

Recent results on the evolution of liquid crystals flows

E. Rocca

Università degli Studi di Milano

WIAS, Berlin, May 15, 2012

Supported by the FP7-IDEAS-ERC-StG Grant “EntroPhase”



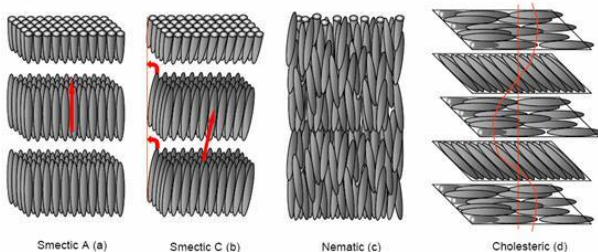
Plan of the Talk

- ▶ The objective: include the **temperature dependence** in models describing the **evolution** of nematic liquid crystal flows within both the Oseen-Frank and Landau-De Gennes theories
- ▶ Our results:
 1. E. Feireisl, M. Frémond, E. R., G. Schimperna, A new approach to non-isothermal models for nematic liquid crystals, ARMA, to appear, preprint arXiv:1104.1339v1 (2011)
 2. E. Feireisl, E.R., G. Schimperna, A. Zarnescu, Evolution of non-isothermal Landau-de Gennes nematic liquid crystals flows, paper in preparation
- ▶ Some future perspectives and open problems

The motivation

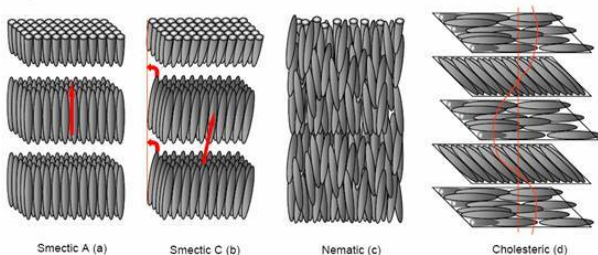
- Liquid crystals are a state of matter that have properties **between** those of a conventional **liquid and** those of a **solid crystal**. A liquid crystal may flow like a liquid, but its molecules may be oriented in a crystal-like way
- Theoretical studies of these types of materials are motivated by **real-world applications**: proper functioning of many practical devices relies on optical properties of certain liquid crystalline substances in the presence or absence of an electric field: **a multi-billion dollar industry**
- At the molecular level, what marks the difference between a liquid crystal and an ordinary, isotropic fluid is that, while the centers of mass of LC molecules do not exhibit any long-range correlation, **molecular orientations do exhibit orientational correlations**

To the present state of knowledge, three main types of liquid crystals are distinguished, termed *smectic*, *nematic* and *cholesteric*



<http://www.laynetworks.com/Molecular-Orientation-in-Liquid-Crystal-Phases.htm>

To the present state of knowledge, three main types of liquid crystals are distinguished, termed *smectic*, *nematic* and *cholesteric*



<http://www.laynetworks.com/Molecular-Orientation-in-Liquid-Crystal-Phases.htm>

The *smectic* phase forms well-defined layers that can slide one over another in a manner very similar to that of a soap

The *nematic* phase: the molecules have long-range orientational order, but no tendency to the formation of layers. Their center of mass positions all point in the **same direction** (within each specific domain)

Crystals in the *cholesteric* phase exhibit a twisting of the molecules perpendicular to the director, with the molecular axis parallel to the director

Our main aim

Our main aim

- We consider the range of temperatures typical for the **nematic phase**



<http://www.netwalk.com/laserlab/lclinks.html>

Our main aim

- We consider the range of temperatures typical for the **nematic phase**



<http://www.netwalk.com/laserlab/lclinks.html>

- The nematic liquid crystals are composed of rod-like molecules, with the long axes of neighboring molecules aligned

Our main aim

- We consider the range of temperatures typical for the **nematic phase**



<http://www.netwalk.com/laserlab/lclinks.html>

- The nematic liquid crystals are composed of rod-like molecules, with the long axes of neighboring molecules aligned
- Most mathematical work has been done on the Oseen-Frank theory, in which the mean orientation of the rod-like molecules is described by a **vector field \mathbf{d}** . However, more popular among physicists is the Landau-de Gennes theory, in which the order parameter describing the orientation of molecules is a matrix, the so-called **Q-tensor**

Our main aim

- We consider the range of temperatures typical for the **nematic phase**



<http://www.netwalk.com/laserlab/lclinks.html>

- The nematic liquid crystals are composed of rod-like molecules, with the long axes of neighboring molecules aligned
- Most mathematical work has been done on the Oseen-Frank theory, in which the mean orientation of the rod-like molecules is described by a **vector field \mathbf{d}** . However, more popular among physicists is the Landau-de Gennes theory, in which the order parameter describing the orientation of molecules is a matrix, the so-called **Q-tensor**
- ▶ The flow **velocity \mathbf{u}** evidently disturbs the alignment of the molecules and also the converse is true: a change in the alignment will produce a perturbation of the velocity field \mathbf{u} . Moreover, we want to include in our model also the **changes of the temperature θ**

Plan

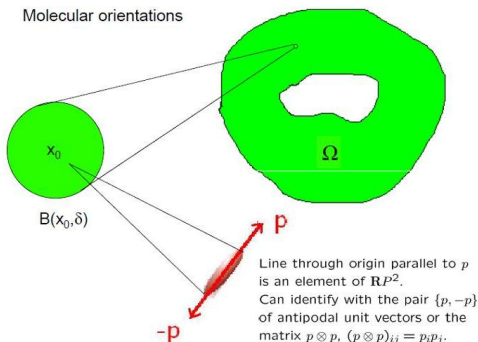
- ▶ Introduce the **Oseen-Frank (Leslie-Ericksen)** and the **Landau-de Gennes** theories for static case (for which the fluid velocity is zero) in the nematic case
- ▶ Discuss the relations between the two models and **the free-energies** in the two cases (cf. the slides by J. Ball [notes for the Summer School, Benin, 2010])
- ▶ The dynamic problem: **include velocities and temperature** dependence in a simplified Leslie-Ericksen model and in a Landau-de Gennes model
- ▶ Our **analytical results in the two cases**
- ▶ Perspectives and open problems

The Landau-de Gennes theory: the molecular orientation

- Consider a nematic liquid crystal filling a bounded connected container Ω in \mathbb{R}^3 with “regular” boundary

The Landau-de Gennes theory: the molecular orientation

- Consider a nematic liquid crystal filling a bounded connected container Ω in \mathbb{R}^3 with “regular” boundary
- The distribution of molecular orientations in a ball $B(x_0, \delta)$, $x_0 \in \Omega$ can be represented as a probability measure μ on the unit sphere \mathbb{S}^2 satisfying $\mu(E) = \mu(-E)$ for $E \subset \mathbb{S}^2$
- For a continuously distributed measure we have $d\mu(p) = \rho(p)dp$ where dp is an element of the surface area on \mathbb{S}^2 and $\rho \geq 0$, $\int_{\mathbb{S}^2} \rho(p)dp = 1$, $\rho(p) = \rho(-p)$



The Landau-de Gennes theory: the Q -tensor

- The first moment $\int_{\mathbb{S}^2} p d\mu(p) = 0$, the second moment $M = \int_{\mathbb{S}^2} p \otimes p d\mu(p)$ is a symmetric non-negative 3×3 matrix (for every $\mathbf{v} \in \mathbb{S}^2$, $\mathbf{v} \cdot M \cdot \mathbf{v} = \int_{\mathbb{S}^2} (\mathbf{v} \cdot p)^2 d\mu(p) = \langle \cos^2 \theta \rangle$, where θ is the angle between p and \mathbf{v}) satisfying $\text{tr}(M) = 1$

The Landau-de Gennes theory: the \mathbb{Q} -tensor

- The first moment $\int_{\mathbb{S}^2} p \, d\mu(p) = 0$, the second moment $M = \int_{\mathbb{S}^2} p \otimes p \, d\mu(p)$ is a symmetric non-negative 3×3 matrix (for every $\mathbf{v} \in \mathbb{S}^2$, $\mathbf{v} \cdot M \cdot \mathbf{v} = \int_{\mathbb{S}^2} (\mathbf{v} \cdot p)^2 \, d\mu(p) = \langle \cos^2 \theta \rangle$, where θ is the angle between p and \mathbf{v}) satisfying $\text{tr}(M) = 1$
- If the orientation of molecules is equally distributed in all directions (the distribution is *isotropic*) and then $\mu = \mu_0$, where $d\mu_0(p) = \frac{1}{4\pi} dS$. In this case the second moment tensor is $M_0 = \frac{1}{4\pi} \int_{\mathbb{S}^2} p \otimes p \, dS = \frac{1}{3} \mathbf{1}$, because $\int_{\mathbb{S}^2} p_1 p_2 \, dS = 0$, $\int_{\mathbb{S}^2} p_1^2 \, dS = \int_{\mathbb{S}^2} p_2^2 \, dS$, etc., and $\text{tr}(M_0) = 1$

