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Function spaces and liquid crystals

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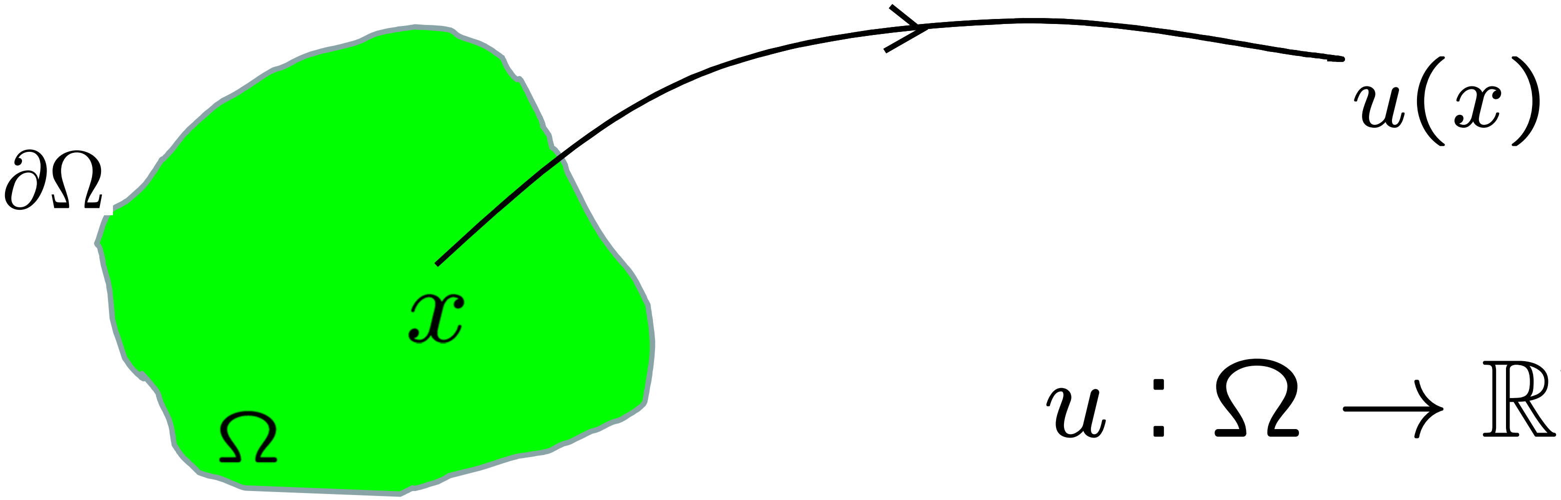
Function spaces



$$u : \Omega \to \mathbb{R}^m$$

$\Omega \subset \mathbb{R}^n$ bounded open set with boundary $\partial\Omega$.

Spaces of smooth maps

$C^r(\Omega : \mathbb{R}^m) = \{r$ times continuously differentiable maps $u : \Omega \to \mathbb{R}^m\}$

L^p spaces

$$L^p(\Omega; \mathbb{R}^m) = \{u : \Omega \to \mathbb{R}^m : \|u\|_p < \infty\}$$

$$\|u\|_p = \begin{cases} \left(\int_\Omega |u|^p \, dx\right)^{\frac{1}{p}} & \text{if } 1 \leq p < \infty \\ \text{ess sup}_{x\in\Omega} |u(x)| & \text{if } p = \infty \end{cases}$$

Sobolev spaces

$$W^{1,p}(\Omega;\mathbb{R}^m) = \{u \in L^p(\Omega;\mathbb{R}^m) : \nabla u \in L^p(\Omega;\mathbb{R}^m)\}$$

$$\nabla u(x) = \left(\frac{\partial u_i}{\partial x_\alpha}(x)\right) \in M^{m\times n}$$

weak or distributional derivative.

$$\int_\Omega \frac{\partial u_i}{\partial x_\alpha}\varphi\, dx = -\int_\Omega u_i \frac{\partial \varphi}{\partial x_\alpha}\, dx$$

for all $\varphi \in C_0^\infty(\Omega)$.

We will discuss what are appropriate function spaces in the context of variational models of nematic liquid crystals, specifically the Oseen-Frank and Landau - de Gennes models and modifications of these. Similar considerations apply to dynamic models.

The Oseen-Frank theory

Minimize

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

subject to $|n| = 1$ and suitable boundary conditions.

