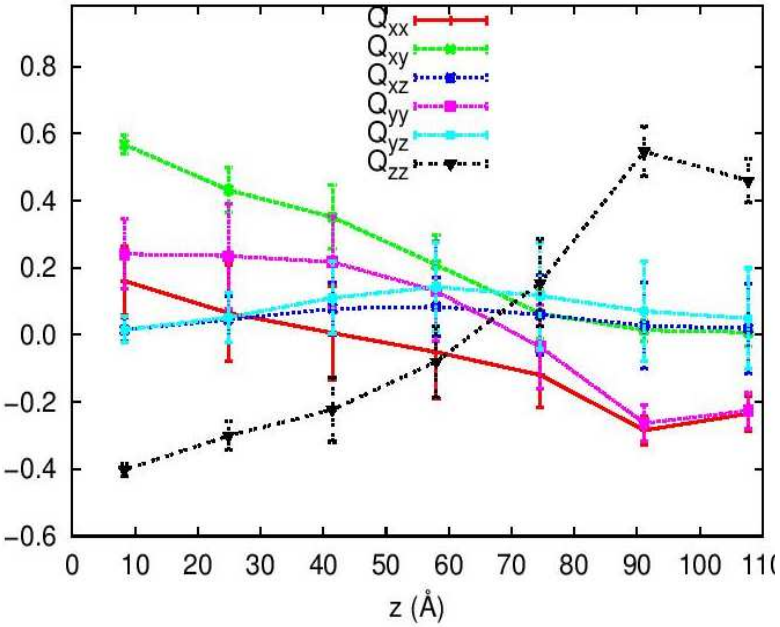
$$\mathbf{Q}(\mathbf{x}) = (1-\delta^{-1}x_3)\mathbf{Q}^{(0)} + \delta^{-1}x_3\mathbf{Q}^{(1)},$$

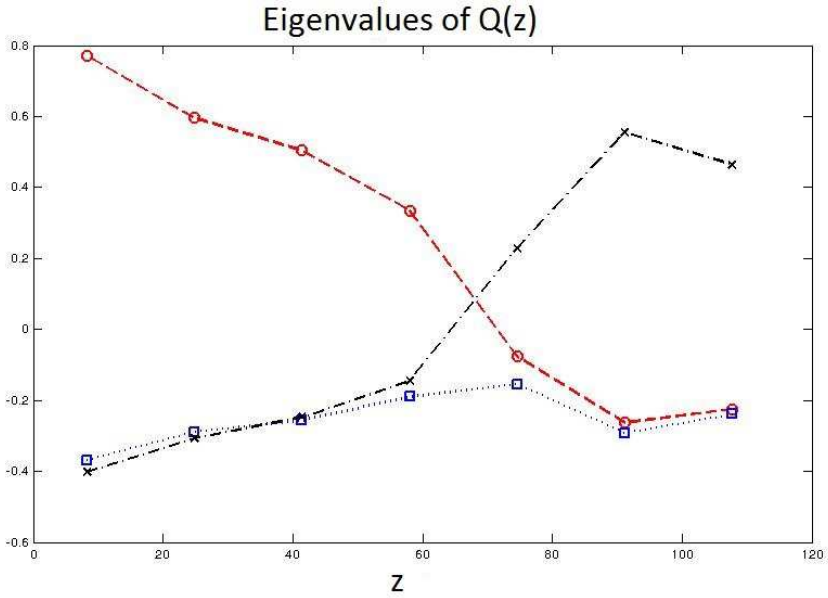
for which the director (the eigenvector of $\mathbf{Q}$ corresponding to the largest eigenvalue)

$$\mathbf{n}(\mathbf{x}) = \begin{cases} \mathbf{e}_1 & \text{if } 0 \le x_3 < \frac{s_1}{s_1+s_2}\delta \\ \mathbf{e}_3 & \text{if } \frac{s_1}{s_1+s_2}\delta < x_3 \le \delta. \end{cases}$$

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

Molecular dynamics simulation of 5CB thin film.





A. Pizzirusso, R. Berardi, L. Muccioli, M. Riccia, and C. Zannoni, Chem. Sci., 3:573579, 2012.

There is an exchange of eigenvalues at $z \simeq 6.81$nm, with a jump in the director $\mathbf{n}$.

