Liquid crystals inertia in the Qian-Sheng model

Arghir Dani Zarnescu

University of Sussex
and
"Simion Stoilow" Institute
of the Romanian Academy

joint work with
Francesco de Anna (Université de Bordeaux)

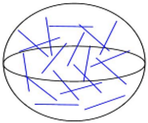
Partial Order: Mathematics, Simulations and Applications
25 January 2016

Liquid crystals modelling: physics

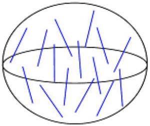
Isotropic liquid phase　　Nematic liquid crystal phase

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

Liquid crystals modelling: physics



Isotropic liquid phase



Nematic liquid crystal phase

- A measure μ such that $0 \leq \mu(A) \leq 1 \; \forall A \subset \mathbb{S}^2$
- The probability that the molecules are pointing in a direction contained in the surface $A \subset \mathbb{S}^2$ is $\mu(A)$

Liquid crystals modelling: physics

- A measure μ such that $0 \leq \mu(A) \leq 1\ \forall A \subset \mathbb{S}^2$
- The probability that the molecules are pointing in a direction contained in the surface $A \subset \mathbb{S}^2$ is $\mu(A)$
- Physical requirement $\mu(A) = \mu(-A)\ \forall A \subset \mathbb{S}^2$

Liquid crystals modelling: physics

Isotropic liquid phase   Nematic liquid crystal phase

- A measure μ such that $0 \leq \mu(A) \leq 1 \ \forall A \subset \mathbb{S}^2$
- The probability that the molecules are pointing in a direction contained in the surface $A \subset \mathbb{S}^2$ is $\mu(A)$
- Physical requirement $\mu(A) = \mu(-A) \ \forall A \subset \mathbb{S}^2$

LdG Q-tensor reduction and earlier theories

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

LdG Q-tensor reduction and earlier theories

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

- The Q-tensor is:
  - isotropic is $Q = 0$
  - uniaxial if it has two equal eigenvalues
  - biaxial otherwise

LdG Q-tensor reduction and earlier theories

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

- 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

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

LdG Q-tensor reduction and earlier theories

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

- 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

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

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

Director theory: stationary aspects and the Oseen-Frank energy

Stationary states obtained as minimisers of the Oseen-Frank free energy:

$$F_{OF}[n, \nabla n] = \int_{\Omega} W(n(x), \nabla n(x))\, dx$$

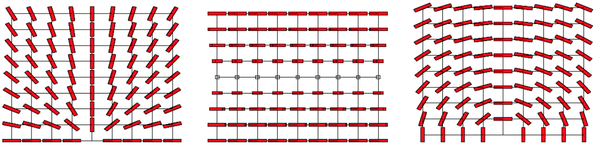
Director theory:
stationary aspects and the Oseen-Frank energy

Stationary states obtained as minimisers of the Oseen-Frank free energy:

$$F_{OF}[n, \nabla n] = \int_{\Omega} W(n(x), \nabla n(x))\, dx$$

where

$$W(n, \nabla n) := K_{11} |\mathrm{div}\, n|^2 + K_{22} |n \cdot \mathrm{curl} n|^2 + K_{33} |n \times \mathrm{curl} n|^2 + (K_{22} + K_{24}) \underbrace{\left(\mathrm{tr}(\nabla n)^2 - (\mathrm{div}\, n)^2\right)}_{\text{saddle-splay(?)}} + K_{13} \underbrace{\mathrm{div}\, [(\mathrm{div}\, n) n]}_{\text{splay-bend(?)}}$$