The Landau-de Gennes theory: the \mathbb{Q} -tensor

- The first moment $\int_{\mathbb{S}^2} p \, d\mu(p) = 0$, the second moment $M = \int_{\mathbb{S}^2} p \otimes p \, d\mu(p)$ is a symmetric non-negative 3×3 matrix (for every $\mathbf{v} \in \mathbb{S}^2$, $\mathbf{v} \cdot M \cdot \mathbf{v} = \int_{\mathbb{S}^2} (\mathbf{v} \cdot p)^2 \, d\mu(p) = \langle \cos^2 \theta \rangle$, where θ is the angle between p and \mathbf{v}) satisfying $\text{tr}(M) = 1$
- If the orientation of molecules is equally distributed in all directions (the distribution is *isotropic*) and then $\mu = \mu_0$, where $d\mu_0(p) = \frac{1}{4\pi} dS$. In this case the second moment tensor is $M_0 = \frac{1}{4\pi} \int_{\mathbb{S}^2} p \otimes p \, dS = \frac{1}{3} \mathbf{1}$, because $\int_{\mathbb{S}^2} p_1 p_2 \, dS = 0$, $\int_{\mathbb{S}^2} p_1^2 \, dS = \int_{\mathbb{S}^2} p_2^2 \, dS$, etc., and $\text{tr}(M_0) = 1$
- ▶ **The de Gennes \mathbb{Q} -tensor** measures the deviation of M from its isotropic value

$$\mathbb{Q} = M - M_0 = \int_{\mathbb{S}^2} \left(p \otimes p - \frac{1}{3} \mathbf{1} \right) d\mu(p)$$

- ▶ Note that (cf. [Ball, Majumdar, Molecular Crystals and Liquid Crystals (2010)])
 1. $\mathbb{Q} = \mathbb{Q}^T$
 2. $\text{tr}(\mathbb{Q}) = 0$
 3. $\mathbb{Q} \geq -\frac{1}{3} \mathbf{1}$

The Landau-de Gennes theory: the \mathbb{Q} -tensor

- The first moment $\int_{\mathbb{S}^2} p \, d\mu(p) = 0$, the second moment $M = \int_{\mathbb{S}^2} p \otimes p \, d\mu(p)$ is a symmetric non-negative 3×3 matrix (for every $\mathbf{v} \in \mathbb{S}^2$, $\mathbf{v} \cdot M \cdot \mathbf{v} = \int_{\mathbb{S}^2} (\mathbf{v} \cdot p)^2 \, d\mu(p) = \langle \cos^2 \theta \rangle$, where θ is the angle between p and \mathbf{v}) satisfying $\text{tr}(M) = 1$
- If the orientation of molecules is equally distributed in all directions (the distribution is *isotropic*) and then $\mu = \mu_0$, where $d\mu_0(p) = \frac{1}{4\pi} dS$. In this case the second moment tensor is $M_0 = \frac{1}{4\pi} \int_{\mathbb{S}^2} p \otimes p \, dS = \frac{1}{3} \mathbf{1}$, because $\int_{\mathbb{S}^2} p_1 p_2 \, dS = 0$, $\int_{\mathbb{S}^2} p_1^2 \, dS = \int_{\mathbb{S}^2} p_2^2 \, dS$, etc., and $\text{tr}(M_0) = 1$
- ▶ **The de Gennes \mathbb{Q} -tensor** measures the deviation of M from its isotropic value

$$\mathbb{Q} = M - M_0 = \int_{\mathbb{S}^2} \left(p \otimes p - \frac{1}{3} \mathbf{1} \right) d\mu(p)$$

- ▶ Note that (cf. [Ball, Majumdar, Molecular Crystals and Liquid Crystals (2010)])
 1. $\mathbb{Q} = \mathbb{Q}^T$
 2. $\text{tr}(\mathbb{Q}) = 0$
 3. $\mathbb{Q} \geq -\frac{1}{3} \mathbf{1}$

1.+2. implies $\mathbb{Q} = \lambda_1 \mathbf{n}_1 \otimes \mathbf{n}_1 + \lambda_2 \mathbf{n}_2 \otimes \mathbf{n}_2 + \lambda_3 \mathbf{n}_3 \otimes \mathbf{n}_3$, where $\{\mathbf{n}_i\}$ is an orthonormal basis of eigenvectors of \mathbb{Q} with corresponding eigenvalues λ_i such that $\lambda_1 + \lambda_2 + \lambda_3 = 0$

2.+3. implies $-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3}$

 - ▶ $\mathbb{Q} = 0$ does not imply $\mu = \mu_0$ (e.g. $\mu = \frac{1}{6} \sum_{i=1}^3 (\delta_{e_i} + \delta_{-e_i})$)

The reduction to the Oseen-Frank model

The reduction to the Oseen-Frank model

- If the eigenvalues of \mathbb{Q} are all distinct then \mathbb{Q} is said to be *biaxial* (biaxiality implies the existence of more than one preferred direction of molecular alignment)
- If two λ_i are equal then \mathbb{Q} is said to be *uniaxial* (liquid crystal materials with a single preferred direction of molecular alignment)

The reduction to the Oseen-Frank model

- If the eigenvalues of \mathbb{Q} are all distinct then \mathbb{Q} is said to be *biaxial* (biaxiality implies the existence of more than one preferred direction of molecular alignment)
- If two λ_i are equal then \mathbb{Q} is said to be *uniaxial* (liquid crystal materials with a single preferred direction of molecular alignment)

Reduction to the Oseen-Frank (1925, 1952) model (Ericksen model, 1991): the uniaxial case: $\lambda_1 = \lambda_2 = -\frac{s}{3}$, $\lambda_3 = \frac{2s}{3}$, setting $\mathbf{n}_3 = \mathbf{n}$ where \mathbf{n}_i is an orthonormal basis of eigenvectors of \mathbb{Q} corresponding to λ_i , we have

$$\mathbb{Q} = -\frac{s}{3}(\mathbf{1} - \mathbf{n} \otimes \mathbf{n}) + \frac{2s}{3}\mathbf{n} \otimes \mathbf{n} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1} \right),$$

where $-\frac{1}{2} \leq s \leq 1$.

Here $s \in \mathbb{R}$ is a real scalar order parameter that measures the degree of orientational ordering and **\mathbf{n} is a vector** representing the direction of preferred molecular alignment

The Landau-De Gennes free energy

The Landau-De Gennes free energy

Suppose (for the moment) that the material is incompressible, homogeneous and at a constant temperature T in Ω . At each $x \in \Omega$ we have an order parameter tensor $\mathbb{Q}(x)$ and **the Landau-de Gennes free energy** (defined in the space of traceless symmetric 3×3 matrixes) is

$$\mathcal{F}_{LG}(\mathbb{Q}) = \int_{\Omega} \left(\frac{L}{2} |\nabla \mathbb{Q}(x)|^2 + f_B(\mathbb{Q}(x)) \right) dx,$$

The Landau-De Gennes free energy

Suppose (for the moment) that the material is incompressible, homogeneous and at a constant temperature T in Ω . At each $x \in \Omega$ we have an order parameter tensor $\mathbb{Q}(x)$ and **the Landau-de Gennes free energy** (defined in the space of traceless symmetric 3×3 matrixes) is

$$\mathcal{F}_{LG}(\mathbb{Q}) = \int_{\Omega} \left(\frac{L}{2} |\nabla \mathbb{Q}(x)|^2 + f_B(\mathbb{Q}(x)) \right) dx,$$

where

- $|\nabla \mathbb{Q}|^2 = \sum_{i,j,k=1}^3 \mathbb{Q}_{ij,k} \mathbb{Q}_{ij,k}$ is the elastic energy density that penalizes spatial inhomogeneities and $L > 0$ is a material-dependent elastic constant
- $f_B(\mathbb{Q})$ is the **bulk free energy density**, e.g., (following [de Gennes, Prost (1995)])

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

where α , b , c are material-dependent positive constants, T is the absolute temperature and T^* is a characteristic liquid crystal temperature. Call $a = \alpha(T - T^*)$

Minimizers of the Landau-de Gennes free energy

Then, from $f_B(\mathbb{Q}) = \frac{\alpha(T-T^*)}{2} \text{tr}(\mathbb{Q}^2) - \frac{b}{3} \text{tr}(\mathbb{Q}^3) + \frac{c}{4} (\text{tr}(\mathbb{Q}^2))^2$, it can be shown that

