

Dissipative solutions for a hyperbolic system arising in liquid crystals modeling

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jointly with

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Outline

- 1 Introduction of the Problem
- 2 The LCs modeling
- 3 The simplified Qian-Sheng model
- 4 The existence of local-in-time smooth solutions
- 5 Existence of global-in-time dissipative solutions
- 6 Weak-strong uniqueness
- 7 Further perspectives

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We present here the results of the following joint work

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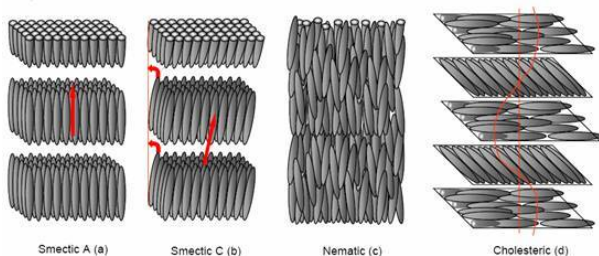
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- The main advantages and the potential future perspectives

The motivation

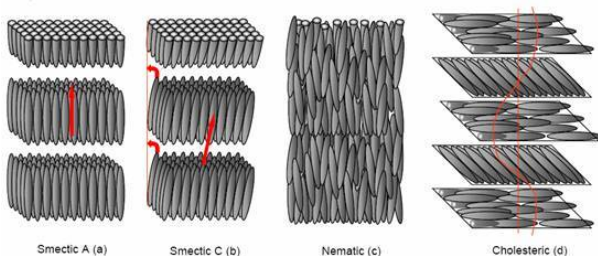
- Liquid crystals are a state of matter that have properties **between** those of a conventional **liquid** and those of a **solid crystal**. A liquid crystal may flow like a liquid, but its molecules may be oriented in a crystal-like way
- Theoretical studies of these types of materials are motivated 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*



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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 **Q -tensor**

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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}**
- Moreover, also changes of the temperature or effects of magnetic and electric fields should be considered (in the future maybe)

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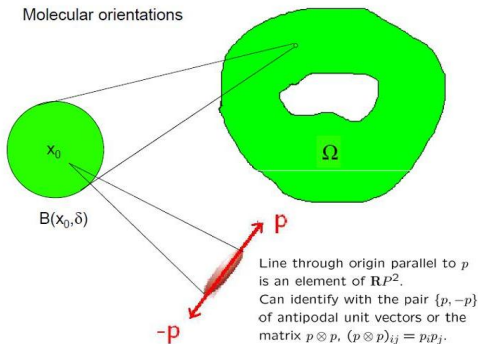
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- Consider a nematic liquid crystal filling a bounded connected container Ω in \mathbb{R}^3 with “regular” boundary
- The distribution of molecular orientations in a ball $B(x_0, \delta)$, $x_0 \in \Omega$ can be represented as a probability measure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

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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 $\text{tr}(M_0) = 1$

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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)])
 1. $\mathbb{Q} = \mathbb{Q}^T$
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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 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. $\mu = \frac{1}{6} \sum_{i=1}^3 (\delta_{\mathbf{e}_i} + \delta_{-\mathbf{e}_i})$)

The reduction to the Oseen-Frank model

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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

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

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 \mathbf{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

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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)])

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

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

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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.

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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

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

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

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

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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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The most characteristic specific feature of this model is the **presence of an inertial term that appears as a second-order material derivative**.

This term provides a **hyperbolic character** to the equations and is the main source of difficulties in the analysis.

It should be noted that this second material derivative also appears in the more commonly used Ericksen-Leslie model of liquid crystals, but there it generates even worse effects due to the additional presence of the unit-length constraint.

The PDEs

The system we are studying is:

$$\operatorname{div}_x \mathbf{v} = 0$$

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- The pressure Π and the factor $\lambda \mathbb{I}$ may be seen as Lagrange multipliers compensating the deviation of the motion from the divergenceless and zero-trace state, respectively

Energy functional

The problem admits a natural energy functional

$$\mathcal{E}[\mathbf{v}, \mathbb{P}, \mathbb{Q}] = \int_{\Omega} \left[\frac{1}{2} |\mathbf{v}|^2 + \frac{1}{2} |\mathbb{P}|^2 + \frac{1}{2} |\nabla_x \mathbb{Q}|^2 + \mathcal{F}(\mathbb{Q}) \right] dx$$

It is easy to check, by multiplying by \mathbf{v} the velocity-equation:

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla_x \mathbf{v} + \nabla_x \Pi = -\operatorname{div}_x (\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q})$$

by $\mathbb{P} (= \partial_t \mathbb{Q} + \mathbf{v} \cdot \nabla_x \mathbb{Q})$ the equation:

$$\partial_t \mathbb{P} + \mathbf{v} \cdot \nabla_x \mathbb{P} = -\frac{\partial \mathcal{F}}{\partial \mathbb{Q}} + \Delta \mathbb{Q} - \lambda \mathbb{I}$$

and integrating the resulting sum by parts, that the total energy is conserved

$$\frac{d}{dt} \mathcal{E}[\mathbf{v}, \mathbb{P}, \mathbb{Q}] = 0$$

for any smooth solution of our system

Qualitative features

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Indeed, if one defines the *extended circulation vector*, where $\mathbb{P}_{ij} \nabla_x Q_{ij}$ represents the circulation associated with the fluid interaction with the nematic order parameter field (here and in the following we assume Einstein summation convention, of summation over repeated indices)

$$\mathcal{C}_{QS} := \mathbf{v} + \mathbb{P}_{ij} \nabla_x Q_{ij}$$

and the *extended vorticity*

$$\bar{\omega}_{QS} := \nabla_x \times \mathcal{C}_{QS}$$

then we have the **Euler-like equation**

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In addition there hold a *circulation theorem*

$$\frac{d}{dt} \oint_{\Gamma(t)} \mathbf{v} + \mathbb{P}_{ij}\nabla_x Q_{ij} d\sigma = 0$$

where $\Gamma(t)$ is a closed path moving with velocity \mathbf{v} and the *helicity conservation*

$$\frac{d}{dt} \int_{\Omega} C_{QS} \cdot \bar{\omega}_{QS} dx = 0$$

as a direct consequence of the Euler-like equation

Our goals and main difficulties

Our goal is to study the existence of **global-in-time** solutions to the problem

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- This may seem a rather ambitious task as the problem is highly non-linear involving the incompressible Euler system for which the existence of *physically admissible* solutions is an open problem even in the class of weak solutions (see [Wiedemann, Ann. Inst. H. Poincaré Anal. Non Linéaire (2011)] and [Székelyhidi–Wiedemann, Arch. Rational Mech. Anal. (2012)])

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The **dissipative solutions** enjoy the following properties:

- Any classical solution of problem above is a dissipative solution
- Any (sufficiently) smooth dissipative solution is a classical solution
- A dissipative solution coincides with the classical solution emanating from the same initial data as long as the latter exists

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5. Finally, we observe that the same procedure used in the construction of local smooth solutions gives rise to a **dissipative solution**

Notations

- For A, B two 3×3 matrices we denote the inner product on the space of matrices as $A : B = \text{tr}(AB)$
- The product $\nabla A \otimes \nabla B$ is a matrix with ij component $\partial_i A : \partial_j B$.
- If $M(x)$ is a 3×3 -matrix, then $|M|$ denotes the Frobenius norm of the matrix, i.e. $|M| = \sqrt{M : M^t}$. Furthermore $\nabla \cdot M$ stands for the vector field $\left(\sum_{j=1}^3 \frac{\partial M_{ij}}{\partial x_j} \right)_{i=1 \dots 3}$
- If \mathbf{v} is a 3-dimensional vector and \mathbb{Q} is a 3×3 matrix then $\mathbf{v} \otimes \mathbb{Q}$ is a third order tensor with components $v_i Q_{kl}$ with $i, k, l \in \{1, 2, 3\}$
- If \mathbb{P} is a 3×3 then $\nabla_x \mathbb{P}$ is a third-order tensor and we denote by $\mathbf{v} \otimes \mathbb{Q} : \nabla_x \mathbb{P}$ the scalar $\sum_{i,j,k=1}^3 v_k Q_{ij} \frac{\partial P_{ij}}{\partial x_k}$

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Assumptions on the potential

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Remarks.

- Assumption (A3) could be generalized and include also potentials with faster (polynomial) growth at infinity, the only complication being the possible appearance of a further defect term in the energy balance. The function $G(Q)$ can be controlled only in L^1 in that case
- Exponential growth at infinity or “singular” potentials (i.e., \mathcal{F} being identically infinity outside a bounded set, like the Ball-Majumdar potential) is more delicate: a further measure-valued term (the limit of $\partial\mathcal{F}(Q)$) would then occur
- Examples of functions that satisfies (A1)-(A3) are

$$\mathcal{F}(Q) = \frac{a}{2}|Q|^2 + \frac{b}{3}\text{tr}(Q^3) + \frac{c}{4}|Q|^4 \quad \text{where } a, b \in R \text{ and } c > 0$$

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Let $s \geq 3$ and $\mathcal{F} \in C^{s+1}(R_{0,\text{sym}}^{3 \times 3}; R)$ satisfying (A1)-(A3). Consider the initial data

$$\mathbf{v}(0, \cdot) = \mathbf{v}_0 \in W^{s,2}(\mathcal{T}^3; R^3), \quad \mathbb{P}(0, \cdot) = \mathbb{P}_0 \in W^{s,2}(\mathcal{T}^3; R_{0,\text{sym}}^{3 \times 3}),$$

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such that $\operatorname{div}_x \mathbf{v}_0 = 0$.

