On a hyperbolic system arising in liquid crystals modeling

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Workshop on Mathematical Fluid Dynamics
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jointly with
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Outline

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We present here the results of the following joint work

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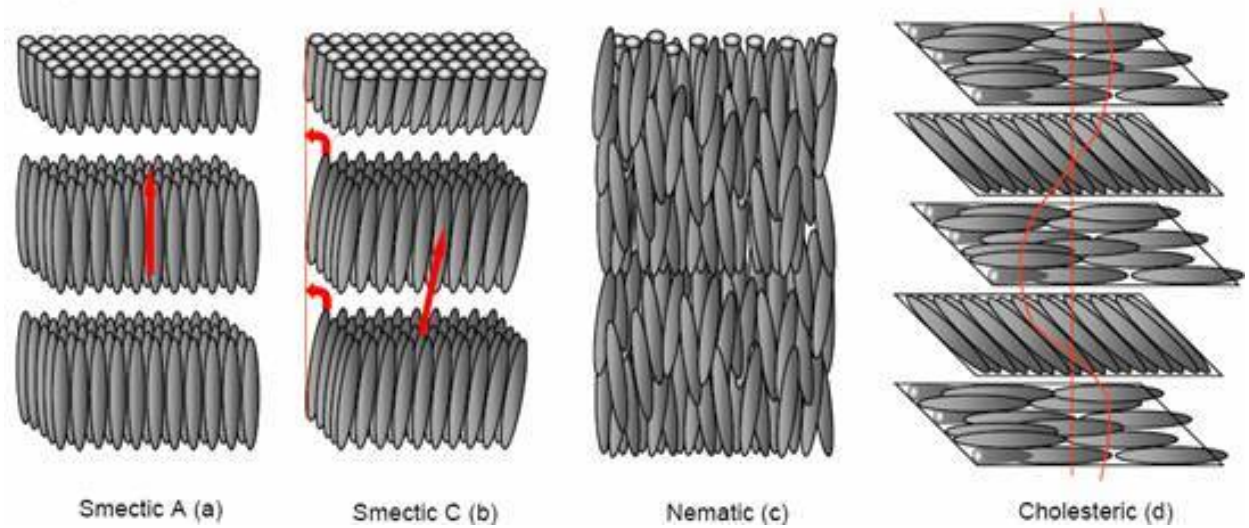
Here is the plan of the talk:

- Introduce the Liquid Crystals modeling and $\mathbb{Q}$-tensors formalism
- Present a simplification of the Qian-Sheng (QS-model) and the resulting PDEs
- Propose the concept of dissipative solution, for which a global-in-time existence theorem is shown
- 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*



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

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

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

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

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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 $\boldsymbol{d}$. 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 $\boldsymbol{u}$ 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 $\boldsymbol{u}$
- Moreover, also changes of the temperature or effects of magnetic and electric fields should be considered (in the future maybe)

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The Landau-de Gennes theory: the molecular orientation