Twist Bend Splay

The dynamic theory and inertia

The derivation of the dynamic equations starts was proposed by Ericksen and then adjusted by Leslie and starts from an energy balance :

$$\frac{d}{dt}\int_V \frac{1}{2}u\cdot u + \frac{1}{2}\sigma n\cdot n + W\,dv$$
$$= \int_V (-\Delta)\,dx + \text{ boundary terms and ``harmless terms''}$$

with u the flow, Δ a dissipation function and W the Oseen-Frank energy

The dynamic theory and inertia

The derivation of the dynamic equations starts was proposed by Ericksen and then adjusted by Leslie and starts from an energy balance :

$$\frac{d}{dt}\int_V \frac{1}{2}u\cdot u + \frac{1}{2}\sigma n\cdot n + W\,dv$$
$$= \int_V (-\Delta)\,dx + \text{ boundary terms and “harmless terms”}$$

with u the flow, Δ a dissipation function and W the Oseen-Frank energy

Concerning σ, F. Leslie in *Adv in Physics, v. 4, 1978* stated:

“the term involving σ represents rotational kinetic energy of the material element and therefore σ is an inertial constant. While this contribution to the kinetic energy is undoubtely negligible in most circumstances we retain it in the general form which follows, since it could conceivably play a nontrivial role when the anisotropic axis is subjected to large accelerations”

General Ericksen-Leslie system

Balance of Momentum:

$$\rho(\partial_t u + u \cdot \nabla u) = \operatorname{div}(-pId + \frac{\partial \Delta}{\partial \nabla u})$$

Balance of Angular Momentum:

$$\sigma \ddot{n} = -\frac{\partial W}{\partial n} + \frac{\partial \Delta}{\partial \dot{n}} + \gamma n$$

We have the *"material derivative"*

$$\dot{n} = (\partial_t + u \cdot \nabla)n$$

and the dissipation function

$$\Delta = \alpha_1 (n \cdot An)^2 + \alpha_4 (\mathrm{tr}(A^2) + \alpha_5 + \alpha_6 \|\Delta \otimes An\|^2 + \gamma_1 \|N\|^2 + 2\gamma_2 N \cdot An$$

with the *"Oldroyd derivative"*

$$N = \dot{n} - \frac{1}{2}(\nabla u - \nabla u^T)n$$

and $A = \frac{1}{2}(\nabla u + \nabla u^T)$.

Remarks on the Ericksen-Leslie system

Balance of Momentum:

$$\rho(\partial_t u + u \cdot \nabla u) = \operatorname{div}(-pId + \frac{\partial \Delta}{\partial \nabla u}) + \rho F$$

Balance of Angular Momentum:

$$\sigma \ddot{n} = -\frac{\partial W}{\partial n} + \frac{\partial \Delta}{\partial n} + \gamma n + G$$

Remarks on the Ericksen-Leslie system

Balance of Momentum:

$$\rho(\partial_t u + u \cdot \nabla u) = \mathrm{div}(-pId + \frac{\partial \Delta}{\partial \nabla u}) + \rho F$$

Balance of Angular Momentum:

$$\sigma \ddot{n} = -\frac{\partial W}{\partial n} + \frac{\partial \Delta}{\partial n} + \gamma n + G$$

- The equations for the stationary states are obtained formally by deleting all the other terms involving u.

Remarks on the Ericksen-Leslie system

Balance of Momentum:

$$\rho(\partial_t u + u \cdot \nabla u) = \operatorname{div}(-pId + \frac{\partial \Delta}{\partial \nabla u}) + \rho F$$

Balance of Angular Momentum:

$$\sigma \ddot{n} = -\frac{\partial W}{\partial n} + \frac{\partial \Delta}{\partial n} + \gamma n + G$$

- The equations for the stationary states are obtained formally by deleting all the other terms involving u.
- We have a double material derivative on n (i.e. a nonlinear operator on n)

$$\ddot{n} = \partial_t^2 n + 2u \cdot \nabla \partial_t n + u \nabla u \nabla n + u(\nabla^2 n) u$$

Remarks on the Ericksen-Leslie system

Balance of Momentum:

$$\rho(\partial_t u + u \cdot \nabla u) = \operatorname{div}(-pId + \frac{\partial \Delta}{\partial \nabla u}) + \rho F$$

Balance of Angular Momentum:

$$\sigma \ddot{n} = -\frac{\partial W}{\partial n} + \frac{\partial \Delta}{\partial n} + \gamma n + G$$

- The equations for the stationary states are obtained formally by deleting all the other terms involving u.
- We have a double material derivative on n (i.e. a nonlinear operator on n)

$$\ddot{n} = \partial_t^2 n + 2u \cdot \nabla \partial_t n + u \nabla u \nabla n + u(\nabla^2 n)u$$

- The most troublesome part is the Lagrange multiplier γ that generates high derivatives!