- the critical points have $\lambda_1 = \lambda_2 = \lambda$, $\lambda_3 = -2\lambda$, where $\lambda = 0$ or $\lambda = \lambda_{\pm} = \frac{-b \pm \sqrt{b^2 - 12ac}}{6c}$
- Hence we find that there is **a phase transformation from an isotropic fluid to a uniaxial nematic phase at the critical temperature $\theta^* = T^* + \frac{2b^2}{27\alpha c}$**
 - ▶ If $T > \theta^*$ then the unique minimizer is $\mathbb{Q} = 0$ (isotropic)
 - ▶ if $T < \theta^*$ then the minimizers are

$$\mathbb{Q} = s_{min}(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1}), \quad \mathbf{n} \in \mathbb{S}^2,$$

with $s_{min} = \frac{b + \sqrt{b^2 - 12ac}}{2c} > 0$ (uniaxial)

The Oseen-Frank free energy

The Oseen-Frank free energy

- It can be shown (cf. [Majumdar, Zarnescu, ARMA (2010)]) that, if L is small in

$$\mathcal{F}_{LG}(\mathbb{Q}) = \int_{\Omega} \left(\frac{L}{2} |\nabla \mathbb{Q}(x)|^2 + f_B(\mathbb{Q}(x)) \right) dx,$$

it is reasonable to consider a theory where \mathbb{Q} is required to be uniaxial with constant scalar order parameter $s > 0$, i.e.

$$\mathbb{Q} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{1} \right).$$

Here $\mathbf{n} = \mathbf{n}(x) \in \mathbb{S}^2$ represents the preferred direction of molecular alignment

The Oseen-Frank free energy

- It can be shown (cf. [Majumdar, Zarnescu, ARMA (2010)]) that, if L is small in

$$\mathcal{F}_{LG}(\mathbb{Q}) = \int_{\Omega} \left(\frac{L}{2} |\nabla \mathbb{Q}(x)|^2 + f_B(\mathbb{Q}(x)) \right) dx,$$

it is reasonable to consider a theory where \mathbb{Q} is required to be uniaxial with constant scalar order parameter $s > 0$, i.e.

$$\mathbb{Q} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{1} \right).$$

Here $\mathbf{n} = \mathbf{n}(x) \in \mathbb{S}^2$ represents the preferred direction of molecular alignment

- In this case f_B is constant and we can consider only the elastic energy and calculating it in terms of \mathbf{n} we obtain the simplest form of the **Oseen-Frank free energy** (1925, 1958)

$$\mathcal{F}_{OF} = Ls^2 \int_{\Omega} |\nabla \mathbf{n}(x)|^2 dx$$

The Ball-Majumdar singular potential

The Ball-Majumdar singular potential

- In the Landau-de Gennes free energy there is **no a-priori bound on the eigenvalues**

The Ball-Majumdar singular potential

- In the Landau-de Gennes free energy there is **no a-priori bound on the eigenvalues**
- In order to **naturally enforce the physical constraints in the eigenvalues of the symmetric, traceless tensors \mathbb{Q}** , Ball and Majumdar have recently introduced in [Ball, Majumdar, Molecular Crystals and Liquid Crystals (2010)] a **singular component**

$$f(\mathbb{Q}) = \begin{cases} \inf_{\rho \in \mathcal{A}_{\mathbb{Q}}} \int_{S^2} \rho(\mathbf{p}) \log(\rho(\mathbf{p})) \, d\mathbf{p} & \text{if } \lambda_i[\mathbb{Q}] \in (-1/3, 2/3), \quad i = 1, 2, 3, \\ \infty & \text{otherwise,} \end{cases}$$

$$\mathcal{A}_{\mathbb{Q}} = \left\{ \rho : S^2 \rightarrow [0, \infty) \mid \int_{S^2} \rho(\mathbf{p}) \, d\mathbf{p} = 1; \mathbb{Q} = \int_{S^2} \left(\mathbf{p} \otimes \mathbf{p} - \frac{1}{3} \mathbb{I} \right) \rho(\mathbf{p}) \, d\mathbf{p} \right\}.$$

to the bulk free-energy f_B enforcing the eigenvalues to stay in the interval $(-\frac{1}{3}, \frac{2}{3})$.

The hydrodynamic theories in the isothermal case

The hydrodynamic theories in the isothermal case

- ⇒ The hydrodynamic theory corresponding to the Oseen-Frank free energy has been developed by Ericksen (1961) and Leslie (1968) (the celebrated **Leslie-Ericksen model**)

The hydrodynamic theories in the isothermal case

- ⇒ The hydrodynamic theory corresponding to the Oseen-Frank free energy has been developed by Ericksen (1961) and Leslie (1968) (the celebrated **Leslie-Ericksen model**)
- ⇒ The **Lin-Liu model** (1995) is obtained by replacing the unit-vector constraint on \mathbf{n} with a Ginzburg-Landau penalization $W(\mathbf{n}) = \frac{1}{4\varepsilon^2} (|\mathbf{n}|^2 - 1)^2$, on the *director field* \mathbf{n} , which should formally converge to the Leslie-Ericksen model when $\varepsilon \rightarrow 0$, but this is an important open issue!

The hydrodynamic theories in the isothermal case

- ⇒ The hydrodynamic theory corresponding to the Oseen-Frank free energy has been developed by Ericksen (1961) and Leslie (1968) (the celebrated **Leslie-Ericksen model**)
- ⇒ The **Lin-Liu model** (1995) is obtained by replacing the unit-vector constraint on \mathbf{n} with a Ginzburg-Landau penalization $W(\mathbf{n}) = \frac{1}{4\varepsilon^2} (|\mathbf{n}|^2 - 1)^2$, on the *director field* \mathbf{n} , which should formally converge to the Leslie-Ericksen model when $\varepsilon \rightarrow 0$, but this is an important open issue!
- ⇒ For the **Landau-de Gennes** free energy with “regular” potential, the hydrodynamic theory has been developed by Paicu and Zarnescu, SIAM (2011) and ARMA (2012)

Our main aims

We study the evolutionary system for liquid crystals including the temperature θ and velocity \mathbf{u} .

Our main aims

We study the evolutionary system for liquid crystals **including the temperature θ and velocity \mathbf{u}** . We deal with two type of models:

1. [E. Feireisl, M. Frémond, E.R., G. Schimperna, ARMA, to appear]: a variant of the Lin-Liu model, introduced by Sun and Liu (2009), for vectorial director field \mathbf{d}
2. [E. Feireisl, E.R., G. Schimperna, A. Zarnescu, paper in preparation]: a recent Ball-Majumdar \mathbb{Q} -tensorial model preserving the physical eigenvalue constraint on the traceless and symmetric matrices \mathbb{Q}

Model 1: the d-vectorial Lin-Liu model

The Mathematical literature on Model 1

The Mathematical literature on Model 1

- The **Leslie-Ericksen model** of liquid crystals is a system of partial differential equations coupling the **Navier-Stokes equations** governing the time evolution of the fluid velocity $\mathbf{u} = \mathbf{u}(t, x)$ with a **Ginzburg-Landau type equation** describing the motion of the director field $\mathbf{d} = \mathbf{d}(t, x)$

The Mathematical literature on Model 1

- The **Leslie-Ericksen model** of liquid crystals is a system of partial differential equations coupling the **Navier-Stokes equations** governing the time evolution of the fluid velocity $\mathbf{u} = \mathbf{u}(t, x)$ with a **Ginzburg-Landau type equation** describing the motion of the director field $\mathbf{d} = \mathbf{d}(t, x)$
- A considerably simplified version of the Leslie-Ericksen model (**Lin and Liu** model) **ignores completely the stretching and rotation effects of the director field** induced by the straining of the fluid, which can be viewed as a serious violation of the underlying physical principles

The Mathematical literature on Model 1

- The **Leslie-Ericksen model** of liquid crystals is a system of partial differential equations coupling the **Navier-Stokes equations** governing the time evolution of the fluid velocity $\mathbf{u} = \mathbf{u}(t, x)$ with a **Ginzburg-Landau type equation** describing the motion of the director field $\mathbf{d} = \mathbf{d}(t, x)$
- A considerably simplified version of the Leslie-Ericksen model (**Lin and Liu** model) **ignores completely the stretching and rotation effects of the director field** induced by the straining of the fluid, which can be viewed as a serious violation of the underlying physical principles
- Such a stretching term was subsequently treated by [**Coutand and Shkoller, C.R. Acad. Sci. Paris. Sér. I, 2001**], who proved a **local well-posedness** result for the corresponding model **without thermal effects**. The main peculiarity of this model is that the presence of the stretching term causes the **loss of the total energy balance**, which, indeed, ceases to hold