Then **there exists** $T_0 > 0$ depending solely on the norm of the initial data **such that our problem**

$$\begin{aligned}\operatorname{div}_x \mathbf{v} &= 0 \\ \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla_x \mathbf{v} + \nabla_x \Pi &= -\operatorname{div}_x (\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q}) \\ \partial_t \mathbb{Q} + \mathbf{v} \cdot \nabla_x \mathbb{Q} &= \mathbb{P} \\ \partial_t \mathbb{P} + \mathbf{v} \cdot \nabla_x \mathbb{P} &= -\frac{\partial \mathcal{F}}{\partial \mathbb{Q}} + \Delta \mathbb{Q} - \lambda \mathbb{I}\end{aligned}$$

admits a strong solution in $[0, T_0] \times \mathcal{T}^3$, **unique** in the class

$$\begin{aligned}\mathbf{v} &\in C([0, T_0]; W^{s,2}(\mathcal{T}^3; R^3)), \\ \mathbb{P} &\in C([0, T_0]; W^{s,2}(\mathcal{T}^3; R_{0,\text{sym}}^{3 \times 3})), \quad \mathbb{Q} \in C([0, T_0]; W^{s+1,2}(\mathcal{T}^3; R_{0,\text{sym}}^{3 \times 3})).\end{aligned}$$

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$$\mathbb{Q} \in C_{\text{weak}}([0, T]; W^{1,2}(\mathcal{T}^3; \mathbb{R}^{3 \times 3})) \cap C([0, T]; L^2(\mathcal{T}^3; \mathbb{R}^{3 \times 3})),$$

they satisfy the relations:

$$\int_{\Omega} \mathbf{v}(\tau, \cdot) \cdot \nabla_x \varphi \, dx = 0 \text{ for any } \varphi \in C_c^\infty(\mathcal{T}^3),$$

$$\left[\int_{\Omega} \mathbf{v} \cdot \varphi \, dx \right]_{t=0}^{t=\tau} = \int_0^\tau \int_{\Omega} \mathbf{v} \cdot \partial_t \varphi + (\mathbf{v} \otimes \mathbf{v}) : \nabla_x \varphi + (\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q}) : \nabla_x \varphi \, dx + \langle \mathbb{R}^1; \nabla_x \varphi \rangle \, dt$$

for any $\varphi \in C_c^\infty([0, T] \times \mathcal{T}^3; \mathbb{R}^3)$, $\text{div}_x \varphi = 0$;

$$\left[\int_{\Omega} \mathbb{Q} : \varphi \, dx \right]_{t=0}^{t=\tau} = \int_0^\tau \int_{\Omega} [\mathbb{Q} : \partial_t \varphi + (\mathbf{v} \otimes \mathbb{Q}) : \nabla_x \varphi + \mathbb{P} : \varphi] \, dx \, dt \text{ for any } \varphi \in C_c^\infty([0, T] \times \mathcal{T}^3; \mathbb{R}_{0,\text{sym}}^{3 \times 3});$$

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for certain $\mathbb{R}^1, \mathbb{R}^2$,

We name by dissipative solutions the trio of functions $[\mathbf{v}, \mathbb{P}, \mathbb{Q}]$ such that

$$\begin{aligned} \mathbf{v} &\in C_{\text{weak}}([0, T]; L^2(\mathcal{T}^3; \mathbb{R}^3)), \quad \mathbb{P} \in C_{\text{weak}}([0, T]; L^2(\mathcal{T}^3; \mathbb{R}^{3 \times 3})), \\ \mathbb{Q} &\in C_{\text{weak}}([0, T]; W^{1,2}(\mathcal{T}^3; \mathbb{R}^{3 \times 3})) \cap C([0, T]; L^2(\mathcal{T}^3; \mathbb{R}^{3 \times 3})), \end{aligned}$$

they satisfy the relations:

$$\int_{\Omega} \mathbf{v}(\tau, \cdot) \cdot \nabla_x \varphi \, dx = 0 \text{ for any } \varphi \in C_c^\infty(\mathcal{T}^3),$$

