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Les mathématiques des cristaux liquides

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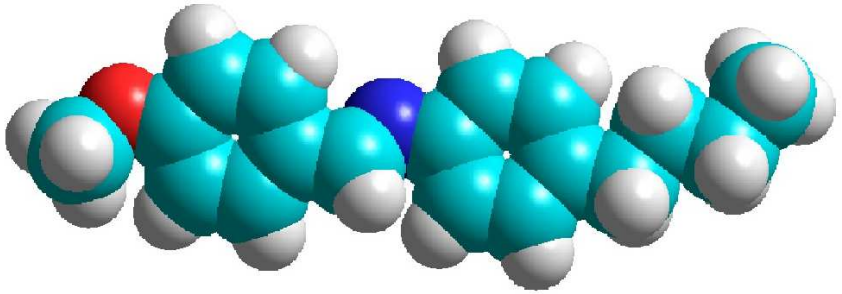
Classes of liquid crystals

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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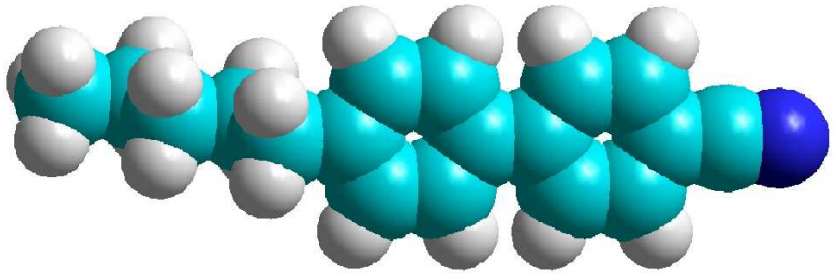

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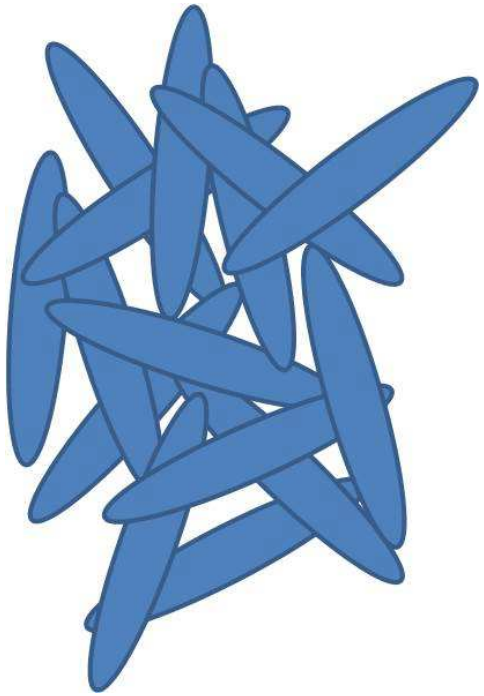
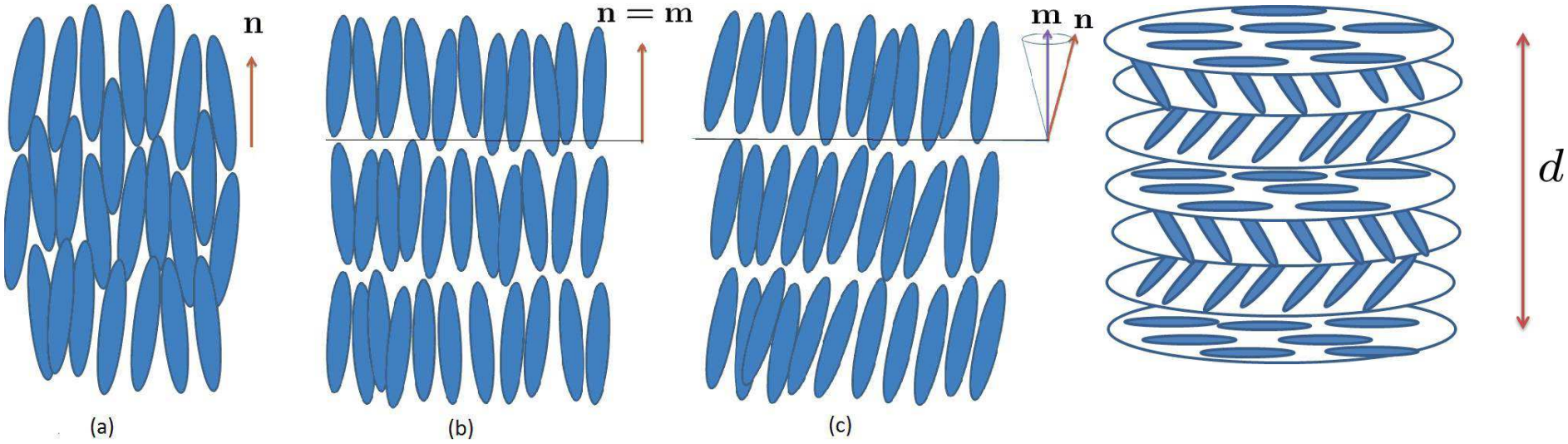
Space-filling models courtesy Claudio Zannoni.