The Mathematical literature on Model 1

- The **Leslie-Ericksen model** of liquid crystals is a system of partial differential equations coupling the **Navier-Stokes equations** governing the time evolution of the fluid velocity $\mathbf{u} = \mathbf{u}(t, x)$ with a **Ginzburg-Landau type equation** describing the motion of the director field $\mathbf{d} = \mathbf{d}(t, x)$
- A considerably simplified version of the Leslie-Ericksen model (**Lin and Liu model**) **ignores completely the stretching and rotation effects of the director field** induced by the straining of the fluid, which can be viewed as a serious violation of the underlying physical principles
- Such a stretching term was subsequently treated by [**Coutand and Shkoller, C.R. Acad. Sci. Paris. Sér. I, 2001**], who proved a **local well-posedness** result for the corresponding model **without thermal effects**. The main peculiarity of this model is that the presence of the stretching term causes the **loss of the total energy balance**, which, indeed, ceases to hold
- In order to prevent this failure, [**Sun and Liu, Disc. Conti. Dyna. Sys., 2009**] introduced a variant of the Lin-Liu model, where **the stretching term is included** and a new component added to the stress tensor in order to **save the total energy balance**

Our recent previous contributions

In two directions:

Our recent previous contributions

In two directions:

- the **isothermal** case
 - [Cavaterra, E.R., in press on Z. Angew. Math. Phys.]: global in time existence of weak solutions in 3D **with the stretching term**

Our recent previous contributions

In two directions:

- the **isothermal** case
 - [Cavaterra, E.R., in press on Z. Angew. Math. Phys.]: global in time existence of weak solutions in 3D **with the stretching term**
 - [Petzeltová, E.R., Schimperna, in press on Calc. Var.] and [S. Frigeri, E.R., preprint arXiv:1205.2534v1 (2012)]: **long-time behaviour** of solutions

Our recent previous contributions

In two directions:

- the **isothermal** case
 - [Cavaterra, E.R., in press on Z. Angew. Math. Phys.]: global in time existence of weak solutions in 3D **with the stretching term**
 - [Petzeltová, E.R., Schimperna, in press on Calc. Var.] and [S. Frigeri, E.R., preprint arXiv:1205.2534v1 (2012)]: **long-time behaviour** of solutions
- the **non-isothermal** case [Feireisl, E.R., Schimperna, Nonlinearity (2011)]: **neglect the stretching effects**

Our new approach

- We propose a **new approach** to the modeling of **non-isothermal** liquid crystals, based on the principles of classical Thermodynamics and **accounting for stretching and rotation effects** of the director field

Our new approach

- We propose a **new approach** to the modeling of **non-isothermal** liquid crystals, based on the principles of classical Thermodynamics and **accounting for stretching and rotation effects** of the director field
- We **incorporate the dependence on the temperature** into the model, obtaining a **complete energetically closed system**, where the total energy is conserved, while the entropy is being produced as the system evolves in time

Our new approach

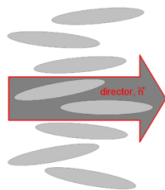
- We propose a **new approach** to the modeling of **non-isothermal** liquid crystals, based on the principles of classical Thermodynamics and **accounting for stretching and rotation effects** of the director field
- We **incorporate the dependence on the temperature** into the model, obtaining a **complete energetically closed system**, where the total energy is conserved, while the entropy is being produced as the system evolves in time
- We apply the Frémond mechanical methodology, deriving the equations by means of a generalized variational principle: the *free energy* \mathcal{F} tends to decrease in a way that is prescribed by the expression of the *pseudopotential of dissipation*, that depends (in a convex way) on a set of *dissipative variables*

Our new approach

- We propose a **new approach** to the modeling of **non-isothermal** liquid crystals, based on the principles of classical Thermodynamics and **accounting for stretching and rotation effects** of the director field
- We **incorporate the dependence on the temperature** into the model, obtaining a **complete energetically closed system**, where the total energy is conserved, while the entropy is being produced as the system evolves in time
- We apply the Frémond mechanical methodology, deriving the equations by means of a generalized variational principle: the *free energy* \mathcal{F} tends to decrease in a way that is prescribed by the expression of the *pseudopotential of dissipation*, that depends (in a convex way) on a set of *dissipative variables*
- The form of **the extra stress in the Navier-Stokes system** obtained by this method coincides with the formula derived from different principles by Sun and Liu in the isothermal case

The state variables

- the mean velocity field \mathbf{u}
- the director field \mathbf{d} , representing preferred orientation of molecules in a neighborhood of any point of a reference domain



- the absolute temperature θ

The evolution

The evolution

- The time evolution of the velocity field is governed by the **incompressible Navier-Stokes** system, with a non-isotropic stress tensor depending on the gradients of the velocity and of the director field \mathbf{d} , where the transport (viscosity) coefficients vary with temperature

The evolution

- The time evolution of the velocity field is governed by the **incompressible Navier-Stokes** system, with a non-isotropic stress tensor depending on the gradients of the velocity and of the director field \mathbf{d} , where the transport (viscosity) coefficients vary with temperature
- The **dynamics of \mathbf{d}** is described by means of a parabolic equation of Ginzburg-Landau type, with a suitable penalization term to relax the constraint $|\mathbf{d}| = 1$

The evolution

- The time evolution of the velocity field is governed by the **incompressible Navier-Stokes** system, with a non-isotropic stress tensor depending on the gradients of the velocity and of the director field \mathbf{d} , where the transport (viscosity) coefficients vary with temperature
- The **dynamics of \mathbf{d}** is described by means of a parabolic equation of Ginzburg-Landau type, with a suitable penalization term to relax the constraint $|\mathbf{d}| = 1$
- A **total energy balance** together with an **entropy inequality**, governing the dynamics of the absolute temperature θ of the system

The evolution

- The time evolution of the velocity field is governed by the **incompressible Navier-Stokes** system, with a non-isotropic stress tensor depending on the gradients of the velocity and of the director field \mathbf{d} , where the transport (viscosity) coefficients vary with temperature
- The **dynamics of \mathbf{d}** is described by means of a parabolic equation of Ginzburg-Landau type, with a suitable penalization term to relax the constraint $|\mathbf{d}| = 1$
- A **total energy balance** together with an **entropy inequality**, governing the dynamics of the absolute temperature θ of the system

⇒ The proposed model is shown compatible with *First and Second laws* of thermodynamics, and the existence of **global-in-time weak solutions** for the resulting PDE system is established, without any essential restriction on the size of the data, or on the space dimension, or on the viscosity coefficient

The director field dynamics

The director field dynamics

- We assume that the driving force governing the dynamics of the director \mathbf{d} is of **“gradient type”** $\partial_{\mathbf{d}}\mathcal{F}$, where the free-energy functional \mathcal{F} is given by

$$\mathcal{F} = \frac{\lambda}{2} |\nabla_x \mathbf{d}|^2 + \lambda W(\mathbf{d}) - \theta \log \theta$$

The director field dynamics

- We assume that the driving force governing the dynamics of the director \mathbf{d} is of **“gradient type”** $\partial_{\mathbf{d}}\mathcal{F}$, where the free-energy functional \mathcal{F} is given by

$$\mathcal{F} = \frac{\lambda}{2} |\nabla_x \mathbf{d}|^2 + \lambda W(\mathbf{d}) - \theta \log \theta$$

- Here λ is a positive constant, W penalizes the deviation of the length $|\mathbf{d}|$ from its natural value 1; generally, W is assumed to be a sum of a dominating convex (and possibly non smooth) part and a smooth non-convex perturbation of controlled growth. E.g. $W(\mathbf{d}) = (|\mathbf{d}|^2 - 1)^2$

The director field dynamics

- We assume that the driving force governing the dynamics of the director \mathbf{d} is of **“gradient type”** $\partial_{\mathbf{d}}\mathcal{F}$, where the free-energy functional \mathcal{F} is given by

$$\mathcal{F} = \frac{\lambda}{2} |\nabla_x \mathbf{d}|^2 + \lambda W(\mathbf{d}) - \theta \log \theta$$

- Here λ is a positive constant, W penalizes the deviation of the length $|\mathbf{d}|$ from its natural value 1; generally, W is assumed to be a sum of a dominating convex (and possibly non smooth) part and a smooth non-convex perturbation of controlled growth. E.g. $W(\mathbf{d}) = (|\mathbf{d}|^2 - 1)^2$
- Consequently, \mathbf{d} satisfies the following equation

$$\mathbf{d}_t + \mathbf{u} \cdot \nabla_x \mathbf{d} - \mathbf{d} \cdot \nabla_x \mathbf{u} = \frac{\lambda}{\eta} (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))$$

where the last term accounts for **stretching of the director field induced by the straining of the fluid** and η is a positive coefficient

The director field dynamics

- We assume that the driving force governing the dynamics of the director \mathbf{d} is of **“gradient type”** $\partial_{\mathbf{d}}\mathcal{F}$, where the free-energy functional \mathcal{F} is given by

$$\mathcal{F} = \frac{\lambda}{2} |\nabla_x \mathbf{d}|^2 + \lambda W(\mathbf{d}) - \theta \log \theta$$