$$\left[\int_{\Omega} \mathbf{v} \cdot \varphi \, dx \right]_{t=0}^{t=\tau} = \int_0^\tau \int_{\Omega} \mathbf{v} \cdot \partial_t \varphi + (\mathbf{v} \otimes \mathbf{v}) : \nabla_x \varphi + (\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q}) : \nabla_x \varphi \, dx + \langle \mathbb{R}^1; \nabla_x \varphi \rangle \, dt$$

for any $\varphi \in C_c^\infty([0, T] \times \mathcal{T}^3; \mathbb{R}^3)$, $\text{div}_x \varphi = 0$;

$$\left[\int_{\Omega} \mathbb{Q} : \varphi \, dx \right]_{t=0}^{t=\tau} = \int_0^\tau \int_{\Omega} [\mathbb{Q} : \partial_t \varphi + (\mathbf{v} \otimes \mathbb{Q}) : \nabla_x \varphi + \mathbb{P} : \varphi] \, dx \, dt \text{ for any } \varphi \in C_c^\infty([0, T] \times \mathcal{T}^3; \mathbb{R}_{0,\text{sym}}^{3 \times 3});$$

$$\left[\int_{\Omega} \mathbb{P} : \varphi \, dx \right]_{t=0}^{t=\tau} = \int_0^\tau \int_{\Omega} \left[\mathbb{P} : \partial_t \varphi + (\mathbf{v} \otimes \mathbb{P}) : \nabla_x \varphi - \frac{\partial \mathcal{F}(\mathbb{Q})}{\partial \mathbb{Q}} : \varphi - \nabla_x \mathbb{Q} : \nabla_x \varphi \right] \, dx + \langle \mathbb{R}^2; \nabla_x \varphi \rangle \, dt$$

for any $\varphi \in C_c^\infty([0, T] \times \mathcal{T}^3; \mathbb{R}_{0,\text{sym}}^{3 \times 3})$;

for certain $\mathbb{R}^1, \mathbb{R}^2$, and the energy balance for any $\tau \in [0, T]$:

$$\left[\int_{\Omega} \left[\frac{1}{2} |\mathbf{v}|^2 + \frac{1}{2} |\mathbb{P}|^2 + \frac{1}{2} |\nabla_x \mathbb{Q}|^2 + \mathcal{G}(\mathbb{Q}) \right] \, dx \right]_{t=0}^{t=\tau} + \mathcal{D}(\tau) = 2\Lambda \int_0^\tau \int_{\Omega} \mathbb{Q} : \mathbb{P} \, dx \, dt$$

for certain $\mathcal{D} \in L^\infty(0, T)$ (dissipation defect), where

$$\int_0^\tau \left[\|\mathbb{R}^1(t, \cdot)\|_{\mathcal{M}(\mathcal{T}^3)} + \|\mathbb{R}^2(t, \cdot)\|_{\mathcal{M}(\mathcal{T}^3)} \right] \, dt \leq c \int_0^\tau \mathcal{D}(t) \, dt, \quad \tau \in [0, T]$$

Theorem 2: dissipative solutions

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Let $\mathcal{F} \in C^2(R_{0,\text{sym}}^{3 \times 3}; \mathbb{R})$ satisfy assumptions (A1)-(A3).

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admits a **dissipative solution** $[\mathbf{v}, \mathbb{P}, \mathbb{Q}]$ in $(0, T) \times \mathcal{T}^3$ for any initial data

$$\mathbf{v}_0 \in L^2(\mathcal{T}^3; \mathbb{R}^3), \operatorname{div}_x \mathbf{v}_0 = 0, \mathbb{P}_0 \in L^2(\mathcal{T}^3; \mathbb{R}_{0,\text{sym}}^{3 \times 3}), \mathbb{Q}_0 \in W^{1,2}(\mathcal{T}^3; \mathbb{R}_{0,\text{sym}}^{3 \times 3}).$$

Remark on the correctors

Remark on the correctors

Apparently no information about the specific form of the correctors $\mathbb{R}^1, \mathbb{R}^2$ in

$$\left[\int_{\Omega} \mathbf{v} \cdot \varphi \, dx \right]_{t=0}^{t=\tau} = \int_0^{\tau} \int_{\Omega} \mathbf{v} \cdot \partial_t \varphi + (\mathbf{v} \otimes \mathbf{v}) : \nabla_x \varphi + (\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q}) : \nabla_x \varphi \, dx + \langle \mathbb{R}^1; \nabla_x \varphi \rangle \, dt$$
$$\left[\int_{\Omega} \mathbb{P} : \varphi \, dx \right]_{t=0}^{t=\tau} = \int_0^{\tau} \int_{\Omega} \left[\mathbb{P} : \partial_t \varphi + (\mathbf{v} \otimes \mathbb{P}) : \nabla_x \varphi - \frac{\partial \mathcal{F}(\mathbb{Q})}{\partial \mathbb{Q}} : \varphi - \nabla_x \mathbb{Q} : \nabla_x \varphi \right] \, dx + \langle \mathbb{R}^2; \nabla_x \varphi \rangle \, dt$$