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

Orientational and some positional order

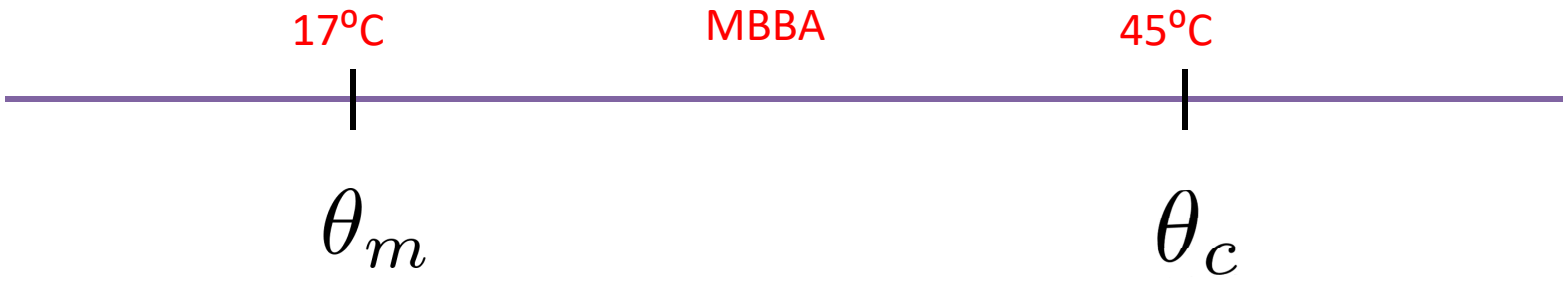
Smectic C phase

Cholesteric phase

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

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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The Oseen-Frank model.

Nematic LC at rest at constant temperature, no EM fields, filling container $\Omega \subset \mathbb{R}^3$, a bounded Lipschitz domain with boundary $\partial\Omega$.

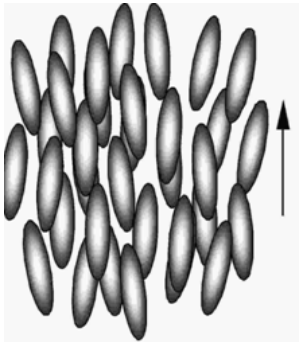
Free energy $$I(\mathbf{n}) = \int_\Omega W(\mathbf{n}, \nabla\mathbf{n})\, d\mathbf{x},$$

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 $\mathbf{n}|_{\partial\Omega}$



$\mathbf{n}(\mathbf{x}) \in S^2$ (unit sphere) is the *director.*

The K_i are the *Frank constants.*

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.

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

Ericksen (1966) inequalities: 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 all $\mathbf{n}$ and some constant $\mu > 0$.

(Proof. Apply the Ericksen inequalities to $W(\mathbf{n}, \nabla\mathbf{n}) - \mu|\nabla\mathbf{n}|^2$.)

Thus the natural function space (finite energy) is $H^1(\Omega; S^2)$.

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

Important identities

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

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

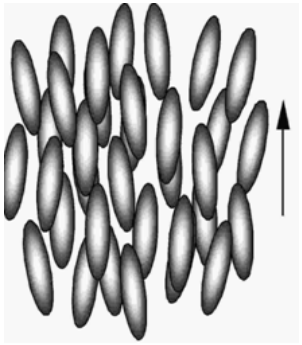
So if $K_1 = K_2 = K_3, K_4 = 0$ (the *one constant approximation*) then

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

which is the energy functional for *harmonic maps* $\mathbf{n} : \Omega \to S^2$.

Orientability

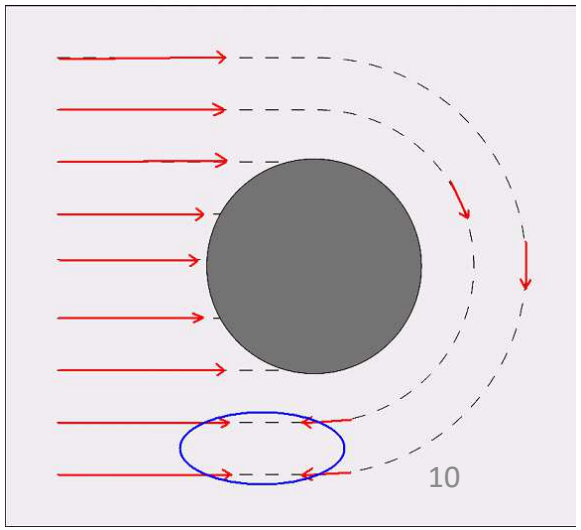
$\mathbf{n}(\mathbf{x})$ and $-\mathbf{n}(\mathbf{x})$ are physically indistinguishable.



So $\mathbf{n}(\mathbf{x})$ is better thought of as a *line field*, or equivalently as a map from Ω to the set of all lines through the origin.

