Analysis of a non-isothermal model for nematic liquid crystals

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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), **Michel Frémond** (Università di Roma Tor Vergata) and **Giulio Schimperna** (Università di Pavia), preprint arXiv:1104.1339v1 (2011)

- Some future perspectives and open problems

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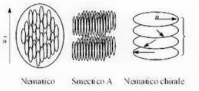
- At the molecular level, what marks the difference between a liquid crystal and an ordinary, isotropic fluid is that, while the centers of mass of LC molecules do not exhibit any long-range correlation, **molecular orientations do exhibit orientational correlations**
- As a result, in the continuum 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

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



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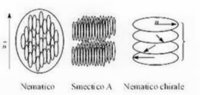

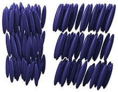

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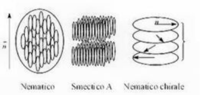

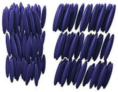

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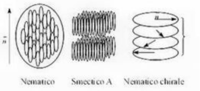

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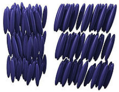

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Crystals in the *cholesteric* phase exhibit a twisting of the molecules perpendicular to the director, with the molecular axis parallel to the director. The main difference between the nematic and cholesteric phases is that the former is invariant 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. But we want to include in our model also the **changes of the temperature** θ.

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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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- A considerably simplified version of the Leslie-Ericksen model was proposed by **[Lin and Liu, Comm. Pure Appl. Math., 1995]** and subsequently analyzed by many authors. The simplified 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.

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- 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 the total energy balance**, which, indeed, ceases to hold.

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- In order to prevent this failure, **[Sun and Liu, Disc. Conti. Dyna. Sys., 2009]** introduced a variant of the model proposed by Lin and Liu, where **the stretching term is included** in the system and a new component added to the stress tensor in order to **save the total energy balance**.

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- the **non-isothermal** case [Feireisl, E.R., Schimperna, Nonlinearity (2011)]: **neglect the stretching effects**

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  - The free energy Ψ of the system, depending on the proper *state variables*, tends to decrease in a way that is prescribed by the expression of a second functional, called pseudopotential of dissipation, that depends (in a convex way) on a set of *dissipative variables*
  - The stress tensor σ, the density of energy vector $\mathbf{B}$ and the energy flux tensor $\mathbb{H}$ are decoupled into their *non-dissipative* and *dissipative* components, whose precise form is prescribed by proper constitutive equations

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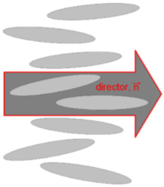
- The form of **the extra stress in the Navier-Stokes system** obtained by this method coincides with the formula derived from different principles by Sun and Liu in the isothermal case

The state variables

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



- the absolute temperature θ

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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.

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- Apart from the fact that the resulting system is mathematically tractable, such an approach seems much closer to the physical background of the problem, being an exact formulation of the *First and Second Laws of thermodynamics*

The director field dynamics

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

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

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- Here λ is a positive constant, F penalizes the deviation of the length $|\mathbf{d}|$ from its natural value 1; generally, F 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. $F(\mathbf{d}) = (|\mathbf{d}|^2 - 1)^2$

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- Consequently, **d** satisfies the following equation

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

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

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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

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

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 and

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- $\mathbf{f}(\mathbf{d}) = \partial_{\mathbf{d}} F(\mathbf{d})$, F being e.g. $F(\mathbf{d}) = (|\mathbf{d}|^2 - 1)^2$
- The presence of **the stretching term $\mathbf{d} \cdot \nabla_x \mathbf{u}$** in the **d**-equation prevents us from applying any maximum principle. Hence, we cannot find any L^∞ bound on **d**. We will need a **weak formulation of the momentum balance**

The total energy balance

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

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

with the internal energy

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

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

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

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

with the internal energy

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

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

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

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

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

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

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

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

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

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We assume that

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

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- The transport coefficients μ, k, and h are continuously differentiable functions of the absolute temperature satisfying

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

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

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

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

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

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

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

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

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

with the pressure p,

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

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- 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

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Integrating over Ω the energy balance (with $e = \frac{\lambda}{2}|\nabla_x \mathbf{d}|^2 + \lambda F(\mathbf{d}) + \theta$)

