A non-isothermal model for nematic liquid crystals

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of the foundation of Jindrich Necas Center for Mathematical Modeling

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Plan of the Talk

- The objective of our modelling approach: include the **temperature dependence** in a model describing the evolution of nematic liquid crystal flows
- Our mathematical results:
  - The results: joint work with **Eduard Feireisl** (Institute of Mathematics, Czech Academy of Sciences, Prague) and **Giulio Schimperna** (University of Pavia), accepted for publication on *Nonlinearity*.
- Some future perspectives and open problems

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- 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
- 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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- 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
- 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**
- As a result, in the continuum description of a liquid crystal, at any point in space it is possible to define a **preferred direction** along which LC molecules tend to be aligned: the **unit vector d** associated with this direction is called **the director**, with a term borrowed from optics

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- An attempt to posit a set of dynamical equations for liquid crystals on a manifold was made a few years ago by **[Shkoller, Comm. Part. Diff. Eq., 2002]**. He employed the director model proposed by **[Lin and Liu, Comm. Pure Appl. Math., 1995]**, which implies a drastic simplification of the Ericksen-Leslie equations, especially in the description of dissipation

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- Several textbooks have been devoted to the presentation of mathematical LC models (cf., e.g., **Chandrasekhar (1977), de Gennes (1974)**). The survey articles by **Ericksen (1976) and Leslie (1978)**, which present in a very comprehensive fashion the "classical" continuum theories used for static and flow problems

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- The first one was originally introduced by **[Leslie, Arch. Rational Mech. Anal., 1963] and [Ericksen, Arch. Rational Mech. Anal., 1991]** and subsequently studied in the isothermal case in **[Sun and Liu, Disc. Conti. Dyna. Sys., 2009]**, where well-posedness is proved in the 2D case or in 3D under the condition that the viscosity coefficient is sufficiently large. The long-time behavior of that system is analyzed in a recent preprint by **[Wu, Xu, Liu, 2010]**.

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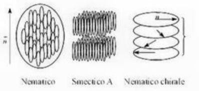
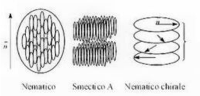
- The second model is a simplification of the Ericksen-Leslie model and has been introduced in **[Lin and Liu, Comm. Pure Appl. Math., 1995]**, where the authors proved existence and uniqueness of global classical solutions in 2D as well as some corresponding results in 3D (in the case of large viscosity).

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





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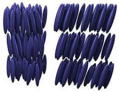

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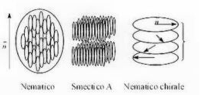

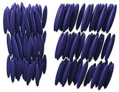

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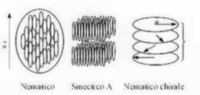

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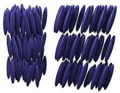

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Crystals in the *cholesteric* phase exhibit a twisting of the molecules perpendicular to the director, with the molecular axis parallel to the director. The main difference between the nematic and cholesteric phases is that the former is invariant with respect to certain reflections while the latter is not

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- 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 $\mathbf{u}$. Hence, both $\mathbf{d}$ and $\mathbf{u}$ are relevant in the dynamics, and also the **changes of the temperature** ϑ (internal energy).

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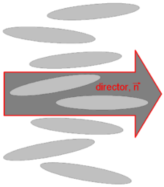
$\Longrightarrow$ We introduce a very simple **non-isothermal model for nematic liquid crystals** in the spirit of the simplified version of the Leslie-Ericksen model proposed by Lin and Liu in 1995.

The state variables

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



- the absolute temperature ϑ

The evolution

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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

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- To avoid this apparent difficulty, we **use the idea proposed in [Feireisl, J. Málek, Differ. Equ. Nonlinear Mech., 2006] replacing the heat equation by the total energy balance and an entropy inequality**. Of course, the price to pay is the explicit appearance of the pressure in the total energy balance that must be handled by refined arguments

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- Another difficulty: the proof of sufficiently strong **estimates on the director field d** in order to pass to the limit in the approximate problem. In particular, the celebrated Gagliardo-Nirenberg inequality is needed in order to control the strongly nonlinear terms containing $\nabla_x \mathbf{d}$ in both the momentum equation and the internal energy balance

The momentum balance

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- The **mass conservation** reads

$$\partial_t \varrho + \mathrm{div}(\varrho \mathbf{u}) = 0\,.$$

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- Motivated by Lin and Liu, we consider the stress tensor in the form

$$\mathbb{T} = \mathbb{S} - \varrho \lambda(\vartheta) \left(\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}\right) - p\mathbb{I}\,,$$

  where p denotes the pressure and $\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} := \sum_k \partial_i d_k \partial_j d_k$.