A typical such line with direction $\pm\mathbf{n}$ can be represented by the matrix $\mathbf{N} = \mathbf{n} \otimes \mathbf{n}$ having components $n_i n_j$. The set of such lines forms the *real projective plane* $\mathbb{R}P^2$.

Smooth line fields need not be orientable, so that it is impossible to assign a direction that turns them into a smooth vector field.



Unoriented Oseen-Frank model

We can write $W(\mathbf{n}, \nabla\mathbf{n}) = \tilde{W}(\mathbf{N}, \nabla\mathbf{N})$, $\mathbf{N} = \mathbf{n} \otimes \mathbf{n}$, with $\tilde{W}$ quadratic in $\nabla\mathbf{N}$.

Indeed, since $N_{ij,k} = n_i n_{j,k} + n_j n_{i,k}$, we have that $N_{ij,k} n_j = n_{i,k}$, using which all the terms in $W(\mathbf{n}, \nabla\mathbf{n})$ can be expressed in terms of $\mathbf{N}, \nabla\mathbf{N}$.

In particular, for the one-constant approximation we have

$$\frac{K_1}{4}|\nabla\mathbf{N}|^2 = \frac{K_1}{4}(n_i n_{j,k} + n_j n_{i,k})(n_i n_{j,k} + n_j n_{i,k}) = \frac{K_1}{2}|\nabla\mathbf{n}|^2.$$

Let $\mathbb{R}P^2 = \{\mathbf{N} \in M^{3\times 3} : \mathbf{N} = \mathbf{n} \otimes \mathbf{n}, \mathbf{n} \in S^2\}$. Equivalently $\mathbb{R}P^2 = \{\mathbf{N} \in M^{3\times 3} : \mathbf{N} = \mathbf{N}^T, \operatorname{tr}\mathbf{N} = 1, |\mathbf{N}|^2 = 1, \det\mathbf{N} = 0\}$.

Unoriented energy minimization problem: find $\mathbf{N} : \Omega \to \mathbb{R}P^2$ that minimizes $\tilde{I}(\mathbf{N}) = \int_\Omega \tilde{W}(\mathbf{N}, \nabla \mathbf{N})\, d\mathbf{x}$ subject to suitable boundary conditions.

Natural function space is $H^1(\Omega; \mathbb{R}P^2)$.

Theorem. (Bethuel & Chiron 2007, JB/Zarnescu 2011)
If Ω is simply-connected and $\mathbf{N} \in H^1(\Omega; \mathbb{R}P^2)$ there exists $\mathbf{n} \in H^1(\Omega; S^2)$ with $\mathbf{N} = \mathbf{n} \otimes \mathbf{n}$.

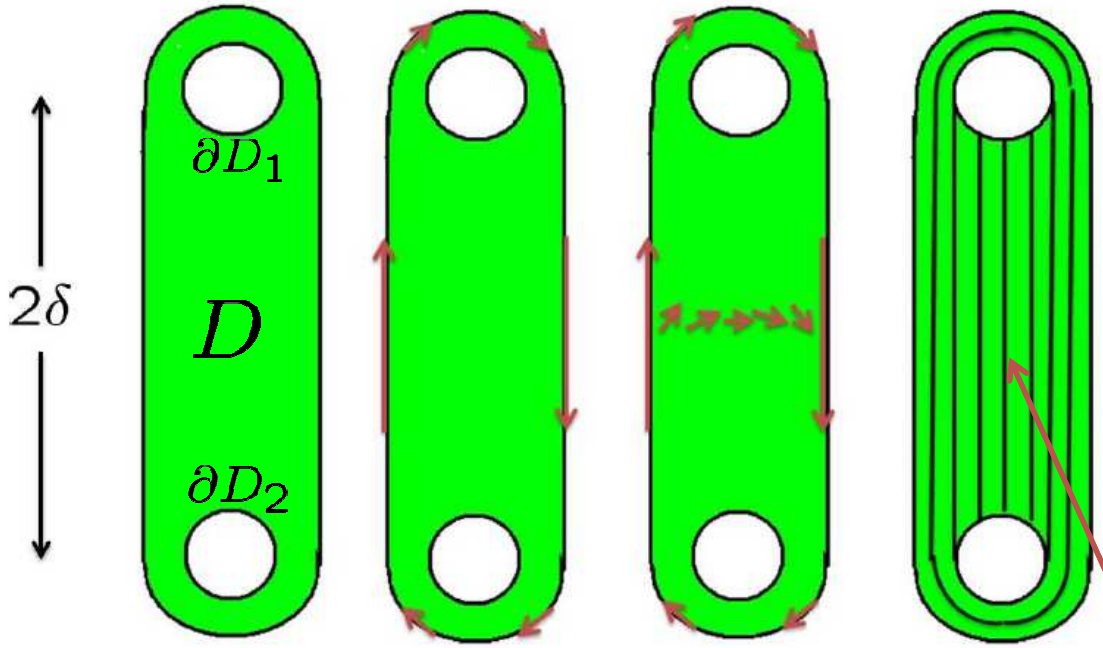
Thus the Oseen-Frank model and its unoriented version are equivalent if Ω is simply-connected.

