IPAM workshop on Partial Order: Mathematics, Simulations and Applications, 29 January 2016

Planar discontinuities for liquid crystals

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EPSRC Pioneering research and skills

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Some questions

Should we allow continuum order parameters (directors, Q-tensors etc) describing liquid crystals to jump across surfaces?

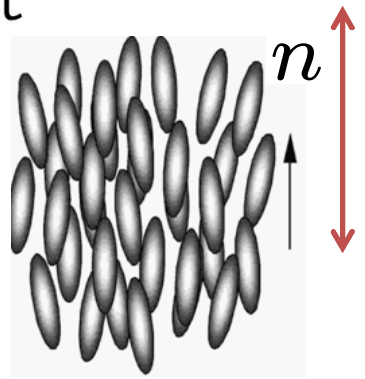
Is there a useful theory of nematic and cholesteric liquid crystals in which the order parameter is a unit vector field and for which observed defects have finite energy?

How do we choose an appropriate function space for mathematical models of continuum physics?

Classical models of nematics and cholesterics

Static models for liquid crystal at constant temperature filling bounded domain $\Omega \subset \mathbb{R}^3$ described in terms of corresponding free-energy functionals.

1. *Oseen-Frank theory*. Order parameter unit vector field $\mathbf{n}$.



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

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

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

2. *Ericksen theory*. Order parameter $(s, \mathbf{n})$, $|\mathbf{n}| = 1$,

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

3. *Landau - de Gennes theory*.

Matrix order parameter $\mathbf{Q}(\mathbf{x}) = (Q_{ij}(\mathbf{x}))$,

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

where $\rho(x, \cdot)$ is probability distribution of molecular orientations, so that

$$\rho(\mathbf{x}, p) \geq 0, \rho(\mathbf{x}, p) = \rho(\mathbf{x}, -p), \int_{S^2} \rho(\mathbf{x}, p)\, dp = 1.$$

Thus, for each $\mathbf{x}$, $\mathbf{Q}(\mathbf{x}) \in \mathcal{E}$, where
$\mathcal{E} = \{\mathbf{Q} : \mathbf{Q} = \mathbf{Q}^T, \operatorname{tr} \mathbf{Q} = 0, \lambda_{\min}(\mathbf{Q}) > -\frac{1}{3}\}$.

Free energy

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

where $\psi(\mathbf{Q}, \nabla\mathbf{Q}) = \psi_B(\mathbf{Q}) + \psi_E(\mathbf{Q}, \nabla\mathbf{Q})$,

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

or the singular potential of Katriel et al, JB/Majumdar which satisfies $\psi_B(\mathbf{Q}) \to \infty$ as $\lambda_{\min}(\mathbf{Q}) \to -\frac{1}{3}$, and, for example,

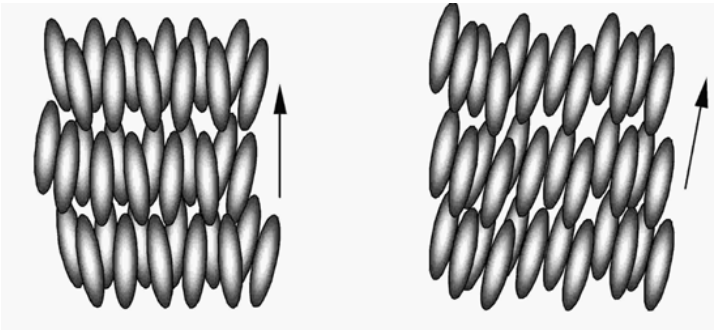
$$\psi_E(\mathbf{Q}, \nabla\mathbf{Q}) = \sum_{i=1}^{4\text{or}5} L_i I_i,$$

where

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

Uniaxial ansatz $\mathbf{Q}(\mathbf{x}) = \mathbf{s}\left(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{\mathbf{1}}{\mathbf{3}}\mathbf{1}\right)$ where $s > 0$ is constant, gives Oseen-Frank, and when $s = s(\mathbf{x})$ we get Ericksen theory.

Models of smectics



1. Assuming each layer has constant thickness

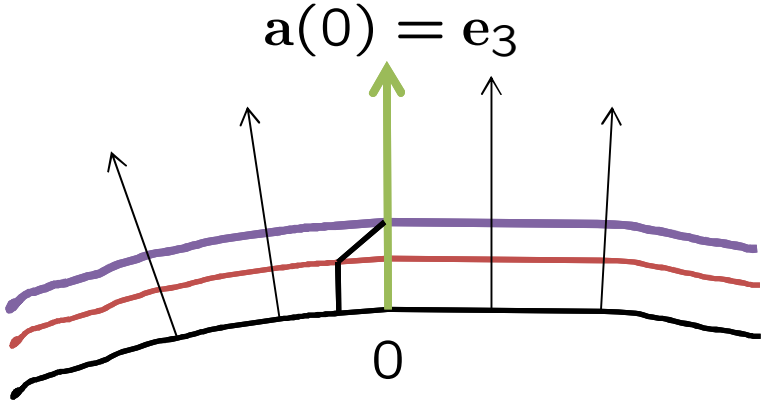
Let $\mathbf{a}(\mathbf{x})$ be the normal to the layer through $\mathbf{x}$.

Claim.

If $\mathbf{a}$ is sufficiently smooth then $\nabla \wedge \mathbf{a} = 0$.

Proof.

Assume that $\mathbf{x} = 0$ and $\mathbf{a}(0) = \mathbf{e}_3$, so that layer surface through $\mathbf{x}$ has equation $x_3 = f(x_1, x_2)$ with $\nabla f(0,0) = 0$. By the IFT the normals at points on surface simply cover a neighbourhood of 0.



For $\mathbf{x}$ on the surface $\mathbf{a}(\mathbf{x}) = \frac{(-f_{,1}, -f_{,2}, 1)}{\sqrt{1+|\nabla f|^2}}$,

so that $\frac{\partial a_1}{\partial x_2}(0) = \frac{\partial a_2}{\partial x_1}(0) = -f_{,12}(0,0)$,

$\frac{\partial a_3}{\partial x_1}(0) = \frac{\partial a_3}{\partial x_2}(0) = 0$, and so

$$(\nabla \wedge \mathbf{a})(0) = \left(-\frac{\partial a_2}{\partial x_3}(0), \frac{\partial a_1}{\partial x_3}(0), 0 \right),$$

which is zero because $\mathbf{a}(0, 0, x_3) = (0, 0, 1)$.

For smectic A could take $\mathbf{n} = \mathbf{a}$, so that setting $K_2 + K_4 = 0$ we have to minimize

$$I(\mathbf{n}) = K_1 \int_\Omega (\operatorname{div} \mathbf{n})^2 d\mathbf{x}$$

subject to $\nabla \wedge \mathbf{n} = 0$, $|\mathbf{n}| = 1$ (Oseen 1933, Orsay group 1971).

If Ω is simply-connected, $\mathbf{n} = \nabla\varphi$ and we have to minimize $I(\mathbf{n}) = K_1 \int_\Omega (\Delta\varphi)^2 d\mathbf{x}$ subject to the eikonal equation $|\nabla\varphi| = 1$. For example, if $\mathbf{n}$ minimizes $\int_\Omega |\nabla \mathbf{n}|^2 d\mathbf{x}$ and $\mathbf{n} = \nabla\varphi$ then φ is a minimizer (e.g. $\mathbf{n}(\mathbf{x}) = \frac{\mathbf{x}}{|\mathbf{x}|}$).

