

On the cubic instability in the Q-tensor theory of nematic liquid crystals

Arghir Zarnescu

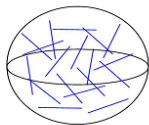
University of Sussex

Joint work with **Gautam Iyer** (*Carnegie Mellon*), **Xiang Xu** (*Carnegie Mellon*)

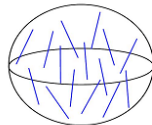
Diffuse Interface Models Workshop

Levico Terme, September 2013

Liquid crystals modelling: physics



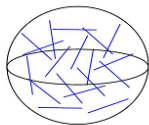
Isotropic liquid phase



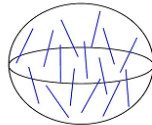
Nematic liquid crystal phase

- A measure μ such that $0 \leq \mu(\mathbf{A}) \leq 1 \ \forall \mathbf{A} \subset \mathbb{S}^2$

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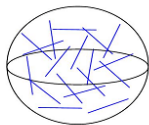
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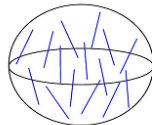
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Liquid crystals modelling: physics



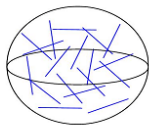
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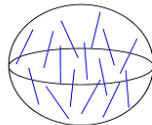
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Q-tensors-statistical mechanics interpretation and constraints



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- Q is a 3×3 symmetric, traceless matrix - a **Q-tensor**
- If $e_i, i = 1, 2, 3$ are eigenvectors of Q , with corresponding eigenvalues $\lambda_i = 1, 2, 3$, we have

$$-\frac{1}{3} \leq \lambda_i = \int_{\mathbb{S}^2} (p \cdot e_i)^2 d\mu(p) - \frac{1}{3} \leq \frac{2}{3}$$

for $i = 1, 2, 3$, since $\int_{\mathbb{S}^2} d\mu(p) = 1$.

Landau-de Gennes Q-tensor reduction and earlier theories



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- **Ericksen's theory (1991)** for **uniaxial** Q-tensors which can be written as

$$Q(x) = s(x) \left(n(x) \otimes n(x) - \frac{1}{3}Id \right), \quad s \in \mathbb{R}, n \in \mathbb{S}^2$$

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- **Oseen-Frank theory (1958)** take s in the uniaxial representation to be a fixed constant s_+

The Q-tensor energy functionals I

- The simplest way to obtain physically relevant configurations is by minimizing an energy functional:

$$\mathcal{F}[Q, D] = \int_{\Omega} \psi(Q(x), D(x)) dx$$

where $(Q_{ij}(x))_{i,j=1,\dots,d}$ is a Q -tensor, i.e. symmetric and traceless $d \times d$ matrix ($d = 2, 3$) and ' $D \sim \nabla Q$ ', is a third order tensor.

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- Physical invariances require that:

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

where $Q^* = RQR^t$ and $D_{ijk}^* = R_{il}R_{jm}R_{kn}D_{lmn}$ for any $R \in O(3)$.

The Q-tensor energy functionals II

- We can decompose:

$$\psi(Q, D) = \psi(Q, 0) + \psi(Q, D) - \psi(Q, 0) = \underbrace{\psi_B(Q)}_{\text{bulk}} + \underbrace{\psi_E(Q, D)}_{\text{elastic}}$$

Then $\psi_B(Q) = \psi_B(RQR^t)$ for $R \in O(3)$ implies that there exists $\bar{\psi}_B$ so that

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- Example of elastic terms that respect the physical invariances:

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

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

The cubic instability

- Take an elastic energy:

$$\psi_E(Q, D) = \sum_{j=1}^4 L_j I_j$$

where $L_j, j = 1, \dots, 4$ are elastic constants.

- If $L_4 \neq 0$ (corresponding to the cubic term) then $F[Q, D] = \int_{\Omega} \psi_B(Q(x)) + \psi_E(Q(x), D(x)) \, dx$ is seen to be **unbounded from below** by taking (J.M. Ball):

$$Q = s(x) \left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} Id \right) \text{ for suitable } s(x) \text{ (then}$$
$$I_4 = \frac{4}{9} s(s'^2 - \frac{3}{r^2} s^2)).$$

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- If $L_4 = 0$ then for $\psi_B \equiv 0$ we have:

$$F[Q] \geq \mu \|\nabla Q\|_{L^2}^2$$

for some $\mu > 0$ if and only if (Longa, Monselesan, and Trebin, 1987):