Landau – de Gennes theory

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

$$\rho(x,p) = \rho(x,-p) \geq 0,$$

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

$$Q(x) = Q^T(x), \mathrm{tr}\, Q(x) = 0$$

$$\lambda_{\mathrm{min}}(Q(x)) \geq -\tfrac{1}{3}$$

Minimize

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

subject to suitable boundary conditions.

For the bulk energy we can take, for example,

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

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

For the elastic energy we can take, for example,

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

where

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

where the coefficients L_i can depend on temperature.

From Landau – de Gennes to Oseen-Frank

Impose the constraint that Q be uniaxial with a constant scalar order parameter $s > 0$, so that

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

Putting this ansatz into the bulk energy

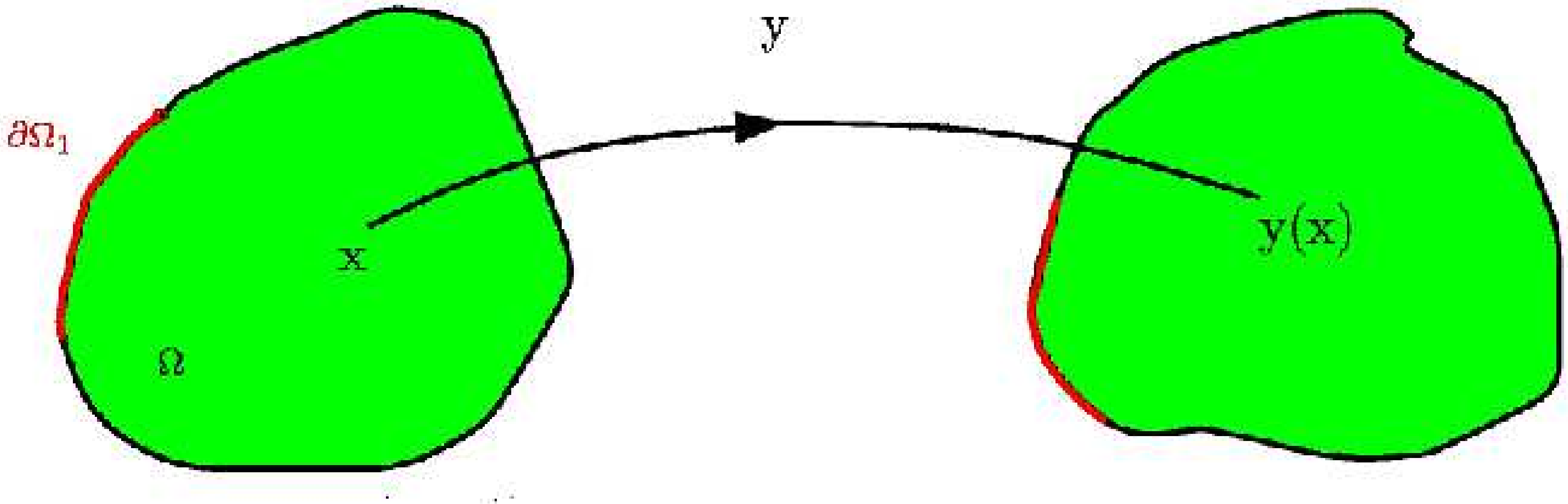
$$I_\theta(Q) = \int_\Omega \psi_E(Q, \nabla Q, \theta)\, dx$$

gives the Oseen-Frank energy with the K_i given in terms of the L_i and s.

The function space to which solutions are required to belong expresses how bad possible singularities of solutions can be and *is part of the mathematical model*.

This must be the case because changing the function space can change the predictions of the model. We give some examples of this, in particular comparing liquid crystals to the theory of nonlinear elasticity.

Nonlinear Elasticity



Minimize

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

among maps $y : \Omega \to \mathbb{R}^3$ satisfying suitable boundary conditions, e.g. $y_{|\partial\Omega_1} = \bar{y}$.

Comparing elasticity and liquid crystals

1. Both give rise to multi-dimensional vectorial problems of the calculus of variations. The fundamental convexity condition for such problems is *quasiconvexity*, which is, for example, more or less necessary and sufficient for the existence of minimizers. In elasticity ψ is *never* convex in ∇y, though it may be quasiconvex (e.g. for realistic models of rubber), whereas for liquid crystals it is perhaps surprising that the usual free energies are convex in ∇Q, ∇n.

2. In both theories there are side constraints. In elasticity there is a global topological constraint that the deformation y be invertible, which implies the local constraint

$$\det \nabla y(x) > 0.$$

For liquid crystals there is the constraint that

$$\lambda_{\mathrm{min}}(Q(x)) \geq -\frac{1}{3}.$$

3. In both theories minimizers can have physically meaningful singularities. In elasticity these include jumps in ∇y (phase boundaries) and discontinuities in y (fracture). In the Oseen-Frank theory minimizers can have discontinuities in n representing defects. In the Landau - de Gennes theory this is not so clear (more about this later).