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- Moreover, $\mathbb{S}$ is the conventional Newtonian viscous stress tensor,

$$\mathbb{S}(\vartheta, \nabla_x \mathbf{u}) = \mu(\vartheta)\left(\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u}\right),$$

μ is the viscosity coefficient assumed always positive, while **λ denotes the thermal dilatation coefficient that is an increasing function of ϑ**

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"** $\partial_{\mathbf{d}} J$, where the potential J is given by

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- Here G is a regular function of ϑ and ϱ, and W **penalizes the deviation of the length $|\mathbf{d}|$ from the value 1**. W may be a general function that can be written as a sum of a convex (possibly non smooth) part, and a smooth, but possibly non-convex one. A typical example is $W(\mathbf{d}) = (|\mathbf{d}|^2 - 1)^2$

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

$$\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} + \partial_{\mathbf{d}} W(\mathbf{d}) = \frac{1}{\varrho} \operatorname{div} \left(\varrho \nabla_x \mathbf{d} \right).$$

The internal energy balance

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- In accordance with the **First law of thermodynamics**, the internal energy balance reads

$$\partial_t(\varrho e_{\rm int}) + {\rm div}(\varrho e_{\rm int}\mathbf{u}) + {\rm div}\,\mathbf{q} = \mathbb{T} : \nabla_x \mathbf{u}\,,$$

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- Following **Ericksen's model**, the flux can be taken in the form

$$\mathbf{q} = -\kappa(\vartheta)\nabla_x\vartheta - (\kappa_{||} - \kappa_{\perp})(\vartheta)\mathbf{d}(\mathbf{d}\cdot\nabla_x\vartheta),$$

  where κ, $\kappa_{||} - \kappa_{\perp}$ are positive functions of the temperature. Finally, we take $e_{\rm int} = c_v\vartheta$, where $c_v > 0$ is the specific heat at constant volume

The PDEs: assuming $\varrho = c_v = 1$, we get the following system:

$$\operatorname{div} \mathbf{u} = 0\,, \tag{INC}$$

$$\partial_t \mathbf{u} + \operatorname{div}(\mathbf{u} \otimes \mathbf{u}) + \nabla_x p = \operatorname{div} \mathbb{S} - \operatorname{div}\left(\lambda(\vartheta)\left(\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}\right)\right) + \mathbf{f}\,, \tag{MOM}$$

$$\partial_t \vartheta + \operatorname{div}(\vartheta \mathbf{u}) + \operatorname{div} \mathbf{q} = \mathbb{S} : \nabla_x \mathbf{u} - \lambda(\vartheta)(\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}) : \nabla_x \mathbf{u}\,, \tag{INT}$$

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$$\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} + \partial W(\mathbf{d}) = \operatorname{div} \nabla_x \mathbf{d}\,. \tag{EQD}$$

The 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:

$$\mathbf{u} \cdot \mathbf{n}|_{\partial\Omega} = 0, \;\; [\mathbb{T}\mathbf{n}] \times \mathbf{n}|_{\partial\Omega} = 0,$$

together with the no-flux boundary condition for the temperature

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

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 $\mathbb{T}\mathbf{n}$ from the director $\mathbf{d}$. It is also suitable for implementation of a numerical scheme.

The total energy balance

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Multiplying momentum equation (MOM) by $\mathbf{u}$ and adding the resulting expression to (INT) we deduce the **total energy balance** in the form

$$\partial_t\Big(\left(\frac{1}{2}|\mathbf{u}|^2 + \vartheta\right) \Big) + \operatorname{div}\Big(\left(\frac{1}{2}|\mathbf{u}|^2 + \vartheta\right) \mathbf{u}\Big) + \operatorname{div}(p\mathbf{u}) + \operatorname{div}\mathbf{q}$$

$$= \operatorname{div}(\mathbb{S}\mathbf{u}) - \operatorname{div}\Big(\lambda(\vartheta)\,(\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d})\,\mathbf{u}\Big) + \mathbf{f}\cdot\mathbf{u}.$$

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$$=\operatorname{div}(\mathbb{S}\mathbf{u})-\operatorname{div}\Big(\lambda(\vartheta)\left(\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d}\right)\mathbf{u}\Big)+\mathbf{f}\cdot\mathbf{u}.$$

Moreover, using the boundary conditions and integrating the last equation over Ω we obtain

$$\partial_t\int_\Omega\Big(\frac{1}{2}|\mathbf{u}|^2+\vartheta\Big)=\int_\Omega\mathbf{f}\cdot\mathbf{u},$$

in particular, the total energy is a constant of motion as soon as $\mathbf{f}\equiv 0$.