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but, actually:

- \mathbb{R}^1 is the tensor of measures whose (i, j) -entry is $\mathcal{R}_{1,1}^{i,j} + \mathcal{R}_{1,2}^{i,j}$ with

- ▶ $v_n^i v_n^j - v^i v^j \rightarrow \mathcal{R}_{1,1}^{i,j}$ weakly-(*) in $L^\infty(0, T; \mathcal{M}(\mathcal{T}^3))$ and

$$\sum_{i,j} \|\mathcal{R}_{1,1}^{i,j}\|_{\mathcal{M}(\mathcal{T}^3)} \leq 3 \int_{\Omega} (|\overline{\mathbf{v}}|^2 - |\mathbf{v}|^2) \, dx.$$

- ▶ $\sum_{\alpha,\beta} (\partial_i Q_n^{\alpha,\beta} \partial_j Q_n^{\alpha,\beta} - \partial_i Q^{\alpha,\beta} \partial_j Q^{\alpha,\beta}) \rightarrow \mathcal{R}_{1,2}^{i,j}$ weakly-(*) in $L^\infty(0, T; \mathcal{M}(\mathcal{T}^3))$ and

$$\sum_{i,j} \|\mathcal{R}_{1,2}^{i,j}\|_{\mathcal{M}(\mathcal{T}^3)} \leq c \int_{\Omega} (|\overline{|\nabla_x \mathbb{Q}|^2} - |\nabla_x \mathbb{Q}|^2) \, dx,$$

- \mathbb{R}^2 is the tensor of measures whose (i, j, k) -entry is $\mathcal{R}_2^{i,j,k}$ with

$$v_n^i P_n^{k,j} - v^i P^{k,j} \rightarrow \mathcal{R}_2^{i,j,k} \text{ weakly-(*) in } L^\infty(0, T; \mathcal{M}(\mathcal{T}^3))$$

and

$$\sum_{i,j} \int_0^{\tau} \|\mathcal{R}_2^{i,j,k}\|_{\mathcal{M}(\mathcal{T}^3)} \, dt \leq c \int_0^{\tau} \int_{\Omega} (|\overline{\mathbf{v}}|^2 - |\mathbf{v}|^2) \, dx \, dt + c \int_0^{\tau} \int_{\Omega} (|\overline{|\mathbb{P}|^2} - |\mathbb{P}|^2) \, dx \, dt.$$

Remark on the dissipation

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The nonnegative function $\mathcal{D} \in L^\infty(0, T)$ in the energy balance:

$$\left[\int_{\Omega} \left[\frac{1}{2} |\mathbf{v}|^2 + \frac{1}{2} |\mathbb{P}|^2 + \frac{1}{2} |\nabla_x \mathbb{Q}|^2 + \mathcal{G}(\mathbb{Q}) \right] dx \right]_{t=0}^{t=\tau} + \mathcal{D}(\tau) = 2\Lambda \int_0^\tau \int_{\Omega} \mathbb{Q} : \mathbb{P} \, dx \, dt$$

is obtained as the limit of the difference in square brackets in

$$\begin{aligned} E[\mathbf{v}(\tau), \mathbb{P}(\tau), \mathbb{Q}(\tau)] + \left[E[\mathbf{v}_n(\tau), \mathbb{P}_n(\tau), \mathbb{Q}_n(\tau)] - E[\mathbf{v}(\tau), \mathbb{P}(\tau), \mathbb{Q}(\tau)] \right] \\ = E[\mathbf{v}_n(0), \mathbb{P}_n(0), \mathbb{Q}_n(0)] + 2\Lambda \int_0^\tau \int_{\Omega} \mathbb{Q}_n : \mathbb{P}_n \, dx \, dt \end{aligned}$$

where the modified energy functional is:

$$E[\mathbf{v}, \mathbb{P}, \mathbb{Q}] := \int_{\Omega} \left[\frac{1}{2} |\mathbf{v}|^2 + \frac{1}{2} |\mathbb{P}|^2 + \frac{1}{2} |\nabla_x \mathbb{Q}|^2 + \mathcal{G}(\mathbb{Q}) \right] dx$$

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Notice that it actually represents a **dissipation defect**