Cavitation

Let $B = \{x \in \mathbb{R}^3 : |x| < 1\}$. Consider the problem of minimizing

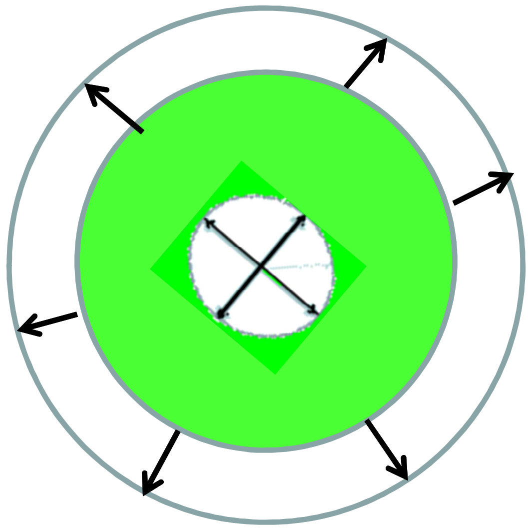
$$I(y) = \int_B [\mu|\nabla y|^2 + h(\det \nabla y)]\, dx$$

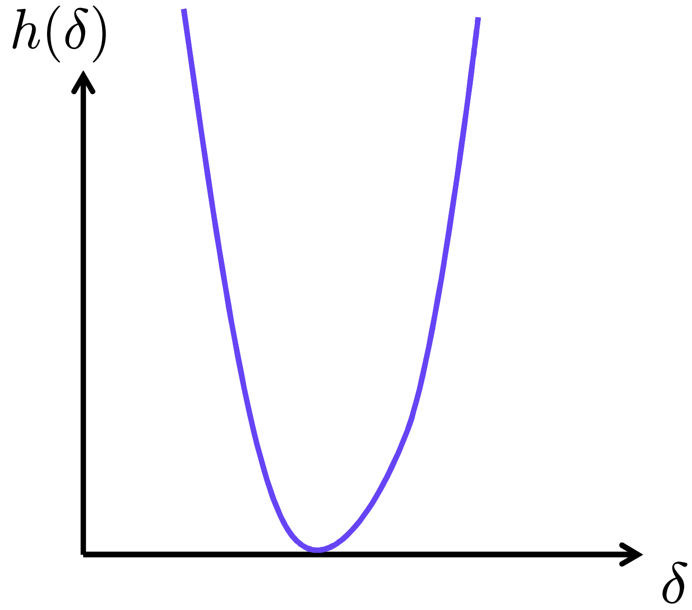
subject to

$$y(x)|_{\partial B} = \lambda x,$$

where $h'' > 0$, $h(\delta) \to \infty$ as $\delta \to \infty$ and $\delta \to 0+$, $h'(1) = -2\mu$, $\mu > 0$ and $\lambda > 1$.

Compressible neo-Hookean material.





If we minimize in the space of smooth maps, or in the space $W^{1,p}$ for $p \geq 3$, then the unique minimizer is $y^*(x) = \lambda x$.

If, however, we minimize in $W^{1,2}$ then the minimizer among radial maps is given by a deformation with a cavity at the origin.

The energy functional stayed the same, but we changed the function space and got different predictions. Indeed the infimum of the energy among smooth maps y is strictly bigger than the infimum among $W^{1,2}$ maps (the Lavrentiev phenomenon).

Note that if we changed the power in the energy, so that

$$I(y) = \int_B [\mu|\nabla y|^p + h(\det \nabla y)]\, dx$$

with $p \geq 3$ then cavitation is impossible (for $p > 3$ this follows from the embedding of $W^{1,p}$ in C^0).

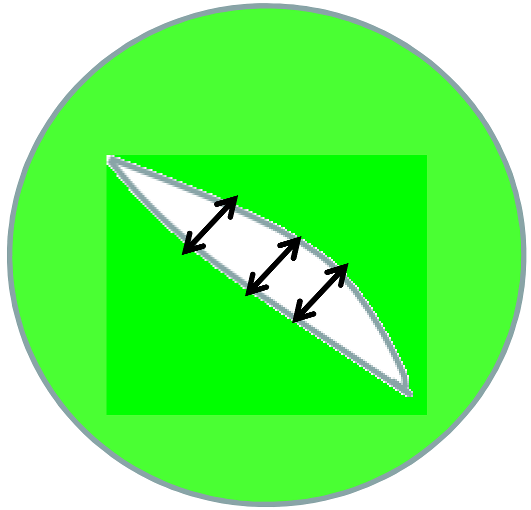
Thus the possible singularities and topology depend on the growth of the energy as $|\nabla y| \to \infty$.

$$I(y) = \int_B [\mu|\nabla y|^2 + h(\det \nabla y)]\, dx$$

How do we choose the function space? We could use the recipe that we choose the largest space on which the energy is defined, i.e. $W^{1,2}$.