The entropy production

The entropy production

Let us denote by $\Lambda(\vartheta)$ a primitive of $1/\lambda(\vartheta)$. Testing (INT) by $1/\lambda(\vartheta)$ and (EQD) by $(\operatorname{div}\nabla_x \mathbf{d} - \partial W(\mathbf{d}))$, integrating the sum over Ω, we get

$$\int_\Omega (\partial_t \mathbf{d} + \mathbf{u}\cdot\nabla_x \mathbf{d})\,(\operatorname{div}\nabla_x \mathbf{d} - \partial W(\mathbf{d})) + \partial_t \int_\Omega (\Lambda(\vartheta)) + \int_\Omega \mathbf{q}\cdot\nabla_x\vartheta\,\frac{\lambda'(\vartheta)}{(\lambda(\vartheta))^2}$$
$$= \int_\Omega |\operatorname{div}\nabla_x \mathbf{d} - \varrho\partial W(\mathbf{d})|^2 + \int_\Omega \frac{1}{\lambda(\vartheta)}\mathbb{S} : \nabla_x \mathbf{u} - \int_\Omega (\nabla_x \mathbf{d}\odot\nabla_x \mathbf{d}) : \nabla_x \mathbf{u}\,,$$

and

$$\int_\Omega (\partial_t \mathbf{d} + \mathbf{u}\cdot\nabla_x \mathbf{d})\,(\operatorname{div}\nabla_x \mathbf{d} - \partial W(\mathbf{d})) = \partial_t \int_\Omega \left(-\frac{|\nabla_x \mathbf{d}|^2}{2} - W(\mathbf{d})\right) - \int_\Omega (\nabla_x \mathbf{d}\odot\nabla_x \mathbf{d}) : \nabla_x \mathbf{u}$$

Thus, finally, we arrive at

$$\partial_t \int_\Omega \left(\Lambda(\vartheta) - \frac{|\nabla_x \mathbf{d}|^2}{2} - W(\mathbf{d})\right) = \int_\Omega |\operatorname{div}(\varrho\nabla_x \mathbf{d}) - \partial W(\mathbf{d})|^2$$
$$+ \int_\Omega \frac{1}{\lambda(\vartheta)}\mathbb{S} : \nabla_x \mathbf{u} - \int_\Omega \mathbf{q}\cdot\nabla_x\vartheta\,\frac{\lambda'(\vartheta)}{(\lambda(\vartheta))^2},$$

where the *entropy density* of the system is $S = \left(\Lambda(\vartheta) - |\nabla_x \mathbf{d}|^2/2 - W(\mathbf{d})\right)$ and, if $\lambda' \geq 0$, then the **Second law of thermodynamics** is satisfied.

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

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

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$$\int_\Omega \mathbf{u}(t,\cdot) \cdot \nabla_x \psi = 0 \text{ for a.a. } t \in (0,T) \quad \forall \psi \in C^\infty(\overline{\Omega}),$$

$$\int_0^T \int_\Omega \Big(\mathbf{u} \cdot \partial_t \varphi + \mathbf{u} \otimes \mathbf{u} : \nabla_x \varphi \Big) = \int_0^T \int_\Omega \mathbb{T} : \nabla_x \varphi - \int_\Omega \mathbf{u}_0 \cdot \varphi(0,\cdot);$$

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- the **equation for d** holding in the strong sense:

$$\partial_t\mathbf{d}+\mathbf{u}\cdot\nabla_x\mathbf{d}+\partial W(\mathbf{d})=\Delta\mathbf{d} \text{ a.e. in } (0,T)\times\Omega, \quad \nabla_x\mathbf{d}_i\cdot\mathbf{n}_{|\partial\Omega}=0\,,\ i=1,2,3\,;$$

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

$$= \int_0^T \int_\Omega (\mathbb{S} - \lambda(\vartheta)(\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}) - p\mathbb{I})\, \mathbf{u} \cdot \nabla_x \varphi - \int_\Omega \left(\frac{1}{2} |\mathbf{u}_0|^2 + \vartheta_0 \right) \varphi(0, \cdot)\,;$$