Compare the Aviles Giga functional (1987)

$$I(\varphi) = \int_{\Omega} [\varepsilon(\Delta\varphi)^2 + (|\nabla\varphi|^2 - 1)^2 d\mathbf{x}$$

For the derivation ...

''Simple examples and physical considerations (Ericksen [17] and Sethna [18]) suggest that the solution of the following relaxition problem explain with acquiricy the phenomena.''

and

[17] Ericksen, J.: private communication.
[1 8] Sethna, J.: private communication.

A more general model would be to minimize an energy of the form

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

For smectic C such a model was proposed by Stewart, Leslie, Nakagawa 1993, who imposed the constraint $\mathbf{a} \cdot \mathbf{n} = \cos\theta$, θ constant, but one could relax this and have a term such as $K((\mathbf{a}.\mathbf{n})^2 - \cos^2\theta)^2$ in the energy, and impose boundary conditions just on $\mathbf{n}$.

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

These models typically introduce the molecular number density $m(\mathbf{x})$ 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

In the de Gennes approach, and that of Chen/Lubensky it is assumed that

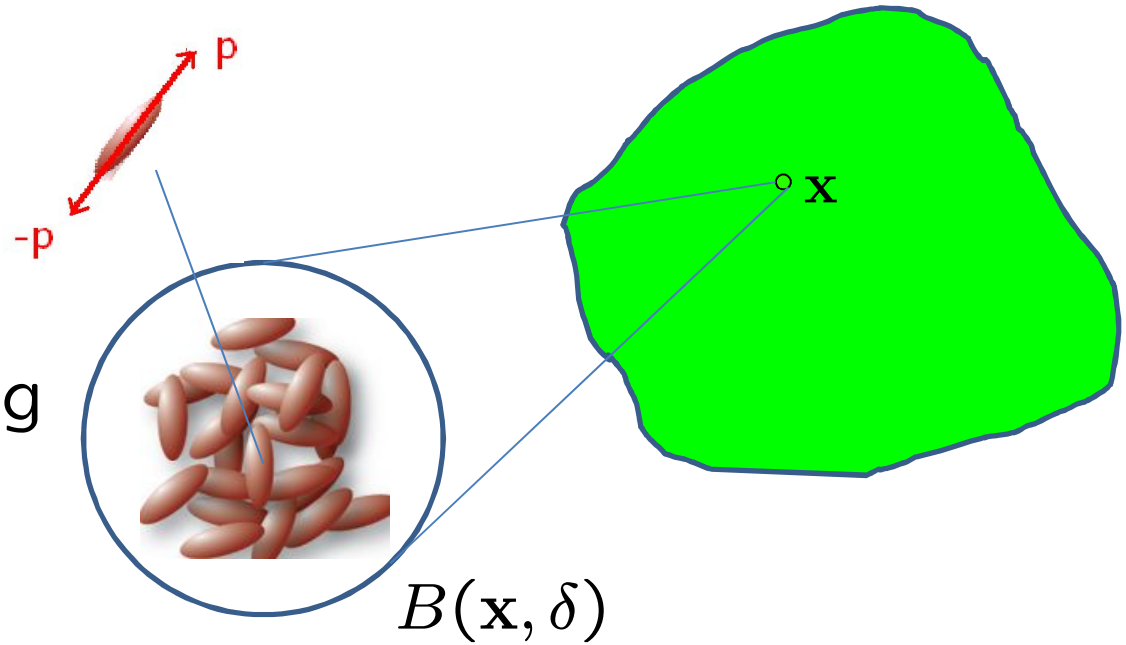
$$m(\mathbf{x}) = \rho_0 + \rho(\mathbf{x}) = \rho_0 + r(\mathbf{x}) \cos \phi(\mathbf{x}),$$

where $\rho_0 > 0$ is a constant average density and $\Psi(\mathbf{x}) = r(\mathbf{x}) e^{i\phi(\mathbf{x})}$ is used as a complex order parameter. Thus $\rho(\mathbf{x})$ describes the fluctuations in the density due to the smectic layers, and $\nabla\phi$ gives the normals to the layers.

But how are we to define $m(\mathbf{x})$ as a macroscopic variable, if it is to vary over distances of the order of a molecular length?

This is related to the interpretation of the probablity distribution of molecular orientations, and how this can be thought of as a macroscopic variable.

First, fix a time t,
a point $\mathbf{x} \in \Omega$,
and a coarse-graining radius $\delta > 0$.



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

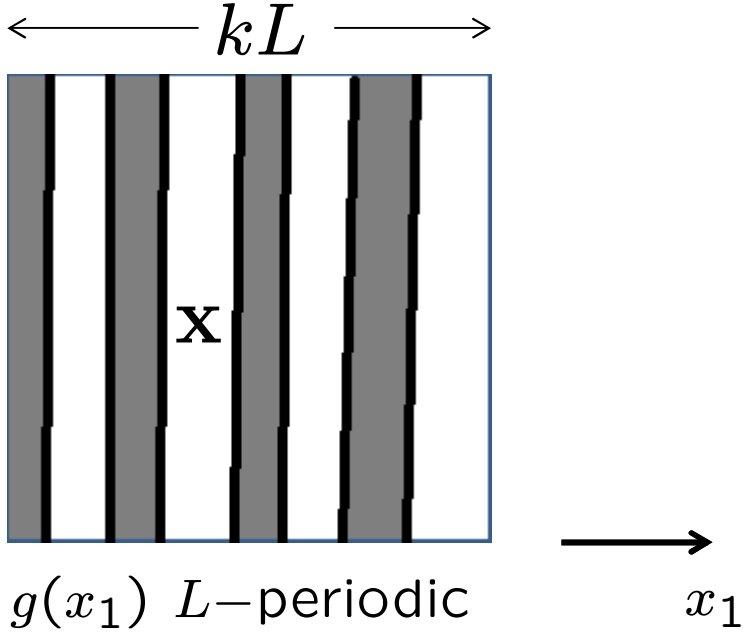
Take the molecule to be a circular cylinder of length d and radius a, and assume the molecules to fill a fraction θ of $B(\mathbf{x}, \delta)$. Then the number of molecules in $B(\mathbf{x}, \delta)$ is $\theta \frac{4}{3} \pi \delta^3 / \pi a^2 d$.

Setting $\theta = \frac{1}{2}$, $a = d/4$, $d = 3$nm, this number is 1 billion for $\delta \sim 10^{-6}$m $= \frac{1}{1000}$mm, and 100 for $\delta \sim 10$nm.

But if we average also over a macroscopically small time interval we could reduce δ, perhaps to $\sim$ 1nm. (Issues: molecules overlapping $\partial B(\mathbf{x}, \delta)$, temperature, dynamics v. equilibrium, ergodicity ...)

Remark concerning spatial averaging for smectics.

If we average over cube with centre $\mathbf{x}$ and side-length kL then the average is *constant.*



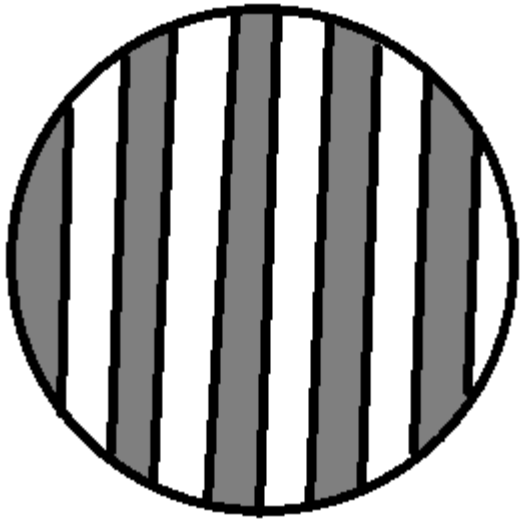
(Corrected slide added after lecture.)