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

No, because the body could develop fracture surfaces across which y is discontinuous.



This is impossible in a Sobolev space, but is possible if we allow $y \in SBV$ and let

$$I(y) = \int_\Omega [\mu|\nabla y|^2 + h(\det \nabla y)]\, dx + \kappa(\text{area}\,(S_y)).$$

Example (B & Mizel)
Minimize

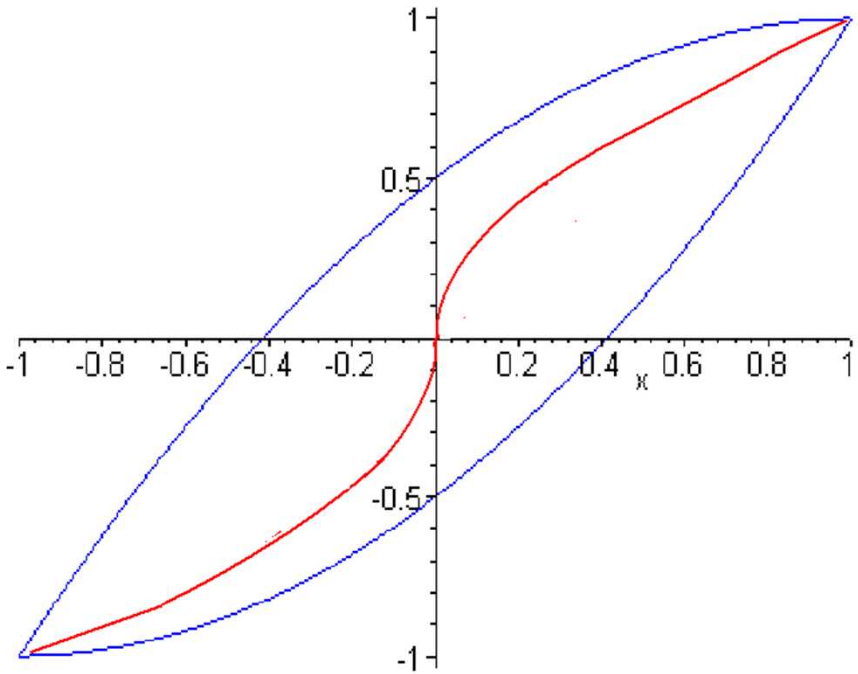
$$I(u) = \int_{-1}^{1} [(x^4 - u^6)^2 u_x^{28} + \epsilon u_x^2]\, dx$$

subject to

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

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

Foss (2003) constructs example with different infimum in each $W^{1,p}$.



Function spaces for Oseen-Frank

Minimize

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

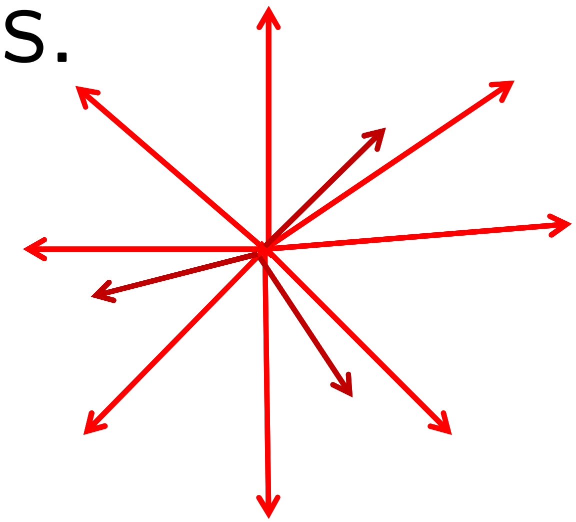
subject to $|n| = 1$ and suitable boundary conditions.

Since the integrand is quadratic in ∇n, the natural function space is

$$W^{1,2}(\Omega; S^2) = \{n \in W^{1,2}(\Omega; \mathbb{R}^3), |n| = 1\}.$$

Get existence of minimizers under usual conditions on the K_i.

Theory allows point defects.