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

Q-tensors versus directors energies

Take

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

with s fixed and $n(x) \in \mathbb{S}^2$. Let

$$K_1 := 2L_1 s^2 + L_2 s^2 + L_3 s^2 - \frac{2}{3}L_4 s^3, \quad K_2 := 2L_1 s^2 - \frac{2}{3}L_4 s^3$$

$$K_3 = 2L_1 s^2 + L_2 s^2 + L_3 s^2 + \frac{4}{3}L_4 s^3, \quad K_4 = L_3 s^2$$

Then $F[Q, D] = G[n, \nabla n]$ with

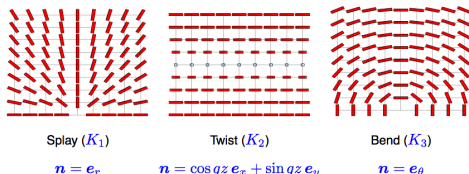
$$\begin{aligned} G[n, \nabla n] = & \int_{\Omega} K_1 (\operatorname{div} n)^2 + K_2 (n \cdot \operatorname{curl} n)^2 + K_3 (n \times \operatorname{curl} n)^2 \, dx \\ & + \int_{\Omega} (K_2 + K_4) (\operatorname{tr}(\nabla n)^2 - (\operatorname{div} n)^2) \, dx \end{aligned}$$

the Oseen-Frank energy functional.

Oseen-Frank energy: interpretation and its darkest secret...the K_{13} term

Recall the Oseen-Frank energy functional:

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



A term **allowed by symmetries**

$$\int_{\Omega} K_{13} \nabla \cdot (n \cdot \nabla n) dx = \int_{\partial\Omega} K_{13} (n \cdot \nu) (\nabla \cdot n) d\sigma$$

would make the energy unbounded from below... Thus it is never included in mathematical studies...

Παντα ρει

Ηερακλειτος

Παντα ρει

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Everything flows

Heraclitus

The L^2 gradient flow

- A gradient flow:

$$\frac{dQ}{dt} = -\text{grad } F[Q, D(Q)]$$

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- We consider the L^2 gradient, taking into account the constraints

$$\frac{\partial Q_{ij}}{\partial t} = - \left(\frac{\delta F}{\delta Q} \right)_{ij} + \lambda \delta_{ij} + \mu_{ij} - \mu_{ji}$$

where λ is a Lagrange multiplier corresponding to the constraint $\text{tr}(Q) = 0$ and $\mu_{ij}, i, j = 1, 2, 3$ are Lagrange multipliers corresponding to the constraint $Q_{ij} = Q_{ji}$.

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- More explicitly **and for the standard potential**

$\psi_B(Q) = \frac{a}{2} \text{tr}(Q^2) + \frac{b}{3} \text{tr}(Q^3) + \frac{c}{4} \text{tr}^2(Q^2)$ this becomes:

$$\begin{aligned} \frac{\partial Q_{ij}}{\partial t} = & 2L_1 \Delta Q_{ij} - aQ_{ij} + b \left(Q_{ik} Q_{kj} - \frac{\text{tr}(Q^2)}{3} \delta_{ij} \right) - c \text{tr}(Q^2) Q_{ij} \\ & + (L_2 + L_3) (\nabla_j \nabla_k Q_{ik} + \nabla_i \nabla_k Q_{jk}) - \frac{2}{3} (L_2 + L_3) \nabla_l \nabla_k Q_{lk} \delta_{ij} \\ & + 2L_4 \nabla_l Q_{ij} \nabla_k Q_{lk} + 2L_4 \nabla_l \nabla_k Q_{ij} Q_{lk} - L_4 \nabla_i Q_{kl} \nabla_j Q_{kl} + \frac{L_4}{3} |\nabla Q|^2 \delta_{ij}. \end{aligned}$$

“Energy conservation” and its use-the L^∞ bound

- Recall the abstract equation:

$$\frac{\partial Q_{ij}}{\partial t} = - \left(\frac{\delta F}{\delta Q} \right)_{ij} + \lambda \delta_{ij} + \mu_{ij} - \mu_{ji}$$

- Multiplying by $-RHS$ and integrating over Ω we get:

$$\frac{d}{dt} F[Q] = - \int_{\Omega} \sum_{i,j=1}^3 \left(\left(\frac{\delta F}{\delta Q} \right)_{ij} + \lambda \delta_{ij} + \mu_{ij} - \mu_{ji} \right)^2 \leq 0 \quad (1)$$

so the energy is apriori bounded, i.e.