The same can happen if we average over a ball. Indeed

$$\frac{1}{\operatorname{vol} B(\mathbf{x},\delta)} \int_{B(\mathbf{x},\delta)} \sin(kz_1)\, dz$$

$$= 3 \sin(kx_1) \left(\frac{\sin k\delta - k\delta \cos k\delta}{(k\delta)^3} \right),$$

which is zero for all $\mathbf{x}$ if $k\delta$ is a root of the equation $\sin\lambda = \lambda\cos\lambda$.



This is related to the Pompeiu problem.

An example of a free-energy functional defined in terms of $\mathbf{n}, \varphi$ is that proposed by Kleman & Parodi is given by

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

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

E (1994) (and later Santangelo & Kamien 2005) argued that a good approximation is given by

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

together with the constraint $\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}$ that rigidly enforces that the director points parallel to the normal.

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

Models using the density ρ rather than φ.

(a) Han, Luo, Wang, Zhang model (2013).

$$
\begin{aligned}
&F[c(\mathbf{x}), Q_2(\mathbf{x})] \\
&= \int_\Omega c(\ln c + B_Q : Q_2 - \ln Z)\mathrm{d}\mathbf{x} + \frac{\alpha}{2}\int_\Omega \{E_{11}c^2 + E_{12}|cQ_2|^2 + E_{13}|cQ_4|^2 \\
&+ E_{21}|\nabla c|^2 + E_{22}|\nabla(cQ_2)|^2 + E_{23}|\nabla(cQ_4)|^2 + E_{24}\,\partial_i(cQ_{2ij})\partial_j(c) \\
&+ E_{25}\,\partial_i(cQ_{ik})\partial_j(cQ_{jk}) + E_{26}\,\partial_i(cQ_{4ijkl})\partial_j(cQ_{2kl}) + E_{27}\,\partial_i(cQ_{4iklm})\partial_j(cQ_{4jklm}) \\
&+ E_{31}|\nabla^2 c|^2 + E_{32}\,\partial_{ij}(cQ_{2pq})\partial_{ij}(cQ_{2pq}) + E_{33}\,\partial_{ij}(cQ_{2ij})\partial_{kl}(cQ_{2kl}) \\
&+ E_{34}\,\partial_{ik}(cQ_{2ip})\partial_{jk}(cQ_{2jp}) + E_{35}\,\partial_{ij}(cQ_{2ij})\partial_{kk}(c) + E_{36}\,\partial_{ij}(cQ_{4ijkl})\partial_{kl}(c) \\
&+ E_{37}\,\partial_{ij}(cQ_{4ijpq})\partial_{kk}(cQ_{2pq}) + E_{38}\,\partial_{ij}(cQ_{4ijkp})\partial_{kl}(cQ_{2lp}) \\
&+ E_{39}\,\partial_{ij}(cQ_{4ijpq})\partial_{kl}(cQ_{4klpq})\}\mathrm{d}\mathbf{x}.
\end{aligned}
$$

(b) Pevnyi, Selinger, Sluckin model

$$I(\rho, \mathbf{n}) = \int_\Omega [K_1|\nabla \mathbf{n}|^2 + B|D^2\rho + q^2\mathbf{n}\otimes\mathbf{n}|^2 + f(\rho]\, dx.$$

Lessons from solid mechanics

Nonlinear elasticity has a similar variational structure to continuum models of liquid crystals, with a free-energy functional of the form

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

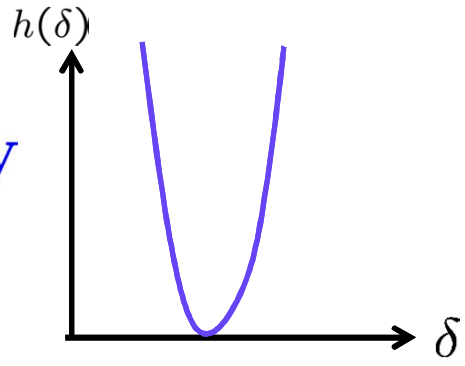
where $\mathbf{y}(\mathbf{x}) \in \mathbb{R}^3$ is the deformed position of a material point having position $\mathbf{x}$ in a reference configuration $\Omega \subset \mathbb{R}^3$.

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

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

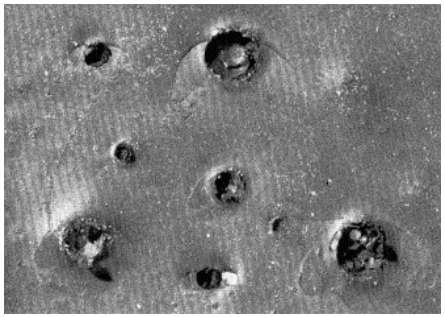
$$I(\mathbf{y}) = \int_{\mathbf{B(0,1)}} [|\nabla \mathbf{y}|^{\mathbf{2}} + \mathbf{h}(\det \nabla \mathbf{y})]\, \mathbf{dx} + \kappa \text{ area } S_{\mathbf{y}}$$

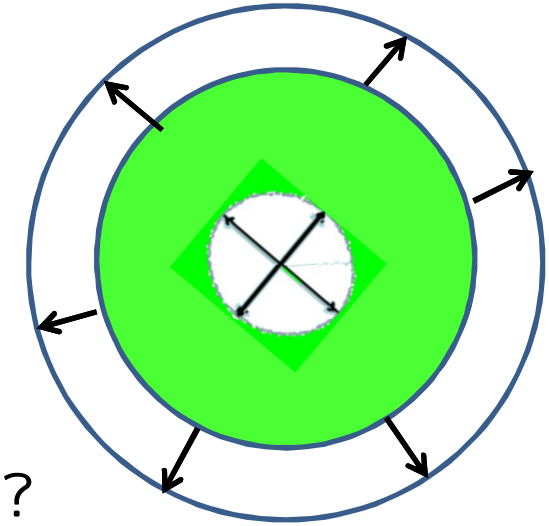
among smooth $\mathbf{y}$ subject to $\mathbf{y}(\mathbf{x}) = \lambda \mathbf{x}$ for $|\mathbf{x}| = \mathbf{1}$ is $\mathbf{y}^*(\mathbf{x}) = \lambda \mathbf{x}$.



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

(Lavrentiev phenomenon)



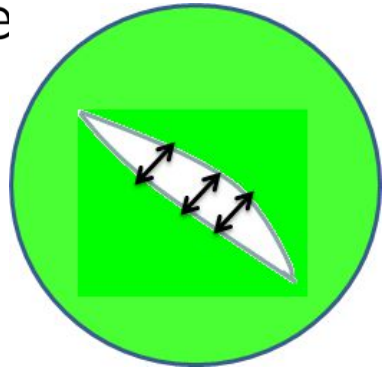


But is $W^{1,2}$ the largest such function space?