The Q-tensor theory: the free energy functional

- Energy functional:

$$\mathcal{F}_{LG}[Q] = \int_\Omega \frac{L}{2} Q_{ij,k}(x) Q_{ij,k}(x) + f_B(Q(x))\, dx$$

with bulk term

$$f_B(Q) = \frac{\alpha(T - T^*)}{2} \mathrm{tr}\left(Q^2\right) - \frac{b}{3} \mathrm{tr}\left(Q^3\right) + \frac{c}{4}\left(\mathrm{tr} Q^2\right)^2$$

where $Q(x) : \Omega \to \{M \in \mathbb{R}^{3\times 3}, M = M^t, \mathrm{tr} M = 0\}$ a Q-tensor

The Q-tensor theory: the free energy functional

- Energy functional:

$$\mathcal{F}_{LG}[Q] = \int_\Omega \frac{L}{2} Q_{ij,k}(x) Q_{ij,k}(x) + f_B(Q(x))\, dx$$

  with bulk term

$$f_B(Q) = \frac{\alpha(T - T^*)}{2} \mathrm{tr}\left(Q^2\right) - \frac{b}{3} \mathrm{tr}\left(Q^3\right) + \frac{c}{4}\left(\mathrm{tr} Q^2\right)^2$$

  where $Q(x) : \Omega \to \{M \in \mathbb{R}^{3\times 3}, M = M^t, \mathrm{tr} M = 0\}$ a Q-tensor

- After a suitable non-dimensionalisation (á la E.Gartland for instance)

$$\tilde{\mathcal{F}}_{LG}[Q] = \int_\Omega \frac{1}{2} Q_{ij,k}(x) Q_{ij,k}(x) + \frac{t}{2} \mathrm{tr}\left(Q^2\right) - \sqrt{6}\mathrm{tr}\left(Q^3\right) + \frac{1}{2}\left(\mathrm{tr} Q^2\right)^2$$

The free energy and the bulk potential

- The bulk potential

$$\tilde{f}_B(Q) = \frac{t}{2}\mathrm{tr}\left(Q^2\right) - \sqrt{6}\mathrm{tr}\left(Q^3\right) + \frac{1}{2}\left(\mathrm{tr}Q^2\right)^2$$

captures the physical specificity. It has three sets of critical points:

- the isotropic points,
- A set of nematic states $\mathcal{S}_- := \{s_-(t)(n \otimes n - \frac{1}{3}Id), n \in \mathbb{S}^2\}$
- Another set of nematic states $\mathcal{S}_+ = \{s_+(t)(n \otimes n - \frac{1}{3}Id), n \in \mathbb{S}^2\}$

The free energy and the bulk potential

- The bulk potential

$$\tilde{f}_B(Q) = \frac{t}{2}\mathrm{tr}\left(Q^2\right) - \sqrt{6}\mathrm{tr}\left(Q^3\right) + \frac{1}{2}\left(\mathrm{tr}Q^2\right)^2$$

  captures the physical specificity. It has three sets of critical points:
  - the isotropic points,
  - A set of nematic states $\mathcal{S}_- := \{s_-(t)(n \otimes n - \frac{1}{3}Id), n \in \mathbb{S}^2\}$
  - Another set of nematic states $\mathcal{S}_+ = \{s_+(t)(n \otimes n - \frac{1}{3}Id), n \in \mathbb{S}^2\}$

