Evolution of non-isothermal nematic liquid crystals flows

E. Rocca

Università degli Studi di Milano

The 9th AIMS Conference on Dynamical Systems, Differential Equations and Applications, Orlando, Florida, USA

SS7 Recent Progress in the Mathematical Theory of Compressible and Incompressible Fluid Flows

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 with singular potential, paper in preparation

- Some future perspectives and open problems

The motivations and the objectives

- The motivations:
  - 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**

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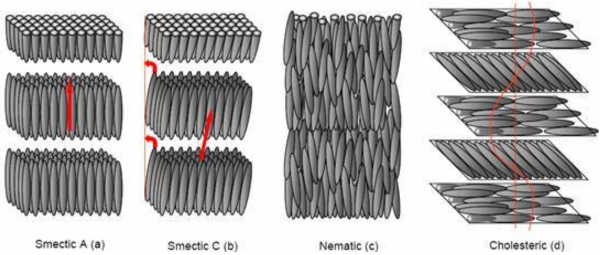

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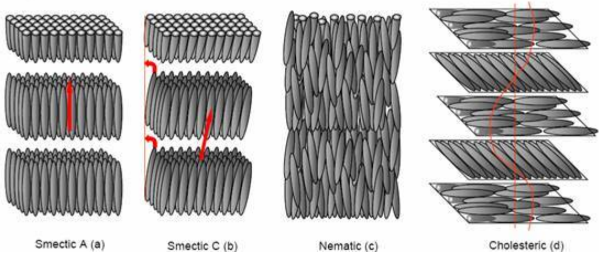

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The *smectic* phase forms well-defined layers that can slide one over another in a manner very similar to that of a soap

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

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- 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 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 **$\mathbb{Q}$-tensor**

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▶ The flow **velocity 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 **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

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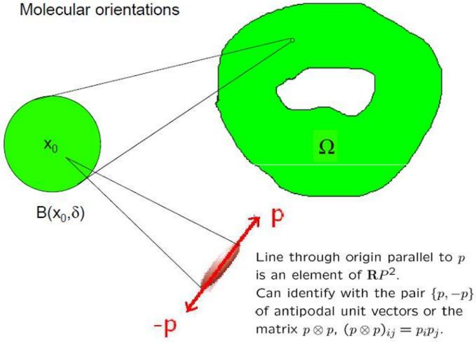
- Consider a nematic liquid crystal filling a bounded connected container Ω in $\mathbb{R}^3$ with "regular" boundary
- The distribution of molecular orientations in a ball $B(x_0, \delta)$, $x_0 \in \Omega$ can be represented as a probability measure μ on the unit sphere $\mathbb{S}^2$ satisfying $\mu(E) = \mu(-E)$ 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 $\mathbb{Q}$-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 $\mathbf{v} \in \mathbb{S}^2$, $\mathbf{v} \cdot M \cdot \mathbf{v} = \int_{\mathbb{S}^2} (\mathbf{v} \cdot p)^2 \, d\mu(p) = < \cos^2 \theta >$, where θ is the angle between p and $\mathbf{v}$) satisfying $\mathrm{tr}(M) = 1$

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- 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 $\mathrm{tr}(M_0) = 1$

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▶ **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)])

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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 othonormal 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. $\mu = \frac{1}{6} \sum_{i=1}^{3} (\delta_{e_i} + \delta_{-e_i})$)

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- 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)
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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 $\mathbf{n}_3 = \mathbf{d}$ where $\mathbf{n}_i$ is an orthonormal basis of eigenvectors of $\mathbb{Q}$ corresponding to λ_i, we have

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

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 **d is a vector** representing the direction of preferred molecular alignment: the **director field**.

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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

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

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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)])

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

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

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

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

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

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

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- 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

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

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

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

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⇒ For the **Landau-de Gennes** free energy with "regular" potential, the hydrodynamic theory has been developed in [Paicu, Zarnescu, SIAM (2011) and ARMA (2012)]

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$\Longrightarrow$ 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

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

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- 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. $W(\mathbf{d}) = (|\mathbf{d}|^2 - 1)^2$

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- Consequently, $\mathbf{d}$ satisfies the following equation

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

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  where the last term accounts for stretching of the director field induced by the straining of the fluid
- 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 $\mathbf{d}$ (useful in order to handle the nonlinearities)

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

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

where p is the pressure, and

- the stress tensors are

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

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

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

where p is the pressure, and

- the stress tensors are

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

  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

$$\partial_t \left(\frac{1}{2}|\mathbf{u}|^2 + e\right) + \mathbf{u}\cdot\nabla_x \left(\frac{1}{2}|\mathbf{u}|^2 + e\right) + \operatorname{div}\left(p\mathbf{u} + \mathbf{q}^d + \mathbf{q}^{nd} - \mathbb{S}\mathbf{u} - \sigma^{nd}\mathbf{u}\right)$$

$$= \mathbf{g}\cdot\mathbf{u} + \operatorname{div}\left(\nabla_x \mathbf{d}\cdot(\Delta\mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d}))\right)$$

with the internal energy

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

and the flux

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

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together with

The entropy inequality

$$H(\theta)_t + \mathbf{u}\cdot\nabla_x H(\theta) + \operatorname{div}(H'(\theta)\mathbf{q}^d)$$

$$\geq H'(\theta)\left(\mathbb{S}:\nabla_x\mathbf{u} + |\Delta\mathbf{d} - \partial_{\mathbf{d}}W(\mathbf{d})|^2\right) + H''(\theta)\mathbf{q}^d\cdot\nabla_x\theta$$