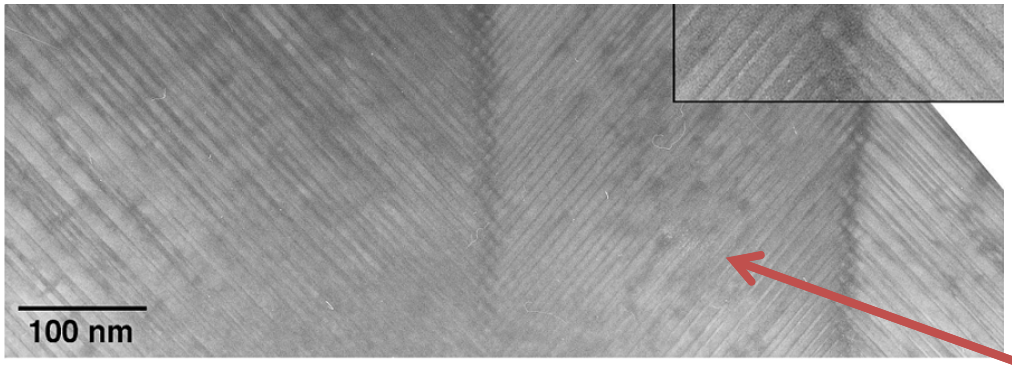
No, because the body could develop fracture surfaces across which $\mathbf{y}$ is discontinuous.

Francfort-Marigo theory of fracture.

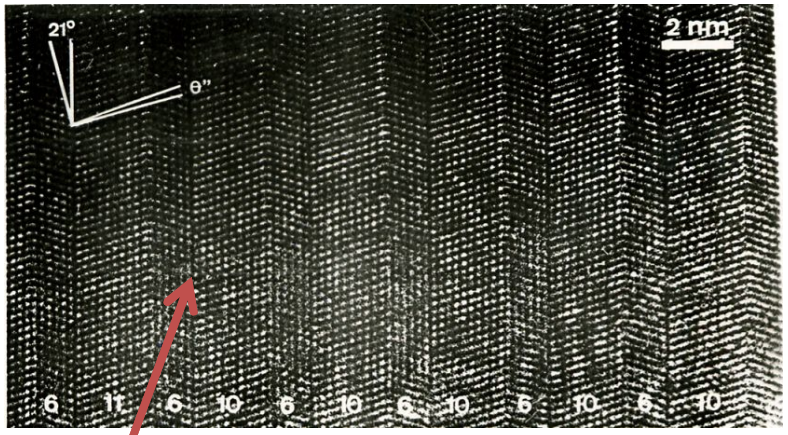
$\mathbf{y} \in \mathbf{SBV}$ (special functions of bounded variation), jump set $S_{\mathbf{y}}$



There can also be planar discontinuities in $\nabla \mathbf{y}$ representing phase boundaries.

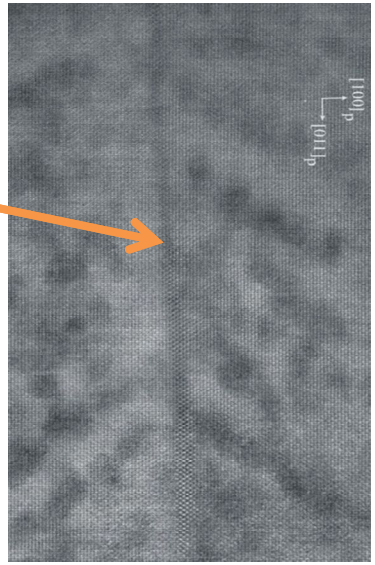


Macrotwins in $Ni_{65}Al_{35}$ single crystal (D. Schryvers)



NiMn, Baele, van Tenderloo, Amelinckx

Sharp, and diffuse interfaces



Perovskite. Salje.

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

$$I(\mathbf{y}) = \int_{\Omega} [\psi(\nabla \mathbf{y}) + \varepsilon |\nabla \nabla \mathbf{y}|^{\mathbf{2}}] \, \mathbf{dx} + \kappa \, \text{area} \, \mathbf{S}_{\nabla \mathbf{y}}.$$

(Ball & Mora-Corral 2009)

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

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

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

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

Description of defects

We first consider the Oseen-Frank model for nematics with $t = 0$:

$$W(\mathbf{n}, \nabla\mathbf{n}) = K_1(\operatorname{div}\mathbf{n})^2 + K_2(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + \mathrm{K}_3(\mathbf{n}\times\operatorname{curl}\mathbf{n})^2 + (K_2 + K_4)(\operatorname{tr}(\nabla\mathbf{n})^2 - (\operatorname{div}\mathbf{n})^2).$$

Then $W(\mathbf{n}, \nabla\mathbf{n}) \leq C|\nabla\mathbf{n}|^2$ for some $C > 0$ whenever $|\mathbf{n}| = 1$, and under the Ericksen inequalities

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

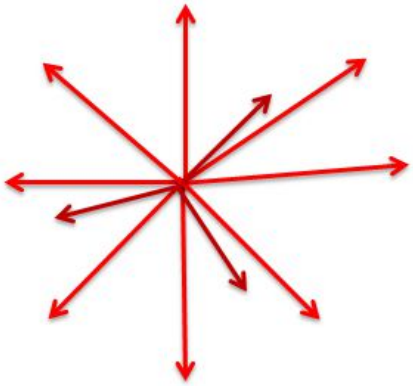
we also have that $C'|\nabla\mathbf{n}|^2 \leq W(\mathbf{n}, \nabla\mathbf{n})$ for some constant $C' > 0$. Hence a natural function space to use is $W^{1,2}(\Omega; S^2)$.

The Euler-Lagrange equation for

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

has solutions representing point defects, e.g.

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



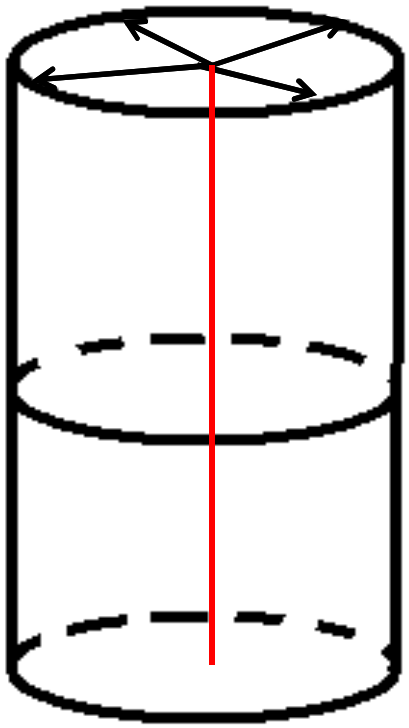
and if $K_1 = K_2 = K_3 = K,\ K_4 = 0$ then $\tilde{\mathbf{n}}$ is the unique minimizer of $I_{OF} = K \int_\Omega |\nabla \mathbf{n}|^2 d\mathbf{x}$ subject to its own boundary conditions (Brezis, Coron, Lieb 1986).

In this case any minimizer is smooth except for a finite number of point defects (Schoen & Uhlenbeck 1982) at points $\mathbf{x}(i)$ such that

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

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

Disclinations



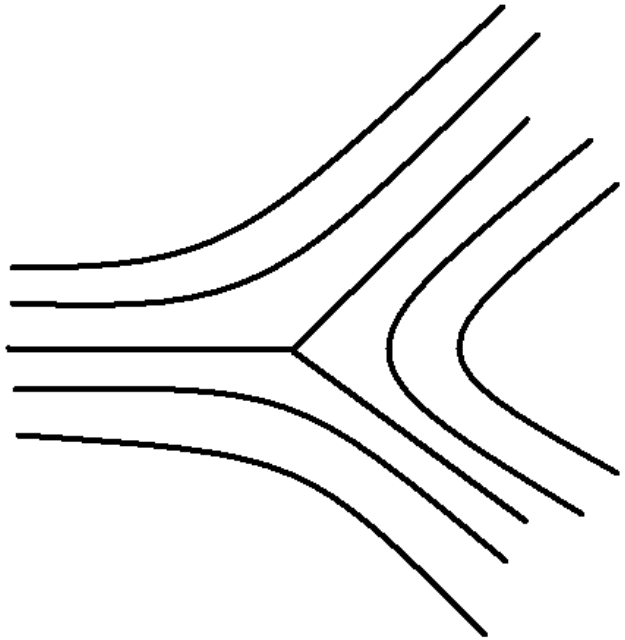
$$\hat{\mathbf{n}}(\mathbf{x}) = (\tfrac{x_1}{r}, \tfrac{x_2}{r}, 0) \quad r = \sqrt{x_1^2 + x_2^2}$$