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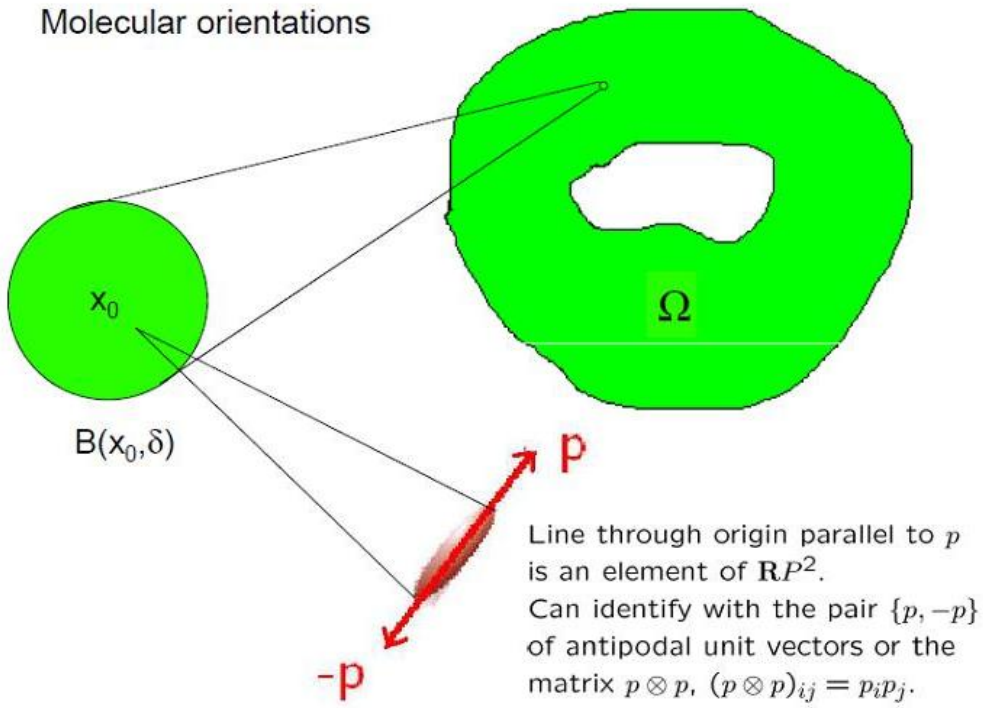
- Consider a nematic liquid crystal filling a bounded connected container Ω in $\mathbb{R}^3$ with "regular" boundary
- The distribution of molecular orientations in a ball $B(x_0, \delta)$, $x_0 \in \Omega$ can be represented as a probability measure μ on the unit sphere $\mathbb{S}^2$ satisfying $\mu(E) = \mu(-E)$ 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 $\mathrm{v} \in \mathbb{S}^2$, $\mathrm{v} \cdot M \cdot \mathrm{v} = \int_{\mathbb{S}^2} (\mathrm{v} \cdot p)^2\, d\mu(p) =< \cos^2\theta >$, where θ is the angle between p and 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 $M_0 = \frac{1}{4\pi} \int_{\mathbb{S}^2} p \otimes p\, dS = \frac{1}{3} 1$, 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

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

- Note that (cf. [Ball, Majumdar, Molecular Crystals and Liquid Crystals (2010)])
  1. $\mathbb{Q} = \mathbb{Q}^T$
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  1.+2. implies $\mathbb{Q} = \lambda_1 \boldsymbol{n}_1 \otimes \boldsymbol{n}_1 + \lambda_2 \boldsymbol{n}_2 \otimes \boldsymbol{n}_2 + \lambda_3 \boldsymbol{n}_3 \otimes \boldsymbol{n}_3$, where $\{\boldsymbol{n}_i\}$ 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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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 $\boldsymbol{n}_3 = \boldsymbol{d}$ where $\boldsymbol{n}_i$ is an orthonormal basis of eigenvectors of $\mathbb{Q}$ corresponding to λ_i, we have

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

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 $\boldsymbol{d}$ 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)])

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

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

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

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

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

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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 $\boldsymbol{d}$ we obtain the simplest form of the Oseen-Frank free energy (1925, 1958)

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

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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

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

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

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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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:

$$\begin{aligned}
&\mathrm{div}_x \boldsymbol{v} = 0 \\
&\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla_x \boldsymbol{v} + \nabla_x \Pi = -\mathrm{div}_x \left(\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q} \right) \\
&\partial_t \mathbb{Q} + \boldsymbol{v} \cdot \nabla_x \mathbb{Q} = \mathbb{P} \\
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\end{aligned}$$

For the sake of simplicity, we restrict ourselves to the periodic boundary conditions, for which the underlying spatial domain may be identified with the flat torus:

$$\mathcal{T}^3 = \left([-\pi, \pi]|_{\{-\pi,\pi\}} \right)^3$$

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- a wave-like equation governing the time evolution of the $\mathbb{Q}$-tensor $\mathbb{Q} = \mathbb{Q}(t,x) \in R^{3\times 3}_{0,\mathrm{sym}}$ - a symmetric traceless matrix
- 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