Relative energy

The dissipative solutions may seem rather weak as we have apparently no information about the specific form of neither the dissipation defect \mathcal{D} nor the correctors $\mathbb{R}^1, \mathbb{R}^2$. Nevertheless, we show that a dissipative solution coincides with the strong solution emanating from the same initial data as long as the latter exists. We consider the modified energy functional

$$E(\mathbf{v}, \mathbb{P}, \mathbb{Q}) = \int_{\Omega} \left[\frac{1}{2} |\mathbf{v}|^2 + \frac{1}{2} |\mathbb{P}|^2 + \frac{1}{2} |\nabla_x \mathbb{Q}|^2 + \mathcal{G}(\mathbb{Q}) \right] dx$$

along with the associated *relative energy functional*

$$\begin{aligned} \mathcal{E}(\mathbf{v}, \mathbb{P}, \mathbb{Q} \mid \tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}) \\ &= \frac{1}{2} \int_{\Omega} \left[|\mathbf{v} - \tilde{\mathbf{v}}|^2 + |\mathbb{P} - \tilde{\mathbb{P}}|^2 + |\nabla_x \mathbb{Q} - \nabla_x \tilde{\mathbb{Q}}|^2 \right] + \mathcal{G}(\mathbb{Q}) - \partial \mathcal{G}(\tilde{\mathbb{Q}}) : (\mathbb{Q} - \tilde{\mathbb{Q}}) - \mathcal{G}(\tilde{\mathbb{Q}}) dx \\ &= E(\mathbf{v}, \mathbb{P}, \mathbb{Q}) + E(\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}) - \int_{\Omega} \left[\mathbf{v} \cdot \tilde{\mathbf{v}} + \mathbb{P} : \tilde{\mathbb{P}} + \nabla_x \mathbb{Q} : \nabla_x \tilde{\mathbb{Q}} \right] - \left[\partial \mathcal{G}(\tilde{\mathbb{Q}}) : (\mathbb{Q} - \tilde{\mathbb{Q}}) + 2\mathcal{G}(\tilde{\mathbb{Q}}) \right] dx \end{aligned}$$

defined for any trio of smooth function $[\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$. The functional \mathcal{E} plays a role of a “distance” between a solution $[\mathbf{v}, \mathbb{P}, \mathbb{Q}]$ and a generic triplet $[\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$.

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defined for any trio of smooth function $[\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$. The functional \mathcal{E} plays a role of a “distance” between a solution $[\mathbf{v}, \mathbb{P}, \mathbb{Q}]$ and a generic triplet $[\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$.

Our goal is to derive the relative entropy inequality - an explicit formula for

$$\left[\mathcal{E}(\mathbf{v}, \mathbb{P}, \mathbb{Q} \mid \tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}) \right]_{t=0}^{t=\tau}$$

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- 1 Introduction of the Problem
- 2 The LCs modeling
- 3 The simplified Qian-Sheng model
- 4 The existence of local-in-time smooth solutions
- 5 Existence of global-in-time dissipative solutions
- 6 Weak-strong uniqueness**
- 7 Further perspectives

Theorem 3: Weak-strong uniqueness

Our ultimate goal is to show that any dissipative solution necessarily coincides with a strong solution originating from the same initial data on the existence interval of the latter. A simple idea is to take the strong solution $[\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$ as “test functions” in the relative energy inequality and to use a Gronwall-type argument.

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Under the hypotheses of Theorem 2 let the initial data enjoy the regularity properties:

$$\begin{aligned}\mathbf{v}(0, \cdot) = \mathbf{v}_0 &\in W^{s,2}(\mathcal{T}^3; \mathbb{R}^3), \quad \mathbb{P}(0, \cdot) = \mathbb{P}_0 \in W^{s,2}(\mathcal{T}^3; \mathbb{R}_{0,\text{sym}}^{3 \times 3}), \\ \mathbb{Q}(0, \cdot) &= \mathbb{Q}_0 \in W^{s+1,2}(\mathcal{T}^3; \mathbb{R}_{0,\text{sym}}^{3 \times 3})\end{aligned}$$

such that $\operatorname{div}_x \mathbf{v}_0 = 0$.

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$$\begin{aligned}\operatorname{div}_x \mathbf{v} &= 0 \\ \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla_x \mathbf{v} + \nabla_x \Pi &= -\operatorname{div}_x (\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q}) \\ \partial_t \mathbb{Q} + \mathbf{v} \cdot \nabla_x \mathbb{Q} &= \mathbb{P} \\ \partial_t \mathbb{P} + \mathbf{v} \cdot \nabla_x \mathbb{P} &= -\frac{\partial \mathcal{F}}{\partial \mathbb{Q}} + \Delta \mathbb{Q} - \lambda \mathbb{I}\end{aligned}$$

and let $[\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$ a the strong solution of the same problem belonging to the regularity class specified in Theorem 1 in the space-time cylinder $(0, T) \times \mathcal{T}^3$.