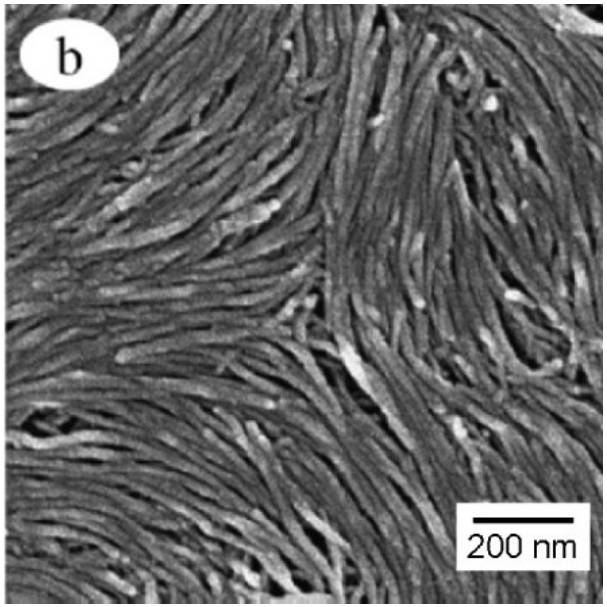
$$|\nabla \hat{\mathbf{n}}(\mathbf{x})|^2 = \tfrac{1}{r^2}$$

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

$$I_{OF}(\hat{\mathbf{n}}) = \infty$$

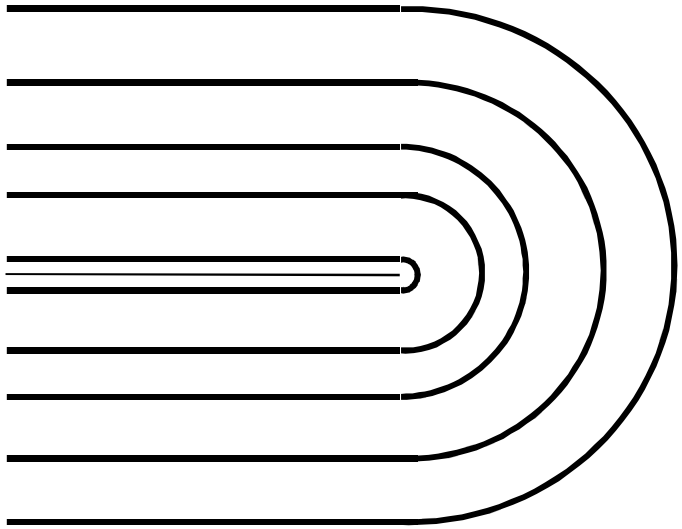
Index $\frac{1}{2}$ singularities.





Zhang/Kumar 2007
Carbon nano-tubes
as liquid crystals

$\mathbf{n} \notin W^{1,2}$ and
$I_{OF}(\mathbf{n}) = \infty$



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 disclinations 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

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

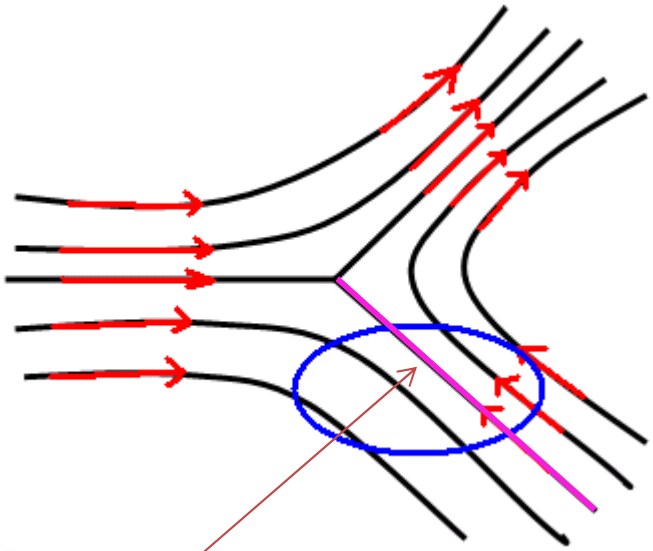
we obtain that $I_\alpha(\hat{\mathbf{n}}) < \infty$ as desired. Also $W_\alpha(\mathbf{n}, \cdot)$ is convex.

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.

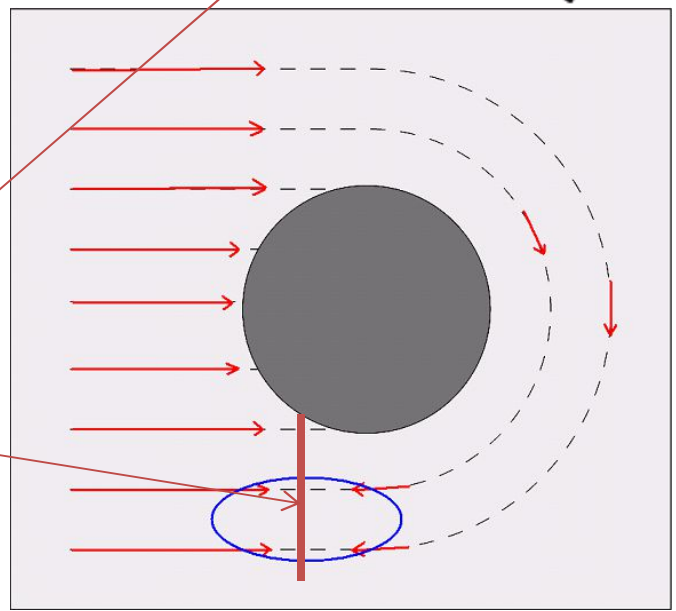
But the index $\frac{1}{2}$ singularities cannot be modelled this way because they are not *orientable*; i.e. they can be described by a line field $\mathbf{n} \otimes \mathbf{n} \in W^{1,p}$ but not by a vector field $\mathbf{n} \in W^{1,p}$.



The same issue arises for smooth line fields in non simply-connected regions.

Ball & Zarnescu 2011 show that any $W^{1,2}$ line field in a simply-connected region is orientable.

This can be handled by allowing $\mathbf{n}$ to jump to $-\mathbf{n}$ across suitable surfaces.



Theorem (Bedford). Assume Ω has Lipschitz boundary and let $\mathbf{n}\otimes\mathbf{n} \in W^{1,2}(\Omega; M^{3\times 3})$, where $\mathbf{n}(\mathbf{x}) \in S^2$ for a.e. $\mathbf{x} \in \Omega$. Then there exists a vector field $\mathbf{m} \in SBV(\Omega; S^2)$ 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.

Bedford also has similar results for the Ericksen model.

Landau - de Gennes theory: Minimizers $\mathbf{Q}$ of the free-energy functional are expected to be smooth (Gartland & Davis 1998) because the Euler-Lagrange equation is elliptic (though there is an issue if the singular potential with $\psi_B(\mathbf{Q}) \to \infty$ as $\lambda_{\mathsf{min}}(\mathbf{Q}) \to -\frac{1}{3}+$ is used, because it is not then clear in general if the Euler-Lagrange equation is satisfied).