- Stability of the critical points:
  - For $t > 1$ the isotropic state is globally stable
  - For $t \in (0, 1)$ the isotropic state is locally stable with $\mathcal{S}_+$ a global minimizer with $\mathcal{S}_-$ unstable
  - Fro $t < 0$ the isotropic state is unstable with $\mathcal{S}_+$ a global minimizer and $\mathcal{S}_-$ local minimizer

The Qian-Sheng model

$$\dot{v} + \nabla p - \frac{\beta_4}{2}\Delta v = \nabla \cdot \Big(-\nabla Q \otimes \nabla Q + \beta_1 Q \mathrm{tr}\{QA\} + \beta_5 AQ + \beta_6 QA \Big) + \nabla \cdot \left(\frac{\mu_2}{2}(\dot{Q} - [\Omega, Q]) + \mu_1 \left[Q, (\dot{Q} - [\Omega, Q])\right] \right)$$

$$J\ddot{Q} + \mu_1 \dot{Q} = \Delta Q - \mathcal{L}\frac{\partial f_B}{\partial Q} - \mu_2 A + \mu_1 [\Omega, Q]$$

where we denoted $[A, B] := AB - BA$ and $\mathcal{L}$ the projection onto the space of trace-free matrices, hence

$$\mathcal{L}\frac{\partial f_B(Q)}{\partial Q} = \frac{\partial f_B(Q)}{\partial Q} - \frac{1}{3}\mathrm{tr}\left(\frac{\partial f_B(Q)}{\partial Q}\right) I_3$$

The Qian-Sheng model

$$\dot{v} + \nabla p - \frac{\beta_4}{2}\Delta v = \nabla\cdot\Big(- \nabla Q \otimes \nabla Q + \beta_1 Q \mathrm{tr}\{QA\} + \beta_5 AQ + \beta_6 QA \Big) + \nabla\cdot\left(\frac{\mu_2}{2}(\dot{Q} - [\Omega, Q]) + \mu_1 \left[Q, (\dot{Q} - [\Omega, Q])\right] \right)$$

$$J\ddot{Q} + \mu_1\dot{Q} = \Delta Q - \mathcal{L}\frac{\partial f_B}{\partial Q} - \mu_2 A + \mu_1[\Omega, Q]$$

where we denoted $[A, B] := AB - BA$ and $\mathcal{L}$ the projection onto the space of trace-free matrices, hence

$$\mathcal{L}\frac{\partial f_B(Q)}{\partial Q} = \frac{\partial f_B(Q)}{\partial Q} - \frac{1}{3}\mathrm{tr}\left(\frac{\partial f_B(Q)}{\partial Q}\right) I_3$$

Note the signs of the μ_2 in the two equations, as we will be lead

soon to the μ_2 conundrum!...

Remarks on the viscosity coefficients

There are six viscosity coefficients $\beta_1, \beta_4, \beta_5, \beta_6$ and μ_1, μ_2.

- We have a "Parodi-type relation"

$$\beta_5 - \beta_6 = \mu_2$$

- The coefficient β_4 corresponds to the Newtonian viscosity so we assume:

$$\beta_4 > 0$$

- All the coefficients are non-dimensional. For a common physical example, the MBBA material, we have:

$$\frac{\mu_2}{\mu_1} \sim -1.92, \frac{\beta_1}{\mu_1} \sim 0.17, \frac{\beta_4}{\mu_1} \sim 0.7, \frac{\beta_5}{\mu_1} \sim 0.7, \frac{\beta_6}{\mu_1} \sim -0.79$$

- Note $\beta_5 + \beta_6 \sim 0$

The energy and its behaviour

One would like to have the energy conservation:

$$\frac{d}{dt}\int |u|^2 + J|\dot{Q}|^2 + \underbrace{\frac{1}{2}|\nabla Q|^2 + f_B(Q)}_{\text{the free energy}}\,dx = 0$$

This is nearly the case and we have:

