On the cubic instability in the Q-tensor theory of nematics

Arghir Zarnescu

University of Sussex

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

Symmetry, bifurcation and order parameters

Cambridge, 9 January 2013

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 $(Q_{ij}(x))_{i,j=1,\ldots,d}$ 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.

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 $(Q_{ij}(x))_{i,j=1,\ldots,d}$ 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.

- 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

$$\psi_B(Q) = \bar{\psi}_B(\mathrm{tr}(Q^2), \mathrm{tr}(Q^3)).$$

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

$$\psi_B(Q) = \bar{\psi}_B(\mathrm{tr}(Q^2), \mathrm{tr}(Q^3)).$$

- Example of elastic terms that respect the physical invariances:

$$I_1 = Q_{ij,k}Q_{ij,k},\ I_2 = Q_{ij,j}Q_{ik,k},$$

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

  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 $L_4 \neq 0$ 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): $Q = s(x)\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} Id\right)$ for suitable $s(x)$ (then $I_4 = \frac{4}{9} s(s'^2 - \frac{3}{r^2} s^2)$).

The cubic instability

- Take an elastic energy:

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

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

- If $L_4 \neq 0$ 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): $Q = s(x)\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} Id\right)$ for suitable $s(x)$ (then $I_4 = \frac{4}{9} s(s'^2 - \frac{3}{r^2} s^2)$).
- 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-statistical mechanics interpretation and constraints

- $$Q = \int_{\mathbb{S}^2} p \otimes p \, d\mu(p) - \frac{1}{3} Id$$

Q-tensors-statistical mechanics interpretation and constraints

- $$Q = \int_{\mathbb{S}^2} p \otimes p \, d\mu(p) - \frac{1}{3} Id$$

- Q is a 3×3 symmetric, traceless matrix - a Q-tensor

Q-tensors-statistical mechanics interpretation and constraints

- $$Q = \int_{\mathbb{S}^2} p \otimes p \, d\mu(p) - \frac{1}{3} Id$$
- 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

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

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

Q-tensors and alternative theories

- Q is a 3×3 symmetric, traceless matrix - a Q-tensor

Q-tensors and alternative theories

- Q is a 3×3 symmetric, traceless matrix - a Q-tensor
- A physical Q-tensor is one for which the eigenvalues are in $(-\frac{1}{3}, \frac{2}{3})$.
- The Q-tensor is:
  - isotropic is $Q = 0$
  - uniaxial if it has two equal eigenvalues
  - biaxial otherwise

Q-tensors and alternative theories

- Q is a 3×3 symmetric, traceless matrix - a Q-tensor
- A physical Q-tensor is one for which the eigenvalues are in $(-\frac{1}{3}, \frac{2}{3})$.
- The Q-tensor is:
  - isotropic is $Q = 0$
  - uniaxial if it has two equal eigenvalues
  - biaxial otherwise
- **Ericksen's theory (1991)** for uniaxial Q-tensors which can be written as

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

Q-tensors and alternative theories

- Q is a 3×3 symmetric, traceless matrix - a Q-tensor
- A physical Q-tensor is one for which the eigenvalues are in $(-\frac{1}{3}, \frac{2}{3})$.
- The Q-tensor is:
  - isotropic is $Q = 0$
  - uniaxial if it has two equal eigenvalues
  - biaxial otherwise
- **Ericksen's theory (1991)** for uniaxial Q-tensors which can be written as

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

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

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

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

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

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

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

$$+ \int_\Omega (K_2 + K_4)(\mathrm{tr}(\nabla n)^2 - (\mathrm{div} n)^2)] \, dx$$

the Oseen-Frank energy functional.

$\Pi\alpha\nu\tau\alpha\ \rho\epsilon\iota$

$H\epsilon\rho\alpha\kappa\lambda\epsilon\iota\tau o\zeta$

$\Pi\alpha\nu\tau\alpha\ \rho\epsilon\iota$

$H\epsilon\rho\alpha\kappa\lambda\epsilon\iota\tau o\zeta$

Everything flows

Heraclitus

The L^2 gradient flow

- A gradient flow:

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

The L^2 gradient flow

- A gradient flow:

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

- 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 $\mathrm{tr}(Q) = 0$ and $\mu_{ij}, i, j = 1, 2, 3$ are Lagrange multipliers corresponding to the constraint $Q_{ij} = Q_{ji}$.

The L^2 gradient flow

- A gradient flow:

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

- 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 $\mathrm{tr}(Q) = 0$ and $\mu_{ij}, i, j = 1, 2, 3$ are Lagrange multipliers corresponding to the constraint $Q_{ij} = Q_{ji}$.

- More explicitly and for the standard potential $\psi_B(Q) = \frac{a}{2} tr(Q^2) + \frac{b}{3} tr(Q^3) + \frac{c}{4} tr^2(Q^2)$ this becomes:

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

“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.

$$F[Q(t)] = \int_\Omega \underbrace{L_1|\nabla Q|^2 + L_2\nabla_j Q_{ik}\nabla_k Q_{ij} + L_3\nabla_j Q_{ij}\nabla_k Q_{ik}}_{\geq \mu\|\nabla Q\|^2_{L^2}} + \underbrace{L_4 Q_{lk}}_{\text{small?}}\nabla_k Q_{ij}\nabla_l Q_{ij}\,dx$$

$$+\int_\Omega \underbrace{\frac{a}{2}tr(Q^2) + \frac{b}{3}tr(Q^3) + \frac{c}{4}tr^2(Q^2)}_{\geq -c_0^2}\,dx \leq F[Q_0]$$

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 $\sqrt{Q_{ij}(t,x)Q_{ij}(t,x)} < M$?

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 $\sqrt{Q_{ij}(t,x)Q_{ij}(t,x)} < M$?
- 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

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

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

Large initial data blow-up: the radial hedgehog ansatz

- We take the ansatz

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

- The gradient flow reduces to:

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

- 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 $\int_{R_0}^{R_1} \theta_-^2 r^2 \, dr$.

"Small" initial data: maximum principle in a restricted case

Proposition

For the evolution system mentioned before, suppose Ω is a smooth, bounded region. If $L_2 + L_3 = 0$, and the initial and boundary data for Q satisfy

$$\|tr(Q_0)\|_{L^\infty} \leq \sqrt{\eta},$$

then

$$\|tr(Q)\|_{L^\infty}(t) \leq \sqrt{\eta}, \ \ \forall \ t \geq 0.$$

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 $\int_\Omega h^2(Q)$.

Physicality in a basic case I: the operator splitting intuition

- Can one understand in an intuitive way if the equation preserves “physicality”?

Physicality in a basic case I: the operator splitting intuition

- Can one understand in an intuitive way if the equation preserves “physicality”?
- 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

Physicality in a basic case I: the operator splitting intuition

- Can one understand in an intuitive way if the equation preserves “physicality”?
- 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
- In general one can expect to obtain the solution $u(t)$ of the equation, starting from initial data u_0 as:

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

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:

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

  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:

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

  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:

$$\int_{\mathbb{R}^3} Q_0(y)d\mu_x(y) = \lim_{k\to\infty} \sum_{j=1}^{N_k} \theta_{k,j} \int_{\mathbb{R}^3} Q_0(y)\delta_{y^{x,t}_{k,j}} \tag{4}$$

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

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

- Thus we have:

$$\left(S(t)Q_0\right)(x) = \lim_{k\to\infty} \sum_{j=1}^{N_k} \theta_{k,j} Q_0(y^{x,t}_{k,j}) \tag{5}$$

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:

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

- 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.
- Physicality preservation is related to the well-posedness of the dynamical model.
- 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.