However, if Ω is not simply-connected the minimizing $\mathbf{N}$ in the unoriented theory may not be orientable.

Example.

Modified from JB/Zarnescu (2011).

$$\Omega = D \times (-1, 1)$$



$$\mathbf{N} = \mathbf{n} \otimes \mathbf{n}$$

Boundary conditions
tangent with $\mathbf{n} \cdot \mathbf{e}_3 = 0$
on outer curved
and flat boundary,
weak anchoring on inner
curved boundary
$(\partial D_1 \cup \partial D_2) \times (-1, 1)$.

less energy when δ large

$$I(\mathbf{n}) = \frac{K_1}{2} \int_\Omega |\nabla \mathbf{n}|^2 \, d\mathbf{x} - \frac{K}{2} \int_{(\partial D_1 \cup \partial D_2) \times (-1,1)} (\mathbf{n} \cdot \boldsymbol{\nu})^2 dS$$

So constrained theory not equivalent to Oseen-Frank for Ω not simply connected.

From now on we consider the standard (oriented) Oseen-Frank model with energy

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

and boundary condition $\mathbf{n}|_{\partial\Omega} = \bar{\mathbf{n}}$.

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

$$\int_\Omega \left(\frac{\partial W}{\partial \nabla \mathbf{n}} \cdot \nabla (P(\mathbf{n}(\mathbf{x}))\mathbf{m}(\mathbf{x})) + \frac{\partial W}{\partial \mathbf{n}} \cdot P(\mathbf{n}(\mathbf{x}))\mathbf{m}(\mathbf{x}) \right) d\mathbf{x} = 0.$$

(WEL)

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

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

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

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

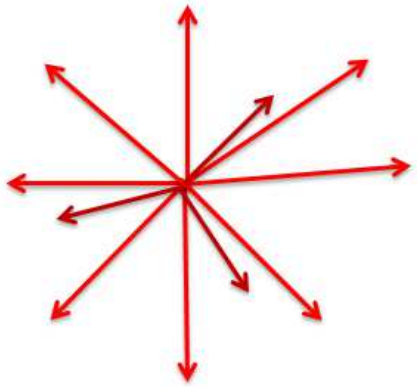
$$\mathbf{n}(\mathbf{x}) = (\cos \mu x_3, \sin \mu x_3, 0),$$

(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

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

so that $\hat{\mathbf{n}} \in H^1(\Omega; S^2)$.

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.

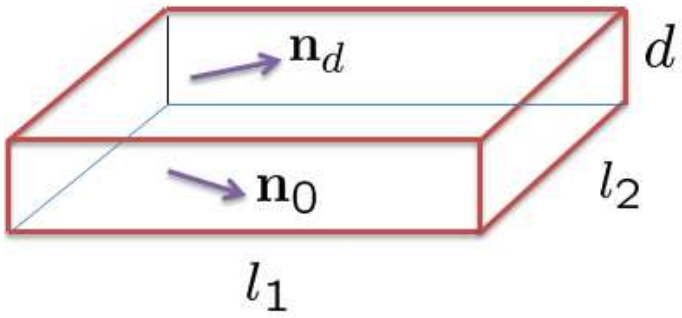
Hence, ignoring the saddle-splay term

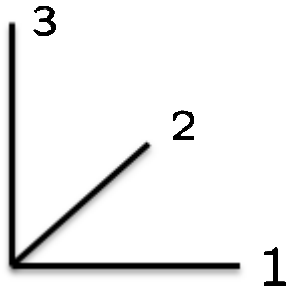
$$\begin{aligned} I(\mathbf{n}) &= \frac{1}{2}\int_\Omega \left(K_1(\mathrm{div}\,\mathbf{n})^2 + K_2(\mathbf{n}\cdot\mathrm{curl}\,\mathbf{n})^2 + K_3|\mathbf{n}\wedge\mathrm{curl}\,\mathbf{n}|^2\right) d\mathbf{x} \\ &\geq K_1\int_\Omega \left((\mathrm{div}\,\mathbf{n})^2 - \mathrm{tr}\,(\nabla\mathbf{n})^2\right)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

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

Pure twist solutions.

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





Boundary conditions:

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

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.

Existence and regularity results for general Frank constants

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).

As we have seen, minimizers can have point defects, so we cannot expect regularity of minimizers. However we can hope for partial regularity.

The best known such 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.

It is not known whether $\mathcal{S}$ consists of finitely many or a countable number of points, or whether minimizers can have a more complicated defect structure.

The one-constant case

In the one-constant case (EL) becomes

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

Thus the Lagrange multiplier, which in general depends on second derivatives of $\mathbf{n}$, is an explicit function $-|\nabla \mathbf{n}|^2$ of first derivatives.