The energy and its behaviour

One would like to have the energy conservation:

$$\frac{d}{dt}\int |u|^2 + J|\dot{Q}|^2 + \underbrace{\frac{1}{2}|\nabla Q|^2 + f_B(Q)}_{\text{the free energy}}\, dx = 0$$

This is nearly the case and we have:

Proposition. *Let (v, Q) be a smooth solution of the Qian-Sheng system in the whole space and decaying sufficiently fast at infinity.*

Assume that the Newtonian viscosity β_4 is positive and large enough compared to the other viscosities $\beta_1, \beta_5, \beta_6, \mu_1$ and μ_2 with $\mu_1 > 0$.

Furthermore assume that the inertia J is sufficiently small compared to μ_1.
Then we have the a priori bounds:

$$\|u\|_{L^\infty(0,T;L^2)\cap L^2(0,T;H^1)}, |\dot{Q}|_{L^\infty(0,T;L^2)}, |\nabla Q|_{L^\infty(0,T;L^2)}, |Q|_{L^\infty((0,T);L^2)} < \infty$$

Weak solutions trouble

Recall that out of the energy law we have the bounds

$$\|u\|_{L^\infty(0,T;L^2)\cap L^2(0,T;H^1)}, |\dot{Q}|_{L^\infty(0,T;L^2)}, |\nabla Q|_{L^\infty(0,T;L^2)}, |Q|_{L^\infty((0,T);L^2)} < \infty$$

Weak solutions trouble

Recall that out of the energy law we have the bounds

$$\|u\|_{L^\infty(0,T;L^2)\cap L^2(0,T;H^1)}, |\dot{Q}|_{L^\infty(0,T;L^2)}, |\nabla Q|_{L^\infty(0,T;L^2)}, |Q|_{L^\infty((0,T);L^2)} < \infty$$

These are not sufficient for passing to the limit in certain terms, such as the stress tensor:

$$\nabla \cdot \Big(-\nabla Q \otimes \nabla Q \Big)$$

(unlike for instance in a parabolic setting where one could use the additional bound $\|Q\|_{L^2(0,T;H^2)}$ and weaken the test functions, to pass to the limit)

Higher regularity solutions

Theorem. *Consider the Qian-Sheng model in dimension two. If we assume the initial data u_0 and Q_0 small enough in H^s and H^{s+1}, with $s > 1$, then there exists an unique classical solutions (v, Q) which is global in time with*

$$v \in L^\infty_t H^s \cap L^2_t H^{s+1}, \quad Q \in L^\infty_t H^{s+1}$$

$$\textit{with} \quad \dot{Q} = \partial_t Q + v \cdot \nabla Q \in L^\infty_t H^s \cap L^2_t H^s.$$

The twist waves of Ericksen and beyond

Question: J.L. Ericksen(1968): could there be solutions of the coupled Ericksen-Leslie system? for which the flow is zero...

The twist waves of Ericksen and beyond

Question: J.L. Ericksen(1968): could there be solutions of the coupled Ericksen-Leslie system? for which the flow is zero...
Answer: yes- **the twist waves**...

The twist waves of Ericksen and beyond

Question: J.L. Ericksen(1968): could there be solutions of the coupled Ericksen-Leslie system? for which the flow is zero...
Answer: yes- **the twist waves**...

What would this mean in our Q-tensor context?

The twist waves of Ericksen and beyond

Question: J.L. Ericksen(1968): could there be solutions of the coupled Ericksen-Leslie system? for which the flow is zero...
Answer: yes- **the twist waves...**

What would this mean in our Q-tensor context?

$$\dot{v} + \nabla p - \frac{\beta_4}{2}\Delta v = \nabla \cdot \Big(-\nabla Q \otimes \nabla Q + \beta_1 Q \mathrm{tr}\{QA\} + \beta_5 AQ + \beta_6 QA \Big) + \nabla \cdot \left(\frac{\mu_2}{2}(\dot{Q} - [\Omega, Q]) + \mu_1 \left[Q, (\dot{Q} - [\Omega, Q])\right] \right)$$

$$J\ddot{Q} + \mu_1 \dot{Q} = \Delta Q - \mathcal{L}\frac{\partial f_B}{\partial Q} - \mu_2 A + \mu_1 [\Omega, Q]$$

Also the $\dot{Q}$, $\ddot{Q}$ simplify to Q_t respectively Q_{tt}.