The graph of the largest eigenvalue $\lambda_{\max}(\mathbf{Q}(z))$ has the same qualitative form as that in Pizzirusoo et al but the values are less, because

$$\lambda_{\max}(\text{average of } \mathbf{Q}(z)) \leq \text{ average of } \lambda_{\max}(\mathbf{Q}(z)).$$

(b) Analysis using director model

Consider for simplicity the functional

$$I(\mathbf{n}) = \int_{\Omega_\delta} K|\nabla \mathbf{n}|^2 \, d\mathbf{x} + k \int_{S_{\mathbf{n}}} (1 - (\mathbf{n}_+ \cdot \mathbf{n}_-)^2)^{\frac{r}{2}} \, d\mathcal{H}^2,$$

where $K > 0$, $k > 0$ and $0 < r < 1$, with boundary conditions $\mathbf{n}(x_1, x_2, 0) = \mathbf{e}_1$, $\mathbf{n}(x_1, x_2, \delta) = \mathbf{e}_3$ and $l_1 = l_2 = 1$ (handled technically by extending $\mathbf{n}$ outside Ω_δ).

Theorem. For any $\delta > 0$ there exists at least one minimizer $\mathbf{n} \in \mathrm{SBV}(\Omega_\delta : S^2)$ of I subject to the boundary conditions.

A candidate for a minimizer of I is the bending solution for the Oseen-Frank theory

$$\bar{\mathbf{n}}(\mathbf{x}) = (\cos \frac{\pi x_3}{2\delta}, 0, \sin \frac{\pi x_3}{2\delta}),$$

with $I(\bar{\mathbf{n}}) = \frac{K\pi^2}{4\delta}$.

However, for δ sufficiently small $\bar{\mathbf{n}}$ is not a minimizer, and minimizers have the form

$$\mathbf{n}^*(\mathbf{x}) = \begin{cases} \mathbf{e}_3, & x_3 > \tau \\ \mathbf{e}_1, & x_3 < \tau \end{cases}$$

where $0 \leq \tau \leq \delta$.

Indeed $I(\mathbf{n}^*) = k$, so that $I(\mathbf{n}^*) < I(\bar{\mathbf{n}})$ provided $\delta < \frac{K\pi^2}{4k}$.

Other possible candidates for physical planar defects.

1. Nematic elastomers

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

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

where

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

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

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

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

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

$$I(\mathbf{y}) = \int_\Omega W(\nabla \mathbf{y})\, d\mathbf{x}, \qquad (1)$$

where

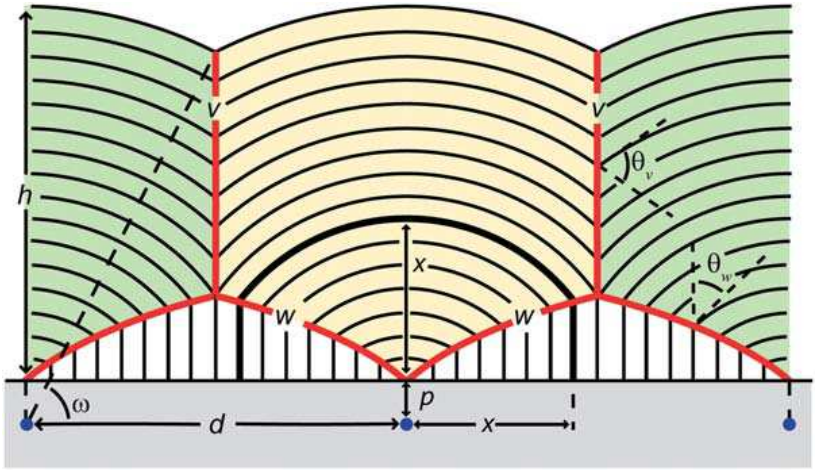
$$W(\mathbf{A}) = \frac{\mu}{2}\left(a^{-\frac{2}{3}} v_1^2(\mathbf{A}) + a^{\frac{1}{3}}(v_2^2(\mathbf{A}) + v_3^2(\mathbf{A}))\right),$$

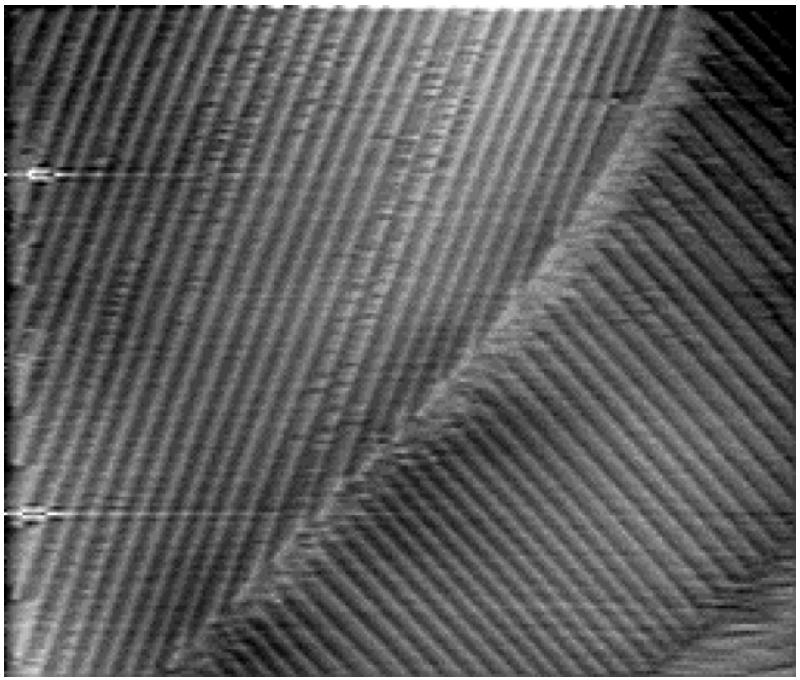
and $v_1(\mathbf{A}) \geq v_2(\mathbf{A}) \geq v_3(\mathbf{A}) > 0$ denote the singular values of $\mathbf{A}$, that is the eigenvalues of $\sqrt{\mathbf{A}^T\mathbf{A}}$.