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and let $[\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$ a the strong solution of the same problem belonging to the regularity class specified in Theorem 1 in the space-time cylinder $(0, T) \times \mathcal{T}^3$. Then we have

$$\mathbf{v} = \tilde{\mathbf{v}}, \quad \mathbb{P} = \tilde{\mathbb{P}}, \quad \mathbb{Q} = \tilde{\mathbb{Q}} \text{ a.a. in } (0, T) \times \mathcal{T}^3.$$

An idea of the proof

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Using the weak formulation, the energy balance, and the bounds for the correctors and taking now as test functions the strong solutions $[\tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$, the relative energy inequality takes the final form

$$\begin{aligned} & \mathcal{E}(\mathbf{v}, \mathbb{P}, \mathbb{Q} \mid \tilde{\mathbf{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}})(\tau) + \mathcal{D}(\tau) \\ & \leq 2\Lambda \int_0^\tau \int_\Omega (\mathbb{Q} - \tilde{\mathbb{Q}}) : (\mathbb{P} - \tilde{\mathbb{P}}) \, dx \, dt - \int_0^\tau \int_\Omega (\mathbf{v} - \tilde{\mathbf{v}}) \cdot \nabla_x \tilde{\mathbf{v}} \cdot (\mathbf{v} - \tilde{\mathbf{v}}) \, dx \, dt \\ & + \int_0^\tau \int_\Omega (\tilde{\mathbf{v}} - \mathbf{v}) \cdot \nabla_x \tilde{\mathbb{P}} \cdot (\mathbb{P} - \tilde{\mathbb{P}}) \, dx \, dt + \int_0^\tau \int_\Omega (\tilde{\mathbf{v}} - \mathbf{v}) \cdot \nabla_x \partial \mathcal{G}(\tilde{\mathbb{Q}}) \cdot (\mathbb{Q} - \tilde{\mathbb{Q}}) \, dx \, dt \\ & + \int_0^\tau \int_\Omega \tilde{\mathbb{P}} : \left(\partial \mathcal{G}(\mathbb{Q}) - \partial^2 \mathcal{G}(\tilde{\mathbb{Q}})(\mathbb{Q} - \tilde{\mathbb{Q}}) - \partial \mathcal{G}(\tilde{\mathbb{Q}}) \right) \, dx \, dt \\ & + \int_0^\tau \int_\Omega \left[(\nabla_x \tilde{\mathbb{Q}} - \nabla_x \mathbb{Q}) \cdot \Delta_x \tilde{\mathbb{Q}} \cdot (\mathbf{v} - \tilde{\mathbf{v}}) - (\nabla_x \mathbb{Q} - \nabla_x \tilde{\mathbb{Q}}) \cdot \nabla_x \tilde{\mathbf{v}} \cdot (\nabla_x \mathbb{Q} - \nabla_x \tilde{\mathbb{Q}}) \right] \, dx \, dt \\ & + c \int_0^\tau \left(\|\nabla_x \tilde{\mathbb{P}}\|_{C(\mathcal{T}^3)} + \|\nabla_x \tilde{\mathbf{v}}\|_{C(\mathcal{T}^3)} \right) \mathcal{D}(\cdot) \, dt. \end{aligned}$$

Applying Gronwall's lemma we get the desired conclusion.

A corollary

Combining Theorem 3 with the local existence result established in Theorem 2 we immediately get the following corollary:

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$$\partial_t \mathbb{P} + \mathbf{v} \cdot \nabla_x \mathbb{P} = -\frac{\partial \mathcal{F}}{\partial \mathbb{Q}} + \Delta \mathbb{Q} - \lambda \mathbb{I}$$

in $(0, T) \times \mathcal{T}^3$ enjoying the regularity specified in Theorem 1.

A corollary

Combining Theorem 3 with the local existence result established in Theorem 2 we immediately get the following corollary: Let $[\mathbf{v}, \mathbb{P}, \mathbb{Q}]$ be a dissipative solution of our problem

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in $(0, T) \times \mathcal{T}^3$ enjoying the regularity specified in Theorem 1.

Then $[\mathbf{v}, \mathbb{P}, \mathbb{Q}]$ is a strong solution, in particular, the dissipation defect \mathcal{D} as well as the defect measures $\mathbb{R}^1, \mathbb{R}^2$ vanish identically in $[0, T] \times \mathcal{T}^3$.