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:

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

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

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$$\int_0^T \int_\Omega \Big(\mathbf{u} \cdot \partial_t \varphi + \mathbf{u} \otimes \mathbf{u} : \nabla_x \varphi + p \,\mathrm{div}\, \varphi\Big)$$

$$= \int_0^T \int_\Omega (\mathbb{S} + \sigma^{nd}) : \nabla_x \varphi - \int_\Omega \mathbf{g} \cdot \varphi - \int_\Omega \mathbf{u}_0 \cdot \varphi(0, \cdot)\,;$$

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

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

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$$\int_0^T \int_\Omega \left(\left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \partial_t \varphi \right) + \int_0^T \int_\Omega \left(\left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \mathbf{u} \cdot \nabla_x \varphi \right)$$

$$+ \int_0^T \int_\Omega \Big(p\mathbf{u} + \mathbf{q} - \mathbb{S}\mathbf{u} - \sigma^{nd} \mathbf{u} \Big) \cdot \nabla_x \varphi$$

$$= \int_0^T \int_\Omega \Big(\nabla_x \mathbf{d} \cdot (\Delta \mathbf{d} - \partial_{\mathbf{d}} W(\mathbf{d})) \Big) \cdot \nabla_x \varphi - \int_0^T \int_\Omega \mathbf{g} \cdot \mathbf{u} \varphi - \int_\Omega \left(\frac{1}{2} |\mathbf{u}_0|^2 + e_0 \right) \varphi(0,\cdot)\,;$$

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

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$$=\int_0^T\int_\Omega(\mathbb{S}+\sigma^{nd}):\nabla_x\varphi-\int_\Omega\mathbf{g}\cdot\varphi-\int_\Omega\mathbf{u}_0\cdot\varphi(0,\cdot)\,;$$

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

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

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

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

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

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

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- The transport coefficients μ, k, and h are continuously differentiable functions satisfying

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

and the initial data satisfy

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

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Then **our problem possesses a weak solution (u, d, θ)** belonging to the class

$$\mathbf{u} \in L^\infty(0,T;L^2(\Omega;\mathbb{R}^3)) \cap L^2(0,T;W^{1,2}(\Omega;\mathbb{R}^3)),$$
$$\mathbf{d} \in L^\infty(0,T;W^{1,2}(\Omega;\mathbb{R}^3)) \cap L^2(0,T;W^{2,2}(\Omega;\mathbb{R}^3)),$$
$$W(\mathbf{d}) \in L^\infty(0,T;L^1(\Omega)) \cap L^{5/3}((0,T)\times\Omega),$$
$$\theta \in L^\infty(0,T;L^1(\Omega)) \cap L^p(0,T;W^{1,p}(\Omega)),\ 1 \leq p < 5/4,\ \theta > 0 \text{ a.e. in } (0,T)\times\Omega,$$

with the pressure p

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- 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 $\mathbb{Q}$-tensorial Ball-Majumdar model

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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
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Theorem [E. Feireisl, E.R., G. Schimperna, A. Zarnescu, paper in preparation] There exists *at least* one weak solution to a system coupling

- a *weak momentum equation* for **u**
- a *gradient-type equation for* $\mathbb{Q}$
- an *entropy inequality+total energy balance* for θ

for finite-energy initial data.

$\mathbb{Q}$-tensor equation

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We assume that the driving force governing the dynamics of the director $\mathbf{d}$ is of **"gradient type"** $\partial_{\mathbf{d}}\mathcal{F}$:

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

- The left hand side is the "generalized material derivative" $D_t\mathbb{Q} = \partial_t \mathbb{Q} + \mathbf{u} \cdot \nabla \mathbb{Q} - \mathbb{S}(\nabla \mathbf{u}, \mathbb{Q})$
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- $\mathbb{H} = \Delta \mathbb{Q} - \frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} + U(\theta)\frac{\partial G(\mathbb{Q})}{\partial \mathbb{Q}}$
- 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 $\frac{2}{3}$

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

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

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

Equation of momentum

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  - 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**:

$$s_t + \mathbf{u} \cdot \nabla s - \operatorname{div}\left(\frac{\kappa(\theta)}{\theta}\nabla\theta\right) \qquad \text{(eq-}\theta\text{)}$$

$$\geq \frac{1}{\theta}\left(\frac{\mu(\theta)}{2}\left|\nabla\mathbf{u} + \nabla^t\mathbf{u}\right|^2 + \Gamma(\theta)|\mathbb{H}|^2 + \frac{\kappa(\theta)}{\theta}|\nabla\theta|^2\right),$$

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

- 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

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

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

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

Total energy balance

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

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

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

- Note the explicit occurrence of the pressure p ("hidden" inside σ). To control it, assuming periodic b.c.'s is essential

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

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

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

  where $e = \mathcal{F} + s\theta$ is the internal energy
- Note the explicit occurrence of the pressure p ("hidden" inside σ). To control it, assuming periodic b.c.'s is essential
- Here the internal energy balance is more complicated than for the vectorial model due to the more sophisticated dependence of ψ_B from θ and $\mathbb{Q} \Longrightarrow$ the entropy s depends also on $\mathbb{Q}$

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)

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

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

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2. E. Feireisl, E.R., G. Schimperna, A. Zarnescu, Evolution of non-isothermal Landau-de Gennes nematic liquid crystals flows with singular potential, paper in preparation

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Thanks for your attention!

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