Another special feature of the one-constant case is that if $\mathbf{n}$ is a minimizer or equilibrium solution then so is $\mathbf{Rn}$ for any $\mathbf{R} \in O(3)$. So, for example, the rotated hedgehog $\mathbf{R}\hat{\mathbf{n}}$ minimizes I subject to its own boundary conditions.

In the one-constant case there is a more precise partial regularity result due to 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 case of planar solutions

$$\mathbf{n}(\mathbf{x}) = (n_1(x_1, x_2), n_2(x_1, x_2), 0)$$

can be treated by complex analysis, writing $z = x_1 + ix_2$ and

$$\tilde{\mathbf{n}} = n_1 + in_2 = e^{i\Phi(\mathbf{x})}.$$

Then the equilibrium equation is equivalent to

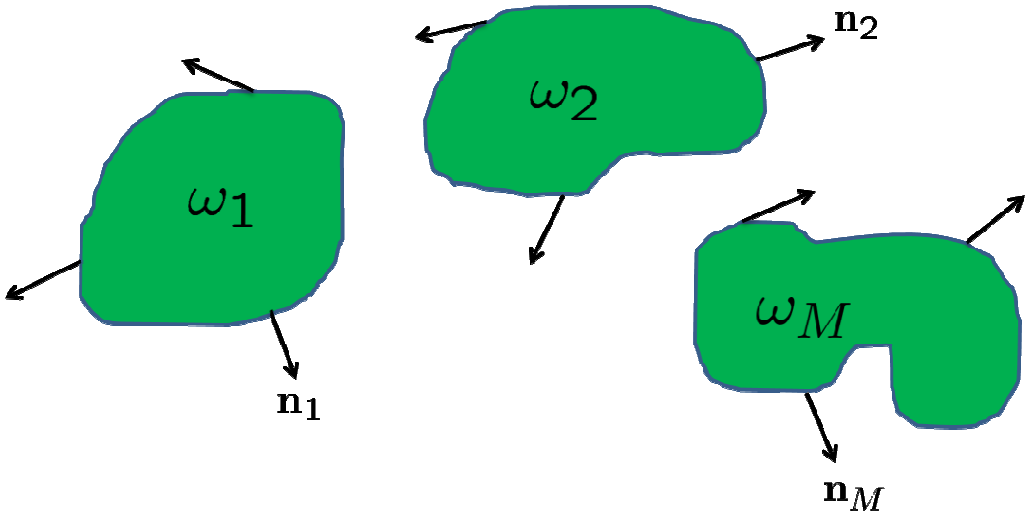
$$\Delta\tilde{\mathbf{n}} + |\nabla\mathbf{n}|^2\tilde{\mathbf{n}} = ie^{i\Phi}\Delta\Phi = \mathbf{0},$$

that is to the linear Laplace equation $\Delta\Phi = 0$, so that in particular equilibrium solutions of locally finite energy are smooth (no defects).

Also, if $\tilde{\mathbf{n}} = \tilde{\mathbf{n}}(z), \tilde{\mathbf{m}} = \tilde{\mathbf{m}}(z)$ are equilibrium solutions so is $\tilde{\mathbf{n}}(z)\tilde{\mathbf{m}}(z)$ as a product of complex numbers, and so is $\tilde{\mathbf{n}}(z)^{-1}$.

We can use this to treat an exterior problem:

$\omega_i \subset \mathbb{R}^2$ disjoint, bounded Lipschitz domains.



$$\Omega = \mathbb{R}^2 \setminus \cup_{i=1}^{M} \bar{\omega}_i$$

$$\bigcup_{i=1}^{M} \bar{\omega}_i \subset B(0, R_0)$$

Let $k = \sum_{i=1}^{M} \deg \mathbf{n}_i$.

What can we say about equilibrium configurations $\mathbf{n}$ in

$$X = \{\mathbf{n} : \Omega \to S^1 : \int_{\Omega \cap B_R} |\nabla \mathbf{n}|^2 \, d\mathbf{x} < \infty$$

for all $R > R_0, \mathbf{n}|_{\partial\omega_i} = \mathbf{n}_i\}$.

and their behaviour at ∞?

Consider the renormalized energy

$$E(\mathbf{n}) = \int_\Omega \left(|\nabla \mathbf{n}|^2 - \frac{k^2}{|\mathbf{x}|^2} \right) d\mathbf{x}.$$

Theorem. (JB/ Lu Liu) There is a unique minimizer $\mathbf{n}_C$ of $E(\mathbf{n})$ in each homotopy class C of X, $\mathbf{n}_C : \bar{\Omega} \to S^1$ is a smooth harmonic map and

$$|\mathbf{n}_C(\mathbf{x}) - \mathbf{n}_C^\infty(\mathbf{x})| \leq \frac{C_0}{r},$$

for some constant $C_0 > 0$, where

$$\mathbf{n}_C^\infty(\mathbf{x}) = (\cos(k\theta + \beta_C), \sin(k\theta + \beta_C))$$

and $\beta_C \in \mathbb{R}$. In each homotopy class C there is also a harmonic map $\hat{\mathbf{n}}_C$ with $E(\hat{\mathbf{n}}_C) = +\infty$.