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

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

$$\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla_x \boldsymbol{v} + \nabla_x \Pi = -\mathrm{div}_x \left(\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q} \right)$$

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

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}[\boldsymbol{v}, \mathbb{P}, \mathbb{Q}] = 0$$

for any smooth solution of our system

Qualitative features

The system can be regarded as an extended Euler system and this was the main motivation for proposing it in the Gay-Balmaz-Tronci paper

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Indeed, if one defines the *extended circulation vector*, where $\mathbb{P}_{ij}\nabla_x\mathbb{Q}_{ij}$ 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)

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

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*

$$\frac{\mathrm{d}}{\mathrm{d}t}\oint_{\Gamma(t)} \boldsymbol{v} + \mathbb{P}_{ij}\nabla_x\mathbb{Q}_{ij}\, d\sigma = 0$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \mathcal{C}_{QS}\cdot\bar{\omega}_{QS}\ \mathrm{d}x = 0$$

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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&\operatorname{div}_x \boldsymbol{v} = 0 \\
&\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla_x \boldsymbol{v} + \nabla_x \Pi = -\operatorname{div}_x \left(\nabla_x \mathbb{Q} \odot \nabla_x \mathbb{Q} \right) \\
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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 $A : B = \mathrm{tr}(AB)$
- 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 $\left(\sum_{j=1}^{3} \frac{\partial M_{ij}}{\partial x_j} \right)_{i=1\ldots3}$
- If $\boldsymbol{v}$ is a 3-dimensional vector and $\mathbb{Q}$ is a 3×3 matrix then $\boldsymbol{v} \otimes \mathbb{Q}$ 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 $v \otimes \mathbb{Q} : \nabla_x \mathbb{P}$ the scalar $\sum_{i,j,k=1}^{3} v_k Q_{ij} \frac{\partial P_{ij}}{\partial x_k}$

Outline

Assumptions on the potential

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(A1) The function $\mathcal{F} : R^{3\times 3}_{0,\mathrm{sym}} \to R$ is isotropic, i.e.

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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 appearence of a further defect term in the energy balance. The function $G(\mathbb{Q})$ 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 $\partial\mathcal{F}(\mathbb{Q})$) would then occur
- Examples of functions that satisfies (A1)-(A3) are

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

Theorem 1: local strong solutions

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

$$\boldsymbol{v}(0,\cdot) = \boldsymbol{v}_0 \in W^{s,2}(\mathcal{T}^3; R^3),\ \mathbb{P}(0,\cdot) = \mathbb{P}_0 \in W^{s,2}(\mathcal{T}^3; R^{3\times 3}_{0,\mathrm{sym}}),$$
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Then there exists $T_0 > 0$ depending solely on the norm of the initial data such that our problem

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

$$\boldsymbol{v} \in C([0,T_0]; W^{s,2}(\mathcal{T}^3; R^3)),$$
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they satisfy the relations:

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

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

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

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

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

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

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

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$$

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

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

Remark on the correctors

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

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

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

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but, actually:

- $\mathbb{R}^1$ is the tensor of measures whose (i,j)-entry is $\mathcal{R}^{i,j}_{1,1} + \mathcal{R}^{i,j}_{1,2}$ with
  - $v^i_n v^j_n - v^i v^j \to \mathcal{R}^{i,j}_{1,1}$ weakly-(*) in $L^\infty(0,T;\mathcal{M}(\mathcal{T}^3))$ and
  $$\sum_{i,j}\|\mathcal{R}^{i,j}_{1,1}\|_{\mathcal{M}(\mathcal{T}^3)} \le 3\int_\Omega\left(\overline{|\boldsymbol{v}|^2} - |\boldsymbol{v}|^2\right)\mathrm{d}x.$$
  - $\sum_{\alpha,\beta}\left(\partial_i Q^{\alpha,\beta}_n \partial_j Q^{\alpha,\beta}_n - \partial_i Q^{\alpha,\beta}\partial_j Q^{\alpha,\beta}\right) \to \mathcal{R}^{i,j}_{1,2}$ weakly-(*) in $L^\infty(0,T;\mathcal{M}(\mathcal{T}^3))$ and
  $$\sum_{i,j}\|\mathcal{R}^{i,j}_{1,2}\|_{\mathcal{M}(\mathcal{T}^3)} \le c\int_\Omega\left(\overline{|\nabla_x\mathbb{Q}|^2} - |\nabla_x\mathbb{Q}|^2\right)\mathrm{d}x,$$
- $\mathbb{R}^2$ is the tensor of measures whose (i,j,k)-entry is $\mathcal{R}^{i,j,k}_2$ with
  $$v^i_n P^{k,j}_n - v^i P^{k,j} \to \mathcal{R}^{i,j,k}_2 \text{ weakly-(*) in } L^\infty(0,T;\mathcal{M}(\mathcal{T}^3))$$
  and
  $$\sum_{i,j}\int_0^\tau\|\mathcal{R}^{i,j,k}_2\|_{\mathcal{M}(\mathcal{T}^3)}\,\mathrm{d}t \le c\int_0^\tau\int_\Omega\left(\overline{|\mathrm{v}|^2} - |\mathrm{v}|^2\right)\mathrm{d}x\,\mathrm{d}t + c\int_0^\tau\int_\Omega\left(\overline{|\mathbb{P}|^2} - |\mathbb{P}|^2\right)\mathrm{d}x\,\mathrm{d}t.$$

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

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

$$\begin{aligned} E[\boldsymbol{v}(\tau), \mathbb{P}(\tau), \mathbb{Q}(\tau)] + \Big[E[\boldsymbol{v}_n(\tau), \mathbb{P}_n(\tau), \mathbb{Q}_n(\tau)] - E[\boldsymbol{v}(\tau), \mathbb{P}(\tau), \mathbb{Q}(\tau)]\Big] \\ = E[\boldsymbol{v}_n(0), \mathbb{P}_n(0), \mathbb{Q}_n(0)] + 2\Lambda \int_0^t \int_\Omega \mathbb{Q}_n : \mathbb{P}_n \,\mathrm{d}x\,\mathrm{d}t \end{aligned}$$

where the modified energy functional is:

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

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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

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along with the associated *relative energy functional*

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

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

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&= E(\boldsymbol{v}, \mathbb{P}, \mathbb{Q}) + E(\tilde{\boldsymbol{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}) - \int_\Omega \left[\boldsymbol{v} \cdot \tilde{\boldsymbol{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] \, \mathrm{d}x
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Our goal is to derive the relative entropy inequality - an explicit formula for

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

Outline

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 $[\tilde{\boldsymbol{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$ 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:

$$\boldsymbol{v}(0,\cdot) = \boldsymbol{v}_0 \in W^{s,2}(\mathcal{T}^3; R^3),\ \mathbb{P}(0,\cdot) = \mathbb{P}_0 \in W^{s,2}(\mathcal{T}^3; R^{3\times 3}_{0,\mathrm{sym}}),$$
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and let $[\tilde{\boldsymbol{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$ 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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$$\boldsymbol{v} = \tilde{\boldsymbol{v}},\ \mathbb{P} = \tilde{\mathbb{P}},\ \mathbb{Q} = \tilde{\mathbb{Q}} \text{ a.a. in } (0, T)\times\mathcal{T}^3.$$

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 $[\tilde{\boldsymbol{v}}, \tilde{\mathbb{P}}, \tilde{\mathbb{Q}}]$, the relative energy inequality takes the final form

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

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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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 $[\boldsymbol{v}, \mathbb{P}, \mathbb{Q}]$ 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 $[\boldsymbol{v}, \mathbb{P}, \mathbb{Q}]$ 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 $[0, T] \times \mathcal{T}^3$.