The twist waves as an overconstrained wave system

Just a damped nonlinear wave system:

$$JQ_{tt} + \mu_1 Q_t = \Delta Q - \mathcal{L}\frac{\partial f_B}{\partial Q}$$

but with an additional constraint....

$$\nabla \cdot \Big(-\nabla Q \otimes \nabla Q \Big) + \nabla \cdot \left(\frac{\mu_2}{2} Q_t + \mu_1 \left[Q, Q_t \right] \right) = \nabla p$$

The twist waves as an overconstrained wave system

Just a damped nonlinear wave system:

$$JQ_{tt} + \mu_1 Q_t = \Delta Q - \mathcal{L}\frac{\partial f_B}{\partial Q}$$

but with an additional constraint....

$$\nabla \cdot \Big(-\nabla Q \otimes \nabla Q \Big) + \nabla \cdot \left(\frac{\mu_2}{2} Q_t + \mu_1 \left[Q, Q_t \right] \right) = \nabla p$$

Natural question: is there at least one such system?

An expected twist wave: the melting hedgehog wave...

We take

$$T(t,x) := s(t,|x|)\bar{H}(x)$$

with $s : \mathbb{R}_+ \times R \to R$ a function to be determined and $\bar{H}$ the "hedgehog" function:

$$H_{ij}(x) := \frac{x_i x_j}{|x|^2} - \frac{\delta_{ij}}{3}, i,j = 1,2,3$$

Then one can check that the wave system for Q reduces to an equation for s only, namely:

$$Js_{tt} + \mu_1 s_t = s_{rr} + \frac{2s_r}{r} - \frac{6s}{r^2} - as + \frac{2b}{3}s^2 - \frac{2c}{3}s^3$$

for which one can show global existence for arbitrary data.

An expected twist wave: the melting hedgehog wave...

We take

$$T(t,x) := s(t,|x|)\bar{H}(x)$$

with $s : \mathbb{R}_+ \times R \to R$ a function to be determined and $\bar{H}$ the "hedgehog" function:

$$H_{ij}(x) := \frac{x_i x_j}{|x|^2} - \frac{\delta_{ij}}{3}, i,j = 1,2,3$$

Then one can check that the wave system for Q reduces to an equation for s only, namely:

$$Js_{tt} + \mu_1 s_t = s_{rr} + \frac{2s_r}{r} - \frac{6s}{r^2} - as + \frac{2b}{3}s^2 - \frac{2c}{3}s^3$$

for which one can show global existence for arbitrary data.

Still, this is somewhat disappointing as it does not require inertia to exist...(just like Ericksen original example).

An expected twist wave: the melting hedgehog wave...

We take

$$T(t,x) := s(t,|x|)\bar{H}(x)$$

with $s : \mathbb{R}_+ \times R \to R$ a function to be determined and $\bar{H}$ the "hedgehog" function:

$$H_{ij}(x) := \frac{x_i x_j}{|x|^2} - \frac{\delta_{ij}}{3}, i,j = 1,2,3$$

Then one can check that the wave system for Q reduces to an equation for s only, namely:

$$Js_{tt} + \mu_1 s_t = s_{rr} + \frac{2s_r}{r} - \frac{6s}{r^2} - as + \frac{2b}{3}s^2 - \frac{2c}{3}s^3$$

for which one can show global existence for arbitrary data.

Still, this is somewhat disappointing as it does not require inertia to exist...(just like Ericksen original example).
Natural question remaining: are there other examples of twist waves?

THANK YOU!