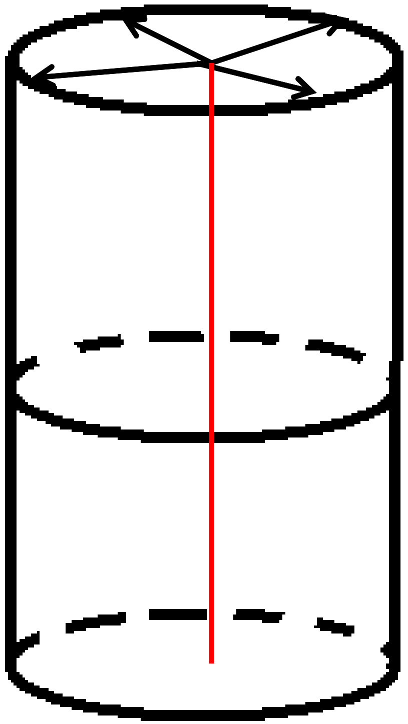
Hedgehog $$n(x) = \frac{x}{|x|}$$

$$\nabla n(x) = \tfrac{1}{|x|}(\mathbf{1} - n \otimes n)$$
$$|\nabla n(x)|^2 = \tfrac{2}{|x|^2}$$
$$\textstyle\int_0^1 r^{2-p} dr < \infty$$

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

Finite energy

Bad news: it can't describe other defects e.g. disclinations.



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

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

infinite energy for quadratic models

Related bad news. The theory cannot support some physical boundary conditions. For example, while there are maps $n \in W^{1,2}(\Omega; S^2)$ satisfying homeotropic boundary condtions (i.e. n normal to boundary) if Ω is a ball, say, there are no such n if Ω is a cube (Bedford).

What could we do about these problems while retaining some of the advantages of the Oseen-Frank theory?

Two possibilities motivated by elasticity for which we would still have existence of minimizers are:

1. Change the growth of the elastic energy as $|\nabla n| \to \infty$ so that it is subquadratic, analogous to replacing $|\nabla n|^2$ by $2(\sqrt{1+|\nabla n|^2}-1)$. This can certainly be done without affecting the elastic constants.

2. Allow n to be discontinuous, so that $n \in SBV$, adding an energy term such as

$$\int_{S_n} f(1-(n^+ \cdot n^-)^2)\, dA,$$

where $f \geq 0$, with $f(\tau) = 0$ if and only if $\tau = 0$.

Orientability
(JB/ Arghir Zarnescu, 2011)

$Q \in W^{1,1}$, $Q(x) = s\left(n(x) \otimes n(x) - \frac{1}{3}\mathbf{1}\right)$, is *orientable* if we can write