Furthermore E attains a minimum $\mathbf{n}^*$ in X, but $\mathbf{n}^*$ is not in general unique.

Remark: The case of nonorientable line fields $\mathbf{n} \otimes \mathbf{n}$ can be handled by the trick of considering $\tilde{\mathbf{n}}(z)^2$.

Main idea of proof.

Carbou's trick. Pick $\mathbf{a}_i \in \omega_i$, $i = 1, \ldots, M$.

Let $d_i = \deg \mathbf{n}_i$. Then we can write any equilibrium solution $\tilde{\mathbf{n}}$ as

$$\tilde{\mathbf{n}}(z) = \left(\frac{z - \mathbf{a}_1}{|z - \mathbf{a}_1|}\right)^{d_1} \ldots \left(\frac{z - \mathbf{a}_M}{|z - \mathbf{a}_M|}\right)^{d_M} e^{i\varphi(z)},$$

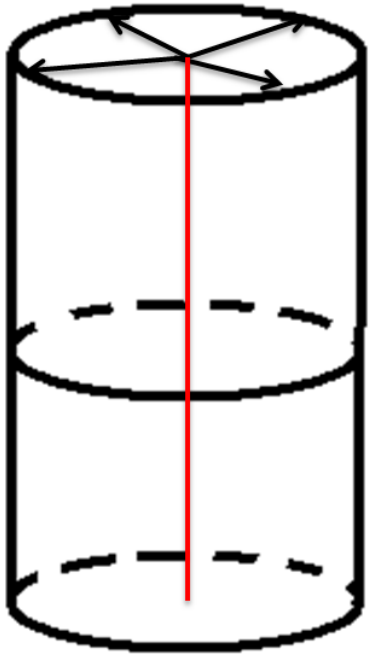
where φ is a smooth solution of $\Delta\varphi = 0$ in Ω.

Rough proof:

$$\tilde{\mathbf{n}}(z) \left(\frac{z - \mathbf{a}_1}{|z - \mathbf{a}_1|}\right)^{-d_1} \ldots \left(\frac{z - \mathbf{a}_M}{|z - \mathbf{a}_M|}\right)^{-d_M}$$

is an equilibrium solution of degree zero.

Line defects



2D hedgehog

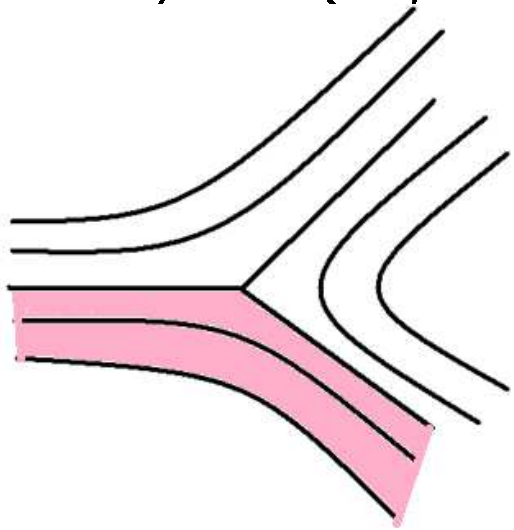
$$\mathbf{n}^\sharp(\mathbf{x}) = (\tfrac{x_1}{r}, \tfrac{x_2}{r}, 0), \quad r = \sqrt{x_1^2 + x_2^2}$$

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

$$I(\mathbf{n}^\sharp) \geq C \int_0^1 r \cdot \frac{1}{r^2}\, dr = \infty$$

$$\mathbf{n}^\sharp \notin H^1(\Omega; S^2).$$

Index $\frac{1}{2}$ defects fail to be described by Oseen-Frank for two reasons



These problems could potentially be fixed by modifying the growth of $W(\mathbf{n}, \nabla \mathbf{n})$ for large $|\nabla \mathbf{n}|$ to be *subquadratic*.