Outline

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 usefull 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 $\boldsymbol{v}$
- 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" $\partial_{\mathbb{Q}}\mathcal{F}$:

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

- The left hand side is the "generalized material derivative" $D_t\mathbb{Q} = \partial_t \mathbb{Q} + \boldsymbol{v} \cdot \nabla \mathbb{Q} - \mathbb{S}(\nabla \boldsymbol{v}, \mathbb{Q})$
- $\mathbb{S}$ represents deformation and stretching effects of the crystal director along the flow

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

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

where

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- $\Gamma(\theta)$ represents a collective rotational viscosity coefficient

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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

$$s_t + \boldsymbol{v} \cdot \nabla s - \operatorname{div}\left(\frac{\kappa(\theta)}{\theta}\nabla\theta\right) \tag{eq-θ}$$

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

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- $\kappa(r) = A_0 + A_k r^k$, A_0, $A_k > 0$, $\frac{3k+2m}{3} > 9$, $\frac{3}{2} < m \leq \frac{6k}{5}$
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- 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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$$= \operatorname{div}(\sigma \boldsymbol{v}) + \operatorname{div} \left(\Gamma(\theta) \nabla \mathbb{Q} : \left(\Delta \mathbb{Q} - \theta \frac{\partial f(\mathbb{Q})}{\partial \mathbb{Q}} + \lambda \theta \right) \right) + \boldsymbol{g} \cdot \boldsymbol{v}$$

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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

$$\theta_0 \in L^\infty(\Omega),\ \operatorname{essinf}_{x\in\Omega} \theta_0(x) = \underline{\theta} > 0,$$
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$$\vartheta_t + \boldsymbol{v}\cdot\nabla_x\vartheta + \operatorname{div}\mathrm{q} = \vartheta\big(\partial_t f(\mathbb{Q}) + \boldsymbol{v}\cdot\nabla_x f(\mathbb{Q})\big) + \nu(\theta)\left|\nabla_x\boldsymbol{v} + \nabla_x^t\boldsymbol{v}\right|^2 + \Gamma(\vartheta)|\mathbb{H}|^2$$

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

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/

Convergences of the defect measures

Examining the difference

$$v_n^i v_n^j - v^i v^j = (v_n^i - v^i)(v_n^j - v^j) - v^i(v^j - v_n^j) - v^j(v^i - v_n^i), \tag{7.1}$$

we find out that

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

Let now $\zeta \in C(\mathcal{T}^3)$ with $\|\zeta\|_\infty \leq 1$. Then, testing (7.1) by ζ, we obtain

$$\int_\Omega (v_n^i v_n^j - v^i v^j)\zeta \, \mathrm{d}x \leq \frac{1}{2}\int_\Omega (v_n^i - v^i)^2|\zeta| \, \mathrm{d}x + \frac{1}{2}\int_\Omega (v_n^j - v^j)^2|\zeta| \, \mathrm{d}x \tag{7.2}$$

$$- \int_\Omega \big(v^i(v^j - v_n^j) + v^j(v^i - v_n^i)\big)\zeta \, \mathrm{d}x$$

Hence, letting $n \nearrow \infty$, we obtain

$$\int_\Omega \mathcal{R}_{1,1}^{i,j}\zeta \, \mathrm{d}x \leq \frac{1}{2}\lim_{n\nearrow\infty}\int_\Omega (v_n^i - v^i)^2|\zeta| \, \mathrm{d}x + \frac{1}{2}\lim_{n\nearrow\infty}\int_\Omega (v_n^j - v^j)^2|\zeta| \, \mathrm{d}x,$$

where the first integral has in fact to be intended as the integral of the function ζ with respect to the measure $\mathcal{R}_{1,1}^{i,j}$. This convention will be extensively used also in the sequel.
Hence, passing to the supremum with respect to ζ, and summing over i, j, we arrive at

$$\sum_{i,j} \|\mathcal{R}_{1,1}^{i,j}\|_{\mathcal{M}(\mathcal{T}^3)} \leq 3\int_\Omega \left(\overline{|\boldsymbol{v}|^2} - |\boldsymbol{v}|^2\right) \, \mathrm{d}x. \tag{7.3}$$

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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 $G = \text{range}[u]$, $1 \leq |\alpha| \leq s$,

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