$$\begin{aligned} F[Q(t)] = \int_{\Omega} & \underbrace{L_1 |\nabla Q|^2 + L_2 \nabla_j Q_{ik} \nabla_k Q_{ij} + L_3 \nabla_j Q_{ij} \nabla_k Q_{ik}}_{\geq \mu \|\nabla Q\|_{L^2}^2} + \underbrace{L_4 Q_{lk}}_{\text{small?}} \nabla_k Q_{ij} \nabla_l Q_{ij} dx \\ & + \int_{\Omega} \underbrace{\frac{a}{2} \text{tr}(Q^2) + \frac{b}{3} \text{tr}(Q^3) + \frac{c}{4} \text{tr}^2(Q^2)}_{\geq -c_0^2} dx \leq F[Q_0] \end{aligned}$$

Small initial data: maximum principle in 2D

Proposition

Consider the 2D gradient flow on a bounded smooth domain $\Omega \subset \mathbb{R}^2$. Suppose the coercivity condition holds. There exists an explicitly computable constant η_1 (depending on $L_i, i = 1, \dots, 4$) so that if

$$\|\tilde{Q}\|_{L^\infty(\partial\Omega)} \leq \|Q_0\|_{L^\infty(\Omega)} < \sqrt{2\eta_1} \quad (2)$$

and

$$|a| \leq 2c\eta_1, \quad (3)$$

then for any $T > 0$, we have

$$\|Q\|_{L^\infty((0,T) \times \Omega)} \leq \sqrt{2\eta_1}. \quad (4)$$

- The proof is done by taking the inner product of the equation with $Qh(Q)$ with $h(Q) = (|Q|^2 - \eta)^+$ and closing an estimate for $\int_\Omega h^2(Q)$.
- It allows to prove existence of solutions with $Q \in L^\infty(0, T; H^1 \cap L^\infty) \cap L^2(0, T; H^2)$, $Q \in S^{(2)}$, a.e. in $\Omega \times (0, T)$

Large initial data blow-up: the radial hedgehog ansatz

- We take the ansatz

$$Q_{ij}(t, x) := \theta(t, |x|) S_{ij}, \quad \text{where } S_{ij} = \left(\frac{x_i x_j}{|x|^2} - \frac{\delta_{ij}}{3} \right).$$

- The gradient flow reduces to:

$$\begin{aligned} \partial_t \theta = & \quad 2L_4 \theta' \left(\frac{\theta'}{3} + \frac{2\theta}{r} \right) + \frac{4L_4}{3} \left(\theta'' \theta - \frac{\theta' \theta}{r} \right) + \frac{2L_4 \theta^2}{r^2} + 2L_1 \left(\theta'' + \frac{2\theta'}{r} - \frac{6\theta}{r^2} \right) \\ & - a\theta + \frac{b\theta^2}{3} - \frac{2c}{3} \theta^3 + \frac{4(L_2 + L_3)}{3} \left(\theta'' + \frac{2\theta'}{r} - \frac{6\theta}{r^2} \right). \end{aligned}$$

- We multiply equation by $-\theta_- r^2$, integrate over $\int_{R_0}^{R_1}$ and by parts to obtain a blow-up inequality in the quantity $\int_{R_0}^{R_1} \theta_-^2 r^2 dr$.

“The finite time blow-up versus long-time existence” dichotomy and size of initial data

- We have seen a typical dichotomy:
 - for small enough (in L^∞) initial data we have global existence
 - For large enough initial data there exists finite time blow-up
- Natural questions:
 - is there a threshold type of initial data that ensures long-time existence?
 - Is this presumptive threshold related to (suitably normalized) physicality?

The physicality versus L^∞ -bound

- If $\|\bar{Q}\|_{L^\infty} < M$ and $Q(0) = \bar{Q}$ does $\|Q(t)\|_{L^\infty} < M?$, i.e.
does $\sqrt{\bar{Q}_{ij}(x)\bar{Q}_{ij}(x)} < M, \forall x \in \Omega$ imply
 $\sqrt{Q_{ij}(t, x)Q_{ij}(t, x)} < M?$

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- Note that if $\lambda_i(Q(x)) \in (-\frac{1}{3}, \frac{2}{3}), i = 1, 2, 3$ (with $\lambda_i(Q(x))$ denoting eigenvalues of Q) then

$$\sqrt{Q_{ij}(x)Q_{ij}(x)} = \sqrt{\sum_{i=1}^3 \lambda_i^2(Q(x))} < \frac{2}{3}$$

but we do not have that

$$\sqrt{\sum_{i=1}^3 \lambda_i^2(Q(x))} < \frac{2}{3} \underbrace{\Rightarrow}_{?} \lambda_i(Q) \in (-\frac{1}{3}, \frac{2}{3})$$

- Physically implies an L^∞ bound but not the other way around, so it is a more subtle requirement.