- Here λ is a positive constant, W penalizes the deviation of the length $|\mathbf{d}|$ from its natural value 1; generally, W is assumed to be a sum of a dominating convex (and possibly non smooth) part and a smooth non-convex perturbation of controlled growth. E.g. $W(\mathbf{d}) = (|\mathbf{d}|^2 - 1)^2$
- Consequently, \mathbf{d} satisfies the following equation

$$\mathbf{d}_t + \mathbf{u} \cdot \nabla_x \mathbf{d} - \mathbf{d} \cdot \nabla_x \mathbf{u} = \frac{\lambda}{\eta} (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))$$

where the last term accounts for **stretching of the director field induced by the straining of the fluid** and η is a positive coefficient

- The presence of **the stretching term** $\mathbf{d} \cdot \nabla_x \mathbf{u}$ in the \mathbf{d} -equation prevents us from applying any maximum principle. Hence, we cannot find any L^∞ bound on \mathbf{d}

The momentum balance

The momentum balance

- ◇ In the context of nematic liquid crystals, we have the **incompressibility** constraint

$$\operatorname{div} \mathbf{u} = 0$$

The momentum balance

- ◇ In the context of nematic liquid crystals, we have the **incompressibility** constraint

$$\operatorname{div} \mathbf{u} = 0$$

- ◇ By virtue of Newton's second law, **the balance of momentum** reads

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla_x \mathbf{u} + \nabla_x p = \operatorname{div} \mathbb{S} + \operatorname{div} \boldsymbol{\sigma}^{nd} + \mathbf{g}$$

where p is the pressure, and

- the stress tensors are

$$\mathbb{S} = \frac{\mu(\theta)}{2} (\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u}), \quad \boldsymbol{\sigma}^{nd} = -\lambda \nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} + \lambda (\partial_d W(\mathbf{d}) - \Delta \mathbf{d}) \otimes \mathbf{d}$$

where $\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} := \sum_k \partial_i d_k \partial_j d_k$, μ is a temperature-dependent viscosity coefficient

The momentum balance

- ◇ In the context of nematic liquid crystals, we have the **incompressibility** constraint

$$\operatorname{div} \mathbf{u} = 0$$

- ◇ By virtue of Newton's second law, **the balance of momentum** reads

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla_x \mathbf{u} + \nabla_x p = \operatorname{div} \mathbb{S} + \operatorname{div} \boldsymbol{\sigma}^{nd} + \mathbf{g}$$

where p is the pressure, and

- the stress tensors are

$$\mathbb{S} = \frac{\mu(\theta)}{2} (\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u}), \quad \boldsymbol{\sigma}^{nd} = -\lambda \nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} + \lambda (\partial_d W(\mathbf{d}) - \Delta \mathbf{d}) \otimes \mathbf{d}$$

where $\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} := \sum_k \partial_i d_k \partial_j d_k$, μ is a temperature-dependent viscosity coefficient

- The presence of **the stretching term** $\mathbf{d} \cdot \nabla_x \mathbf{u}$ in the \mathbf{d} -equation prevents us from applying any maximum principle. Hence, we cannot find any L^∞ bound on \mathbf{d} . We will need a **weak formulation of the momentum balance**

The total energy balance

The total energy balance

$$\begin{aligned} \partial_t \left(\frac{1}{2} |\mathbf{u}|^2 + e \right) + \mathbf{u} \cdot \nabla_x \left(\frac{1}{2} |\mathbf{u}|^2 + e \right) + \operatorname{div} \left(p\mathbf{u} + \mathbf{q}^d + \mathbf{q}^{nd} - \mathbb{S}\mathbf{u} - \boldsymbol{\sigma}^{nd} \mathbf{u} \right) \\ = \mathbf{g} \cdot \mathbf{u} + \lambda \gamma \operatorname{div} \left(\nabla_x \mathbf{d} \cdot (\Delta \mathbf{d} - \partial_d W(\mathbf{d})) \right) \end{aligned}$$

with the internal energy

$$e = \frac{\lambda}{2} |\nabla_x \mathbf{d}|^2 + \lambda W(\mathbf{d}) + \theta$$

and the flux

$$\mathbf{q} = \mathbf{q}^d + \mathbf{q}^{nd} = -k(\theta) \nabla_x \theta - h(\theta) (\mathbf{d} \cdot \nabla_x \theta) \mathbf{d} - \lambda \nabla_x \mathbf{d} \cdot \nabla_x \mathbf{u} \cdot \mathbf{d}$$

together with

The total energy balance

$$\begin{aligned} \partial_t \left(\frac{1}{2} |\mathbf{u}|^2 + e \right) + \mathbf{u} \cdot \nabla_x \left(\frac{1}{2} |\mathbf{u}|^2 + e \right) + \operatorname{div} \left(\mathbf{p}\mathbf{u} + \mathbf{q}^d + \mathbf{q}^{nd} - \mathbb{S}\mathbf{u} - \boldsymbol{\sigma}^{nd}\mathbf{u} \right) \\ = \mathbf{g} \cdot \mathbf{u} + \lambda\gamma \operatorname{div} \left(\nabla_x \mathbf{d} \cdot (\Delta \mathbf{d} - \partial_d W(\mathbf{d})) \right) \end{aligned}$$

with the internal energy

$$e = \frac{\lambda}{2} |\nabla_x \mathbf{d}|^2 + \lambda W(\mathbf{d}) + \theta$$

and the flux

$$\mathbf{q} = \mathbf{q}^d + \mathbf{q}^{nd} = -k(\theta) \nabla_x \theta - h(\theta) (\mathbf{d} \cdot \nabla_x \theta) \mathbf{d} - \lambda \nabla_x \mathbf{d} \cdot \nabla_x \mathbf{u} \cdot \mathbf{d}$$

together with

The entropy inequality

$$\begin{aligned} H(\theta)_t + \mathbf{u} \cdot \nabla_x H(\theta) + \operatorname{div}(H'(\theta) \mathbf{q}^d) \\ \geq H'(\theta) \left(\mathbb{S} : \nabla_x \mathbf{u} + \lambda\gamma |\Delta \mathbf{d} - \partial_d W(\mathbf{d})|^2 \right) + H''(\theta) \mathbf{q}^d \cdot \nabla_x \theta \end{aligned}$$

holding for any smooth, non-decreasing and concave function H .

The initial and boundary conditions

In order to avoid the occurrence of boundary layers, we suppose that the boundary is impermeable and perfectly smooth imposing the **complete slip** boundary conditions:

$$\mathbf{u} \cdot \mathbf{n}|_{\partial\Omega} = 0, \quad [(\mathbb{S} + \sigma^{nd})\mathbf{n}] \times \mathbf{n}|_{\partial\Omega} = 0$$

together with the **no-flux** boundary condition for the temperature

$$\mathbf{q}^d \cdot \mathbf{n}|_{\partial\Omega} = 0$$

and the **Neumann** boundary condition for the director field

$$\nabla_x d_i \cdot \mathbf{n}|_{\partial\Omega} = 0 \text{ for } i = 1, 2, 3$$

The last relation accounts for the fact that there is no contribution to the surface force from the director \mathbf{d} . It is also suitable for implementation of a numerical scheme.

A **weak solution** is a triple $(\mathbf{u}, \mathbf{d}, \theta)$ satisfying:

- the **momentum equations** ($\varphi \in C_0^\infty([0, T) \times \bar{\Omega}; \mathbb{R}^3)$, $\varphi \cdot \mathbf{n}|_{\partial\Omega} = 0$):

A **weak solution** is a triple $(\mathbf{u}, \mathbf{d}, \theta)$ satisfying:

- the **momentum equations** ($\varphi \in C_0^\infty([0, T) \times \bar{\Omega}; \mathbb{R}^3)$, $\varphi \cdot \mathbf{n}|_{\partial\Omega} = 0$):

$$\begin{aligned} & \int_0^T \int_{\Omega} (\mathbf{u} \cdot \partial_t \varphi + \mathbf{u} \otimes \mathbf{u} : \nabla_x \varphi + p \operatorname{div} \varphi) \\ &= \int_0^T \int_{\Omega} (\mathbb{S} + \sigma^{nd}) : \nabla_x \varphi - \int_{\Omega} \mathbf{g} \cdot \varphi - \int_{\Omega} \mathbf{u}_0 \cdot \varphi(0, \cdot); \end{aligned}$$

A **weak solution** is a triple $(\mathbf{u}, \mathbf{d}, \theta)$ satisfying:

- the **momentum equations** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega}; \mathbb{R}^3)$, $\varphi \cdot \mathbf{n}|_{\partial\Omega} = 0$):

$$\begin{aligned} & \int_0^T \int_{\Omega} (\mathbf{u} \cdot \partial_t \varphi + \mathbf{u} \otimes \mathbf{u} : \nabla_x \varphi + p \operatorname{div} \varphi) \\ &= \int_0^T \int_{\Omega} (\mathbb{S} + \sigma^{nd}) : \nabla_x \varphi - \int_{\Omega} \mathbf{g} \cdot \varphi - \int_{\Omega} \mathbf{u}_0 \cdot \varphi(0, \cdot); \end{aligned}$$

- the **director equation**: $\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} - \mathbf{d} \cdot \nabla_x \mathbf{u} = \gamma (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))$ a.e., $\nabla_x \mathbf{d}_i \cdot \mathbf{n}|_{\partial\Omega} = 0$;

A **weak solution** is a triple $(\mathbf{u}, \mathbf{d}, \theta)$ satisfying:

- the **momentum equations** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega}; \mathbb{R}^3)$, $\varphi \cdot \mathbf{n}|_{\partial\Omega} = 0$):

$$\begin{aligned} & \int_0^T \int_{\Omega} (\mathbf{u} \cdot \partial_t \varphi + \mathbf{u} \otimes \mathbf{u} : \nabla_x \varphi + p \operatorname{div} \varphi) \\ &= \int_0^T \int_{\Omega} (\mathbb{S} + \sigma^{nd}) : \nabla_x \varphi - \int_{\Omega} \mathbf{g} \cdot \varphi - \int_{\Omega} \mathbf{u}_0 \cdot \varphi(0, \cdot); \end{aligned}$$

- the **director equation**: $\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} - \mathbf{d} \cdot \nabla_x \mathbf{u} = \gamma (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))$ a.e., $\nabla_x \mathbf{d}_i \cdot \mathbf{n}|_{\partial\Omega} = 0$;
- the **total energy balance** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega})$, $e_0 = \frac{\lambda}{2} |\nabla_x \mathbf{d}_0|^2 + \lambda W(\mathbf{d}_0) + \theta_0$):

A **weak solution** is a triple $(\mathbf{u}, \mathbf{d}, \theta)$ satisfying:

- the **momentum equations** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega}; \mathbb{R}^3)$, $\varphi \cdot \mathbf{n}|_{\partial\Omega} = 0$):

$$\begin{aligned} & \int_0^T \int_{\Omega} (\mathbf{u} \cdot \partial_t \varphi + \mathbf{u} \otimes \mathbf{u} : \nabla_x \varphi + p \operatorname{div} \varphi) \\ &= \int_0^T \int_{\Omega} (\mathbb{S} + \sigma^{nd}) : \nabla_x \varphi - \int_{\Omega} \mathbf{g} \cdot \varphi - \int_{\Omega} \mathbf{u}_0 \cdot \varphi(0, \cdot); \end{aligned}$$

- the **director equation**: $\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} - \mathbf{d} \cdot \nabla_x \mathbf{u} = \gamma (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))$ a.e., $\nabla_x \mathbf{d}_i \cdot \mathbf{n}|_{\partial\Omega} = 0$;

- the **total energy balance** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega})$, $e_0 = \frac{\lambda}{2} |\nabla_x \mathbf{d}_0|^2 + \lambda W(\mathbf{d}_0) + \theta_0$):

$$\begin{aligned} & \int_0^T \int_{\Omega} \left(\left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \partial_t \varphi \right) + \int_0^T \int_{\Omega} \left(\left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \mathbf{u} \cdot \nabla_x \varphi \right) \\ & \quad + \int_0^T \int_{\Omega} (\mathbf{p}\mathbf{u} + \mathbf{q} - \mathbb{S}\mathbf{u} - \sigma^{nd}\mathbf{u}) \cdot \nabla_x \varphi \\ &= \lambda \gamma \int_0^T \int_{\Omega} (\nabla_x \mathbf{d} \cdot (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))) \cdot \nabla_x \varphi - \int_0^T \int_{\Omega} \mathbf{g} \cdot \mathbf{u} \varphi - \int_{\Omega} \left(\frac{1}{2} |\mathbf{u}_0|^2 + e_0 \right) \varphi(0, \cdot); \end{aligned}$$

- the **entropy production inequality** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega})$, $\varphi \geq 0$):

A **weak solution** is a triple $(\mathbf{u}, \mathbf{d}, \theta)$ satisfying:

- the **momentum equations** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega}; \mathbb{R}^3)$, $\varphi \cdot \mathbf{n}|_{\partial\Omega} = 0$):

$$\begin{aligned} & \int_0^T \int_{\Omega} (\mathbf{u} \cdot \partial_t \varphi + \mathbf{u} \otimes \mathbf{u} : \nabla_x \varphi + p \operatorname{div} \varphi) \\ &= \int_0^T \int_{\Omega} (\mathbb{S} + \sigma^{nd}) : \nabla_x \varphi - \int_{\Omega} \mathbf{g} \cdot \varphi - \int_{\Omega} \mathbf{u}_0 \cdot \varphi(0, \cdot); \end{aligned}$$

- the **director equation**: $\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} - \mathbf{d} \cdot \nabla_x \mathbf{u} = \gamma (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))$ a.e., $\nabla_x \mathbf{d}_i \cdot \mathbf{n}|_{\partial\Omega} = 0$;

- the **total energy balance** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega})$, $e_0 = \frac{\lambda}{2} |\nabla_x \mathbf{d}_0|^2 + \lambda W(\mathbf{d}_0) + \theta_0$):

$$\begin{aligned} & \int_0^T \int_{\Omega} \left(\left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \partial_t \varphi \right) + \int_0^T \int_{\Omega} \left(\left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \mathbf{u} \cdot \nabla_x \varphi \right) \\ & \quad + \int_0^T \int_{\Omega} (\mathbf{p}\mathbf{u} + \mathbf{q} - \mathbb{S}\mathbf{u} - \sigma^{nd}\mathbf{u}) \cdot \nabla_x \varphi \\ &= \lambda \gamma \int_0^T \int_{\Omega} (\nabla_x \mathbf{d} \cdot (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))) \cdot \nabla_x \varphi - \int_0^T \int_{\Omega} \mathbf{g} \cdot \mathbf{u} \varphi - \int_{\Omega} \left(\frac{1}{2} |\mathbf{u}_0|^2 + e_0 \right) \varphi(0, \cdot); \end{aligned}$$

- the **entropy production inequality** ($\varphi \in C_0^\infty([0, T] \times \bar{\Omega})$, $\varphi \geq 0$):

$$\begin{aligned} & \int_0^T \int_{\Omega} H(\theta) \partial_t \varphi + \int_0^T \int_{\Omega} (H(\theta) \mathbf{u} + H'(\theta) \mathbf{q}^d) \cdot \nabla_x \varphi \\ & \leq - \int_0^T \int_{\Omega} (H'(\theta) (\mathbb{S} : \nabla_x \mathbf{u} + \lambda \gamma |\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d})|^2) + H''(\theta) \mathbf{q}^d \cdot \nabla_x \theta) \varphi - \int_{\Omega} H(\theta_0) \varphi(0, \cdot) \end{aligned}$$

for any smooth, non-decreasing and concave function H .

The assumptions

The assumptions

We assume that

- $W \in C^2(\mathbb{R}^3)$, $W \geq 0$, W convex for all $|\mathbf{d}| \geq D_0$, $\lim_{|\mathbf{d}| \rightarrow \infty} W(\mathbf{d}) = \infty$, for a certain $D_0 > 0$

The assumptions

We assume that

- $W \in C^2(\mathbb{R}^3)$, $W \geq 0$, W convex for all $|\mathbf{d}| \geq D_0$, $\lim_{|\mathbf{d}| \rightarrow \infty} W(\mathbf{d}) = \infty$, for a certain $D_0 > 0$
- The transport coefficients μ , k , and h are continuously differentiable functions of the absolute temperature satisfying

$$0 < \underline{\mu} \leq \mu(\theta) \leq \bar{\mu}, \quad 0 < \underline{k} \leq k(\theta), \quad h(\theta) \leq \bar{k} \quad \text{for all } \theta \geq 0$$

for suitable constants \underline{k} , \bar{k} , $\underline{\mu}$, $\bar{\mu}$

The assumptions

We assume that

- $W \in C^2(\mathbb{R}^3)$, $W \geq 0$, W convex for all $|\mathbf{d}| \geq D_0$, $\lim_{|\mathbf{d}| \rightarrow \infty} W(\mathbf{d}) = \infty$, for a certain $D_0 > 0$
- The transport coefficients μ , k , and h are continuously differentiable functions of the absolute temperature satisfying

$$0 < \underline{\mu} \leq \mu(\theta) \leq \bar{\mu}, \quad 0 < \underline{k} \leq k(\theta), \quad h(\theta) \leq \bar{k} \quad \text{for all } \theta \geq 0$$

for suitable constants \underline{k} , \bar{k} , $\underline{\mu}$, $\bar{\mu}$

- $\Omega \subset \mathbb{R}^3$ is a bounded domain of class $C^{2+\nu}$ for some $\nu > 0$, $\mathbf{g} \in L^2((0, T) \times \Omega; \mathbb{R}^3)$