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- the **entropy production inequality** (in the sense of distributions):

$$\partial_t \left(\Lambda(\vartheta) - \frac{|\nabla_x \mathbf{d}|^2}{2} - W(\mathbf{d}) \right) \geq -\operatorname{div} \left(\mathbf{u}\Lambda(\vartheta) + \frac{\mathbf{q}}{\lambda(\vartheta)} + \mathbf{u} \cdot (\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}) - \mathbf{u} W(\mathbf{d}) \right)$$

$$+ |\Delta \mathbf{d} - \partial W(\mathbf{d})|^2 + \frac{1}{\lambda(\vartheta)} \mathbb{S} : \nabla_x \mathbf{u} - \mathbf{q} \cdot \nabla_x \vartheta \frac{\lambda'(\vartheta)}{(\lambda(\vartheta))^2}$$

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We assume that

- $W \in C^2(\mathbb{R}^3), \quad W \geq 0, \quad \partial W(\mathbf{d}) \cdot \mathbf{d} \geq 0$ for all $|\mathbf{d}| \geq D_0$ for a certain $D_0 > 0$

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- The transport coefficients are continuously differentiable functions of the absolute temperature satisfying

$$0 < \underline{\mu} \leq \mu(\vartheta) \leq \overline{\mu}, \quad 0 < \underline{\kappa} \leq \kappa(\vartheta), \ (\kappa_{||} - \kappa_{\perp})(\vartheta) \leq \overline{\kappa} \ \text{ for all } \vartheta \geq 0$$

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- $\lambda \in C^1([0, +\infty))$ be such that

$$\lambda'(\vartheta) \geq 0, \quad \lambda'(0) > 0, \quad \lambda(0) = 0, \quad \lambda(\vartheta) \leq \overline{\lambda} \ \text{ for all } \vartheta \geq 0$$

  for a certain $\overline{\lambda} > 0$.

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Let $\Omega \subset \mathbb{R}^3$ be a bounded domain of class $C^{2+\nu}$ for some $\nu > 0$. Assume that the previous hypotheses are satisfied. Finally, let the initial data be such that

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

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

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

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

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

with the pressure p,

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

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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

Total dissipation balance

Total dissipation balance

Combining the energy balance (multiplied by a positive constant $K > 0$) with the entropy inequality we obtain the **total dissipation balance** in the form

$$\int_\Omega \left(\frac{K}{2}|\mathbf{u}|^2 + (K\vartheta - \Lambda(\vartheta)) + \frac{|\nabla_x \mathbf{d}|^2}{2} + W(\mathbf{d}) \right)(\tau, \cdot)$$

$$+ \int_0^\tau \int_\Omega \left(|\Delta \mathbf{d} - \partial W(\mathbf{d})|^2 + \frac{1}{\lambda(\vartheta)} \mathbb{S} : \nabla_x \mathbf{u} - \mathbf{q} \cdot \nabla_x \vartheta \frac{\lambda'(\vartheta)}{\lambda^2(\vartheta)} \right)$$

$$\leq \int_\Omega \left(\frac{K}{2}|\mathbf{u}_0|^2 + (K\vartheta_0 - \Lambda(\vartheta_0)) + \frac{|\nabla_x \mathbf{d}_0|^2}{2} + W(\mathbf{d}_0) \right).$$

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For K sufficiently large, the terms on the left hand side turn out to be non-negative, and the integral on the right-hand side is bounded; hence we deduce the **a priori bounds**

$$\mathbf{u} \in L^\infty(0,T;L^2(\Omega;\mathbb{R}^3)) \cap L^2(0,T;W^{1,2}(\Omega;\mathbb{R}^3)) \cap L^{10/3}((0,T)\times\Omega;\mathbb{R}^3),$$

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Moreover, we also get

$$\Lambda(\vartheta) \in L^\infty(0, T; L^1(\Omega)), \quad (\Lambda(\vartheta))^+ \in L^2(0, T; W^{1,2}(\Omega)).$$

Director field estimate

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Take the scalar product of the **d**-equation equation with **d** yielding

$$\partial_t |\mathbf{d}|^2 + \mathbf{u} \cdot \nabla_x |\mathbf{d}|^2 + 2\partial W(\mathbf{d}) \cdot \mathbf{d} = \Delta |\mathbf{d}|^2 - 2|\nabla_x \mathbf{d}|^2.$$

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By means of our assumptions on W, we may apply the standard **maximum principle to $|\mathbf{d}|^2$** obtaining

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

and so also

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

which, together with **Gagliardo-Nirenberg interpolation inequality**

$$\|\nabla_x \mathbf{d}\|_{L^4(\Omega)} \le c_1 \|\Delta \mathbf{d}\|_{L^2(\Omega)}^{1/2} \|\mathbf{d}\|_{L^\infty(\Omega)}^{1/2} + c_2 \|\mathbf{d}\|_{L^\infty(\Omega)} \,,$$

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This estimate turns out to be "crucial" in order to obtain a bound for the pressure and, in general, for the proof of existence of solutions.