Therefore defects are not described by singularities of $\mathbf{Q}$, but rather by regions where $|\nabla \mathbf{Q}|$ is very high, in which a continuous choice of eigenvectors for $\nabla \mathbf{Q}$ may not possible.

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

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

Planar defects

Let us explore whether it might be reasonable to consider a free-energy functional for nematic and cholesteric 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 $\mathbf{n} \in SBV(\Omega; S^2)$, where $\boldsymbol{\nu}$ is the normal to the jump set $S_\mathbf{n}$. Here $W(\mathbf{n}, \nabla \mathbf{n})$ is assumed to have the Oseen-Frank form or be modified so as to have subquadratic growth as suggested previously.

Admissible interfacial energies

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

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

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 nematic and cholesteric molecules, so that

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

Theorem. For these conditions to be satisfied it is necessary and sufficient 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

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

An equivalent representation is in terms of the matrices $\mathbf{M}_+ = \mathbf{n}_+ \otimes \mathbf{n}_+, \mathbf{M}_- = \mathbf{n}_- \otimes \mathbf{n}_-$, $\mathbf{N} = \boldsymbol{\nu} \otimes \boldsymbol{\nu}$, namely

$$f(\mathbf{n}_+, \mathbf{n}_-, \boldsymbol{\nu}) = g(\mathbf{M}_+ \cdot \mathbf{M}_-, \mathbf{M}_+ \cdot \mathbf{N}, \mathbf{M}_- \cdot \mathbf{N}, \mathrm{tr}\,(\mathbf{M}_+ \mathbf{M}_- \mathbf{N})).$$

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

Possible candidates for planar defects.

1. Nematic elastomers

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

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

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.

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

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

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

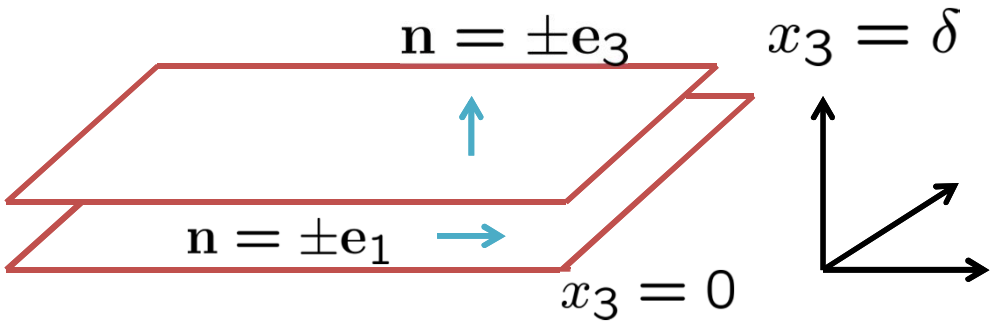
$$W(\mathbf{A}) = \frac{\mu}{2}\left(a^{-\frac{2}{3}} v_1^2(\mathbf{A}) + a^{\frac{1}{3}}(v_2^2(\mathbf{A}) + v_3^2(\mathbf{A}))\right),$$

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 $\mathbf{n} \in SBV$ may be a useful approximation.

Order reconstruction

$\Omega_\delta = (0, l_1) \times (0, l_2) \times (0, \delta)$



Barbero & Barberi (1983)

Palffy-Muhoray, Gartland & Kelly (1994), Ambrosio & Virga (1991)

(a) Analysis using Landau - de Gennes

Boundary conditions:

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

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

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

and $\mathbf{Q}$ periodic in x_1, x_2.

Assume that $L_4 = 0$ with the Longa inequalities

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

which imply that

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

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

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

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 $\delta \to 0$

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

where

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

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

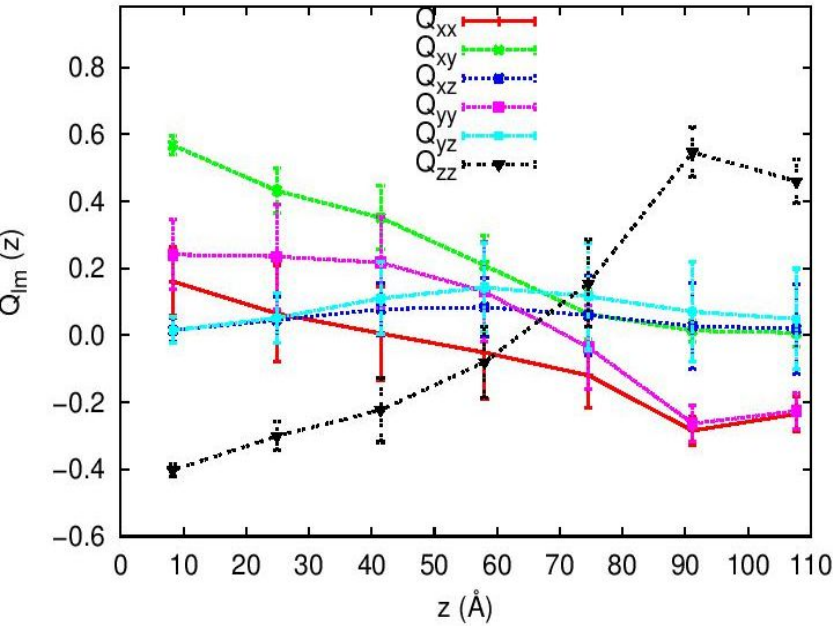
So for sufficiently small δ, $\mathbf{Q}$ is given approximately by

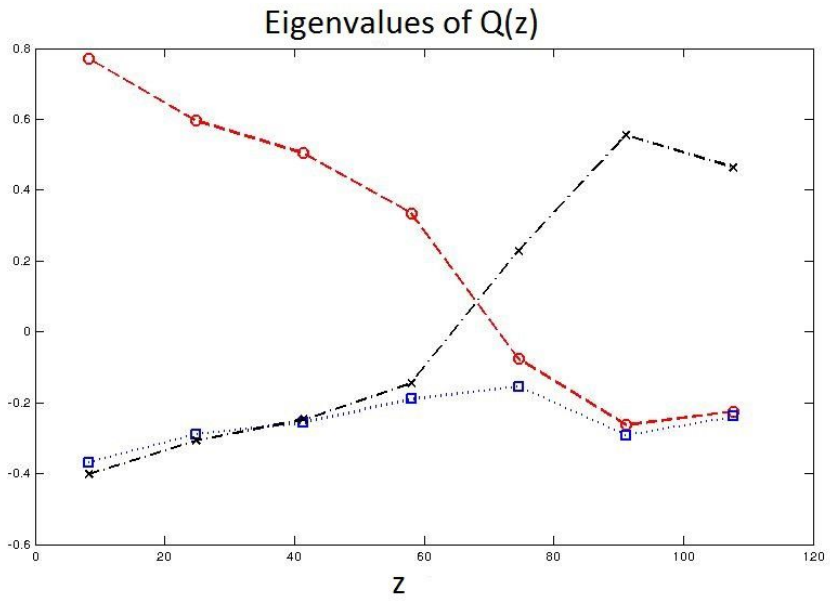
$$\mathbf{Q}(\mathbf{x}) = (1-\delta^{-1}x_3)\mathbf{Q}^{(0)} + \delta^{-1}x_3\mathbf{Q}^{(1)},$$

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

$$\mathbf{n}(\mathbf{x}) = \begin{cases} \mathbf{e}_1 & \text{if } 0 \le x_3 \le \frac{s_1}{s_1+s_2}\delta \\ \mathbf{e}_3 & \text{if } \frac{s_1}{s_1+s_2}\delta \le x_3 \le 1. \end{cases}$$

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





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

(b) Analysis using director model

Consider for simplicity the functional

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

where $k' > 0$ and $0 < r < 1$, with boundary conditions $\mathbf{n}(x_1, x_2, 0) = \pm \mathbf{e}_1$, $\mathbf{n}(x_1, x_2, \delta) = \pm \mathbf{e}_3$.