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$$= \mathbf{g} \cdot \mathbf{u} + \lambda\gamma \operatorname{div} \left(\nabla_x \mathbf{d} \cdot (\Delta \mathbf{d} - \mathbf{f}(\mathbf{d})) \right),$$

and using the Gronwall lemma, we get immediately the following bounds:

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

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Similarly, choosing $H(\theta) = \theta$ in the entropy balance

$$\int_0^T \int_\Omega H(\theta)\partial_t \varphi + \int_0^T \int_\Omega \left(H(\theta)\mathbf{u} + H'(\theta)\mathbf{q}^d \right) \cdot \nabla_x \varphi$$

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we obtain

$$\varepsilon(\mathbf{u}) \in L^2((0, T) \times \Omega, \mathbb{R}^{3\times 3}), \ \Delta \mathbf{d} - \mathbf{f}(\mathbf{d}) \in L^2((0, T) \times \Omega; \mathbb{R}^3).$$

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yielding, by virtue of Korn's inequality,

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

Interpolation

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It follows from the previous estimate $\Delta \mathbf{d} - \mathbf{f}(\mathbf{d}) \in L^2((0,T) \times \Omega)$ and the convexity of F that

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$$\mathbf{d} \in L^{10}((0,T)\times\Omega;\mathbb{R}^3),\ \nabla_x \mathbf{d} \in L^{10/3}((0,T)\times\Omega;\mathbb{R}^{3\times3}),$$

whence

$$\sigma^{nd}(= -\lambda\nabla_x \mathbf{d}\odot\nabla_x \mathbf{d} + \lambda(\mathbf{f}(\mathbf{d}) - \Delta\mathbf{d})\otimes\mathbf{d}) \in L^{5/3}((0,T)\times\Omega;\mathbb{R}^{3\times3}).$$

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By the same token, by means of convexity of F, we have

$$|F(\mathbf{d})| \le c(1 + |\mathbf{f}(\mathbf{d})||\mathbf{d}|),$$

yielding

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

Pressure estimate

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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

$$\Delta p = \operatorname{div}\operatorname{div}\left(\mathbb{S} + \sigma^{nd} - \mathbf{u}\otimes\mathbf{u}\right) + \operatorname{div}\mathbf{g},$$

supplemented with the boundary condition

$$\nabla_x p \cdot \mathbf{n} = \left(\operatorname{div}\left(\mathbb{S} + \sigma^{nd} - \mathbf{u}\otimes\mathbf{u}\right) + \mathbf{g}\right)\cdot\mathbf{n} \text{ on } \partial\Omega\,.$$

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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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The choice $H(\theta) = (1+\theta)^\eta,\ \eta \in (0,1)$, in the entropy equation yields

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

Now, we apply an interpolation argument we immediately get

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

Furthermore, seeing that

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

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

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

Entropy estimate

The choice $H(\theta) = (1+\theta)^\eta,\ \eta \in (0,1)$, in the entropy equation yields

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

Now, we apply an interpolation argument we immediately get

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

Furthermore, seeing that

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

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

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

Finally, the same argument and $H(\theta)=\log\theta$ give rise to

$$\log\theta \in L^2((0,T);W^{1,2}(\Omega))\cap L^\infty(0,T;L^1(\Omega))\,.$$

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- The **key point** of this approach **is replacing the heat equation**, commonly used in models of heat conducting fluids, **by the total energy balance+the entropy inequality**: the resulting system of equations is free of dissipative terms that are difficult to handle, due to the **low regularity of the weak solutions**

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- The price we have to pay: **we have to control the pressure** appearing explicitly in the total energy flux $\Longrightarrow$ we need to assume **the complete slip boundary conditions** on $\mathbf{u}$

Future perspectives and open problems

- The **isothermal** liquid crystal model **accounting for the stretching** contribution has also recently been analyzed in [Petzeltová, E.R., Schimperna, preprint arXiv:1107.5445v1, 2011], where the **long time behaviour of solutions** is investigated in the 3D case:

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  - These results generalize the ones obtained in [Wu, Xu, Liu, preprint arXiv:0901.1751v2, 2010]
- An open problem could be to investigate the **existence of the global attractor** for this system at least in the isothermal case (work in progess with Sergio Frigeri (postdoc at the Università degli Studi di Milano – ERC-StG project "EntroPhase"))