Pressure estimate

Pressure estimate

Thanks to our choice of the slip boundary conditions for the velocity, **the pressure p can be "computed" directly from our equations** as the unique solution of the elliptic problem

$$\Delta p = \operatorname{div}\operatorname{div}\Big(\mathbb{S} - \lambda(\vartheta)\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} - \mathbf{u} \otimes \mathbf{u}\Big),$$

supplemented with the boundary condition

$$\partial_{\mathbf{n}} p = (\operatorname{div}(\mathbb{S} - \lambda(\vartheta)\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} - \mathbf{u} \otimes \mathbf{u})) \cdot \mathbf{n} \quad \text{on } \partial\Omega\,.$$

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To be precise, the last two relations have to be interpreted in a "very weak" sense. Namely, the pressure p is determined through a family of integral identities

$$\int_\Omega p\Delta\varphi = \int_\Omega \Big(\mathbb{S} - \lambda(\vartheta)\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} - \mathbf{u} \otimes \mathbf{u}\Big) : \nabla_x^2 \varphi$$

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for any test function $\varphi \in C^\infty(\overline{\Omega})$, $\nabla_x \varphi \cdot \mathbf{n}|_{\partial\Omega} = 0$. Consequently, the bounds already established may be used, together with the standard elliptic regularity results, to conclude that

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

Entropy estimate

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Multiplying the ϑ-equation by $H'(\vartheta)$ (for a generic $H \in C^2([0,+\infty))$) we deduce its **"renormalized" form**

$$\partial_t H(\vartheta) + \operatorname{div}(H(\vartheta)\mathbf{u}) + \operatorname{div}(H'(\vartheta)\mathbf{q})$$
$$+H''(\vartheta)\Big(\kappa(\vartheta)|\nabla_x\vartheta|^2 + (\kappa_{||} - \kappa_\perp)(\vartheta)|\mathbf{d}\cdot\nabla_x\vartheta|^2\Big)$$
$$= H'(\vartheta)\Big(\mathbb{S} - \lambda(\vartheta)\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d}\Big) : \nabla_x\mathbf{u} \quad \text{in } \mathcal{D}'((0,T)\times\Omega).$$

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The choice $H(\vartheta) = (1+\vartheta)^\eta,\ \eta \in (0,1)$, together with the uniform bounds obtained before, yield

$$\nabla_x(1+\vartheta)^\nu \in L^2((0,T)\times\Omega;\mathbb{R}^3) \text{ for any } 0 < \nu < \frac{1}{2}\,.$$

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$$+H''(\vartheta)\Big(\kappa(\vartheta)|\nabla_x\vartheta|^2 + (\kappa_{||}-\kappa_{\perp})(\vartheta)|\mathbf{d}\cdot\nabla_x\vartheta|^2\Big)$$
$$= H'(\vartheta)\Big(\mathbb{S} - \lambda(\vartheta)\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d}\Big) : \nabla_x\mathbf{u} \quad \text{in } \mathcal{D}'((0,T)\times\Omega).$$

The choice $H(\vartheta) = (1+\vartheta)^\eta$, $\eta \in (0,1)$, together with the uniform bounds obtained before, yield

$$\nabla_x(1+\vartheta)^\nu \in L^2((0,T)\times\Omega;\mathbb{R}^3) \text{ for any } 0 < \nu < \frac{1}{2}\,.$$

Now, we apply an interpolation argument between $\vartheta \in L^\infty(0,T;L^1(\Omega))$ and $\vartheta^\nu \in L^1(0,T;L^3(\Omega))$, for $\nu \in (0,1]$, getting

$$\vartheta \in L^q((0,T)\times\Omega) \text{ for any } 1 \le q < 5/3\,.$$

Entropy estimate

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Further, observing that, for all $p \in [1,5/4)$ and $\nu > 0$,

$$\int_{(0,T)\times\Omega} |\nabla_x\vartheta|^p \le \left(\int_{(0,T)\times\Omega} |\nabla_x\vartheta|^2\vartheta^{\nu-1}\right)^{\frac{p}{2}} \left(\int_{(0,T)\times\Omega} \vartheta^{(1-\nu)\frac{p}{2-p}}\right)^{\frac{2-p}{2}},$$

we conclude that

$$\nabla_x\vartheta \in L^p((0,T)\times\Omega;\mathbb{R}^3), \quad \nabla_x(\Lambda(\vartheta)) \in L^p((0,T)\times\Omega;\mathbb{R}^3) \text{ for any } 1 \le p < 5/4.$$