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

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

by making the uniaxial ansatz

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

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

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

$$\mathbf{Q}(x_1, x_2, x_3) = s\left(\mathbf{e}_1 \otimes \mathbf{e}_1 - \frac{1}{3}\mathbf{1}\right) \text{ for } -1 < x_3 < 0,$$

$$\mathbf{Q}(x_1, x_2, x_3) = s\left(\mathbf{e}_3 \otimes \mathbf{e}_3 - \frac{1}{3}\mathbf{1}\right) \text{ for } \delta < x_3 < \delta+1,$$

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

Candidates for minimizers of I are the two smooth $\mathbf{Q}$ given by

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

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

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

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

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

$$\hat{\mathbf{Q}}(\mathbf{x}) = \begin{cases} s\left(\mathbf{e}_1 \otimes \mathbf{e}_1 - \frac{1}{3}\mathbf{1}\right) & \text{if } 0 < x_3 < \frac{\delta}{2} \\ s\left(\mathbf{e}_3 \otimes \mathbf{e}_3 - \frac{1}{3}\mathbf{1}\right) & \text{if } \frac{\delta}{2} < x_3 < \delta \end{cases}$$

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

Related problems for cholesterics

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

$$I(\mathbf{n}) = \int_\Omega [|\nabla \mathbf{n}|^2 + 2t\mathbf{n} \cdot \nabla \wedge \mathbf{n} + t^2|\mathbf{n}|^2]\, d\mathbf{x}$$

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

$\mathbf{n}(x_1, x_2, 0) = \mathbf{e}_1$, $\mathbf{n}(x_1, x_2, \delta) = \mathbf{e}_3$, $\mathbf{n}$ periodic in x_1, x_2.

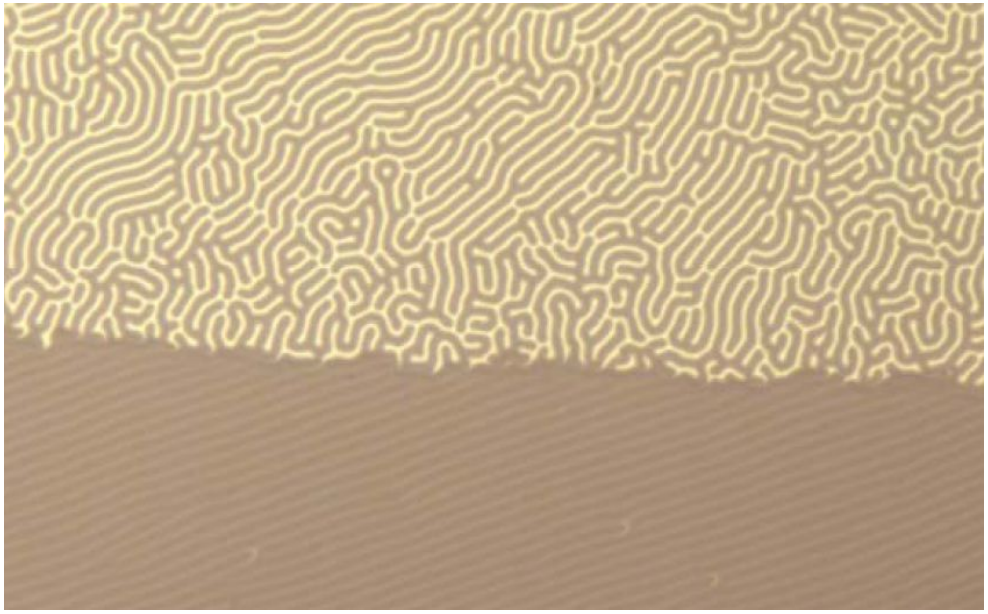
He proves that there is an explicit unique global minimizer $\mathbf{n}^* = \mathbf{n}^*(x_3)$ among $\mathbf{n}$ depending only on x_3, and there exists $\tau > 0$ such that $\mathbf{n}^*$ is the unique global minimizer in $W^{1,2}$ among all admissible $\mathbf{n}$ for $t \in [0, \tau]$.

Similarly, for the boundary conditions

$\mathbf{n}(x_1, x_2, 0) = \mathbf{e}_3, \mathbf{n}(x_1, x_2, \delta) = \mathbf{e}_3, \mathbf{n}$ periodic in x_1, x_2,

Bedford proves that $\mathbf{n} = \mathbf{e}_3$ is for some $\tau > 0$ the unique minimizer in $W^{1,2}$ for $t \in [0, \tau]$, a strong local minimizer if $t \in [0, \pi)$ and not a weak local minimizer if $t > \pi$.

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



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

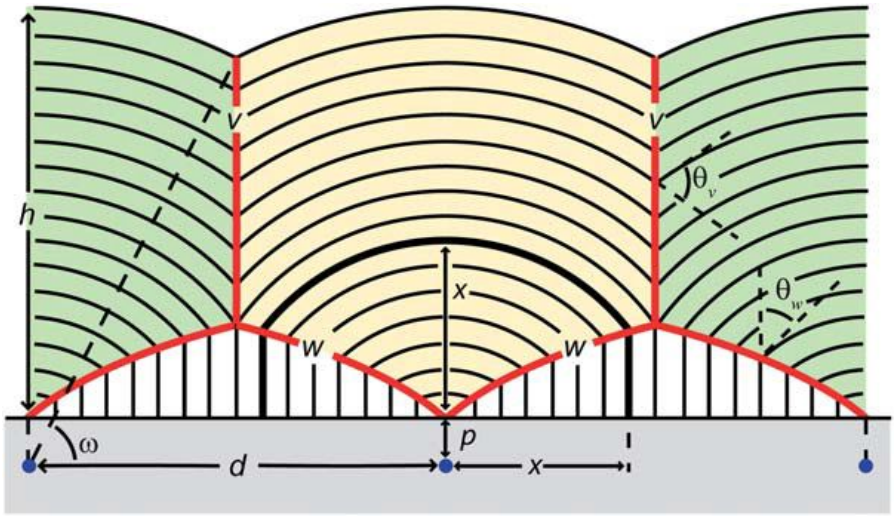
$$I(\mathbf{n}) = \int_\Omega [|\nabla \mathbf{n}|^2 + 2t\mathbf{n}\cdot\nabla\wedge\mathbf{n} + t^2|\mathbf{n}|^2]\, d\mathbf{x} + K\mathcal{H}^2(S_{\mathbf{n}})$$