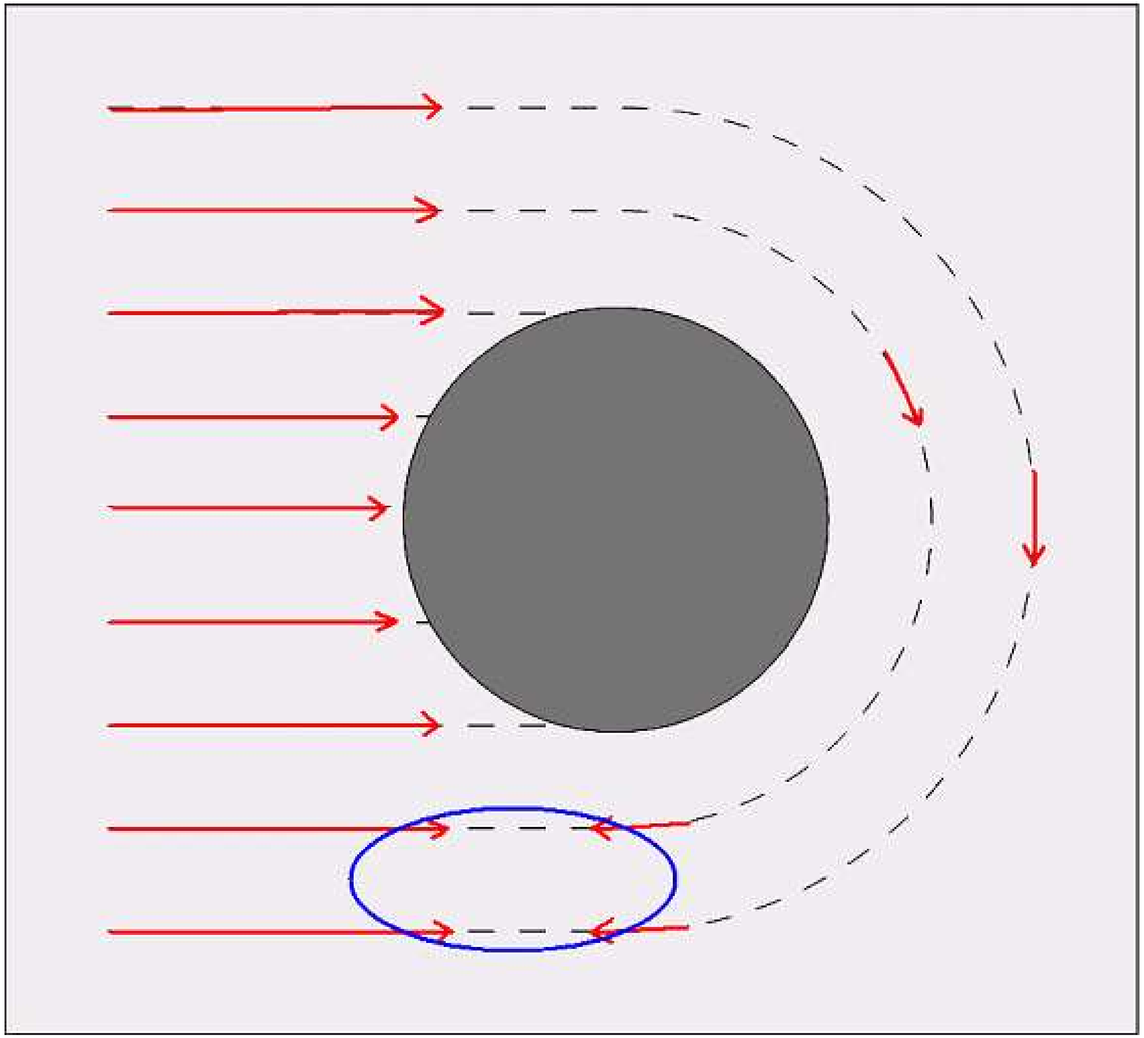
$$Q(x) = s\left(\tilde{n}(x) \otimes \tilde{n}(x) - \frac{1}{3}\mathbf{1}\right),$$

where $\tilde{n} \in W^{1,1}(\Omega, S^2)$. That is for each x we can choose $\tilde{n}(x) = \pm n(x) \in S^2$ so that $\tilde{n}(\cdot)$ has sufficient regularity to have a well-defined gradient $\nabla\tilde{n}$. Hence $\tilde{n}$ is a (Sobolev) *lifting* of $Q : \Omega \to \mathbb{R}P^2$ to $\tilde{n} : \Omega \to S^2$.

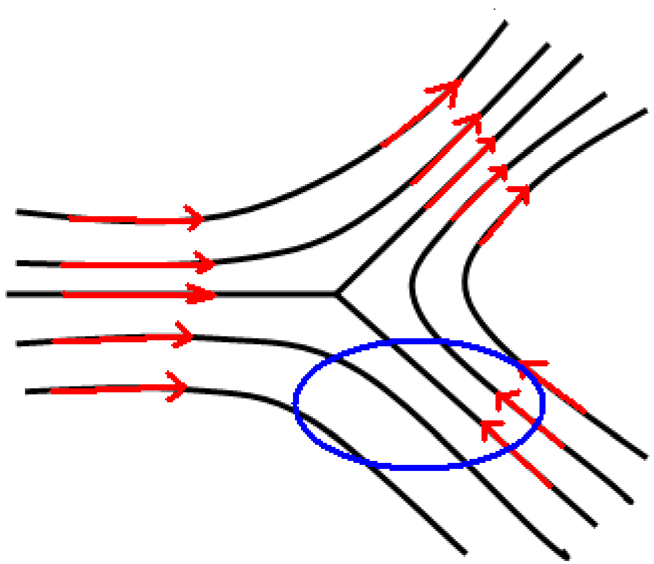
Theorem

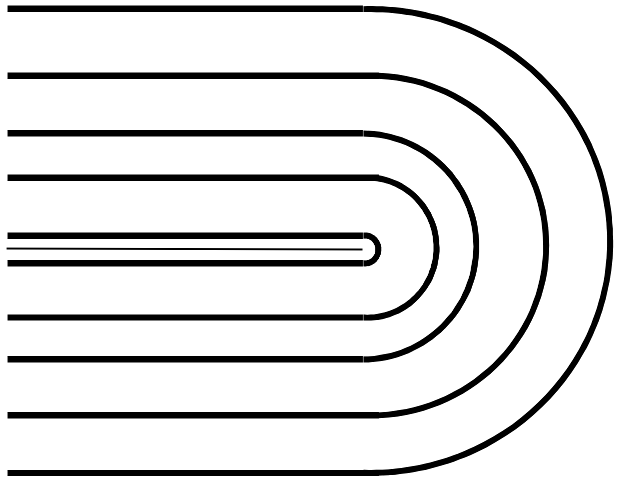
An orientable Q has exactly two orientations.