The existence theorem

The existence theorem

Assume that the previous hypotheses are satisfied. Finally, let the initial data be such that

$$\mathbf{u}_0 \in L^2(\Omega; \mathbb{R}^3), \operatorname{div} \mathbf{u}_0 = 0, \mathbf{d}_0 \in W^{1,2}(\Omega; \mathbb{R}^3), W(\mathbf{d}_0) \in L^1(\Omega),$$

$$\theta_0 \in L^1(\Omega), \operatorname{ess\,inf}_\Omega \theta_0 > 0.$$

The existence theorem

Assume that the previous hypotheses are satisfied. Finally, let the initial data be such that

$$\mathbf{u}_0 \in L^2(\Omega; \mathbb{R}^3), \operatorname{div} \mathbf{u}_0 = 0, \mathbf{d}_0 \in W^{1,2}(\Omega; \mathbb{R}^3), W(\mathbf{d}_0) \in L^1(\Omega),$$

$$\theta_0 \in L^1(\Omega), \operatorname{ess\,inf}_\Omega \theta_0 > 0.$$

Then **our problem possesses a weak solution $(\mathbf{u}, \mathbf{d}, \theta)$ in $(0, T) \times \Omega$** belonging to the class

$$\mathbf{u} \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{1,2}(\Omega; \mathbb{R}^3)),$$

$$\mathbf{d} \in L^\infty(0, T; W^{1,2}(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{2,2}(\Omega; \mathbb{R}^3)),$$

$$W(\mathbf{d}) \in L^\infty(0, T; L^1(\Omega)) \cap L^{5/3}((0, T) \times \Omega),$$

$$\theta \in L^\infty(0, T; L^1(\Omega)) \cap L^p(0, T; W^{1,p}(\Omega)), \quad 1 \leq p < 5/4, \quad \theta > 0 \text{ a.e. in } (0, T) \times \Omega,$$

with the pressure p ,

$$p \in L^{5/3}((0, T) \times \Omega).$$

An idea of the proof

An idea of the proof

- We perform suitable **a-priori estimates** which coincide with the regularity class stated in the Theorem

An idea of the proof

- We perform suitable **a-priori estimates** which coincide with the regularity class stated in the Theorem
- It can be shown that **the solution set of our problem is weakly stable (compact) with respect to these bounds**, namely, any sequence of (weak) solutions that complies with the uniform bounds established above has a subsequence that converges to some limit

An idea of the proof

- We perform suitable **a-priori estimates** which coincide with the regularity class stated in the Theorem
- It can be shown that **the solution set of our problem is weakly stable (compact) with respect to these bounds**, namely, any sequence of (weak) solutions that complies with the uniform bounds established above has a subsequence that converges to some limit
- Hence, we construct a suitable family of **approximate problems (via Faedo-Galerkin scheme + regularizing terms in the momentum equation)** whose solutions weakly converge (up to subsequences) to limit functions which solve the problem in the weak sense

Model 2: the Q -tensorial Ball-Majumdar model

The physical variables

We work in the three-dimensional torus $\Omega \subset \mathbb{R}^3$ in order to avoid complications connected with boundary conditions.

Our model will consider the evolution of the following variables:

- the mean velocity field \mathbf{u}
- the tensor field \mathbb{Q} , representing preferred (local) orientation of the crystals
- the absolute temperature θ

Energy and dissipation

- The free energy density takes the form

$$\mathcal{F} = \frac{1}{2} |\nabla \mathbb{Q}|^2 + f_B(\theta, \mathbb{Q}) - \theta \log \theta,$$

Energy and dissipation

- The free energy density takes the form

$$\mathcal{F} = \frac{1}{2} |\nabla \mathbb{Q}|^2 + f_B(\theta, \mathbb{Q}) - \theta \log \theta,$$

where f_B is bulk the configuration potential:

- ▶ $f_B(\theta, \mathbb{Q}) = f(\mathbb{Q}) - U(\theta)G(\mathbb{Q})$
- ▶ f is the convex l.s.c. and singular Ball-Majumdar potential
- ▶ U changes in sign at a critical temperature: $U(\theta) = \alpha(\theta - \theta^*)$ for $\theta \sim \theta^*$ with a controlled growth for large θ
- ▶ e.g. $G(\mathbb{Q}) = \text{tr}(\mathbb{Q}^2)$

Energy and dissipation

- The free energy density takes the form

$$\mathcal{F} = \frac{1}{2} |\nabla \mathbb{Q}|^2 + f_B(\theta, \mathbb{Q}) - \theta \log \theta,$$

where f_B is bulk the configuration potential:

- ▶ $f_B(\theta, \mathbb{Q}) = f(\mathbb{Q}) - U(\theta)G(\mathbb{Q})$
 - ▶ f is the convex l.s.c. and singular Ball-Majumdar potential
 - ▶ U changes in sign at a critical temperature: $U(\theta) = \alpha(\theta - \theta^*)$ for $\theta \sim \theta^*$ with a controlled growth for large θ
 - ▶ e.g. $G(\mathbb{Q}) = \text{tr}(\mathbb{Q}^2)$
- The dissipation pseudo-potential is given by

$$\mathcal{P} = \frac{\mu(\theta)}{4} |\nabla \mathbf{u} + \nabla^t \mathbf{u}|^2 + I_{\{0\}}(\text{div } \mathbf{u}) + \frac{\kappa(\theta)}{2\theta} |\nabla \theta|^2 + \frac{1}{2\Gamma(\theta)} |D_t \mathbb{Q}|^2$$

with the viscosity μ , the heat conductivity κ , the collective rotational coefficient Γ smooth. $D_t \mathbb{Q}$ "generalized material derivative"

Q-tensor equation

Q-tensor equation

We assume that the driving force governing the dynamics of the director \mathbf{d} is of “gradient type” $\partial_d \mathcal{F}$:

$$\partial_t \mathbb{Q} + \mathbf{u} \cdot \nabla \mathbb{Q} - \mathbb{S}(\nabla \mathbf{u}, \mathbb{Q}) = \Gamma(\theta) \mathbb{H}, \quad (\text{eq-Q})$$

- The left hand side is the “generalized material derivative”

$$D_t \mathbb{Q} = \partial_t \mathbb{Q} + \mathbf{u} \cdot \nabla \mathbb{Q} - \mathbb{S}(\nabla \mathbf{u}, \mathbb{Q})$$

- \mathbb{S} represents deformation and stretching effects of the crystal director along the flow

Q-tensor equation

We assume that the driving force governing the dynamics of the director \mathbf{d} is of “gradient type” $\partial_d \mathcal{F}$:

$$\partial_t \mathbb{Q} + \mathbf{u} \cdot \nabla \mathbb{Q} - \mathbb{S}(\nabla \mathbf{u}, \mathbb{Q}) = \Gamma(\theta) \mathbb{H}, \quad (\text{eq-Q})$$

- The left hand side is the “generalized material derivative”
 $D_t \mathbb{Q} = \partial_t \mathbb{Q} + \mathbf{u} \cdot \nabla \mathbb{Q} - \mathbb{S}(\nabla \mathbf{u}, \mathbb{Q})$
- \mathbb{S} represents deformation and stretching effects of the crystal director along the flow
- $\mathbb{H} = \Delta \mathbb{Q} - \frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} + U(\theta) \frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}}$
- The function f represents the convex part of a singular potential of **[Ball-Majumdar]** type
- The functions U and G are smooth and satisfy suitable growth conditions

The Ball-Majumdar potential

The Ball-Majumdar potential (cf. [Ball, Majumdar (2010)]) exhibit a logarithmic divergence as the eigenvalues of \mathbb{Q} approaches $-\frac{1}{3}$ and $\frac{2}{3}$

$$f(\mathbb{Q}) = \begin{cases} \inf_{\rho \in \mathcal{A}_{\mathbb{Q}}} \int_{S^2} \rho(\mathbf{p}) \log(\rho(\mathbf{p})) \, d\mathbf{p} & \text{if } \lambda_i[\mathbb{Q}] \in (-1/3, 2/3), \quad i = 1, 2, 3, \\ \infty & \text{otherwise,} \end{cases}$$

$$\mathcal{A}_{\mathbb{Q}} = \left\{ \rho : S^2 \rightarrow [0, \infty) \mid \int_{S^2} \rho(\mathbf{p}) \, d\mathbf{p} = 1; \mathbb{Q} = \int_{S^2} \left(\mathbf{p} \otimes \mathbf{p} - \frac{1}{3} \mathbb{I} \right) \rho(\mathbf{p}) \, d\mathbf{p} \right\}.$$

\Rightarrow It explodes as one of the eigenvalues of \mathbb{Q} approaches the limiting values $-1/3$ or $2/3$.