(i) they are not orientable

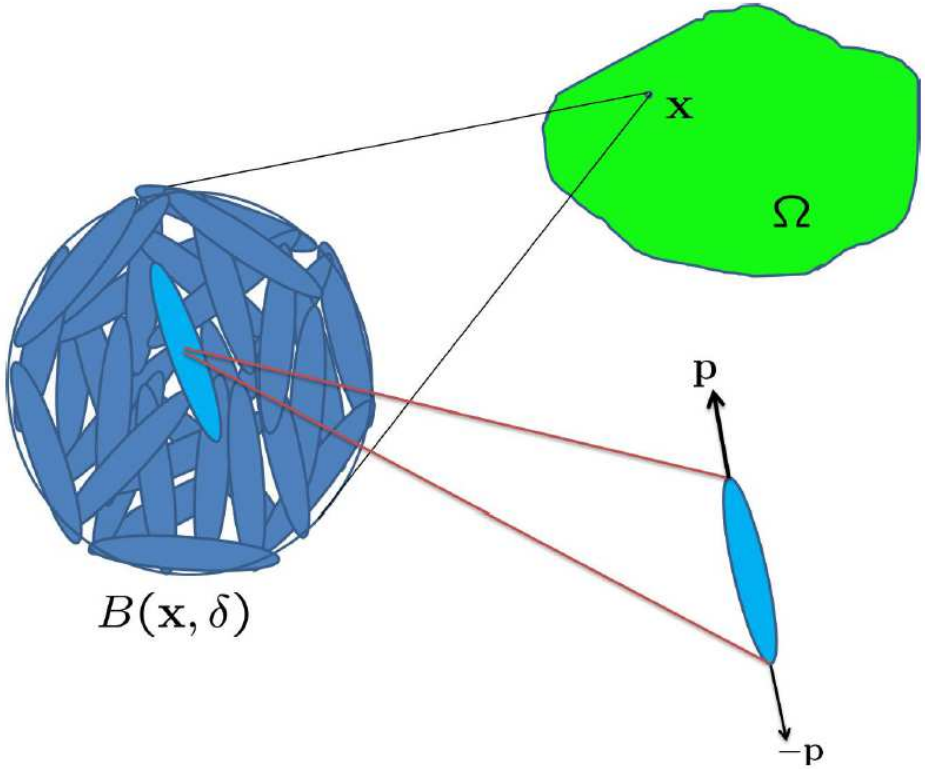
(ii) Energy ∞ in each sector

Can also consider *surface defects* ($\mathbf{n} \in SBV$).

The Landau - de Gennes model

The Landau - de Gennes model uses a tensor order parameter based on the probability distribution $\rho(\mathbf{x}, \mathbf{p})$ of molecular orientations at a point $\mathbf{x}$.

It gives structure to defects, so that in particular line defects have finite energy, and in a natural ansatz reduces to the unoriented Oseen-Frank model.



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

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

First moment

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

Second moment

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

If $\rho(\mathbf{x}, \mathbf{p}) = \frac{1}{4\pi}$ is isotropic, then $\mathbf{M}(\mathbf{x}) = \frac{1}{3}\mathbf{1}$.

The de Gennes $\mathbf{Q}$ tensor is defined as

$$\begin{aligned} \mathbf{Q}(\mathbf{x}) &= \mathbf{M}(\mathbf{x}) - \frac{1}{3}\mathbf{1} \\ &= \int_{S^2} (\mathbf{p} \otimes \mathbf{p} - \frac{1}{3}\mathbf{1}) \rho(\mathbf{x}, \mathbf{p})\, d\mathbf{p}. \end{aligned}$$

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

Free-energy for nematic (constant temperature)

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

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

If $a < \frac{b^2}{27c}$ then ψ_B minimized by uniaxial $\mathbf{Q} = s(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{1})$, $\mathbf{n} \in S^2$, $s = \frac{b+\sqrt{b^2-24ac}}{4c} > 0$.

Often assumed that

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

linear in temperature

where $b > 0, c > 0$.

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

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

One of 6 possible linearly independent cubic terms that are quadratic in $\nabla\mathbf{Q}$ (see Longa, Monselesan, Trebin (1987)).

Note that
$I_2 - I_3 = (Q_{ij}Q_{ik,k})_{,j} - (Q_{ij}Q_{ik,j})_{,k}$
is a null Lagrangian.

We assume that

If $L_2 = L_3 = L_4 = 0$ then $\psi_E = \frac{L_1}{2}|\nabla\mathbf{Q}|^2$

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

where the L_i are material constants.

From Landau - de Gennes to Oseen-Frank

Since ψ_B is minimized for uniaxial

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

in the limit of small elastic constants L_i we expect minimizers of $I(\mathbf{Q})$ to be nearly uniaxial. This motivates the *constrained theory* in which we minimize $I(\mathbf{Q})$ subject to $(*)$.

Putting $(*)$ into ψ_E we obtain the (unoriented) Oseen-Frank energy $\tilde{W}(\mathbf{N}, \nabla\mathbf{N})$ with Frank constants given by

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \\ K_4 \end{pmatrix} = s^2 \begin{pmatrix} 2 & 1 & 1 & -\frac{2}{3}s \\ 2 & 0 & 0 & -\frac{2}{3}s \\ 2 & 1 & 1 & \frac{4}{3}s \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} L_1 \\ L_2 \\ L_3 \\ L_4 \end{pmatrix}.$$

From the Onsager model to the bulk energy

Consider a homogeneous nematic liquid crystal at constant temperature, with probability distribution of molecular orientations $\rho(\mathbf{x}, \mathbf{p}) = \rho(\mathbf{p})$ independent of $\mathbf{x}$.