Physicality in a basic case I: the operator splitting intuition

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- The operator splitting idea: Consider an equation

$$\partial_t u = Au + Bu.$$

- Let $\mathcal{A}(t)u_0$ denote the solution of the equation, at time t and initial data u_0 **assuming that $B = 0$ in the previous equation**
- Let $\mathcal{B}(t)u_0$ denote the solution of the equation, at time t and initial data u_0 **assuming that $A = 0$ in the previous equation**

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- Let $\mathcal{B}(t)u_0$ denote the solution of the equation, at time t and initial data u_0 **assuming that $A = 0$ in the previous equation**
- In general one can expect to obtain the solution $u(t)$ of the equation, starting from initial data u_0 as:

$$\lim_{n \rightarrow \infty} \underbrace{\mathcal{A}(t/n)\mathcal{B}(t/n)\mathcal{A}(t/n)\mathcal{B}(t/n) \dots \mathcal{A}(t/n)\mathcal{B}(t/n)}_{n \text{ times}} u_0$$

Physicality in a basic case II: diffusion preserves the closed convex hull of the initial data

- First let us denote by $S(t)f$ the solution of the heat equation with initial data f . Then in the whole space we have the following formula:

$$(S(t)f)(x) = \frac{1}{(4\pi t)^{3/2}} \int_{\mathbb{R}^3} f(y) e^{-\frac{|x-y|^2}{4t}} dy \quad (5)$$

where f can be a matrix as well, and the formula is interpreted then component-wise.

- Let us observe that the formula can be alternatively written as:

$$S(t)f(x) = \int_{\mathbb{R}^3} f(y) d\mu_{x,t}(y) \quad (6)$$

where the measure $d\mu_{x,t}$ is an absolutely continuous probability measure (with respect to the Lebesgue measure) with probability density function

$$\Phi(t, x, y) = \frac{e^{-\frac{|x-y|^2}{4t}}}{(4\pi t)^{3/2}}.$$

Let us note that this is a probability measure precisely because

$$\int_{\mathbb{R}^3} \Phi(t, x, y) dy = 1.$$

Physicality in a basic case III: diffusion preserves the convex hull

- On the other hand one can show that a probability measure can be obtained as the weak-star limit of convex combinations of delta measures, i.e. for $Q_0(\cdot)$ continuous one has:

$$\int_{\mathbb{R}^3} Q_0(y) d\mu_x(y) = \lim_{k \rightarrow \infty} \sum_{j=1}^{N_k} \theta_{k,j} \int_{\mathbb{R}^3} Q_0(y) \delta_{y_{k,j}^{x,t}} \quad (7)$$

for suitable $\{\theta_{k,j} \in [0, 1], y_{k,j} \in \mathbb{R}^3\}_{j \in \{1, \dots, N_k\}}, \forall k \in \mathbb{N}$ and $\sum_{j=1}^{N_k} \theta_{k,j} = 1$ where $\delta_{y_{k,j}^{x,t}}$ denotes a delta measure:

$$\delta_{y_{k,j}^{x,t}}(E) = \begin{cases} 1 & \text{if } y_{k,j} \in E \\ 0 & \text{if } y_{k,j} \notin E \end{cases}$$

- Thus we have:

$$(S(t)Q_0)(x) = \lim_{k \rightarrow \infty} \sum_{j=1}^{N_k} \theta_{k,j} Q_0(y_{k,j}^{x,t}) \quad (8)$$

where for each $k \in \mathbb{N}$ we have $\sum_{j=1}^{N_k} \theta_{k,j} = 1$, i.e. $S(t)Q_0(x)$ is in the convex hull of Q_0 .

Physicality in a basic case IV: nonlinearity preserves the convex hull

- Consider the ODE:

$$\frac{dQ}{dt} = -aQ + b(Q^2 - \frac{\text{tr}}{3}Q^2) + cQ\text{tr}(Q^2)$$

- If the initial data is Q_0 , then there exists an orthogonal matrix so that $RQ_0R^t = D$ where D is a diagonal matrix (with eigenvalues of Q_0 on the diagonal)
- One can apply R on the left hand side and R^t on the right hand side of the ODE, and using $R^tR = RR^t = Id$ to get a system for a diagonal matrix (in terms of eigenvalues of Q only)
- One can check that the restriction on the range of eigenvalues is preserved by the flow (as the flow is still a gradient one).

Concluding remarks

- A dynamic theory might provide a substitute for the failure of a static one.
- Typical dichotomy: long time well-posedness for small data, blow-up for large data.
- The threshold size might be related to the physicality.
- Maximum principle can be seen as a cruder version of physicality.
- Physicality preservation seems to be related to the well-posedness of the part of the flow generated by the (purely) quadratic (in gradient) terms.