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



The index one half singularities are non-orientable





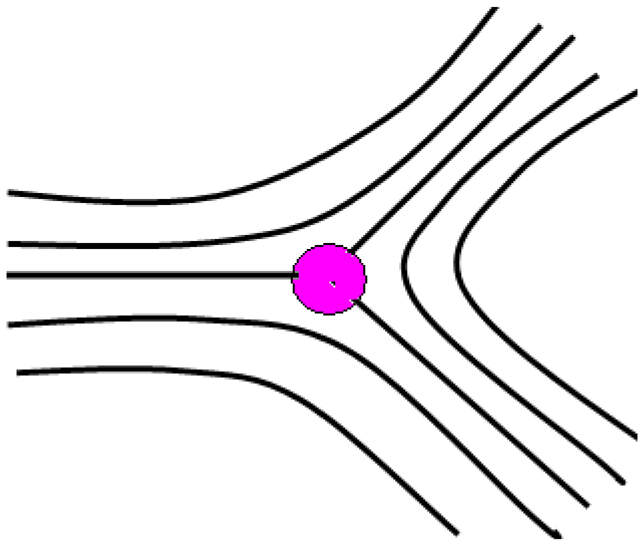
$$Q \notin W^{1,2}$$

Theorem

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

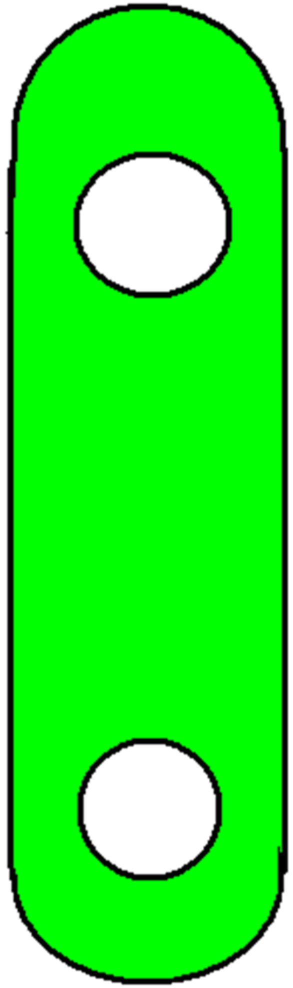
(See also a recent topologically more general lifting result of Bethuel and Chiron for maps $u:\Omega\rightarrow N$.)