The Onsager model with the Maier-Saupe molecular interaction has free energy proportional to

$$E(\rho) = \int_{S^2} \rho(\mathbf{p}) \ln \rho(\mathbf{p}) \, d\mathbf{p} - \frac{\kappa}{2} |\mathbf{Q}(\rho)|^2,$$

with

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

Following Katriel et al (1986), JB/Majumdar (2010, 2019?) we define for $\mathbf{Q} = \mathbf{Q}^T, \mathrm{tr}\,\mathbf{Q} = 0$

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

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

Theorem (JB/Majumdar) $f(\mathbf{Q})$ is strictly convex and

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

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

Critical points of $E(\rho)$

Since $|\mathbf{Q}(\rho)|^2 = |\mathbf{M}(\rho) - \frac{1}{3}\mathbf{1}|^2 = |\mathbf{M}(\rho)|^2 - \frac{1}{3}$, critical points of E correspond to solutions of the Euler-Lagrange equation

$$1 + \ln \rho(\mathbf{p}) = \kappa \mathbf{M}(\rho) \cdot \mathbf{p} \otimes \mathbf{p} + \text{constant},$$

and so are given by

$$\rho(\mathbf{p}) = \frac{\exp \kappa(\mathbf{M}(\rho) \cdot \mathbf{p} \otimes \mathbf{p})}{Z(\rho)},$$

where $Z(\rho) = \int_{S^2} \exp \kappa(\mathbf{M}(\rho) \cdot \mathbf{p} \otimes \mathbf{p})\, d\mathbf{p}$.

Writing $\mathbf{M}(\rho) = \sum_{i=1}^{3} \gamma_i \mathbf{e}_i \otimes \mathbf{e}_i$, where $\gamma_i > 0$, $\sum_{i=1}^{3} \gamma_i = 1$, we thus have to solve the equations

$$\int_{S^2} p_i^2 \exp \kappa \left(\sum_{j=1}^{3} \gamma_j p_j^2 \right) d\mathbf{p} = \gamma_i Z, \quad i = 1, 2, 3,$$

where $Z = \int_{S^2} \exp \kappa \left(\sum_{j=1}^{3} \gamma_j^2 p_j^2 \right) d\mathbf{p}$.

$$\int_{S^2} p_i^2 \exp \kappa \left(\sum_{j=1}^{3} \gamma_j p_j^2 \right) \, d\mathbf{p} = \gamma_i Z, \quad i = 1, 2, 3 \quad \text{(EL)}$$

$$Z = \int_{S^2} \exp \kappa \left(\sum_{j=1}^{3} \gamma_j^2 p_j^2 \right) \, d\mathbf{p}$$

Fatkullin & Slastikov (2005), Liu, Zhang & Zhang(2005) (see also Zhou, Wang, Forest & Wang (2005)) characterize all solutions, and in particular show that they are *axisymmetric*. That is, there are no solutions with the γ_i all different.

Proof of axial symmetry

Lemma.

$$\int_{S^2}(p_1^2-p_3^2)\exp\kappa\left(\sum_{j=1}^{3}\gamma_j p_j^2\right)\,d\mathbf{p}$$

$$=2\kappa(\gamma_1-\gamma_3)\int_{S^2}p_1^2p_3^2\exp\kappa\left(\sum_{j=1}^{3}\gamma_j p_j^2\right)\,d\mathbf{p}.$$

Proof. Apply the divergence theorem on $B(0,1)$ to the divergence free vector field

$$\mathbf{u}(\mathbf{p})=(p_1,0,-p_3(1+2\kappa(\gamma_1-\gamma_3)p_1^2))$$
$$\exp\kappa[\gamma_3+(\gamma_1-\gamma_3)p_1^2+(\gamma_2-\gamma_3)p_2^2].$$

Suppose all the γ_i are distinct. By the lemma and (EL), and since $\gamma_1 \neq \gamma_3$,

$$2\kappa \int_{S^2} p_1^2 p_3^2 \exp \kappa \left(\sum_{j=1}^{3} \gamma_j p_j^2 \right) \, d\mathbf{p} = Z.$$

Therefore

$$\int_{S^2} p_1^2 (p_3^2 - p_2^2) \exp \kappa \left(\sum_{j=1}^{3} \gamma_j p_j^2 \right) \, d\mathbf{p} = 0.$$

But the LHS equals

$$\int_{S^2} p_1^2 (p_2^2 - p_3^2) \exp \kappa (\gamma_1 p_1^2 + \gamma_2 p_3^2 + \gamma_3 p_2^2) \, d\mathbf{p}.$$

Adding, we get that

$$\int_{S^2} p_1^2(p_3^2 - p_2^2) \exp(\kappa\gamma_1 p_1^2) g(p_2, p_3) d\mathbf{p} = 0,$$

where $g(p_2, p_3) = \exp \kappa(\gamma_2 p_2^2 + \gamma_3 p_3^2) - \exp \kappa(\gamma_3 p_2^2 + \gamma_2 p_3^2)$.

But $g(p_2, p_3) > 0$ iff $\kappa(\gamma_2 - \gamma_3)(p_2^2 - p_3^2) > 0$, so since $\gamma_2 \neq \gamma_3$ the integrand has one sign. Contradiction.