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$$\vartheta\mathbf{u},\ \Lambda(\vartheta)\mathbf{u} \text{ bounded in } L^{q}((0,T)\times\Omega;\mathbb{R}^3)) \text{ for any } q\in[1,10/9)\,,$$

$$\mathbb{S}\mathbf{u},\ \lambda(\vartheta)(\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d})\mathbf{u} \ \text{ bounded in } L^{5/4}(0,T;L^{5/4}(\Omega;\mathbb{R}^3))\,,$$

$$\frac{\mathbf{q}}{\lambda(\vartheta)} \text{ bounded in } L^{s}((0,T)\times\Omega;\mathbb{R}^3) \text{ for any } s\in[1,5/4)\,.$$

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We pass to the limit in the **total energy balance** and to the lim sup in the **entropy inequality** (thanks also to the positivity and convexity of some terms)

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

$$=\int_0^T\int_\Omega(\mathbb{S}-\lambda(\vartheta)\left(\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d}\right)-p\mathbb{I})\,\mathbf{u}\cdot\nabla_x\varphi-\int_\Omega\left(\frac{1}{2}|\mathbf{u}_0|^2+\vartheta_0\right)\varphi(0,\cdot)\,;$$

$$\partial_t\left(\Lambda(\vartheta)-\frac{|\nabla_x\mathbf{d}|^2}{2}-W(\mathbf{d})\right)\geq-\operatorname{div}\left(\mathbf{u}\Lambda(\vartheta)+\frac{\mathbf{q}}{\lambda(\vartheta)}+\mathbf{u}\cdot(\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d})-\mathbf{u}W(\mathbf{d})\right)$$

$$+|\Delta\mathbf{d}-\partial W(\mathbf{d})|^2+\frac{1}{\lambda(\vartheta)}\mathbb{S}:\nabla_x\mathbf{u}-\mathbf{q}\cdot\nabla_x\vartheta\frac{\lambda'(\vartheta)}{(\lambda(\vartheta))^2}\,.$$

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$$
\begin{aligned}
&\mathbf{u}_t - \operatorname{div}(\mathbf{u} \otimes \mathbf{u}) - \nu \Delta \mathbf{u} = \operatorname{div} \mathbb{S}, \\
&\mathbb{S} = -p\mathbb{I} - L(\nabla \mathbf{d} \odot \nabla \mathbf{d}) - \delta(L\Delta \mathbf{d} - \mathbf{f}(\mathbf{d})) \otimes \mathbf{d}, \\
&\operatorname{div} \mathbf{u} = 0, \\
&\mathbf{d}_t + \mathbf{u} \cdot \nabla \mathbf{d} - \delta \mathbf{d} \cdot \nabla \mathbf{u} - L\Delta \mathbf{d} + \mathbf{f}(\mathbf{d}) = 0,
\end{aligned}
$$

where we have set

$$
\mathbf{f}(\mathbf{d}) := \big(\psi(|\mathbf{d}|^2) - 1\big)\mathbf{d} = \frac{1}{2}\partial_{\mathbf{d}}\big(\widehat{\psi}(|\mathbf{d}|^2) - |\mathbf{d}|^2\big)
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and the coefficient ν, L, δ satisfy $\nu, L > 0$ and $\delta \geq 0$

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- In **[Sun and Liu, Disc. Conti. Dyna. Sys., 2009]** global well-posedness is proved in the **2D case or in 3D under the condition that the viscosity coefficient is sufficiently large**. To the best of our knowledge, **global-in-time existence for this 3D model is entirely open**, even within the class of weak solutions. The case of Dirichlet boundary conditions both for **u** and **d** are under study in a recent **joint work with C. Cavaterra**

Open problems and perspectives

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- The study the singular limit of our system with $W_\varepsilon(\mathbf{d}) = \frac{1}{\varepsilon^2}(|\mathbf{d}|^2 - 1)^2$, where the physically meaningful condition $|\mathbf{d}| = 1$ is obtained: non convex problem (cf. **[Chen, Math. Z. (1989)] for nematic liquid crystals**).