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



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

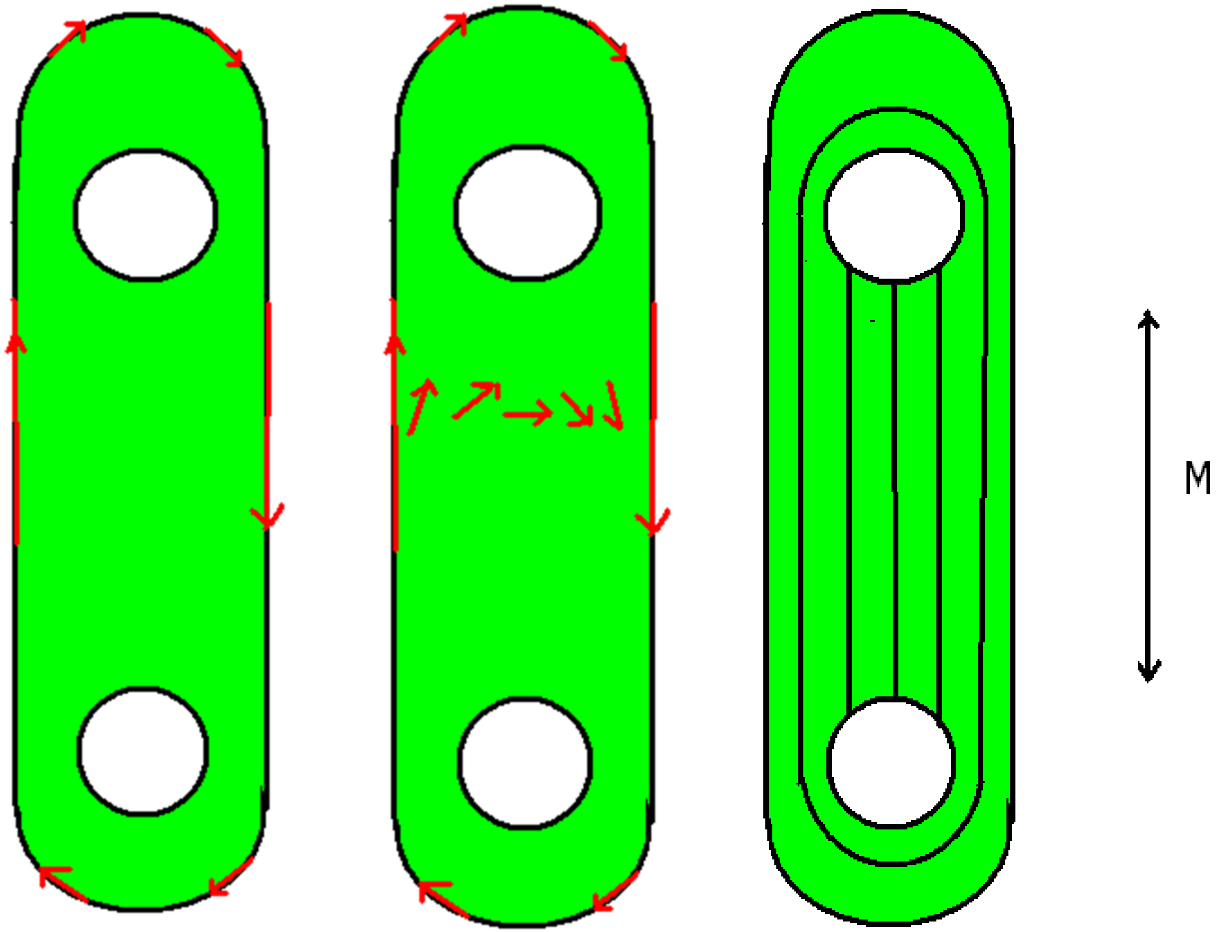
A two-dimensional example



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

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

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



For M large enough (in fact for any M) the minimum energy configuration is unoriented, even though there is a minimizer among oriented maps.

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

Landau – de Gennes theory

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

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

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

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

attains a minimum on

symmetric trace-free tensors

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

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

But what if $L_4 \neq 0$?

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

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

is unbounded below.

The reason for this is that there is no way of controlling the term

$$L_4 Q_{kl} Q_{ij,k} Q_{ij,l}$$

in terms of $|\nabla Q|^2$ unless you know that the eigenvalue constraints $\lambda_{\mathrm{min}}(Q) > -\frac{1}{3}$ are satisfied.

This can be ensured if

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

as proposed by Ericksen in the context of his theory.

Such an ψ_B can be constructed from the Onsager/Maier-Saupe model (JB/Majumdar) following a similar prescription to that of Katriel, Kventsel, Luckhurst and Sluckin (1986), and then you have existence of a minimizer even for $L_4 \neq 0$.

In elasticity a similar thing is done to ensure that $\det \nabla y > 0$, namely to assume that

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

How are defects described in the Landau - de Gennes model? According to the regularity result of Davis & Gartland minimizers are smooth, so that in contrast to the Oseen-Frank theory defects are not described by singularities of Q, but rather by discontinuous behaviour of the eigenvectors of Q which can occur when eigenvalues coalesce (de Gennes, Biscari/Peroli, Zarnescu ...).

However there is another possibility, if one accepts the idea that $\psi_E(\nabla Q, \theta)$ might not be quadratic in ∇Q.

There is an important example of Šverák & Yan (2000) of a smooth strongly convex $\psi : M^{5\times 3} \to [0, \infty)$ such that

$$I(u) = \int_B \psi(\nabla u(x))\, dx$$

a unique minimizer $u : B \to \mathbb{R}^5$ (subject to its own smooth boundary values) that is Lipschitz but not C^1).

Remarkably the minimizer is given by

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

It seems possible that ψ can be constructed to be isotropic, and perhaps the singularity remains when a lower-order bulk energy is added. This would mean that defects might sometimes be representable as singularities of Q.

Summary

1. The function space is part of the mathematical model. The same energy functional can have different minimizers in different spaces.

2. It should be a target to derive the appropriate function space at the same time as the energy functional (or dynamic equations). For elasticity there are some atomic-to-continuum derivations in this spirit using Γ-convergence (Braides et al).