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

2. Smectic thin films

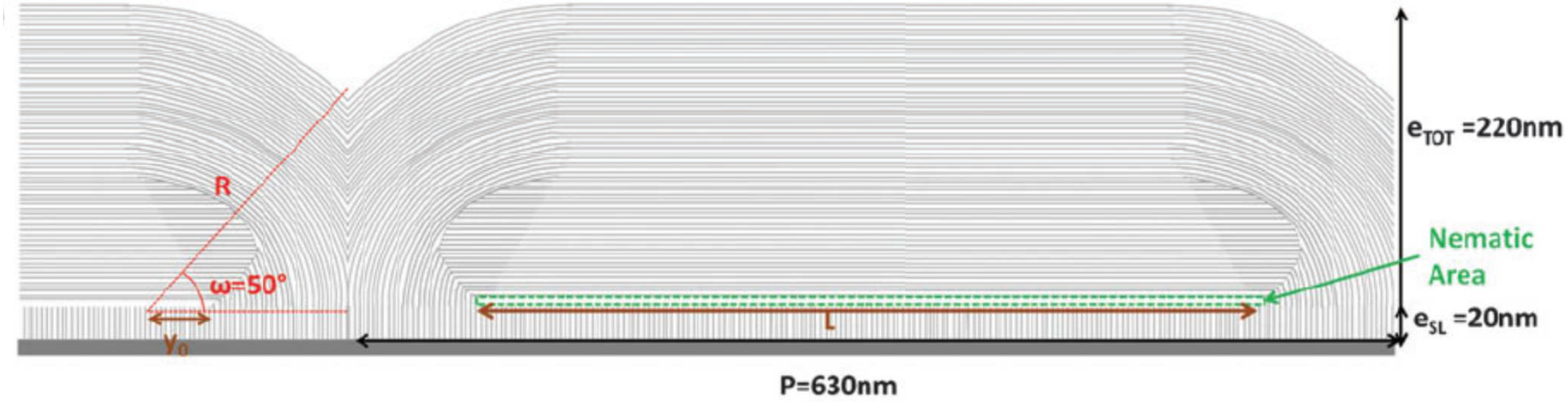
AFM image
Michel, Lacaze
et al, 2004



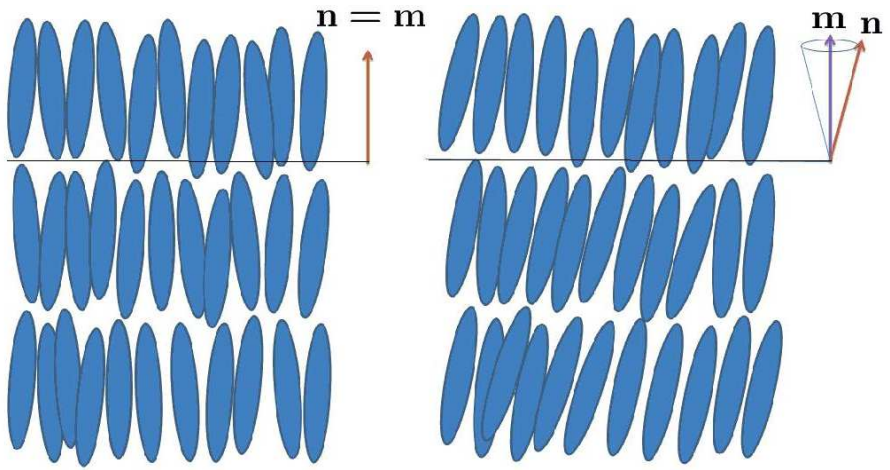


8CB smectic thin films
Zappone, Lacaze et al, 2010

Coursault, ... , Lacaze, Soft Matter (2016)



Models of smectics



1. Assuming constant layer thickness.

e.g. Leslie, Stewart, Nakagama (1993)

Minimize

$$I(\mathbf{n},\mathbf{m}) = \int_\Omega \psi(\mathbf{n},\mathbf{m},\nabla\mathbf{n},\nabla\mathbf{m})\,d\mathbf{x}$$

subject to $|\mathbf{n}| = |\mathbf{m}| = 1$, $\operatorname{curl}\mathbf{m} = \mathbf{0}$.