Equation of momentum

Equation of momentum

- In the context of nematic liquid crystals, we have the **incompressibility** constraint

$$\operatorname{div} \mathbf{u} = 0$$

Equation of momentum

- In the context of nematic liquid crystals, we have the **incompressibility** constraint

$$\operatorname{div} \mathbf{u} = 0$$

- By virtue of Newton's second law, **the balance of momentum** reads

$$\partial_t \mathbf{u} + \operatorname{div}(\mathbf{u} \otimes \mathbf{u}) = \operatorname{div} \sigma + \mathbf{g}, \quad (\text{eq-u})$$

Equation of momentum

- In the context of nematic liquid crystals, we have the **incompressibility** constraint

$$\operatorname{div} \mathbf{u} = 0$$

- By virtue of Newton's second law, **the balance of momentum** reads

$$\partial_t \mathbf{u} + \operatorname{div}(\mathbf{u} \otimes \mathbf{u}) = \operatorname{div} \boldsymbol{\sigma} + \mathbf{g}, \quad (\text{eq-u})$$

- ▶ The stress $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma} = \frac{\mu(\theta)}{2} (\nabla \mathbf{u} + \nabla^t \mathbf{u}) - p \mathbb{I} + \mathbb{T}$$

Equation of momentum

- In the context of nematic liquid crystals, we have the **incompressibility** constraint

$$\operatorname{div} \mathbf{u} = 0$$

- By virtue of Newton's second law, **the balance of momentum** reads

$$\partial_t \mathbf{u} + \operatorname{div}(\mathbf{u} \otimes \mathbf{u}) = \operatorname{div} \boldsymbol{\sigma} + \mathbf{g}, \quad (\text{eq-u})$$

- The stress $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma} = \frac{\mu(\theta)}{2} (\nabla \mathbf{u} + \nabla^t \mathbf{u}) - p \mathbb{I} + \mathbb{T}$$

- The **coupling term (or "extra-stress")** \mathbb{T} depends both on θ and \mathbb{Q} :

$$\mathbb{T} = 2\xi (\mathbb{H} : \mathbb{Q}) \left(\mathbb{Q} + \frac{1}{3} \mathbb{I} \right) - \xi \left[\mathbb{H} \left(\mathbb{Q} + \frac{1}{3} \mathbb{I} \right) + \left(\mathbb{Q} + \frac{1}{3} \mathbb{I} \right) \mathbb{H} \right] + (\mathbb{Q} \mathbb{H} - \mathbb{H} \mathbb{Q}) - \nabla \mathbb{Q} \odot \nabla \mathbb{Q},$$

where ξ is a fixed scalar parameter.

Entropy equation

Entropy equation

The evolution of temperature is prescribed by stating the **entropy balance**:

$$s_t + \mathbf{u} \cdot \nabla s - \operatorname{div} \left(\frac{\kappa(\theta)}{\theta} \nabla \theta \right) \quad (\text{eq-}\theta)$$
$$\geq \frac{1}{\theta} \left(\frac{\mu(\theta)}{2} |\nabla \mathbf{u} + \nabla^t \mathbf{u}|^2 + \Gamma(\theta) |\mathbb{H}|^2 + \frac{\kappa(\theta)}{\theta} |\nabla \theta|^2 \right),$$

where $s = 1 + \log \theta + U'(\theta)G(\mathbb{Q})$

Entropy equation

The evolution of temperature is prescribed by stating the **entropy balance**:

$$\begin{aligned} & s_t + \mathbf{u} \cdot \nabla s - \operatorname{div} \left(\frac{\kappa(\theta)}{\theta} \nabla \theta \right) \\ & \geq \frac{1}{\theta} \left(\frac{\mu(\theta)}{2} |\nabla \mathbf{u} + \nabla^t \mathbf{u}|^2 + \Gamma(\theta) |\mathbb{H}|^2 + \frac{\kappa(\theta)}{\theta} |\nabla \theta|^2 \right), \end{aligned} \tag{eq-}\theta$$

where $s = 1 + \log \theta + U'(\theta)G(\mathbb{Q})$

- The coefficients μ , κ and Γ are smooth and bounded
- The “heat” balance can be recovered by (formally) multiplying by θ
- Due to the quadratic terms, we can only interpret (eq- θ) as an inequality

Total energy balance

Total energy balance

- Passing from the heat equation to the entropy inequality gives rise to some information loss

Total energy balance

- Passing from the heat equation to the entropy inequality gives rise to some information loss
- Following an idea by [Bulíček, Feireisl, & Málek (2009)], we can complement the system with the total energy balance

$$\partial_t \left(\frac{1}{2} |\mathbf{u}|^2 + e \right) + \operatorname{div} \left(\left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \mathbf{u} \right) + \operatorname{div} \mathbf{q} \quad (\text{eq-bal})$$

$$= \operatorname{div}(\boldsymbol{\sigma} \mathbf{u}) + \operatorname{div} \left(\Gamma(\theta) \nabla \mathbb{Q} : \left(\Delta \mathbb{Q} - \frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} + U(\theta) \frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}} \right) \right) + \mathbf{g} \cdot \mathbf{u},$$

where $e = \mathcal{F} + s\theta$ is the internal energy

Total energy balance

- Passing from the heat equation to the entropy inequality gives rise to some information loss
- Following an idea by [Bulíček, Feireisl, & Málek (2009)], we can complement the system with the total energy balance

$$\begin{aligned} & \partial_t \left(\frac{1}{2} |\mathbf{u}|^2 + e \right) + \operatorname{div} \left(\left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \mathbf{u} \right) + \operatorname{div} \mathbf{q} && \text{(eq-bal)} \\ & = \operatorname{div}(\boldsymbol{\sigma} \mathbf{u}) + \operatorname{div} \left(\Gamma(\theta) \nabla \mathbb{Q} : \left(\Delta \mathbb{Q} - \frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} + U(\theta) \frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}} \right) \right) + \mathbf{g} \cdot \mathbf{u}, \end{aligned}$$

where $e = \mathcal{F} + s\theta$ is the internal energy

- Note the explicit occurrence of the pressure p (“hidden” inside $\boldsymbol{\sigma}$). To control it, assuming periodic b.c.’s is essential

Main result

Theorem: existence of global in time weak solutions

We can prove existence of at least one weak solution to system (eq-u)+(eq-Q)+(eq- θ)+(eq-bal) for finite-energy initial data , namely

$$\theta_0 \in L^\infty(\Omega), \quad \theta_0(x) \geq \underline{\theta} > 0,$$

$$Q_0 \in H^1(\Omega), \quad f(Q_0) \in L^1(\Omega),$$

$$\mathbf{u}_0 \in L^2(\Omega), \quad \operatorname{div} \mathbf{u}_0 = 0.$$

Main mathematical difficulties

- Operating a **minimum principle argument** to prove, in a rigorous way, that the temperature remains strictly positive
- Proving the **total energy balance**. In particular, estimating the terms involving the pressure ($p\mathbf{u}$) and the singular potential ($\Gamma(\theta)\nabla\mathbb{Q} : \partial f(\mathbb{Q})$)
- Obtaining sufficiently strong estimates for **the temperature θ** (we need growth conditions on U , but can consider general latent heat and both heat conductivity and viscosity coefficients with any growth condition)

Possible extensions

- The system we described may be modified in several ways, giving rise to further interesting mathematical problems
- In particular, we are interested in the case when the configuration potential has the form (proposed also by Ball and Majumdar)

$$\Lambda(\theta)f(\mathbb{Q}) + G(\mathbb{Q})$$

- We have preliminary results both in the case when $\Lambda(\theta) = \theta$ and in the case when Λ is nondegenerate at 0.

References

1. E. Feireisl, M. Frémond, E.R., G. Schimperna, A new approach to non-isothermal models for nematic liquid crystals, ARMA, to appear, preprint arXiv:1104.1339v1 (2011)
2. E. Feireisl, E.R., G. Schimperna, A. Zarnescu, Evolution of non-isothermal Landau-de Gennes nematic liquid crystals flows, paper in preparation

References

1. E. Feireisl, M. Frémond, E.R., G. Schimperna, A new approach to non-isothermal models for nematic liquid crystals, ARMA, to appear, preprint arXiv:1104.1339v1 (2011)
2. E. Feireisl, E.R., G. Schimperna, A. Zarnescu, Evolution of non-isothermal Landau-de Gennes nematic liquid crystals flows, paper in preparation

Thanks for your attention!