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The study of more refined models

We should include more effects in the model, like:

The study of more refined models

We should include more effects in the model, like:

1. changes of the **temperature** (we have results for the Landau-de Gennes nematic liquid crystals flows)
2. effects of **magnetic and electric fields** (this is only a work in progress):
LCs behave differently depending on what direction electric or magnetic fields are applied relative to the director and so the introduction of the dependence on the magnetic and electric field in the mathematical models and analysis would be particularly challenging and useful in view of applications

Point 1. Our main contributions in the Landau-de Gennes case

We study the **non-isothermal** evolutionary system for nematic liquid crystals within the recent Ball-Majumdar \mathbb{Q} -tensorial model preserving the physical eigenvalue constraint on the **traceless and symmetric matrices \mathbb{Q}** :

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We still work in the three-dimensional torus $\Omega \subset \mathbb{R}^3$ in order to avoid complications connected with boundary conditions. We consider the evolution of the following variables:

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

The free energy and the \mathbb{Q} -tensor equation

The free energy density takes the form

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

where

- $f_B(\theta, \mathbb{Q}) = \theta f(\mathbb{Q}) + G(\mathbb{Q})$ is bulk the configuration potential
- f is the convex l.s.c. and singular Ball-Majumdar potential, G is a smooth function of \mathbb{Q}
- $a\theta^m$ prescribes a power-like specific heat

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We assume that the driving force governing the dynamics of the director \mathbb{Q} is of “gradient type” $\partial_{\mathbb{Q}} \mathcal{F}$:

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

- The left hand side is the “generalized material derivative” $D_t \mathbb{Q} = \partial_t \mathbb{Q} + \mathbf{v} \cdot \nabla \mathbb{Q} - \mathbb{S}(\nabla \mathbf{v}, \mathbb{Q})$
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- $\Gamma(\theta)$ represents a collective rotational viscosity coefficient

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 inequality

Entropy inequality

The evolution of temperature is prescribed by stating the **entropy inequality**

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

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

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- The viscosity ν is smooth and bounded - without any growth condition
- $\kappa(r) = A_0 + A_k r^k$, $A_0, A_k > 0$, $\frac{3k+2m}{3} > 9$, $\frac{3}{2} < m \leq \frac{6k}{5}$
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- $\Gamma(r) = \Gamma_0 + \Gamma_1 r$, $\Gamma_0, \Gamma_1 > 0$
- 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**

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

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

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- To control it, assuming periodic b.c.'s is essential

Main result: the “Entropic formulation”

Theorem: existence of global in time “Entropic solutions”

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

$$\theta_0 \in L^\infty(\Omega), \text{essinf}_{x \in \Omega} \theta_0(x) = \underline{\theta} > 0,$$

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- Notice that, if the solution is more regular, the **entropy inequality** becomes an **equality** and, multiplying it by θ we just get the standard **internal energy balance**

$$\vartheta_t + \mathbf{v} \cdot \nabla_x \vartheta + \text{div } \mathbf{q} = \vartheta (\partial_t f(\mathbb{Q}) + \mathbf{v} \cdot \nabla_x f(\mathbb{Q})) + \nu(\theta) |\nabla_x \mathbf{v} + \nabla_x^t \mathbf{v}|^2 + \Gamma(\vartheta) |\mathbb{H}|^2$$

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- However, this regularity is out of reach for this model: that is why this solution notion is significant

Open problems for the QS-model

- Include the temperature dependence
- Deal with the singular potential case
- ...

Many thanks to all of you for the attention!

<http://matematica.unipv.it/rocca/>

The existence of local-in-time smooth solutions

We establish the existence of local-in-time solutions in the Sobolev framework $W^{s,2}(\mathcal{T}^N)$ of functions with derivatives up to order s square integrable in \mathcal{T}^N .

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1. For $u, v \in W^{s,2} \cap L^\infty(\mathcal{T}^3)$ and α a multi-index with $|\alpha| \leq s$

$$\|\partial_x^\alpha(uv)\|_{L^2(\mathcal{T}^3)} \leq c_s \left(\|u\|_{L^\infty(\mathcal{T}^3)} \|\nabla_x^s v\|_{L^2(\mathcal{T}^3)} + \|v\|_{L^\infty(\mathcal{T}^3)} \|\nabla_x^s u\|_{L^2(\mathcal{T}^3)} \right).$$

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3. For $u \in W^{s,2} \cap C(\mathcal{T}^3)$, and F s -times continuously differentiable function on an open neighborhood of the compact set $G = \text{range}[u]$, $1 \leq |\alpha| \leq s$,

$$\|\partial_x^\alpha F(u)\|_{L^2(\mathcal{T}^3)} \leq c_s \|\partial_u F\|_{C^{s-1}(G)} \|u\|_{L^\infty(\mathcal{T}^3)}^{|\alpha|-1} \|\partial_x^\alpha u\|_{L^2(\mathcal{T}^3)}.$$