For smectic A set $\mathbf{m} = \mathbf{n}$.

2. Models allowing variable layer thickness, dislocations ...

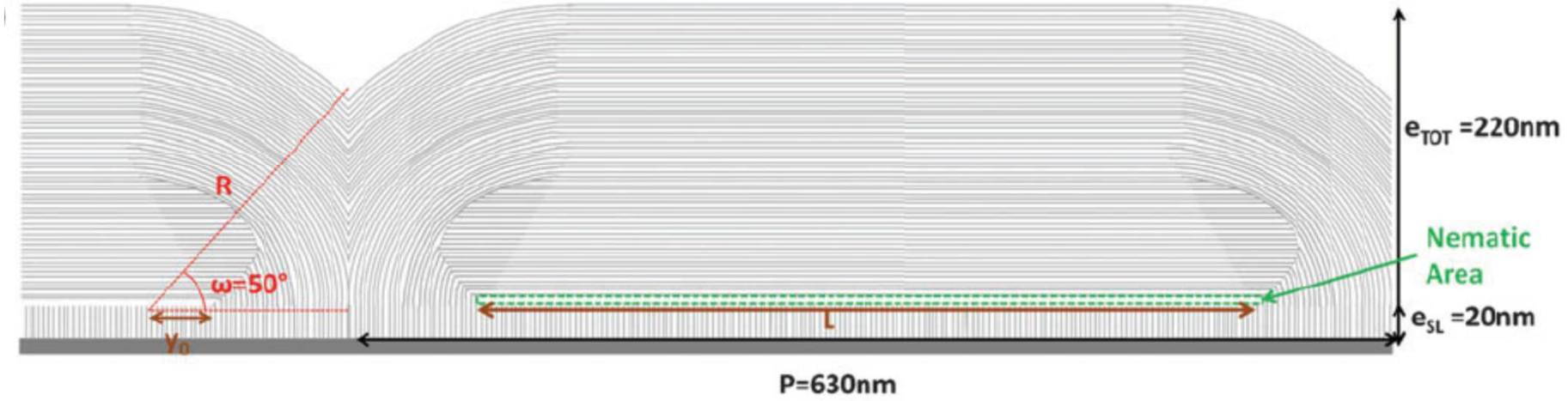
These models typically introduce the molecular number density $\rho(\mathbf{x})$ as a new macroscopic variable, with the smectic layers being seen as density waves.

C. Zhang, A. M. Grubb, A. J. Seed, P. Sampson, A. Jákli, O. D. Lavrentovich, 2015

de Gennes (1972), Chen & Lubensky (1976)
Han, Luo, Wang & Zhang (2014)
Pevnyi, Selinger & Sluckin (2014) ...

Question: how to understand the macroscopic variable $\rho(\mathbf{x})$ varying over a molecular length-scale.

Smectic A thin films (Canevari, Stroffolini, JB)



Minimize

$$I(\mathbf{n}) = \frac{1}{2}\int_\Omega |\nabla \mathbf{n}|^2\, d\mathbf{x} + \mathcal{H}^1(S_{\mathbf{n}})$$

where $\Omega = (0, L) \times (0, \delta) \subset \mathbb{R}^2$, in the class

$$\mathcal{A} = \{\mathbf{n} \in \mathrm{SBV}(\Omega, S^1) : \mathrm{curl}\, \mathbf{n} = 0 \text{ a.e.}\}.$$

Really this needs to be formulated as a free-boundary problem for a fixed volume of fluid, but as a beginning suppose we are on the fixed domain Ω with the same boundary conditions as for the order reconstruction problem, i.e.

$$\mathbf{n}(x_1, 0) = \mathbf{e}_1,\ \mathbf{n}(x_1, \delta) = \mathbf{e}_2,\ \mathbf{n} \text{ periodic in } x_1.$$

Theorem. For any $\tau \in (0, \delta)$ the map

$$\mathbf{n}^*(\mathbf{x}) = \begin{cases} \mathbf{e}_2, & x_2 > \tau \\ \mathbf{e}_1, & x_2 < \tau \end{cases}$$

is a minimizer for I subject to the boundary conditions.

The proof uses the auxiliary problem of minimizing

$$I_k(\mathbf{n}) = \frac{1}{2} \int_\Omega \left(|\nabla \mathbf{n}|^2 + k |\mathrm{curl}\, \mathbf{n}|^2 \right) d\mathbf{x} + \mathcal{H}^1(S_\mathbf{n})$$

in the limit $k \to \infty$.