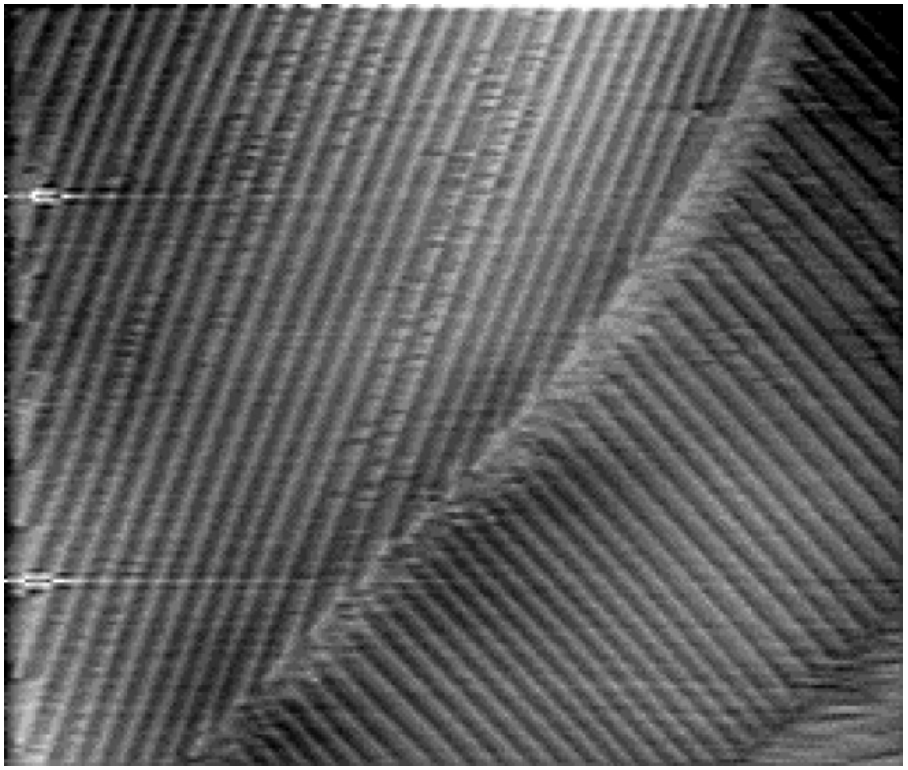
over $\mathbf{n} \in SBV(\Omega; \{0\} \cup S^2)$ satisfying $\mathbf{n}(x_1, x_2, 0) = \mathbf{e}_1, \mathbf{n}(x_1, x_2, \delta) = \mathbf{e}_3$ and $\mathbf{n}$ periodic in x_1, x_2.

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

3. Smectic thin films

AFM image
Michel, Lacaze
et al, 2004





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

Modified Pevnyi, Selinger & Sluckin model (2014)

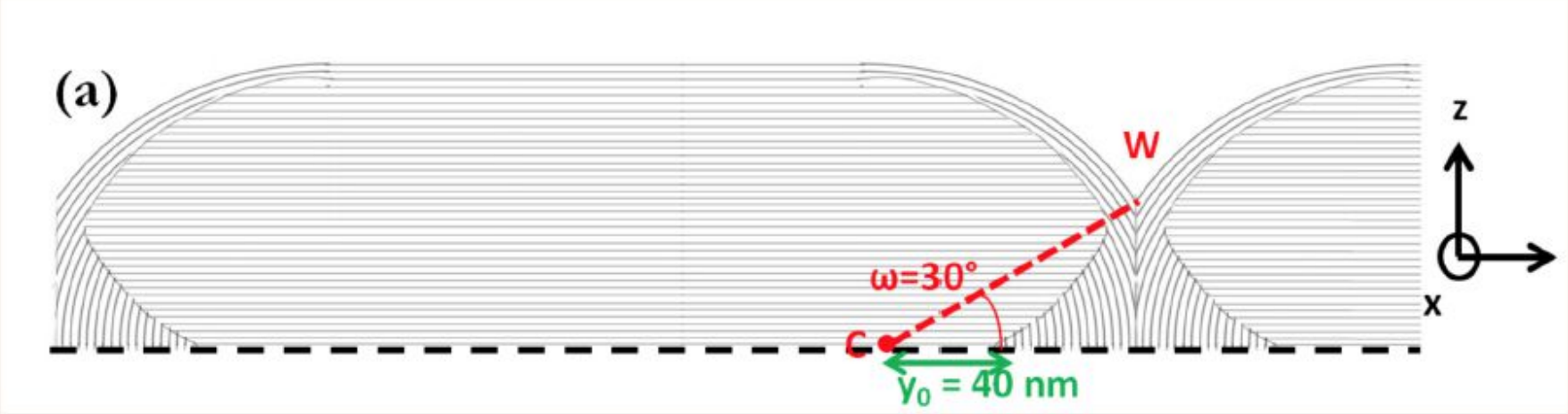
$$I(\mathbf{Q},\rho)=\int_\Omega\left(\psi_E(\mathbf{Q},\nabla\mathbf{Q})+B\left|D^2\rho+\frac{q^2}{3s}\left(3\mathbf{Q}+s\mathbf{1}\right)\rho\right|^2+f(\rho)\right)d\mathbf{x}$$
$$+k\int_{S_\mathbf{Q}}\left|\mathbf{Q}_+-\mathbf{Q}_-\right|^r d\mathcal{H}^2$$

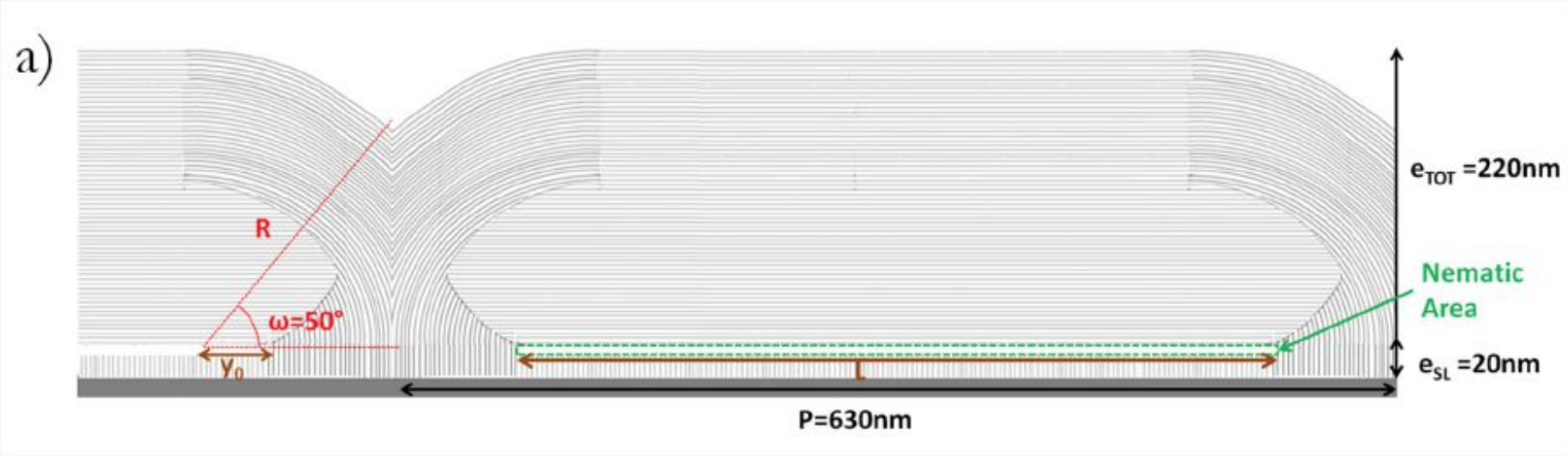
$$\mathbf{Q}(\mathbf{x})=s\left(\mathbf{n}(\mathbf{x})\otimes\mathbf{n}(\mathbf{x})-\tfrac{1}{3}\mathbf{1}\right)$$

probably need dependence on ν

Then under suitable hypotheses on ψ_E and f one can prove the existence of a minimizing pair $\mathbf{Q},\rho$ in

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





Coursault, ... , Lacaze (2015)

Ongoing computations of A. León Baldelli.